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Quantum Simulation of Inflationary Cosmology: Probing Analogue Trans-Planckian Spectra in Dipolar Bose-Einstein Condensates

인플레이션 우주론의 양자역학적 시뮬레이션: 쌍극자 보스-아인슈타인 응축체 내에서의 유추 초 플랑크 스펙트럼의 탐구

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Quantum Simulation of Inflationary Cosmology: Probing Analogue Trans-Planckian Spectra in Dipolar Bose-Einstein Condensates

Seok-Yeong Chä

Supervised by

Associate Professor **Uwe R. Fischer**

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Department of Physics and Astronomy
The Graduate School
Seoul National University

Abstract

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Seok-Yeong Chä
Department of Physics and Astronomy
The Graduate School
Seoul National University

This study concerns the emergence of effective curved spacetime in the quasi two dimensional dipolar Bose-Einstein condensates, in which Bogoliubov quasiparticle excitation spectrum displays, at sufficiently large gas density, a deep roton minimum due to the spatially anisotropic behavior of the dipolar two-body potential.

The study can generally be divided into two parts. Firstly, an analogue de Sitter cosmos in an expanding dipolar condensate is considered. It is demonstrated that a hallmark signature of inflationary cosmology, the scale invariance of the power spectrum (SIPS) of inflaton field correlations, experiences strong modifications when, at the initial stage of expansion, the excitation spectrum displays roton minimum. This exemplifies that dipolar quantum gases furnish a viable laboratory tool to experimentally investigate, with well-defined and controllable initial conditions, whether excitation spectra deviating from Lorentz invariance at trans-Planckian momenta violate standard predictions of inflationary cosmology.

Secondly, it is investigated whether a rapid quench, performed on the speed of sound of excitations propagating on the condensate background, leads to the dynamical Casimir effect (DCE), which can be characterized by measuring the density-density correlation function. It is shown, for both zero and finite initial temperatures, that the continuous-variable bipartite quantum state of quasiparticle pairs with opposite momenta, resulting from the quench, displays an enhanced potential for the presence of entanglement, when compared to a gas with repulsive contact interactions only. Entangled quasiparticle pairs contain momenta close to the roton, and hence the quantum correlation significantly increases in the presence of deep roton minimum.

Keywords : Bose-Einstein Condensation, Dipole-Dipole Interaction, Inflation, Dynamical Casimir Effect, Trans-Planckian Physics, Analogue Gravity, Roton Minimum
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Chapter 1

Introduction

Quantum field theory in curved spacetime (QFTCS) predicts that pairs of correlated particles are created from the vacuum when classical background rapidly varies in time [1]. This process can take place in expanding (or contracting) universe, where it is coined as cosmological particle production [2, 3]. This occurs analogously in the dynamical Casimir effect for photons generated from the electrodynamical quantum vacuum in a vibrating cavity [4]. Correlated pairs of particles can also be produced by the phenomenon of Hawking radiation in the presence of an event horizon [5, 6].

As a major result from QFTCS, the hypothesis of a rapid initial expansion of the cosmos in the inflationary scenario [7–9] resolved many vexing cosmological questions plaguing other theories, such as the observed flatness and homogeneity of the universe, as well as the nonexsistence of monopoles. However the resolution of these issues came at the price of creating another potential prolem [10]: Generally the period of inflation lasts so long that, at the beginning of the inflationary period, the physical wavelengths of comoving scales which correspond to the present large-scale structure of the universe were smaller than the Planck length. Thus necessarily trans-Planckian energies become involved, for which the physics is at present speculative. Similar issues regarding kinematical phenomena for quantum fields propagating on a fixed curved spacetime arise when tracing back Hawking radiation emission all the way down to the black hole horizon [11–14].

On the other hand, by temporal variations of a homogeneous background, quasiparticle pairs with opposite momenta can be produced and form (continuous-variable) bipartite quantum states: They are entangled. The degree of quantum entanglement can be understood in hierarchical way. States exhibiting "Bell nonlocality" form a strict subset of "steerable" quantum states. And the steerable states form a strict subset of "nonseparable" states [15–17]. Steering [18] refers to the quantum correlations that can be observed between the outcomes of measurements applied on a half of the entangled state (Alice) and on the resulting post-measurement state left with the other party (Bob). A criterion testing quantum steering can be seen as an entanglement test where one of the parties (Alice) performs uncharacterized measurements, i.e., with a procedure not accessible (hidden in a black box) to the other party (Bob) [19]. With all these intriguing features, however, directly observing pair creation in relativistic quantum field theory is notoriously difficult due to the challenging experimental requirements for achieving sizable pair production rates.

To render these problems under rather general conditions accessible to experiments, the idea of quantum simulation [20] was applied to relativistic quantum fields on an effective curved spacetime [21, 22]. This is frequently classified under the notion of "analogue gravity," see for an extensive review and a comprehensive list of references [23]. The analogue gravity program [21, 23–25] has been successfully theoretically implemented in ultracold matter for various cosmological phenomena, e.g., inflaton quantum fluctuations [26, 27], the Gibbons-Hawking effect [28], cosmological particle production [29–31], the cosmological constant problem [25, 32, 33], or false vacuum decay [34]. Also, several quantum simulation experiments, in which quasiparticles propagate on a rapidly changing background, leading to the dynamical Casimir effect, have been proposed, e.g., in [30, 35–39].

Importantly, recent experimental advances have allowed for groundbreaking observations of analogues of cosmological particle production, Sakharov oscillations, black hole lasers, and Hawking radiation [40–44], as well as those experiments conducted for observing dynamical Casimir effect, c.f., e.g., [40, 41, 45, 46]. In the same vein, to investigate the analogue event or cosmological horizons and the associated entanglement effects, several experiments have been proposed [24, 26, 47–51] and some were realized in the lab [42, 44, 52–54]. These experiments held promises to realize experimental cosmology: A quantum simulation of inflationary scenario with reproducible initial conditions, which is distinct from the current purely observational cosmology of a pregiven state of the universe.

A major original motivation of analogue gravity, so far not experimentally investigated, is to probe consequences of trans-Planckian physics in a microscopically well understood setup in a regime inaccessible for quantum fields in the presence of strong real (Einsteinian or other) gravity. We here propose to realize this aim with *dipolar* Bose-Einstein condensates, addressing the trans-Planckian problem of inflationary cosmology.

Going beyond contact interactions (in field theory language ϕ^4), magnetic dipole-dipole interaction (DDI) dominated condensates [55] have been created with chromium [56], dysprosium [57], and erbium [58] atoms, and the realization of BECs made up of molecules with permanent electric dipoles [59] is now at the forefront of ongoing research cf., e.g., [60, 61]. The excitation spectrum of DDI-dominated BECs displays a *roton min-*

imum [62–64]. Various ramifications of the dipolar BEC roton, originally defined for and observed in the strongly interacting superfluid helium II [65,66], have been recently experimentally investigated in ultracold dipolar quantum gases [67–70]. In addition, the significant progress in probing correlation functions to increasing accuracy [41, 71] pave the way for an exploration of the intricate many-body correlations due to DDI.

In dipolar Bose-Einstein condensates, the (analogue) trans-Planckian large-momentum sector of the excitation spectrum (containing in particular the roton) is well controlled by adjusting the relative strength of contact and dipolar interactions. We will demonstrate that, for the creation of quasiparticle pairs in a time-dependent background, the existence of a deep roton minimum in the excitation spectrum plays a dominant role [72, 73].

For certain classes of inflaton dispersion relations, displaying deviations from Lorentz invariance at trans-Planckian scales, the predictions of inflation, in particular the scale invariance of the power spectrum (SIPS) of inflaton field correlations, remain robust, while for others, they change significantly, cf., e.g., [74–78]. In our study, it is shown that dipolar BECs, possessing trans-Planckian spectra leading to strong departures from Lorentz invariance, yield significant changes of the standard inflationary prediction of SIPS. This represents the first example within analogue gravity where violations of SIPS can become experimentally manifest.

We also exploit that the (analogue) trans-Planckian sector can be engineered to explore the consequences for the quantum many-body state of the quasiparticles created by quench. The entanglement, here represented by the nonseparability and steerability present in a bipartite continuous variable system, are significantly enhanced in the presence of a deep roton minimum, that is, for sufficiently large densities of a DDI dominated gas. In quantum simulation–analogue gravity language, this is the quasiparticle production due to the dynamical Casimir effect for a relativistic quantum field of phonons in the low-momentum corner.

Chapter 2

Bose-Einstein Condensation

2.1 Time Line of Bose-Einstein Condensation

- 1925 : A. Einstein, on the basis of a paper by the Indian physicist S. N. Bose (1924), devoted to the statistical description of the quanta of light, predicted the occurrence of a phase transition in a gas of noninteracting atoms.

  $\Rightarrow$ This phase transition is associated with the condensation of atoms in the state of lowest energy and is the consequence of quantum statistical effects.

- 1938 : F. London, immediately after the discovery of superfluidity in liquid helium (Allen and Misener, 1938; Kapitza, 1938), had the intuition that superfluidity could be a manifestation of Bose-Einstein condensation.

- 1941 : The first self-consistent theory of superfluids was developed by Landau in terms of the spectrum of elementary excitations of the fluid.

- 1947 : N. N. Bogoliubov developed the first microscopic theory of interacting Bose gases, based on the concept of Bose-Einstein condensation.

- 1949, 1955, 1956 : The prediction of quantized vortices by Onsager (1949) and Feynman and their experimental discovery by Hall and Vinen (1956).

- 1951, 1956 : Landau and Lifshitz (1951), Penrose (1951) and Penrose and Onsager (1956) introduced the concept of the off-diagonal long-range order and discussed its relationship with BEC.

- 1970s : The experimental studies on the dilute atomic gases started from 1970s, profiting from new techniques developed in atomic physics based on magnetic and optical trapping, and advanced cooling mechanisms(evaporative cooling) to obtain temperatures very close to BEC.

- 1980s : Laser-based techniques, such as laser cooling and magneto-optical trapping, were developed to cool and trap neutral atoms. Alkali atoms were well suited to laser-based methods because their optical transition can be excited by available lasers and because they have a favourable internal energy-level structure for cooling to very low temperatures. Once they are trapped, their temperature can be lowered further by evaporative cooling.

- 1995 : By combining the different cooling techniques, the experimental teams of Cornell and Wiemann at Boulder and of Ketterle at MIT eventually succeeded in 1995 in reaching the temperatures and densities required to observe BEC in vapours of ^{87}Rb (Anderson *et al.*, 1995) and ^{23}Na (Davis *et al.*, 1995).

  $\Rightarrow$ Despite the huge literature on the theory of Bose-Einstein condensation developed in previous years, the experiments of 1995 have opened a new variety of important questions. In particular the predictions of meanfield theory, based on the extension of Bogoliubov theory to nonuniform gases, are now rather well settled and provide a satisfactory description of many physical phenomena exhibited by these quantum gases.

2.2 Off-Diagonal Long-Range Order

Long-range order, symmetry breaking and order parameter are key concepts underlying the phenomenon of Bose-Einstein condensation. Let us start our discussion by introducing a very general definition which applies to any system, independent of statistics, in equilibrium as well as out of equillibrium. We consider **single-particle density matrix** defined by

$$\rho_1(\mathbf{r},\mathbf{r}') \equiv \langle \mathbf{r}'|\hat{\rho}_1|\mathbf{r}\rangle = \frac{1}{N}\langle \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r}')\rangle, \tag{2.1}$$

where $\hat{\Psi}^\dagger(\mathbf{r})$ ($\hat{\Psi}(\mathbf{r})$) is the field operator creating (annihilating) a particle at the point $\mathbf{r}$. For a system of Bosons, the field operators of (2.1) satisfy the well-known commutation relations

$$[\hat{\Psi}(\mathbf{r}), \hat{\Psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r}-\mathbf{r}'), \qquad [\hat{\Psi}(\mathbf{r}), \hat{\Psi}(\mathbf{r}')] = 0. \tag{2.2}$$

If the system occupies a pure state, described by the N-body wave function $\varphi_n(\mathbf{r}_1, \cdots, \mathbf{r}_N)$, then the average is taken as follows:

$$\rho_1^{(n)}(\mathbf{r}, \mathbf{r}') = \int d\mathbf{r}_2 \cdots d\mathbf{r}_N \; \varphi_n^*(\mathbf{r}, \mathbf{r}_2, \cdots, \mathbf{r}_N)\varphi_n(\mathbf{r}', \mathbf{r}_2, \cdots, \mathbf{r}_N), \tag{2.3}$$

involving integration over the $N-1$ variables $\mathbf{r}_2, \cdots, \mathbf{r}_N$.

For the more general case of a statistical mixture, expression (2.3) should be averaged according to the probability for a system to occupy the different states. The most important example is a system in thermodynamic equilibrium. In this case the states φ_n are eigenstates of the Hamiltonian with energy E_n and the weight of each state is fixed by the factor $\exp(-E_n/kT)$, so that the density matrix becomes

$$\rho_1(\mathbf{r}, \mathbf{r}') = \frac{1}{Q}\sum_n e^{-E_n/kT}\rho_1^{(n)}(\mathbf{r}, \mathbf{r}'),$$

where $Q = \sum_n \exp(-E_n/kT)$ is the partition function.

By setting $\mathbf{r} = \mathbf{r}'$ in the eq.(2.1), one finds the diagonal density of the system:

$$N\rho_1(\mathbf{r}, \mathbf{r}) = \langle \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})\rangle \equiv \rho(\mathbf{r}),$$

where $\rho(\mathbf{r})$ is the particle density of the system at point $\mathbf{r}$. The total number of particles is then

$$N = \int d\mathbf{r}\; \rho(\mathbf{r}) = \int d\mathbf{r}\; N\rho_1(\mathbf{r}, \mathbf{r}).$$

This equation defines the normalization of the single-particle density matrix.

Off-Diagonal Long-Range Order (ODLRO) is a concept that C. N. Yang [79] introduced to analyze the occurrence of order in a system. A system is said to possess an ODLRO if the single-particle density matrix

$$N\rho_1(\mathbf{r}, \mathbf{r}') = \mathrm{Tr}(\hat{\rho}\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r}')) = \langle \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r}')\rangle \tag{2.4}$$

remains on the order of N/V as $|\mathbf{r} - \mathbf{r}'|$ increases. The expression (2.4) says that the single-particle density matrix gives the probability ampitudes that the quantum state of the system remains unperturbed if a particle is removed from the system at $\mathbf{r}'$ and added to it at $\mathbf{r}$. ODLRO implies that a particle can travel a long distance without disturbing the system.

Let's consider a system of Bosons described by the density operator $\hat{\rho}$. Let $\hat{\rho}_1$ be the reduced single-particle density operator. For convenience, let's define

$$\hat{\sigma}_1 \equiv N\hat{\rho}_1.$$

In a nonequilibrium situations in which the state of a system changes in time, the density operators can have time dependence. Since $\hat{\rho}_1$(and so $\hat{\sigma}_1$) is still Hermitian, we can consider the representation in which the single-particle density operator is diagonal at all times:

$$\hat{\sigma}_1(t) = \sum_\nu n_\nu(t)|\psi_\nu(t)\rangle\langle\psi_\nu(t)|$$

$$\text{or} \quad \sigma_1(\mathbf{r},\mathbf{r}';t) := \langle\mathbf{r}'|\hat{\sigma}_1(t)|\mathbf{r}\rangle = \sum_\nu n_\nu(t)\psi^*_\nu(\mathbf{r},t)\psi_\nu(\mathbf{r}',t). \tag{2.5}$$

For the construction of the state vectors ψ_ν, one can reformulate the argument as follows. Since $\sigma_1(\mathbf{r},\mathbf{r}') = (\sigma_1(\mathbf{r}',\mathbf{r}))^*$, the matrix σ_1 is Hermitian and can be diagonalized. The long-range order exhibited by the single-particle density matrix is strongly connected to the behavior of its eigenvalues n_i defined by the solution of the eigenvalue equation,

$$\int d\mathbf{r}' \; \sigma_1(\mathbf{r},\mathbf{r}')\psi_i(\mathbf{r}') = n_i\psi_i(\mathbf{r}). \tag{2.6}$$

The solutions of (2.6) provide a natural basis of orthonormal wave functions $\varphi_i(\mathbf{r})$ normalized to unity. By multiplying (2.6) by $\varphi^*_i(\mathbf{r})$ and integrating over $\mathbf{r}$, one finds

$$\int d\mathbf{r}d\mathbf{r}'\sigma_1(\mathbf{r},\mathbf{r}')\psi^*_i(\mathbf{r})\psi_i(\mathbf{r}') = n_i. \tag{2.7}$$

Taking summation over i, we obtain

$$N = \sum_i n_i,$$

which follows from the completeness relation $\sum_i \psi^*_i(\mathbf{r})\psi_i(\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')$.

Note that the single-particle wave functions ψ_i are well defined not only for ideal gases, but also for interacting and nonuniform systems. The knowledge of the functions ψ_i and of the eigenvalues n_i permits us to write the density matrix in the diagonalized form

$$\sigma_1(\mathbf{r},\mathbf{r}') = \sum_i n_i\psi^*_i(\mathbf{r})\psi_i(\mathbf{r}'). \tag{2.8}$$

A major consequence of the diagonalization (2.8) is given by the possibility of identifying in an unambiguous way the single-particle wave functions ψ_i for both interacting and nonuniform systems. These functions can be used to write the field operator $\hat{\Psi}(\mathbf{r})$ in the form

$$\hat{\Psi}(\mathbf{r}) = \sum_i \psi(\mathbf{r})\hat{a}_i, \tag{2.9}$$

where $\hat{a}_i$ are defined by

$$\hat{a}_i = \int d\mathbf{r}\ \psi_i^*(\mathbf{r})\hat{\Psi}(\mathbf{r}). \tag{2.10}$$

It is easy to check that their commutation relations are

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}, \qquad [\hat{a}_i, \hat{a}_j] = 0.$$

Using the definition (2.1) and the eigenvalue equation (2.6), one finds that the expectation value of the operators $\hat{a}_j^\dagger \hat{a}_i$ is given by

$$\langle \hat{a}_i^\dagger \hat{a}_j \rangle = \delta_{ij} n_i.$$

We introduce an interpreation that the operators $\hat{a}_i$ ($\hat{a}_i^\dagger$) are annihilation (creation) operators of a particle in the state φ_i.

2.3 Definition of Bose-Einstein Condensation

Let $|\psi_0(t)\rangle$ be the state with maximum eigenvalue. The condition for the occurance of **Bose-Einstein condensasation** is formulated as [80]:

$$n_0 = \mathcal{O}(N).$$

If BEC occures only in the $\nu = 0$ mode, $n_{\nu \neq 0} = \mathcal{O}(1)$. In other words, Bose-Einstein condensation occurs when one (or several) of the single-particle states (hereafter called the condensate, $i = 0$) is occupied in a macroscopic way, i.e. when $n_0 \equiv N_0$ is a number of order N, while the other single-particle states have a microscopic occupation of order 1.

In this case eq.(2.8) can conveniently be rewritten in the separated form

$$\sigma_1(\mathbf{r}, \mathbf{r}') = N_0 \psi_0^*(\mathbf{r})\psi_0(\mathbf{r}') + \sum_{i \neq 0} n_i \psi_i^*(\mathbf{r})\psi_i(\mathbf{r}'). \tag{2.11}$$

At large distances $s = |\mathbf{r} - \mathbf{r}'|$, the only contribution that remains finite is that from the condensate. The contribution remains finite up to distances $|\mathbf{r} - \mathbf{r}'|$ fixed by the extension of the function ψ_0.

Suppose that BEC didn't exist, i.e., there is no macroscopically occupied state. Then in the limit $|\mathbf{r} - \mathbf{r}'| \to \infty$, every terms in (2.5) do not add up but rather cancel each other, since ψ_ν's are orthogonal to each other. Thus $\sigma_1(\mathbf{r}, \mathbf{r}'; t)$ will not remain on the order of N/V, i.e., the system will not show ODLRO. We have just proved that ODLRO implies the onset of BEC.

If BEC occurred only in the $\nu = 0$ mode, that is, $n_0 = \mathcal{O}(N)$ and $n_{\nu\neq 0} = \mathcal{O}(1)$, then, in the limit $|\mathbf{r} - \mathbf{r}'| \to \infty$, we have

$$\begin{aligned}\sigma_1(\mathbf{r}, \mathbf{r}'; t) &\to n_0 \psi_0^*(\mathbf{r}, t)\psi_0(\mathbf{r}', t) \\ &\equiv \Psi^*(\mathbf{r}, t)\Psi(\mathbf{r}', t).\end{aligned}$$

We refer to

$$\Psi(\mathbf{r}, t) := \sqrt{n_0}\psi_0(\mathbf{r}, t)$$

as **condensate wavefunction** or **order parameter** and n_0 as the number of condensed Bosons. $\Psi(\mathbf{x}, t)$ can be understood as an eigenfunction of the single-particle reduced density matrix $\sigma_1(\mathbf{x}, \mathbf{y}; t)$:

$$\int d\mathbf{x}\, \sigma_1(\mathbf{x}, \mathbf{y})\Psi(\mathbf{x}, t) \simeq n_0 \Psi(\mathbf{y}, t), \qquad n_0 = \int d\mathbf{x}\, |\Psi(\mathbf{x}, t)|^2. \tag{2.12}$$

We note that if $\Psi(\mathbf{x}, t)$ is a solution to the eigenvalue problem (2.12), $\Psi(\mathbf{x}, t)e^{i\phi}$ is also a solution to it, where ϕ is an arbitrary real number. The global phase of the condensate wavefunction is therefore arbitrary. Making an explicit choice for the value of the order parameter corresponds to a formal breaking of gauge symmetry, the **U(1) symmetry breaking**.

2.4 Uniform and Isotropic Case

Let us consider the case of uniform and isotropic system of N particles occupying a volume V in the absence of external potentials. In the thermodynamic limit, where $N, V \to \infty$ with the density $n = N/V$ kept fixed, the single-particle density matrix depends only on the modulus of the relative position $\mathbf{s} = \mathbf{r} - \mathbf{r}'$, and the solutions of (2.6) are plane waves:

$$\psi_{\mathbf{p}}(\mathbf{r}) = \frac{1}{\sqrt{V}} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \tag{2.13}$$

with the value of $\mathbf{p}$ being determined by the boundary consitions and the eigenvalues are given by

$$n_{\mathbf{p}} = \int_V d\mathbf{r}' \; \sigma_1(r') e^{i\mathbf{p}\cdot\mathbf{r}'/\hbar}.$$

The expansion (2.11) now becomes

$$\sigma_1(s) = N_0/V + \frac{1}{V} \sum_{\mathbf{p}\neq 0} n_{\mathbf{p}} e^{-i\mathbf{p}\cdot\mathbf{s}/\hbar}. \tag{2.14}$$

One finds that, in the presence of BEC, the single-particle density matrix does not vanish at large distances but approaches a finite value: $\sigma_1(s) \to N_0/V \quad \text{as} \quad s \to \infty$. This behaviour was pointed out by Landau(1951), Penrose(1951) and Penrose and Onsager (1956) and is often referred to as off-diagonal long-range order, since it involves the nondiagonal components ($\mathbf{r} \neq \mathbf{r}'$) of the single-particle density matrix (2.1).

The above considerations also hold in the presence of interactions. For example, while in the ideal gas all the particles are in the condensate at $T = 0$ and $N_0 = N$, in the presence of interactions one has $N_0 < N$ even at $T = 0$. The condensate fraction N_0/N depends on the temperature of the sample and vanishes above the critical temperature T_c for Bose-Einstein condensation. In Fig. 2.1 the behaviour of $\sigma_1(s)$ at different temperatures is shown.

2.5 Bogoliubov Approximation

The wave function relative to the macroscopic eigenvalue N_0 plays a crucial role in the theory of BEC and characterizes the so-called wave function of the condensate. We separate in the field operator (2.9) the 'condensate' term $i = 0$ from the other components:

$$\hat{\Psi}(\mathbf{r}) = \psi_0(\mathbf{r})\hat{a}_0 + \sum_{i\neq 0} \psi_i(\mathbf{r})\hat{a}_i. \tag{2.15}$$

The **Bogoliubov approximation** is to treating the macroscopic component $\varphi_0\hat{a}_0$ of the field operator (2.15) as a classical field be the approximation $\hat{a}_0 \approx \sqrt{N_0}$ so that eq.(2.15) can be

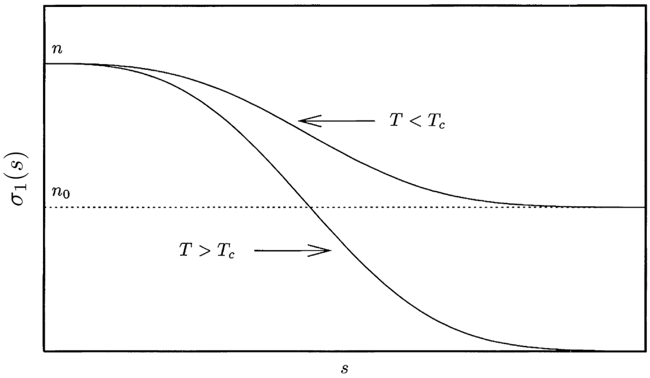


Figure 2.1: Off-diagonal single-particle density as a function of the relative distance s. For temperatures below the critical temperature, $\sigma_1(s)$ approaches, for large s, the value $n_0 = N_0/V$, where N_0 is the number of particles in the condensate. At $s = 0$, $\sigma_1(s)$ coincides with the diagonal density $n = N/V$.

rewritten as

$$\hat{\Psi}(\mathbf{r}) = \Psi_0(\mathbf{r}) + \delta\hat{\Psi}(\mathbf{r}), \tag{2.16}$$

where we have defined $\Psi_0 = \sqrt{N_0}\psi_0$ and $\delta\hat{\Psi} = \sum_{i\neq 0}\psi_i\hat{a}_i$.

The function $\Psi_0(\mathbf{r})$ is called the wave function of the condensate or the order parameter. It is a complex quantity, characterized by its modulus and phase:

$$\Psi_0(\mathbf{r}) = |\Psi_0(\mathbf{r})|e^{i\Phi(\mathbf{r})}. \tag{2.17}$$

The phase $\Phi(\mathbf{r})$ plays a major role in characterizing the coherence and superfluid phenomena. The order parameter (2.17) characterizes the Bose-Einstein condensed phase and vanishes above the critical temperature. As one can see from its definition (2.11), the order parameter $\Psi_0 = \sqrt{N_0}\psi_0$ is defined only up to a constant phase factor. One can always multiply this function by the numerical factor $e^{i\alpha}$ without changing any physical property. Making an explicit choice for the value of the order parameter corresponds to a formal breaking of gauge symmetry.

One can write $\Psi_0 = \langle\hat{\Psi}\rangle$, having in mind that the states on the left have one less particle in the condensate than the states on the right.

If we take this average over stationary states whose time dependence is governed by the law $e^{-iEt/\hbar}$, it is easy to see that the time dependence of the order parameter is given by the law

$$\Psi_0(\mathbf{r}, t) = \Psi_0(\mathbf{r}) e^{-i\mu t/\hbar},$$

where $\mu = E(N) - E(N-1) \sim \partial E/\partial N$ is the chemical potential. It is interesting to remark that the time evolution of the order parameter is not governed by the energy, as happens with usual wave functions, but by the chemical potential which emerges as a key parameter in the physics of Bose-Einstein condensates.

Chapter 3

Description of the System

3.1 Lagrangian Density of the System

We start our discussion with the Lagrangian density of a Bose gas comprising atoms or molecules of mass m,

$$\mathcal{L} = \frac{i\hbar}{2}\big(\Psi^*\partial_t\Psi - \partial_t\Psi^*\Psi\big) - \frac{\hbar^2}{2m}|\nabla\Psi|^2 - V_{\rm ext}|\Psi|^2 - \frac{1}{2}|\Psi|^2 \int d^3\mathbf{R}'\, V_{\rm int}(\mathbf{R}-\mathbf{R}')|\Psi(\mathbf{R}')|^2, \tag{3.1}$$

where $\mathbf{R} = (\mathbf{r}, z)$ are spatial 3D coordinates. The system is trapped by an external trapping potential of the form

$$V_{\rm ext}(\mathbf{R}, t) = \frac{1}{2}m\omega_\perp^2\mathbf{r}^2 + \frac{1}{2}m\omega_z^2 z^2,$$

where both $\omega_\perp$ and ω_z can in general be time-dependent. We will assume that, over the whole time evolution, the gas is strongly confined in z direction, with aspect ratio $\kappa = \omega_z/\omega_\perp \gg 1$. We also assume quasi-homogeneity in the plane, i.e. that the relevant wavelengths of quasiparticle excitations are much shorter than the inhomogeneity scale caused by the in-plane harmonic trapping.

The two-body interaction is given by

$$V_{\rm int}(\mathbf{R}-\mathbf{R}') = g_c\delta^3(\mathbf{R}-\mathbf{R}') + V_{dd}(\mathbf{R}-\mathbf{R}'),$$

where g_c is the contact interaction coupling which is given by the s-wave scattering length a_s via

$$g_c = \frac{4\pi\hbar^2 a_s}{m}.$$

The scattering length arises in describing collision or scattering between particles. In scattering theory, the asymptotic wavefunction for scattered particle reads

$$\psi(r,\theta) = e^{ikz} + f(\theta)\frac{e^{ikr}}{r}.$$

The differential cross section, i.e. the probability per unit time to scatter into the direction $\mathbf{k}$ can be obtained as

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 .$$

In case of θ independent s-wave scattering, the total cross section becomes

$$\sigma = 4\pi |f|^2 =: 4\pi a_s^2 .$$

The contact coupling g_c or s-wave scattering length a_s is positive/negative when the interaction between atoms is repulsive/attractive. On the other hand, $V_{dd}(\mathbf{R} - \mathbf{R}')$ describes the dipole-dipole interaction (DDI) assuming the dipoles to be polarized along z-direction by an external field, so that their interaction is given by

$$V_{dd}(\mathbf{R}, t) = \frac{3g_d}{4\pi} \frac{1 - 3z^2/|\mathbf{R}|^2}{|\mathbf{R}|^3}, \tag{3.2}$$

where $g_d = \mu d_m^2/3$ for magnetic and $g_d = d_e^2/3\varepsilon$ for electric dipoles. Contrary to the contact interaction, DDI is long-ranged and anisotropic. We note that, for the stability of the condensate, the interaction should be dominantly repulsive. Thus we need the strong confinement in z-direction so that DDI is dominantly repulsive.

In general, g_c and g_d can be time-dependent, depending on the protocol of condensate expansion or contraction which is implemented, see below. We denote by $g_{c,0}$ and $g_{d,0}$ their initial, $t = 0$, values. We have a scaling law $V_{\rm int}(\Lambda \mathbf{R}) = \Lambda^\alpha V_{\rm int}(\mathbf{R})$ [81] for a combined 3D contact and dipolar potential with $\alpha = -3$. Note that the scaling equation (3.12) below is thus 3D.

We note here that the analysis can equivalently be formulated in Heisenberg formalism, in which the system is described by the Hamiltonian in second quantized form,

$$\begin{aligned}\hat{\mathcal{H}} = \int d^3\mathbf{R} \left[-\frac{\hbar^2}{2m} \hat{\Psi}^\dagger(\mathbf{R}) \nabla^2 \hat{\Psi}(\mathbf{R}) + \hat{\Psi}^\dagger(\mathbf{R}) V_{\rm ext}(\mathbf{R}) \hat{\Psi}(\mathbf{R}) \right] \\ + \frac{1}{2} \int d^3\mathbf{R}\, d^3\mathbf{R}'\, \hat{\Psi}^\dagger(\mathbf{R}) \hat{\Psi}^\dagger(\mathbf{R}') V_{\rm int}(\mathbf{R} - \mathbf{R}') \hat{\Psi}(\mathbf{R}') \hat{\Psi}(\mathbf{R}).\end{aligned}$$

The unitary time evolution in the Heisenberg picture, i.e., the Heisenberg equation of motion for the field operator reads,

$$i\hbar\frac{\partial\hat{\Psi}}{\partial t} = [\hat{\Psi},\hat{\mathcal{H}}] = \Big[-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{ext}}(\mathbf{R}) + \int d^3\mathbf{R}'\, V_{\text{int}}(\mathbf{R}-\mathbf{R}')\hat{\Psi}^\dagger(\mathbf{R}')\hat{\Psi}(\mathbf{R}')\Big]\hat{\Psi}.$$

3.2 Dimensional Reduction

To ensure stability in the DDI dominated regime [63], we impose the system to stay sufficiently close to the quasi-2D regime during expansion. In the limit of zero-point energy of the axial harmonic oscillator greatly exceeding the chemical potential, and for large aspect ratio, the longitudinal and transversal degrees of freedom decouple and we factorize the order parameter $\Psi(\mathbf{R},t)$ as follows.

$$\Psi(\mathbf{R},t) = \Psi_\perp(\mathbf{r},t)\Phi_z(z)e^{-i\omega_z t/2}. \tag{3.3}$$

Here $\Phi_z(z)$ describes the zero point oscillations in a harmonic oscillator potential, and is given by

$$\Phi_z(z) = \frac{1}{(\pi d_z^2)^{1/4}}\exp\Big[-\frac{z^2}{2d_z^2}\Big],$$

where $d_z = \sqrt{\hbar/m\omega_z}$ is the oscillator length. Improved estimates for d_z can be found by treating d_z as a parameter minimizing the Gross-Pitaevskiĭ ground-state energy [63, 82].

Substituting (3.3) into the action (3.1), and integrating out the z dependence, we obtain the reduced Lagrangian for the horizontal in-plane mode:

$$\begin{aligned}\mathcal{L}_\perp = \frac{i\hbar}{2}(\Psi_\perp^*\partial_t\Psi_\perp - \partial_t\Psi_\perp^*\Psi_\perp) - \frac{\hbar^2}{2m}|\nabla_\perp\Psi_\perp|^2 - \frac{m}{2}\omega_\perp^2 r^2|\Psi_\perp|^2 \\ - \frac{1}{2}|\Psi_\perp|^2\int d^2\mathbf{r}'\, V_{\text{int}}^{\text{2D}}(\mathbf{r}-\mathbf{r}')|\Psi_\perp(\mathbf{r}')|^2,\end{aligned}$$

where $\nabla_\perp = (\partial_x,\partial_y)$. The interaction potential is reduced to

$$V_{\text{int}}^{\text{2D}}(\mathbf{r}-\mathbf{r}') = \int dzdz'\, V_{\text{int}}(\mathbf{R}-\mathbf{R}')\rho_z(z)\rho_z(z'), \tag{3.4}$$

where $\rho_z = |\Phi_z|^2$ The nature of interactions can be seen clearly by looking at their Fourier space representations. Here and below, we will use asymmetric Fourier convention in which the inverse transform incorporates the whole prefactor. The Fourier transform of the density profile in z-direction ρ_z, for homogeneous density in the 2D plane, is given by

$$\rho_z(\mathbf{Q}) = V\delta^{(2)}_{\mathbf{q},0}\exp\left[-\frac{q_z^2 d_z^2}{4}\right],$$

where V is the area of the plane and $\mathbf{Q} = (\mathbf{q}, q_z)$. Substituting the inverse Fourier transforms of these expressions into (3.4), we obtain [63]

$$V^{\mathrm{2D}}_{\mathrm{int}}(\mathbf{r}-\mathbf{r}') = \frac{1}{\sqrt{2\pi}d_z}(g_c + 2g_d)\delta^{(2)}(\mathbf{r}-\mathbf{r}') - \frac{3}{2}\frac{g_d}{V}\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} q w\left[\frac{qd_z}{\sqrt{2}}\right]. \tag{3.5}$$

Here we made use of an integral representation of the error function [83]

$$w(z) \equiv e^{z^2}\mathrm{erfc}(z) = \frac{2z}{\pi}\int_0^\infty \frac{e^{-t^2}}{z^2+t^2}dt \quad (z>0), \tag{3.6}$$

where the complementary error function is defined as $\mathrm{erfc}(z) = 1 - \mathrm{erf}(z)$ and $\mathrm{erf}(z) = (2/\sqrt{\pi})\int_0^z \exp(-t^2)dt$. From (3.5), we see that the DDI contributes to the delta-function-like interaction. As a result, the interaction potential has the Fourier representation,

$$\begin{aligned} V^{\mathrm{2D}}_{\mathrm{int}}(q) &= \frac{1}{\sqrt{2\pi}d_z}(g_c + 2g_d) - \frac{3}{2}g_d\, q\, w\left[\frac{qd_z}{\sqrt{2}}\right] \\ &\equiv g^{\mathrm{eff}} - \frac{3}{2}g_d\, q\, w\left[\frac{qd_z}{\sqrt{2}}\right]. \end{aligned}$$

It is convenient to decompose the total (contact and dipolar) interaction into a sum of effective contact interaction and nonlocal interaction:

$$V^{\mathrm{2D}}_{\mathrm{int}}(\mathbf{r}-\mathbf{r}') = g^{\mathrm{eff}}\delta^{(2)}(\mathbf{r}-\mathbf{r}') + U^{\mathrm{2D}}(\mathbf{r}-\mathbf{r}'), \tag{3.7}$$

where the effective contact coupling strength is defined by

$$g^{\mathrm{eff}} \equiv g_c^{\mathrm{2D}} + \frac{2g_d}{\sqrt{2\pi}d_z} = \frac{1}{\sqrt{2\pi}d_z}(g_c + 2g_d),$$

and the nonlocal interaction is written as

$$U^{\mathrm{2D}}(\mathbf{r}-\mathbf{r}') = -\frac{3}{2}\frac{g_d}{V}\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} q w\left[\frac{qd_z}{\sqrt{2}}\right].$$

As a result, the action of the system becomes

$$\mathcal{L} = \frac{i\hbar}{2}(\Psi^*\partial_t\Psi - \partial_t\Psi^*\Psi) - \frac{\hbar^2}{2m}|\nabla\Psi|^2 - \frac{m}{2}\omega^2 r^2|\Psi|^2 - \frac{g^{\rm eff}}{2}|\Psi|^4 \\ - \frac{1}{2}|\Psi|^2\int d^2\mathbf{r}'\, U^{\rm 2D}(\mathbf{r}-\mathbf{r}')|\Psi(\mathbf{r}')|^2, \quad (3.8)$$

where we dropped subscripts for conciseness.

3.3 Scaling Transformation

We can prescribe an external time dependences not only with a temporal profile of the trap frequencies but also to $g_c = 4\pi\hbar^2 a_s/m$ and g_d by changing the s-wave scattering length a_s via Feshbach resonances [84, 85] and using a rotating polarizing field to change g_d [86], respectively. As a result, the gas cloud will adapt to these changes and will either expand or contract. Under the usual scaling transformation [87, 88], laid down in a very general form in [81], which is applicable to BECs with both time-dependent trapping and coupling constants, one imposes that the *scaling variables* $\mathbf{x}$, τ, and ψ obey

$$\mathbf{x} \equiv \frac{\mathbf{r}}{b(t)}, \qquad \tau \equiv \int_0^t \frac{1}{b^2(t')}dt', \qquad \Psi(\mathbf{r},t) \equiv e^{i\Phi(\mathbf{x},t)}\frac{\psi(\mathbf{x},\tau)}{b}, \quad (3.9)$$

with a scale factor $b(t)$. Here $\Phi(\mathbf{x},t) = \frac{1}{2}\frac{m}{\hbar}r^2\frac{\partial_t b}{b}$ is chosen so as to describe the bulk velocity $\mathbf{v} = \dot{\mathbf{x}} = -\frac{1}{b}\frac{\hbar}{m}\nabla\Phi$, while the phase of ψ will represent the residual velocity potential, which can be regarded as small. The Lab time t is different from the (analogue) cosmic time τ. See below for more details.

Insertion of these ansatz into the action (3.8) yields

$$\mathcal{L} = \frac{i\hbar}{2}(\psi^*\partial_\tau\psi - \partial_\tau\psi^*\psi) - \frac{\hbar^2}{2m}|\nabla_{\mathbf{x}}\psi|^2 - \frac{m}{2}x^2\left(\frac{d^2b}{dt^2}b^3 + \omega^2 b^4\right)|\psi|^2 - \frac{g^{\rm eff}}{2}|\psi|^4 \\ - \frac{g_d}{2g_{d,0}b}\int d^2\mathbf{x}'\, U_0^{\rm 2D}(\mathbf{x}-\mathbf{x}')|\psi(\mathbf{x})|^2|\psi(\mathbf{x}')|^2, \quad (3.10)$$

where $\nabla_{\mathbf{x}} = (\partial_x, \partial_y)$. Note that the measure $dtd^2\mathbf{r}$ gives an additional factor of b^4 by the relation $dtd^2\mathbf{r} = b^4 d\tau d^2\mathbf{x}$. The scaled nonlocal interaction is written as

$$U_0^{\rm 2D}(\mathbf{x}-\mathbf{x}') = -\frac{3}{2}\frac{g_{d,0}}{V}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}kw\left[\frac{kd_{z,0}}{\sqrt{2}}\right],$$

where $g_{d,0}$ and $d_{z,0}$ are initial values. In order to obtain this expression, we have assumed a scaling condition

$$d_z(t) = d_{z,0} b(t) \quad \text{or} \quad \omega_z(t) = \frac{\omega_{z,0}}{b^2(t)}. \tag{3.11}$$

We combine the remaining time dependences into a single factor $f(t)$ by imposing [73, 81, 89] $[b(0) = f(0) = 1]$

$$f^2 = \frac{b^3 \partial_t^2 b + b^4 \omega^2(t)}{\omega_0^2} = \frac{g_c(t)}{g_{c,0} b} = \frac{g_d(t)}{g_{d,0} b}, \tag{3.12}$$

to obtain the action of the form

$$\mathcal{L} = \frac{i\hbar}{2}(\psi^* \partial_\tau \psi - \psi \partial_\tau \psi^*) - \frac{\hbar^2}{2m} |\nabla_{\mathbf{x}} \psi|^2 - f^2 \left[\frac{m}{2} \omega_0^2 x^2 |\psi|^2 + \frac{g_0^{\text{eff}}}{2} |\psi|^4 \right. \\ \left. + \frac{1}{2} \int d^2\mathbf{x}' \, U_0^{\text{2D}}(\mathbf{x} - \mathbf{x}') |\psi(\mathbf{x})|^2 |\psi(\mathbf{x}')|^2 \right]. \tag{3.13}$$

Given experimentally prescribed time dependences of trapping and couplings, the above relations determine the scaling expansion. On the other hand, given a desired scaling expansion or contraction $b = b(t)$, to which, e.g., the time dependence of the speed of sound $c = c(t)$ is related via $f(t)$, one can determine the required trapping frequencies, imposing possibility in addition a temporal dependence of the coupling constants. Note that for the scaling approach to accurately yield the expansion or contraction dependence of the field operator in a gas with both contact and dipolar interactions present (i.e., for the scaling evolution to follow a symmetry), the contact g_c and dipole g_d couplings are required to either have an identical time dependence, or to both remain constant. We remark that when one of the $g_{c,0},\ g_{d,0}$ equals zero, the terms $g_c(t)/g_{c,0}b$ or $g_d(t)/g_{d,0}b$, respectively, do not appear as a constraint on the right hand side of the equation (3.12) for f^2.

We recombine the interaction terms and rewrite the action (3.13) as

$$\mathcal{L} = \frac{i\hbar}{2}(\psi^* \partial_\tau \psi - \psi \partial_\tau \psi^*) - \frac{\hbar^2}{2m} |\nabla_{\mathbf{x}} \psi|^2 - f^2 \left[\frac{m}{2} \omega_0^2 x^2 \right. \\ \left. + \frac{1}{2} \int d^2\mathbf{x}' \, V_{\text{int},0}^{\text{2D}}(\mathbf{x} - \mathbf{x}') |\psi(\mathbf{x}')|^2 \right] |\psi|^2, \tag{3.14}$$

where $V_{\text{int},0}^{\text{2D}}(\mathbf{x} - \mathbf{x}') = (1/V) \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} V_{\text{int},0}^{\text{2D}}(k)$ with V the area of the plane, and the quasi-2D Fourier transform of the interaction potential is, for the stationary initial state, given by the analytic expression [63]

$$V^{\mathrm{2D}}_{\mathrm{int},0}(k) = g_0^{\mathrm{eff}} \left\{ 1 - \frac{3R}{2} \zeta w \left[\frac{\zeta}{\sqrt{2}} \right] \right\}, \tag{3.15}$$

where $w[z] = \exp[z^2](1 - \mathrm{erf}[z])$ denotes the w function and $\zeta = kd_{z,0}$ is a dimensionless wavenumber. Furthermore,

$$g_0^{\mathrm{eff}} = \frac{1}{\sqrt{2\pi} d_{z,0}} (g_{c,0} + 2g_{d,0}) \tag{3.16}$$

is an effective contact coupling. We also defined

$$R = \frac{\sqrt{\pi/2}}{1 + g_{c,0}/2g_{d,0}}. \tag{3.17}$$

The parameter R ranges from $R = 0$ if $g_{d,0}/g_{c,0} \to 0$, to $R = \sqrt{\pi/2}$ for $g_{d,0}/g_{c,0} \to \infty$ and expresses the relative strength of contact and dipolar interactions. In the remainder of the thesis, we put either $R = 0$ (contact dominance) or $R = \sqrt{\pi/2}$ (DDI dominance).

Chapter 4

Analyzing the System

4.1 Zeroth-Order Analysis

From the action (3.14), we obtain the nonlocal Gross-Pitaevskiĭ equation

$$i\hbar\partial_\tau\psi = -\frac{\hbar^2}{2m}\nabla^2_{\mathbf{x}}\psi + f^2\left[\frac{m}{2}\omega_0^2\mathbf{x}^2 + \int d^2\mathbf{x}'\,V^{\rm 2D}_{\rm int,0}(\mathbf{x}-\mathbf{x}')|\psi(\mathbf{x}')|^2\right]\psi. \tag{4.1}$$

In terms of the Madelung representation for the scaled order parameter, $\psi = \sqrt{\rho}e^{i\phi}$, the equation of motion (4.1) can be recast as

$$\partial_\tau\rho = -\frac{\hbar}{m}(\nabla_{\mathbf{x}}\phi\cdot\nabla_{\mathbf{x}}\rho + \rho\nabla^2_{\mathbf{x}}\phi), \tag{4.2}$$
$$-\hbar\partial_\tau\phi = -\frac{\hbar^2}{2m\sqrt{\rho}}\nabla^2_{\mathbf{x}}\sqrt{\rho} + \frac{\hbar^2}{2m}(\nabla_{\mathbf{x}}\phi)^2 + f^2\left[\frac{m}{2}\omega_0^2\mathbf{x}^2 + \int d^2\mathbf{x}'\,V^{\rm 2D}_{\rm int,0}(\mathbf{x}-\mathbf{x}')\rho(\mathbf{x}')\right],$$

If we linearize the fields around stationary background solutions, $\rho = \rho_0+\delta\rho$, $\phi = \phi_0+\delta\phi$, the zeroth order equations are the same as (4.2) with subscripts 0 attached to the fields, and the first order equations are the Bogoliubov equations (4.10).

We solve the zeroth order equations assuming vanishingly small residual comoving frame velocity ($\mathbf{v}_{\rm com} \equiv \frac{\hbar}{m}\nabla_x\phi_0 = 0$) by the ansatz $\psi_0(\mathbf{x},\tau) = \sqrt{\rho_0(\mathbf{x})}e^{i\phi_0(\tau)}$ [27], and neglect the kinetic energy term, which is equivalent to neglecting terms proportional to $\nabla^2_x\sqrt{\rho_0}$. Then we obtain a spatially constant phase function

$$\phi_0(\tau) = -\frac{\mu_0}{\hbar}\int_0^\tau d\tau'\,f^2(\tau'), \tag{4.3}$$

where μ_0 is initial chemical potential, and an integral equation for time independent density profile

$$\int d^2\mathbf{x}'\,V^{\rm 2D}_{\rm int,0}(\mathbf{x}-\mathbf{x}')\rho_0(\mathbf{x}') = \mu_0 - \frac{m}{2}\omega_0^2\mathbf{x}^2, \tag{4.4}$$

which can be solved numerically. Because of the partially attractive nature of DDI, the profile shows enhanced concentration at the center compared to the pure contact case, cf.

Fig. 4.1. Also, the anisotropy of the interaction results in the appearance of small wiggles in the density profile [90, 91].

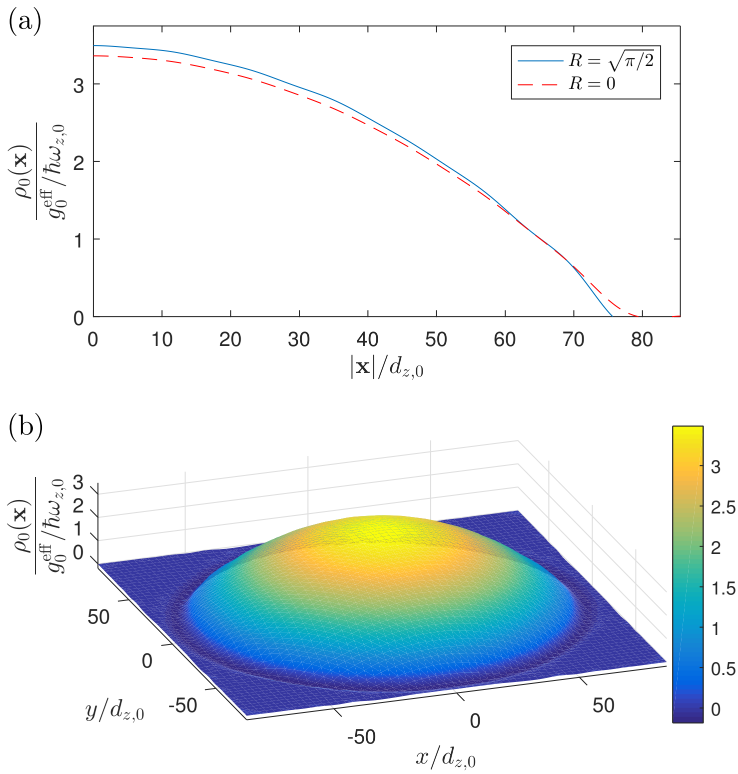


Figure 4.1: The density profile of the gas in units of $g_0^{\text{eff}}/\hbar\omega_{z,0}$ as a function of radial distance in units of $d_{z,0}$. In (a), blue solid and red dashed line corresponds to DDI-dominant and contact-dominant cases, repectively. We also present a visualization of the gas in (b), using parameters appropriate for erbium atoms [92]. Namely, particle number $N = 9.5 \times 10^4$, magnetic moment $d_m = 7\,\mu_B$, Boson mass $m = 168\,\text{u}$, aspect ratio $\kappa_0 = 30$, and transverse trapping frequency $\omega_{z,0} = 2\pi \times 5435\,\text{Hz}$.

4.2 First-Order Analysis

Now we consider the first order equations. We assume that the planar cloud size greatly exceeds the wavelengths of relevant Bogoliubov excitations in the plane. Especially near the center of cloud, density gradients are thus negligible, and we approximate the 2D comoving density $\rho_0 \simeq$ const. The Bogoliubov equations for density and phase fluctuations read,

$$(\partial_\tau + \mathbf{v}_{\rm com}\cdot\nabla_{\mathbf{x}})\,\delta\rho = -\frac{\hbar\rho_0}{m}\nabla^2_{\mathbf{x}}\delta\phi - \frac{\hbar}{m}\nabla_{\mathbf{x}}\rho_0\cdot\nabla_{\mathbf{x}}\delta\phi - (\nabla_{\mathbf{x}}\cdot\mathbf{v}_{\rm com})\delta\rho, \tag{4.5}$$

$$(\partial_\tau + \mathbf{v}_{\rm com}\cdot\nabla_{\mathbf{x}})\,\delta\phi = -\frac{f^2 g_0^{\rm eff}}{\hbar}\mathcal{W}\delta\rho + \frac{\hbar}{2m\rho_0}\nabla_{\mathbf{x}}\cdot\big[\frac{\delta\rho}{\sqrt{\rho_0}}\nabla_{\mathbf{x}}\sqrt{\rho_0}\big], \tag{4.6}$$

where $\mathcal{W}$ is an integral operator defined by

$$\mathcal{W} \equiv \int d^2\mathbf{x}'\left[\frac{1}{V}\sum_{\mathbf{k}}\mathcal{W}_k e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}\right]\star(\mathbf{x}'), \tag{4.7}$$

$$\mathcal{W}_k = 1 - \frac{3R}{2}\zeta w\left[\frac{\zeta}{\sqrt{2}}\right] + \frac{\zeta^2}{4Af^2}, \qquad A = \frac{mc_0^2}{\hbar\omega_{z,0}}, \tag{4.8}$$

where $\star$ stands for the argument upon which the integral operator acts. Here, $c_0 = \sqrt{g_0^{\rm eff}\rho_0/m}$ is the speed of sound and $\mathbf{v}_{\rm com} = (\hbar/m)\nabla_{\mathbf{x}}\phi_0$ is the commoving frame velocity.

Rewriting in the momentum space, the Bogoliubov equations become, with comoving momentum $\mathbf{k}$, assuming vanishingly small comoving velocity and quasi-homogeneity,

$$(\partial_\tau + i\mathbf{v}_{\rm com}\cdot\mathbf{k})\delta\rho_{\mathbf{k}} = \frac{\hbar\rho_0}{m}k^2\delta\phi_{\mathbf{k}}, \tag{4.9}$$

$$(\partial_\tau + i\mathbf{v}_{\rm com}\cdot\mathbf{k})\delta\phi_{\mathbf{k}} = -\frac{f^2 g_0^{\rm eff}}{\hbar}\mathcal{W}_k\delta\rho_{\mathbf{k}},, \tag{4.10}$$

Solving (4.10) for $\delta\rho_{\mathbf{k}}$ and substituting into (4.9) yields

$$(\partial_\tau + i\mathbf{v}_{\rm com}\cdot\mathbf{k})^2\delta\phi_k + \left(2\frac{\dot a}{a} - \frac{\dot{\mathcal{W}}_k}{\mathcal{W}_k}\right)(\partial_\tau + i\mathbf{v}_{\rm com}\cdot\mathbf{k})\delta\phi_k + \left(\frac{c_0 k}{a}\right)^2\mathcal{W}_k\delta\phi_k = 0, \tag{4.11}$$

where overdot denotes τ derivatives. We have introduced the Friedmann-Robertson-Walker (FRW) cosmological scale factor by $a(t) \equiv 1/f(t)$, see below for a detailed discussion.

In an adiabatic regime [89], momentarily ignoring time derivatives of a and $\mathcal{W}_k$, and assuming vanishingly small comoving velocity, $\mathbf{v}_{\rm com} = 0$, the dispersion relation of Bogoliubov excitations reads

$$\frac{\varepsilon^2}{(\hbar\omega_{z,0})^2} = \frac{A\zeta^2}{a^2}\left(1 - \frac{3R}{2}\zeta w\left[\frac{\zeta}{\sqrt{2}}\right]\right) + \frac{\zeta^4}{4}, \tag{4.12}$$

where the the dimensionless parameter, $R = g_{d,0}/(d_{z,0}g_0^{\rm eff}) = \sqrt{\pi/2}/(1 + g_{c,0}/2g_{d,0})$,

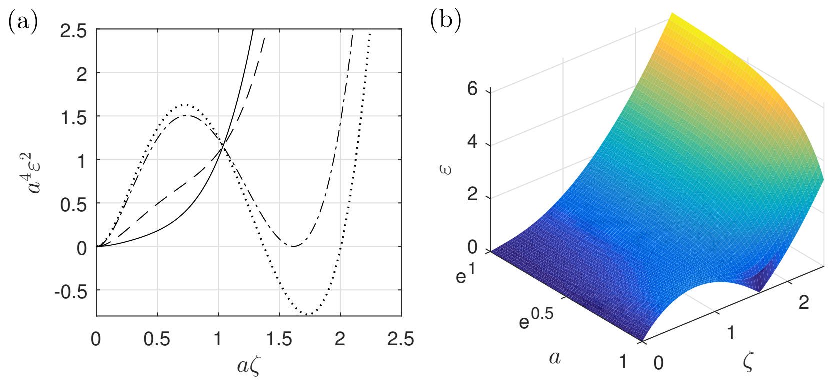


Figure 4.2: (a) Squared Bogoliubov excitation energy in units of $\hbar^4/4m^2d_{z,0}^4$, for DDI dominance, $R = \sqrt{\pi/2}$. Counting from bottom to top at small ζ, A in (4.8) is $A_c/10$, $A_{\min}$, A_c, and $1.1A_c$. For $A > A_{\min} = 1.249$, the spectrum develops a roton minimum, and becomes unstable for $A > A_c = 3.4454$. (b) Time evolution of the Bogoliubov spectrum in the course of expansion at criticality $A = A_c$. Initially, a roton minimum occurs, disappearing at late times.

ranges from $R = 0$ if $g_{d,0}/g_{c,0} \to 0$ to $R = \sqrt{\pi/2}$ for $g_{d,0}/g_{c,0} \to \infty$. In the latter DDI dominated case, the spectrum displays a **"roton" minimum** [62–64], which touches zero when A is equal to the critical value $A_c = 3.4454$, see Fig.4.2. Various ramifications of the dipolar BEC roton, originally defined for and observed in the strongly interacting superfluid helium II [65, 66], have been recently experimentally investigated in ultracold dipolar quantum gases [67–70].

Note here that, when working in Heisenberg formulation, we define the density and phase perturbation fields as

$$\delta\hat{\rho} := \psi_0^*\delta\hat{\psi} + \delta\hat{\psi}^\dagger\psi_0, \quad \delta\hat{\phi} := \frac{1}{2i\rho_0}[\psi_0^*\delta\hat{\psi} - \psi_0\delta\hat{\psi}^\dagger], \quad [\delta\hat{\rho}(\mathbf{x}), \delta\hat{\phi}^\dagger(\mathbf{x}')] = i\delta^{(2)}(\mathbf{x} - \mathbf{x}').$$

Then, the density $\hat{\rho} = \hat{\psi}^\dagger\hat{\psi}$ and current $\hat{\mathbf{j}} = \frac{\hbar}{2mi}\left[\hat{\psi}^\dagger\nabla_{\mathbf{x}}\hat{\psi} - \nabla_{\mathbf{x}}\hat{\psi}^\dagger\hat{\psi}\right]$ operators have the following expansion.

$$\hat{\rho} = \rho_0 + \delta\hat{\rho}, \qquad \hat{\mathbf{j}} = \rho_0\mathbf{v}_{\rm com} + \delta\hat{\rho}\mathbf{v}_{\rm com} + \rho_0\delta\mathbf{v}, \qquad \delta\mathbf{v} := \frac{\hbar}{m}\nabla_{\mathbf{x}}\delta\hat{\phi},$$

where $\rho_0 = |\psi_0|^2$ and $\mathbf{v}_{com} = (\hbar/m)\nabla_{\mathbf{x}}\phi_0$. The density and phase perturbation operators defined above satisfy the same Bogoliubov equations (4.5) and (4.6).

Chapter 5

Gravitational Analogy

5.1 Effective FRW Universe in the Condensate

In the long-wavelength limit, $\mathcal{W}_k \to 1$, and (4.11) becomes

$$(\partial_\tau + i\mathbf{v}_{\mathrm{com}} \cdot \mathbf{k})^2 \delta\phi_k + 2\frac{\dot{a}}{a}(\partial_\tau + i\mathbf{v}_{\mathrm{com}} \cdot \mathbf{k})\delta\phi_k + \left(\frac{c_0 k}{a}\right)^2 \delta\phi_k = 0. \tag{5.1}$$

Rewriting the equation (5.1) in real space, the resulting equation is equivalent to the phases only Lagrangian,

$$\overline{\mathcal{L}^{(2)}} = \frac{\hbar^2/2}{f^2 g_0^{\mathrm{eff}}}(D\delta\phi)^2 - \frac{\hbar^2 \rho_0}{2m}(\nabla_{\mathbf{x}}\delta\phi)^2, \tag{5.2}$$

where $D = \partial_\tau + \mathbf{v}_{\mathrm{com}} \cdot \nabla_{\mathbf{x}}$ is the comoving derivative. Now the gravitational analogy can be drawn by introducing a dimensionless symmetric rank 2 tensor

$$g_{\mu\nu} = \frac{a^2}{\Omega^2}\begin{pmatrix} (c_s^2 - \mathbf{v}_{\mathrm{com}}^2)/c_0^2 & \mathbf{v}_{\mathrm{com}}/c_0 \\ \mathbf{v}_{\mathrm{com}}/c_0 & -\mathbf{1} \end{pmatrix} \tag{5.3}$$

where $c_s(\tau) = (1/a)\sqrt{g_0^{\mathrm{eff}}\rho_0/m}$ is the speed of sound and $c_0 = c_s(0)$. The conformal factor Ω is dimensionless and defined by

$$\Omega = \frac{c_0^2 m^2}{\hbar^2 \rho_0}. \tag{5.4}$$

With the metric tensor (5.3), the Lagrangian becomes that of a minimally coupled free scalar field in a curved spacetime

$$\overline{\mathcal{L}^{(2)}} = \frac{mc_0^2}{2}\sqrt{|g|}g^{\mu\nu}\partial_\mu\delta\phi\partial_\nu\delta\phi, \tag{5.5}$$

where repeated indices imply summation over $\mu = 0,\, 1,\, 2$ and $x^0 = c_0\tau$.

For the background solutions (4.3) and (4.4), $\mathbf{v}_{\mathrm{com}} = (\hbar/m)\nabla_{\mathbf{x}}\phi_0 = \mathbf{0}$ and ρ_0 is time independent. In this case the line element (5.3) becomes

$$ds^2 = \Omega^{-2}\big(c_0^2 d\tau^2 - a^2 d\mathbf{x}^2\big), \quad a = \frac{1}{f}. \tag{5.6}$$

Herein, we assume that the density ρ_0 is essentially homogeneous near the center of cloud. This implies that ω_0, the trapping frequency in the scaled coordinate system, is negligible compared to the time scale of the effective spacetime (that is the Hubble constant H, cf. (5.14)). Then Ω as defined in (5.6) becomes spatially constant, and the action (5.5) is invariant under the conformal transformation

$$\tilde{g}_{\mu\nu} = \Omega^2 g_{\mu\nu} \quad \text{and} \quad \delta\tilde{\phi} = \Omega^{-1/2}\delta\phi, \tag{5.7}$$

and the resulting metric $\tilde{g}_{\mu\nu}$ assumes the form of FRW universe

$$ds^2 = c_0^2 d\tau^2 - a^2 d\mathbf{x}^2 = \tilde{g}_{\mu\nu} dx^\mu dx^\nu, \tag{5.8}$$

where $\tilde{g}_{\mu\nu} = \mathrm{diag}(1, -a^2, -a^2)$. Now we can apply standard techniques of quantum field theory in a FRW universe to obtain independent solutions for $\delta\tilde{\phi}$. Then the independent solutions for original field $\delta\phi$ will be obtained by $\delta\phi = \Omega^{1/2}\delta\tilde{\phi}$.

In this effective spacetime, the Klein-Gordon (KG) equation for massless, minimally coupled free scalar field,

$$\Box\delta\tilde{\phi} = (1/\sqrt{|\tilde{g}|})\partial_\mu(\sqrt{|\tilde{g}|}\tilde{g}^{\mu\nu}\partial_\nu\delta\tilde{\phi}) = 0, \tag{5.9}$$

takes the form

$$\delta\ddot{\tilde{\phi}}_k + 2\frac{\dot{a}}{a}\delta\dot{\tilde{\phi}}_k + \left(\frac{c_0 k}{a}\right)^2 \delta\tilde{\phi}_k = 0, \tag{5.10}$$

which is the same as (5.1) provided $\mathbf{v}_{\mathrm{com}} = 0$ and $\delta\phi = \Omega^{1/2}\delta\tilde{\phi}$. Here, for ease of connecting the current discussion to a standard cosmological context, we introduce the conformal time

$$\eta \equiv \int_\infty^\tau \frac{c_0}{a(\tau')} d\tau', \tag{5.11}$$

which ranges from $-\infty$ $(\tau \to -\infty)$ to 0 $(\tau \to \infty)$. Then the metric (5.6) takes the conformally flat form $ds^2 = a^2[d\eta^2 - d\mathbf{x}^2]$, and the equation (5.1) can be recast in terms of an auxiliary field $\chi_k \equiv \sqrt{a}\delta\tilde{\phi}_k$ by

$$\partial_\eta^2 \chi_k + \left[k^2 - \frac{\partial_\eta^2 a}{2a} + \frac{(\partial_\eta a)^2}{4a^2}\right]\chi_k = 0 \quad \Leftrightarrow \quad \partial_\eta^2 \chi_k + \omega_\eta^2(\eta)\chi_k = 0. \tag{5.12}$$

Comparing this equation with Eq. (1) in [74], one identifies ω_η as an effective comoving frame mode frequency. The choice of auxiliary field χ_k is motivated by removing the first derivative term in (5.10).

5.2 Ideal de Sitter Expansion

We consider de Sitter spacetime by setting $a(\tau) = 1/f(\tau) = e^{H\tau}$. There are several simple analytic solutions to the scaling equation (3.12) for the realization of analogue de Sitter spacetime. For example one can consider $b \equiv 1 \,\forall\, t$, so that scaling time equals lab time, $\tau = t$, and obtain the scale factor evolution

$$a^{-2}(t) = e^{-2Ht} = \frac{\omega^2}{\omega_0^2} = \frac{g_c}{g_{c,0}} = \frac{g_d}{g_{d,0}}. \tag{5.13}$$

While this expansion has the advantage that the gas does not need to expand [$b(t) = 1 \,\forall\, t$ and thus $\tau \equiv t$], comes with the experimental difficulty that both couplings need to vary exponentially rapidly in lab time, see Eqs. (5.13). While this is, in principle, possible [86], also cf. Ref. [93], we keep for the below discussion g_c as well as g_d constant; then $a^2(t) = b(t)$. For de Sitter expansion, $a(\tau) = 1/f(\tau) = e^{H\tau}$, and thence in the lab,

$$b(t) = \sqrt{4Ht + 1}, \quad \omega^2(t) = \omega_0^2/b^5 + 4H^2/b^4. \tag{5.14}$$

The radial condensate velocity then scales as $v = 2Hr/b^2$ and the kinetic energy per particle, relative to $\omega_{z,0}$, as A/b^2. It thus decreases $\propto \omega_z$, ensuring proximity to the quasi-2D limit $\forall\, t$. Our numerical analysis is based on this solution. Note that we assume ω_0 to be negligible compared to H in the quasihomogeneous limit. The much slower (in comoving τ space) pre-de Sitter stage of cosmic expansion, $t < 0$, is conceived such that it $\approx$ adiabatically leads to $\partial_t b(0) = 2H$, and can be used to simulate as well the radiation- [$a(\tau) \propto \tau^{1/2}$] and matter-dominated [$a(\tau) \propto \tau^{2/3}$] eras [94], by appropriately tuning $\omega(t)$ and/or $g_{c,d}(t)$.

A simple parameter can help us understand the underlying physical process and characterize appropriate asymptotic regimes. Define

$$s \equiv \frac{c_0/H}{a/k} = \frac{c_0 k}{Ha}, \tag{5.15}$$

which is the ratio of Hubble radius to the physical wavelength of a chosen mode. The parameter s starts from ∞ and approaches zero when τ runs from $-\infty$ to ∞, that is when conformal time $\eta \equiv \int_\infty^\tau d\tau' c_0/a(\tau')$, ranges from $-\infty$ to 0. Note that, in the de Sitter analogue $a = e^{H\tau}$, the conformal time becomes $\eta = -c_0/Ha$, and the parameter s can be written employing conformal time simply as $s = -k\eta$. One can see that the horizon crossing time η_k of a chosen wavenumber k is determined by $s = 1$ or $k = a(\eta_k)H/c_0$. In the de Sitter analogue, $a = -c_0/H\eta$, the horizon crossing time is the moment when

$$k\eta_k = -1. \tag{5.16}$$

The equation (5.1) can now be written as

$$\delta\tilde{\phi}_k'' - \frac{1}{s}\delta\tilde{\phi}_k' + \delta\tilde{\phi}_k = 0, \tag{5.17}$$

where prime denotes taking derivative with respect to s.

Large s implies that the mode is well inside the Hubble radius and does not feel the curvature of the analogue spacetime. When a is small, i.e., before the inflation, the condition $s \gg 1$ is satisfied for wide range of k and so all the relevant modes are well inside the Hubble radius. At this epoch, the second term in (5.17) can be neglected and we get the WKB solution for time varying frequency $\omega_k = c_0 k/a$:

$$\delta\tilde{\phi}_k \longrightarrow \sqrt{\frac{\hbar V}{2ma^2 Hs}}\exp(is) = \sqrt{\frac{\hbar V}{2ma^2\omega_k}}\exp\left(-i\int_\infty^\tau \omega_k(\tau')d\tau'\right), \tag{5.18}$$

where coefficients are chosen by imposing a normalization condition. Define the conserved Klein-Gordon (KG) innerproduct by [95, 96]

$$\begin{aligned}(f,g)_{\mathrm{KG}} &= i\frac{mc_0^2}{\hbar}\int d^2\mathbf{x}\,\sqrt{|\gamma|}f^*(\mathbf{x},\tau)\overleftrightarrow{\partial_n}g(\mathbf{x},\tau)\\ &= i\frac{mc_0^2}{\hbar}\int d^2\mathbf{x}\,\frac{a^2}{c_0^2}f^*(\mathbf{x},\tau)\overleftrightarrow{\partial_\tau}g(\mathbf{x},\tau).\end{aligned} \tag{5.19}$$

Here, γ is the determinant of the metric in the spatial slice $\tau = \text{const.}$, n^μ is its normal, and $\partial_n = n^\mu \partial_\mu$. Then the normalization conditions can be stated in terms of KG innerproduct:

$$\left(\frac{1}{V} \delta\tilde{\phi}_k e^{i\mathbf{k}\cdot\mathbf{x}},\ \frac{1}{V} \delta\tilde{\phi}_k e^{i\mathbf{k}'\cdot\mathbf{x}} \right)_{\text{KG}} = \delta^{(2)}_{\mathbf{k},\mathbf{k}'}.$$

We note that, with this choice of coefficients, the canonical commutation relation,

$$\left[\delta\hat{\tilde{\phi}}(\mathbf{x},\tau),\ \delta\hat{\tilde{\pi}}(\mathbf{y},\tau)\right] = i\hbar\delta^{(2)}(\mathbf{x}-\mathbf{y}),$$

with conjugate momentum $\delta\tilde{\pi} = \partial\overline{\mathcal{L}^{(2)}}/\partial(\partial_\tau \delta\tilde{\phi}) = ma^2 \partial_\tau \delta\tilde{\phi}$ holds, and the proper (diagonalized) expression for the energy $\overline{H^{(2)}} = \sum_{\mathbf{k}} \hbar\omega_k (\hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}} + 1/2)$ can be obtained.

It is possible to obtain an analytic solution to (5.17) over the whole range of time. Following [97, 98], we define a function F by $F(s) = \frac{1}{s}\delta\tilde{\phi}_k$. Then (5.17) becomes the Bessel equation of order 1:

$$s^2 F'' + sF' + (s^2 - 1)F = 0,$$

whose general solution can be written as a linear combination of Bessel functions J_1 and Y_1 [83]. Thus we obtain

$$\delta\tilde{\phi}_k(s) = s\Big[A(k)J_1(s) + B(k)Y_1(s)\Big]. \tag{5.20}$$

We can determine the coefficients $A(k)$ and $B(k)$ by matching this solution with the WKB solution (5.18) in the $s \to \infty$ limit. Recalling the asymptotic behavior of Bessel functions [83], we see that, for fixed η,

$$B(k) \to iA(k), \quad A(k) \to \sqrt{\frac{\pi\hbar V H}{4mc_0^2 k^2}} \quad \text{as } k \to \infty,$$

must be fulfilled in order to match the WKB solution (5.18) up to a constant phase.

We invoke de Sitter invariance to determine $A(k)$ and $B(k)$ for all k. We observe that the metric (5.8) with $a(\tau) = e^{H\tau}$ is invariant under the transformation

$$\tau \to \tau' = \tau + \tau_1, \qquad \mathbf{x} \to \mathbf{x}' = e^{-H\tau_1}\mathbf{x},$$

where τ_1 is arbitrary. If we define $\mathbf{k}' \equiv \mathbf{k}e^{H\tau_1}$, we have $\mathbf{k}'/a(\tau') = \mathbf{k}/a(\tau)$ and $\mathbf{k}\cdot\mathbf{x} = \mathbf{k}'\cdot\mathbf{x}'$. Thus we obtain

$$\delta\tilde{\phi}_{k'}(s) = s\Big[A(k')J_1(s) + B(k')Y_1(s)\Big],$$

since s is unchanged when $\tau \to \tau'$ and $k \to k'$. From the invariance of the metric, it follows that $\delta\tilde{\phi}_{k'}(s)e^{i\mathbf{k}'\cdot\mathbf{x}'}/V' = \delta\tilde{\phi}_k(s)e^{i\mathbf{k}\cdot\mathbf{x}}/V$ and so

$$\frac{A(k)}{V} = \frac{A(k')}{V'}$$

for any k and any τ_1. Taking $\tau_1 \to \infty$, the r.h.s. converges to $(1/V)\sqrt{\pi\hbar VH/4mc_0^2k^2}$. Therefore we conclude that $A(k) = \sqrt{\pi\hbar VH/4mc_0^2k^2}$ for any k. The mode function now becomes

$$\delta\tilde{\phi}_k(s) = s\sqrt{\frac{\pi\hbar VH}{4mc_0^2k^2}}\Big[J_1(s) + iY_1(s)\Big] =: h_k(s), \tag{5.21}$$

where the variable $s = (c_0/H)/(a/k)$ measures the ratio of Hubble radius to the cosmic expansion-rescaled wavelength.

We quantize the field in the FRW Universe by imposing the canonical commutation relation,

$$\Big[\delta\hat{\tilde{\phi}}(\mathbf{x},\tau),\, \delta\hat{\tilde{\pi}}(\mathbf{y},\tau)\Big] = i\hbar\delta^{(2)}(\mathbf{x}-\mathbf{y}), \qquad \delta\tilde{\pi} = \frac{\partial\overline{\mathcal{L}^{(2)}}}{\partial(\partial_\tau\delta\tilde{\phi})} = ma^2\partial_\tau\delta\tilde{\phi}.$$

The algebra can be shown to be equivalent to that of Bogoliubov quasiparticle operators, $\hat{\tilde{a}}^\dagger_{\mathbf{k}},\ \hat{\tilde{a}}_{\mathbf{k}}$. Now, We finally obtain the mode expansion for the phase fluctuation field:

$$\delta\hat{\tilde{\phi}}(\mathbf{x},\tau) = \sum_{\mathbf{k}} \hat{\tilde{a}}_{\mathbf{k}} f^{(0)}_{\mathbf{k}}(\mathbf{x},\tau) + \hat{\tilde{a}}^\dagger_{\mathbf{k}} f^{(0)*}_{\mathbf{k}}(\mathbf{x},\tau), \tag{5.22}$$

where $\hat{\tilde{a}}_{\mathbf{k}}$ and $\hat{\tilde{a}}^\dagger_{\mathbf{k}}$ are time independent creation/annihilation operators obeying the commutation relations $[\hat{\tilde{a}}_{\mathbf{k}},\, \hat{\tilde{a}}^\dagger_{\mathbf{k}'}] = \delta^{(2)}_{\mathbf{k},\mathbf{k}'}$. The mode function is written as

$$f^{(0)}_{\mathbf{k}}(\mathbf{x},\tau) = \frac{1}{V}h_k(s)e^{i\mathbf{k}\cdot\mathbf{x}}.$$

The vacuum corresponding to the basis $\hat{\tilde{a}}_{\mathbf{k}}$ is the Bunch-Davies vacuum [99]. Note that at this stage the relation between what $\hat{\tilde{a}}^\dagger_{\mathbf{k}}$ creates and the Bogoliubov quasiparticles is not clear. We will establish a direct connection between them below in (8.15).

The Bunch-Davies vacuum yields an asymptotic Minkowski vacuum in the (formally) infinite past equivalent to the lab's quasiparticle vacuum. It is assumed that the initial Bunch-Davies vacuum $|0\rangle$ at $\eta = -c_0/H$ ($t = \tau = 0$) is during the pre-de Sitter stage smoothly connected to this asymptotic vacuum. We emphasize that "cosmological" quasiparticles are measurable: Below we establish the equivalence of representations using cosmological co-moving or scaling and lab frame Bogoliubov quasiparticles, also cf. [95, 96], and elaborate on the measurement process when the expansion is stopped.

The modes oscillate almost freely for $\eta \to -\infty$. At $k\eta = -1$ and horizon crossing, the mode freezes, leading to the standard theory of inhomogeneity or galaxy formation during inflation [9]. At late times, $s \to 0$, and the modes do effectively not evolve anymore. Fig. 5.1 shows the evolution of kh_k as a function of $k\eta$; (b)$\sim$(d) illustrate the fact that when trans-Planckian defomation of the spectrum is included (see below), horizon crossing and mode freezing nontrivially still occur.

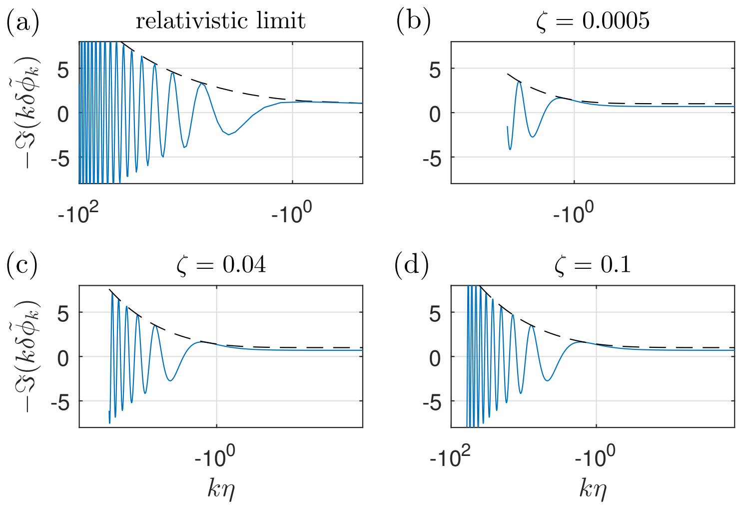


Figure 5.1: (a) Freezing process of the inflaton mode function kh_k in units of $\sqrt{\hbar HV/\pi mc_0^2} = \sqrt{HV/\pi A\omega_{z,0}}$ in terms of the wavenumber dependent logarithmic conformal time $k\eta$. Blue solid line represents the imaginary part of kh_k and black dashed line represents the absolute value of kh_k. (a) Lorentz-invariant relativistic regime. (b)$\sim$(d) demonstrate that when the trans-Planckian spectrum is taken into account, solving Eq.(7.11), freezing still occurs ($A = A_c/10$ and $R = \sqrt{\pi/2}$).

Chapter 6

Real Space Realization

6.1 Correlation Function

We investigate the spatially Fourier-transformed two-point correlation function, which is defined by [26]

$$C_{\delta\tilde{\phi}}(\mathbf{k},\tau) = \int_V d^2\mathbf{x}\, e^{-i\mathbf{k}\cdot\mathbf{x}} \langle \delta\hat{\tilde{\phi}}(0,\tau)\delta\hat{\tilde{\phi}}(\mathbf{x},\tau)\rangle.$$

Now the mode expansion (5.22) is to be substituted. Recalling the asymptotic behavior of the Bessel functions, we have

$$h_k(s) \to -i\sqrt{\frac{\hbar V H}{\pi m c_0^2}}\frac{1}{k}, \qquad \text{as } s \to 0,$$

and therefore we obtain

$$C_{\delta\tilde{\phi}}(\mathbf{k},\tau) = \frac{|h_k|^2}{V} \;\to\; \frac{\hbar H}{\pi m c_0^2}\frac{1}{k^2}. \tag{6.1}$$

Note that the mode function and correlation function become time independent at late times. Thus the density fluctuations determined by (4.10) vanish at zeroth order. In order to obtain nontrivial density fluctuations, one has to take the time dependence of the phase fluctuations into account, which is beyond the zeroth-order frozen part.

6.2 Definition of Power Spectrum

The amplitude of quantum fluctuations is always well defined irrespective of whether the particle interpretation of a given field is available [97]. One way to characterize the typical fluctuations on scales L is to calculate the variance $\delta\chi_L^2(\tau) = \langle 0|[\hat{\chi}_L(\tau)]^2|0\rangle$ of the field operator averaged over a region of size L:

$$\hat{\chi}_L(\tau) \equiv \int d^2\mathbf{x}\, \delta\hat{\tilde{\phi}}(\mathbf{x},\tau) W_L(\mathbf{x}),$$

where $W_L(\mathbf{x})$ is a window function which is of order 1 for $|\mathbf{x}| \lesssim L$ and rapidly decays for $|\mathbf{x}| \gg L$. It is prototypically specified in terms of Gaussian function $W_L(\mathbf{x}) = (1/2\pi L^2)\exp(-|\mathbf{x}|^2/2L^2)$. Given the mode expansion (5.22), after straightforward algebra with an approximation to the Fourier transform of the unit ($L = 1$) window function, $w(\mathbf{k}) \simeq 2\pi[1 - \theta(k-1)]$, one can find

$$\delta\chi_L^2(\tau) \simeq \int_0^{L^{-1}} \frac{dk}{k} \frac{k^2|h_k|^2}{V}.$$

We define the (two-dimensional version of) power spectrum $P(k)$ to be proportional to the variance per $\ln k$:

$$k^2 P(k) \equiv \frac{d\delta\chi_L^2}{d\ln k} = \frac{k^2|h_k|^2}{V}, \quad k = L^{-1}.$$

Another equivalent characterization of the power spectrum is as the Fourier transform of the correlation function [94]:

$$\xi(\mathbf{x}-\mathbf{y}) = \langle 0|\delta\hat{\tilde{\phi}}(\mathbf{x},\tau)\delta\hat{\tilde{\phi}}(\mathbf{y},\tau)|0\rangle =: \frac{1}{V}\sum_{\mathbf{k}} P(k) e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}. \tag{6.2}$$

from which we have $P(k) = \langle \delta\hat{\tilde{\phi}}_{\mathbf{k}}\delta\hat{\tilde{\phi}}_{\mathbf{k}}^\dagger\rangle/V = |h_k|^2/V$, where $\delta\hat{\tilde{\phi}}_{\mathbf{k}}$ is the Fourier transform of the mode expansion (5.22). Note that $P(k)$ is nothing but the correlation function obtained in (6.1). At late times, $\eta \to 0$, the power spectrum $P(k)$ converges to $\hbar H/\pi m c_0^2 k^2$ and we see that the quantity

$$\Delta^2(k) = k^2 P(k)$$

becomes independent of k. We thus obtain, after the freezing process, a spectrum in which $\Delta^2(k)$, the variance per $\ln k$ [94], is constant. This is called a scale-invariant power spectrum (SIPS): The universe has the same degree of 'wrinkliness' on each resolution scale. One can also understand this concept by observing that $|\delta\tilde{\phi}_k|^2 \propto \frac{1}{k^2}$, namely the probability amplitude of a fluctuation is proportional to the wavelength of the fluctuation, so that the shape is always the same regardless of which scale we see. Note that SIPS is not *per se* related to the scaling approach to describe expansion of the gas.

It is commonly argued that the prediction of scale invariance arises because de Sitter space is invariant under time translation: there is no natural origin of time under exponential expansion [94]. At a given moment of time, the only length scale in the model is the horizon size c_0/H, so it is inevitable that the fluctuations that exist on this scale are the same at

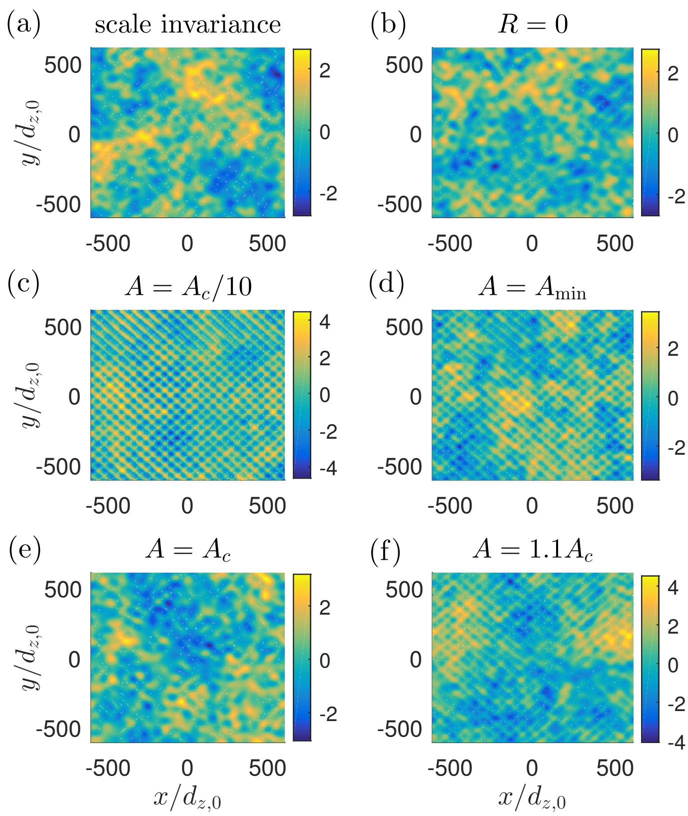


Figure 6.1: (a) Coordinate space representation of the (real) field $\delta\tilde{\phi}(\mathbf{x}, \tau)$, in units of $\sqrt{\hbar HV/\pi m c_0^2 d_{z,0}^2}$ after the completion of the freezing process, where the 2D volume of the system $V = (2\kappa_0 d_{z,0})^2$, with initial aspect ratio κ_0, and the wavevector separation is chosen to be $\Delta k = 2\pi/2\kappa_0 d_{z,0}$. The statistical self-similarity reveals itself by the same degree of "wrinkliness" on each scale. (b) The field obtained from numerical implementation of the full Bogoliubov equations ($A = A_c/10$, $R = 0$). Plots (c) through (f) are for increasing A and dominating DDI ($R = \sqrt{\pi/2}$).

all time. If one ignores their evolution while they are outside the horizon, the resulting fluctuations give us the scale-invariant or Harrison-Zel'dovich-Peebles spectrum [100–102].

6.3 Gaussian Random Field Method

Regarding the phase fluctuation field $\delta\hat{\tilde{\phi}}(\mathbf{x}, \tau)$ as a homogeneous and isotropic Gaussian random field [9], i.e. a field whose Fourier coefficients $\delta\tilde{\phi}_{\mathbf{k}} = a_{\mathbf{k}} + ib_{\mathbf{k}}$ are random variables with probability function of the form,

$$p(a_{\mathbf{k}}, b_{\mathbf{k}}) = \frac{1}{\pi\sigma_k^2} e^{-a_{\mathbf{k}}^2/\sigma_k^2} e^{-b_{\mathbf{k}}^2/\sigma_k^2}, \tag{6.3}$$

the correlation function can be expressed as

$$\xi(\mathbf{x}-\mathbf{y}) = \frac{1}{V^2} \sum_{\mathbf{k},\mathbf{k}'} \langle \delta\tilde{\phi}_{\mathbf{k}}(\tau) \delta\tilde{\phi}^*_{\mathbf{k}'}(\tau) \rangle e^{i\mathbf{k}\cdot\mathbf{x} - i\mathbf{k}'\cdot\mathbf{y}} = \frac{1}{V} \sum_{\mathbf{k}} \sigma_k^2 e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}, \tag{6.4}$$

where one has to take into account that $a_{-\mathbf{k}} = a_{\mathbf{k}}$ and $b_{-\mathbf{k}} = -b_{\mathbf{k}}$. From (6.3), one can see that $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$ are real random variables with standard deviation $\sigma_k/\sqrt{2}$.

Comparing (6.2) and (6.4), we see that the variance of the random variable $\delta\tilde{\phi}_{\mathbf{k}}$ is given by $\sigma_k^2 = P(k) = |h_k|^2/V \to \hbar H/\pi m c_0^2 k^2$, from which we can obtain a real-space realization of the phase fluctuation field $\delta\hat{\tilde{\phi}}(\mathbf{x}, \tau)$ in the scale-invariant fully relativistic limit, see Fig. 6.1 (a).

Chapter 7

Incorporating Trans-Planckian Deformation

7.1 Generalized Klein-Gordon Equation

The solution (5.21) represents phonons residing in the low-momentum corner of the Bogoliubov dispersion relation [see Fig. 4.2 (a)]. In order to incorporate trans-Planckian dispersion and to describe its influence on the small k regime, we consider the more general Bogoliubov equations (4.5) and (4.6). Solving (4.6) for $\delta\rho$ and substituting into (4.5), we obtain

$$(\partial_\tau + \mathbf{v}_{\rm com}\cdot\nabla_{\mathbf{x}})\left[\frac{a^2}{c_0^2}\mathcal{W}^{-1}(\partial_\tau + \mathbf{v}_{\rm com}\cdot\nabla_{\mathbf{x}})\delta\tilde{\phi}\right] = \nabla_{\mathbf{x}}^2\delta\tilde{\phi}, \tag{7.1}$$

This is the 'generalized' Klein-Gordon equation with the local Lorentz invariance being broken [96]. Rewriting (7.1) in momentum space, or equivalently, solving (4.10) for $\delta\rho_{\mathbf{k}}$ and substituting into (4.9) yields (4.11).

The normalization condition is given by

$$(f_{\mathbf{k}}^{(\lambda)}, f_{\mathbf{k}'}^{(\lambda)})_{\mathcal{W}-\rm KG} = \delta^{(2)}_{\mathbf{k},\mathbf{k}'}, \quad (f_{\mathbf{k}}^{(\lambda)}, f_{\mathbf{k}'}^{(\lambda)*})_{\mathcal{W}-\rm KG} = \delta^{(2)}_{\mathbf{k},\mathbf{k}'}, \quad (f_{\mathbf{k}}^{(\lambda)*}, f_{\mathbf{k}'}^{(\lambda)*})_{\mathcal{W}-\rm KG} = -\delta^{(2)}_{\mathbf{k},\mathbf{k}'},$$

where the "generalized" KG inner product is defined by [96]

$$(f,\, g)_{\mathcal{W}-\rm KG} = i\frac{mc_0^2}{\hbar}\int d^2\mathbf{x}\,\frac{a^2}{c_0^2}f^*(\mathbf{x},\tau)\overleftrightarrow{\mathcal{W}^{-1}\partial_\tau}g(\mathbf{x},\tau). \tag{7.2}$$

Let us again introduce an auxiliary field and discuss in the cosmological context. In order to remove the first derivative term of (4.11), we define $\chi_k \equiv \sqrt{a/\mathcal{W}_k}\,\delta\tilde{\phi}_k$, and recast (4.11) as [assuming $\mathbf{v}_{\rm com} = 0$]

$$\partial_\eta^2\chi_k + \Bigg[k^2\mathcal{W}_k - \frac{\partial_\eta^2 a}{2a}\left(1 - \frac{2a\partial_\eta\mathcal{W}_k}{\mathcal{W}_k}\right) + \frac{(\partial_\eta a)^2}{4a^2}\left(1 - \frac{3a^2(\partial_\eta\mathcal{W}_k)^2}{\mathcal{W}_k^2} + \frac{2a^2\partial_\eta^2\mathcal{W}_k}{\mathcal{W}_k} + \frac{4a\partial_\eta\mathcal{W}_k}{\mathcal{W}_k}\right)\Bigg]\chi_k = 0. \tag{7.3}$$

This equation again corresponds to Eq. (1) of [74], cf. the relativistic limit above in (5.12), where now the effective comoving frame mode frequency ω_η is the square root of the expression in the square brackets. It is easily observed that (7.3) converges to (5.12) when $\mathcal{W}_k = 1$, i.e. in the long wavelength limit. Furthermore, (7.3) becomes (5.12) except a factor of $\mathcal{W}_k$ multiplied to k^2 when $\mathcal{W}_k$ is time independent (or a independent). This case is discussed below.

7.2 An Exactly Solvable Case

Solving the general equation (4.11) requires numerical methods. We show herein that an analytic solutions under an approximation to the interaction potential and introducing a momentum cutoff is feasible. We replace the Fourier transform of the interaction $V^{\rm 2D}_{\rm int,0}(\zeta)$ by

$$\bar{V}^{\rm 2D}_{\rm int,0}(\zeta) = \begin{cases} (1-\frac{1}{f^2})\frac{g_0^{\rm eff}\zeta^2}{4A} + V^{\rm 2D}_{\rm int,0}(\zeta) & (\zeta \le \zeta_c), \\ (1-\frac{1}{f^2})\frac{g_0^{\rm eff}\zeta_c^4}{4A\zeta^2} + V^{\rm 2D}_{\rm int,0}(\zeta) & (\zeta > \zeta_c), \end{cases} \tag{7.4}$$

where momentum cutoff ζ_c is set to include a part of trans-Planckian momenta, cf. Eq.(7.10):

$$\zeta_c = \zeta_{\rm Pl} \times \alpha, \tag{7.5}$$

where $\alpha \gtrsim 1$ determines the cutoff location and gives a class of spectrum lines that yields scale invariant power spectra (cf. Eq.(7.8)). Note that initially ($f = 1$) the new potential $\bar{V}^{\rm 2D}_{\rm int,0}$ coincides with the original one $V^{\rm 2D}_{\rm int,0}$ (Fig. 7.1 (a)). As time passes, the excitation spectrum deviates from the true dispersion. However, the deviation is localized around the cutoff momentum ζ_c, and the dispersion law at low energies is secured $\forall t$.

Below the cutoff ($\zeta \le \zeta_c$), $\mathcal{W}_k$ as defined in (4.8) becomes time independent:

$$\mathcal{W}_k = \frac{\zeta^2}{4A} + \frac{1}{g_0^{\rm eff}} V^{\rm 2D}_{\rm int,0}(\zeta),$$

and equation (4.11) becomes

$$(\partial_\tau + i\mathbf{v}_{\rm com}\cdot\mathbf{k})^2\delta\phi_k + 2H(\partial_\tau + i\mathbf{v}_{\rm com}\cdot\mathbf{k})\delta\phi_k + \left(\frac{c_0\mathcal{K}(k)}{a}\right)^2\delta\phi_k = 0, \tag{7.6}$$

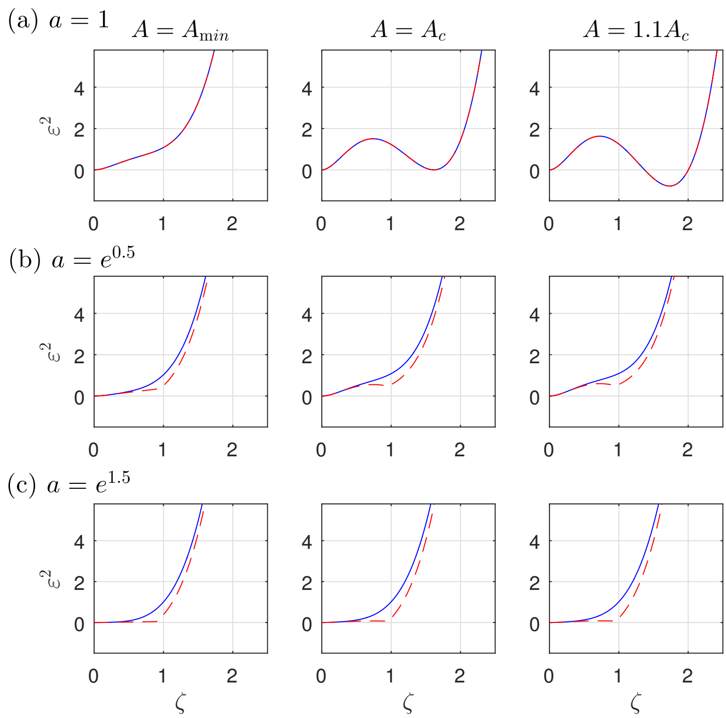


Figure 7.1: The squared excitation spectrum in units of $(\hbar^2/md_{z,0}^2)^2$ at various instants of time. From left to right, the values of A are $A_{\min}$, A_c and $A_c \times 1.1$, repectively. $R = \sqrt{\pi/2}$ for every case. The cutoff momentum is placed at $\alpha = 1.8$ (cf. (7.5)). Blue lines represent the original spectrum while the red dashed lines are approximations carried out to obtain an analytic solution. Initially the two coincide and as time evolves they gradually deviate. Note that the deviation is however localized around the cutoff momentum ζ_c.

which is identical to (5.1) with k now being replaced with $\mathcal{K}(k)$ defined by

$$\mathcal{K}(k)^2 \equiv k^2 \mathcal{W}_k. \tag{7.7}$$

We can then carry out exactly the same procedure for obtaining the mode functions (5.21) with $s = c_0 k/Ha$ being replaced with $\tilde{s} = c_0 \mathcal{K}(k)/Ha$ and with an additional prefactor $\sqrt{\mathcal{W}_k}$.

With these modified mode functions, the Fourier transformed correlation function, or the power spectrum now becomes (after freezing)

$$C_{\delta\tilde{\phi}}(\mathbf{k}, \tau) = \frac{|h_k|^2}{V} \;\rightarrow\; \frac{\hbar H \mathcal{W}_k}{\pi m c_0^2 \mathcal{K}(k)^2},$$

and the variance per $\ln k$ becomes

$$\Delta^2(k) = \frac{2\hbar H \mathcal{W}_k}{mc_0^2} \frac{k^2}{\mathcal{K}(k)^2} = \frac{2\hbar H}{mc_0^2}, \tag{7.8}$$

which still is scale invariant. Therefore, this type of trans-Planckian deformation implied by (7.4) has no effect on the power spectrum and on the matter distribution after the freezing process and SIPS is retained.

7.3 Numerical Implementation

Now we implement numerical analysis of the full Bogolubov equation (4.11). We start by rewriting (4.11) in terms of the variable $s = c_0 k/Ha$ [assuming $\mathbf{v}_{\rm com} = 0$]:

$$\delta\tilde{\phi}_k'' - \frac{G(\zeta)^2 - (a\zeta)^2/4A}{G(\zeta)^2 + (a\zeta)^2/4A}\frac{1}{s}\delta\tilde{\phi}_k' + \left[G(\zeta)^2 + \frac{(a\zeta)^2}{4A}\right]\delta\tilde{\phi}_k = 0, \tag{7.9}$$

$$\delta\tilde{\phi}_k = \frac{1}{\sqrt{\Omega}}\delta\phi_k, \qquad G(\zeta)^2 \equiv \frac{1}{g_0^{\rm eff}} V_{\rm int,0}^{\rm 2D}(\zeta).$$

Here prime($'$) denotes s derivatives. Taking into account (4.12) and (4.8), the linear dispersion occurs for wavenumbers satisfying

$$\frac{(a\zeta)^2}{4A} \ll G(\zeta)^2 \quad (\Rightarrow \text{analogue Planck scale } \zeta_{\rm Pl}). \tag{7.10}$$

For small ζ, $G(\zeta)^2 \to 1$, and Eq. (7.10) defines $\zeta_{\rm Pl}$. Let us first analyze the condition (7.10) in detail. Fig. 7.2 shows the plots of $G(\zeta)^2$ and $(a_1\zeta)^2/4A$ for various values of A where a_1 is the final value of the scale factor. We see that, for the validity of the gravitational analogy, one can pose the later time Planck scale to be $\zeta_{\rm Pl} \lesssim 0.1$. If $\zeta < 0.05$, the condition (7.10) is safely satisfied for all cases.

Experiments will generally probe sub-Planckian ζ that satisfy (7.10). Therefore, we consider (7.9) given (7.10) is fulfilled,

$$\delta\tilde{\phi}_k'' - \frac{1}{s}\delta\tilde{\phi}_k' + G(\zeta)^2\delta\tilde{\phi}_k = 0. \tag{7.11}$$

Before inflation, $s \to \infty$ and the second term in (7.11) becomes negligible. Therefore, one

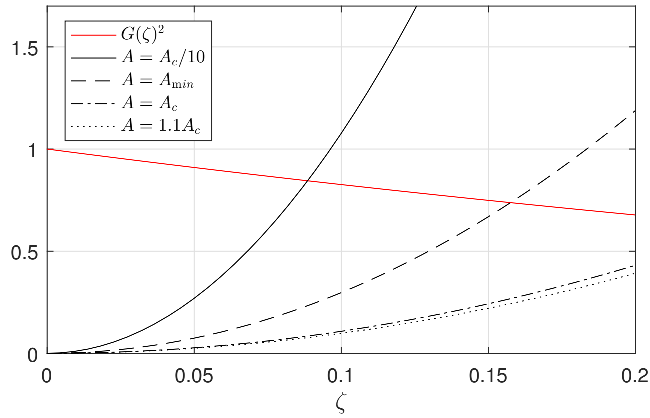


Figure 7.2: Plots of $G(\zeta)^2$ and $(a_1\zeta)^2/4A$ for various values of A. Here the final value of the scale factor a_1 is assumed to be $e^{5/2}$, i.e., 2.5 e-folds of expansion.

finds that the mode functions would converge to a WKB solution as $a \to 0$:

$$\delta\tilde{\phi}_k \to \sqrt{\frac{G(\zeta)\hbar V H s}{2mc_0^2 k^2}} \exp(iG(\zeta)s),$$

where the coefficient is determined by the normalization condition

$$\left(\frac{1}{V}\delta\tilde{\phi}_k e^{i\mathbf{k}\cdot\mathbf{x}},\ \frac{1}{V}\delta\tilde{\phi}_{k'} e^{i\mathbf{k}'\cdot\mathbf{x}}\right)_{\mathcal{W}-\mathrm{KG}} = \delta^{(2)}_{\mathbf{k},\mathbf{k}'}$$

where the Generalized Klein-Gordon ($\mathcal{W}$-KG) inner product is defined by the equation (7.2). This solution and its derivative provides initial conditions to the second order differential equation (7.11). Final values (after inflation) of the mode functions h_k then give the power spectrum via $P(k) = |h_k|^2/V$ and $\Delta^2(k) = k^2 P(k)$.

From (5.14), we have $4H^2 = \omega^2(0)$ (for $\omega_0^2 \ll 4H^2$). Setting $\kappa_0 = 50$, $\omega_{z,0} = 2\pi \times 2921\text{Hz}$ results in $H = 183.5\,\text{sec}^{-1}$. Given n_f e-folds of the scale factor $a(t_f) = \exp[n_f]$, the final lab time is

$$t_f = (\exp[4n_f] - 1)/4H.$$

For 2.5 e-folds, then, $t_f \sim 30\,\text{sec}$ in lab time (for $w_{z,0} = 2\pi \times 3952$ Hz, $H = 248.3\,\text{sec}^{-1}$, and 2 e-folds, $t_f \sim 3\,\text{sec}$). We introduce a momentum cutoff $\zeta_c \lesssim 0.1$ which meets (7.10) at late times. Fig. 7.3 displays $\Delta^2(k)$, and clearly shows the deviations from SIPS, occurring for strongly dipolar interactions. When $R = 0$, Eq. (7.11) becomes identical to the wave

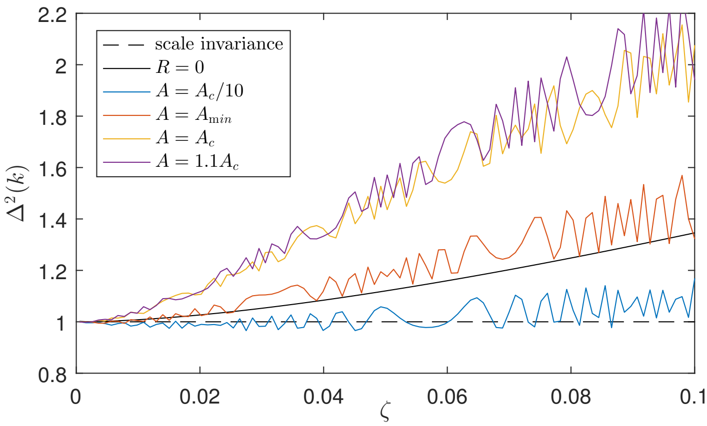


Figure 7.3: $\Delta^2(k) = k^2 P(k)$ as a function of in-plane momentum ζ, for 2.5 e-folds. Black dashed line represent SIPS. The black solid line corresponds to contact interaction, $R = 0$ ($A = A_c/10$). The other lines correspond to DDI dominance ($R = \sqrt{\pi/2}$), with values of A as specified in the inset. In the long-wavelength limit, they all converge to SIPS. The slope of the $R = 0$ curve decreases for increasing number of e-folds, asymptotically yieldding SIPS for pure contact interactions.

equation in analogue curved spacetime (5.1), and SIPS for long wavelengths obtains, cf. Ref. [27] and Fig. 7.3. For high momenta, there is a slight upturn in the spectrum line. As we increase the number of e-folds, this deviation converges to zero; for small wavelengths, it takes longer time to exit the Hubble horizon, and settling down requires longer. Using the power spectrum $\Delta^2(k)$, one again constructs Gaussian random fields, and the coordinate-space realization of Fig. 6.1 (b)–(f) is obtained, demonstrating the violation of SIPS for increasing DDI by introducing short-range correlations. In other words, there is roton minimum imprint in the spatial distribution of the frozon fluctuations. This result becomes the first example within analogue gravity program where violations of SIPS can become experimentally manifest [73].

Whether SIPS is robust to trans-Planckian physics was studied in [74] (also cf. [75]), where scale separation and adiabaticity in conformal time were established as sufficient conditions for SIPS. Scale separation reads $H/c_0 \ll k_{\rm Pl}(\eta_k)/a(\eta_k)$, while adiabaticity holds when $\left|c_0\partial_\eta\omega_\eta/\omega_\eta^2\right| \ll 1 \;\forall\; \eta_i < \eta < \eta_f$, where $\omega_\eta(\eta)$ is an effective comoving frame mode frequency [74]. Furthermore, η_f is the 'nonadiabatic time' lying between η_i, the onset of inflation, and η_k, the horizon crossing, which satisfies $H/c_0 \ll k/a(\eta_f) \ll k_{\rm Pl}(\eta_k)/a(\eta_k)$. Roughly speaking, η_f is the moment when the mode stops to behave WKB-like. For de Sitter spacetime, $a = -c_0/H\eta$, scale separation holds when $k \ll k_{\rm Pl}(\eta_k)$. A given k thus must lie in the linear dispersion regime at horizon crossing $k\eta_k = -1$, which is is equivalent to imposing (7.10) at this point. Therefore, in our numerical implementation of the Bogoliubov equations which employs (7.10), scale separation is satisfied automatically. According to [74], scale separation usually implies adiabaticity, resulting in the robustness of the predictions of the inflationary scenario. However, when the spectrum has (even if only initially) a deep minimum, as here, adiabaticity can be violated even when scale separation holds, and SIPS breaks down.

Chapter 8

Connection to Lab Frame Variables

Quantum excitations in BECs can, on the one hand, be analyzed within the Bogoliubov formalism by directly perturbing the Gross Pitaevskiĭ equation. On the other hand, the phase perturbations of the condensate obey a modified Klein-Gordon equation, and a corresponding quantization can be carried out as in (5.22). Since the de Sitter expansion is not asymptotically flat at late times, a vacuum state cannot be unambiguously defined for late times. However, the experimental verification obviously requires a choice of Fock vacuum and that choice should lead to physically reasonable results. We therefore assume, following [103], that the expansion stops at some chosen moment of time τ_1 and the gas becomes stationary, in other words, $f(\tau) = e^{-H\tau}$ for $\tau < \tau_1$, and $f(\tau) \equiv f_1$ for $\tau \geq \tau_1$.

8.1 Bogoliubov Transformation to Minkowski Vacuum at Late Times

Suppose that we have obtained a complete set of "in" mode functions $f_{\mathbf{k}}^{(0)}$ for $\tau < \tau_1$, e.g. one obtained under (7.7):

$$f_{\mathbf{k}}^{(0)}(\mathbf{x}, \tau) = \frac{1}{V} h_k(\eta) e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{8.1}$$

where the temporal part is given by

$$h_k(\eta) = \sqrt{\frac{\pi\hbar V \mathcal{W}_k}{4ma^2 H}} \Big\{ J_1(-\mathcal{K}(k)\eta) + iY_1(-\mathcal{K}(k)\eta) \Big\},$$

where $\mathcal{K}(k)$ is as defined in (7.7). And suppose that a complete set of "out" mode functions $f_{\mathbf{k}}^{(1)}$ which defines the vacuum state at late times $\tau > \tau_1$ is given, e.g. one consists of

$$f_{\mathbf{k}}^{(1)}(\mathbf{x}, \tau) = \frac{1}{V} \sqrt{\frac{\hbar V \mathcal{W}_k}{2ma_1^2 \omega_{k1}}} e^{-i\omega_{k1}(\tau - \tau_1)} e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{8.2}$$

where $\omega_{k1} \equiv c_0 \mathcal{K}(k)/a_1$. This is a solution to the Bogoliubov equation (7.6) with $a \equiv a_1$ and $H = \frac{\dot{a}}{a}$ set equal to zero, which represents the late time behavior of the equation. The coefficients are fixed by imposing the normalization conditions ($\lambda = 0, 1$)

$$(f_{\mathbf{k}}^{(\lambda)}, f_{\mathbf{k}'}^{(\lambda)})_{\mathcal{W}\text{-KG}} = \delta^{(2)}_{\mathbf{k},\mathbf{k}'}, \quad (f_{\mathbf{k}}^{(\lambda)}, f_{\mathbf{k}'}^{(\lambda)*})_{\mathcal{W}\text{-KG}} = 0, \quad (f_{\mathbf{k}}^{(\lambda)*}, f_{\mathbf{k}'}^{(\lambda)*})_{\mathcal{W}\text{-KG}} = -\delta^{(2)}_{\mathbf{k},\mathbf{k}'}, \tag{8.3}$$

where the generalized KG product ($\mathcal{W}$-KG inner product) is defined by [96]

$$(f, g)_{\mathcal{W}\text{-KG}} = i\frac{mc_0^2}{\hbar}\int d^2\mathbf{x}\, \frac{a^2}{c_0^2} f^*(\mathbf{x}, \tau)\overleftrightarrow{\mathcal{W}^{-1}\partial_\tau} g(\mathbf{x}, \tau). \tag{8.4}$$

Note that $\mathcal{W}$-KG inner product converges to the standard relativistic KG product (5.19) in the limit $\mathcal{W} \to 1$.

The task at hand is to represent the "in" mode functions at $\tau > \tau_1$ as a linear combination of the "out" mode functions, i.e. finding the Bogoliubov coefficients α_k, β_k in the expression

$$f_{\mathbf{k}}^{(0)} = \alpha_k^* f_{\mathbf{k}}^{(1)} + \beta_k^* f_{-\mathbf{k}}^{(1)*} \tag{8.5}$$

for $\tau > \tau_1$. Then the creation/annihilation operators for "in" and "out" states will be related by

$$\hat{\tilde{a}}_{\mathbf{k}}^{(1)} = (f_{\mathbf{k}}^{(1)}, \delta\hat{\tilde{\phi}})_{\mathcal{W}\text{-KG}} = \alpha_k^* \hat{\tilde{a}}_{\mathbf{k}}^{(0)} + \beta_k \hat{\tilde{a}}_{-\mathbf{k}}^{(0)\dagger}.$$

Since $H = \dot{a}/a$ in (7.6) changes at $\tau = \tau_1$ in a discontinuous manner, the mode functions and their derivatives must be matched at this point:

$$f_{\mathbf{k}}^{(0)}(\tau_1) = \alpha_k^* f_{\mathbf{k}}^{(1)}(\tau_1) + \beta_k^* f_{-\mathbf{k}}^{(1)*}(\tau_1),$$
$$\partial_\tau f_{\mathbf{k}}^{(0)}(\tau_1) = \alpha_k^* \partial_\tau f_{\mathbf{k}}^{(1)}(\tau_1) + \beta_k^* \partial_\tau f_{-\mathbf{k}}^{(1)*}(\tau_1),$$

where we suppressed $\mathbf{x}$ dependence for conciseness. In the case of (8.1) and (8.2), solving this equation yields

$$\begin{aligned} \alpha_k^* &= \sqrt{\frac{\pi\omega_{k1}}{8H}}\left\{J_1 + Y_1' + \frac{HY_1}{\omega_{k1}} + i\left[Y_1 - J_1' - \frac{HJ_1}{\omega_{k1}}\right]\right\}, \\ \beta_k^* &= \sqrt{\frac{\pi\omega_{k1}}{8H}}\left\{J_1 - Y_1' - \frac{HY_1}{\omega_{k1}} + i\left[Y_1 + J_1' + \frac{HJ_1}{\omega_{k1}}\right]\right\}, \end{aligned} \tag{8.6}$$

where the arguments of the Bessel functions are $-\mathcal{K}(k)\eta_1$. Note that, if the normalization conditions, (8.3), are applied to (8.5), then one obtains the correct Bosonic Bogoliubov unitarity condition $|\alpha_k|^2 - |\beta_k|^2 = 1$. This relation can also be checked from (8.6) by direct computation.

If the initial state is assumed to have no excitations, the quantum state is the initial vacuum denoted by $|0\rangle_{(0)}$, i.e., $\hat{\hat{a}}_{\mathbf{k}}^{(0)}|0\rangle_{(0)} = 0$. We consider the Heisenberg picture and the state for $\delta\hat{\hat{\phi}}$ is time independent. Then the expected number of quasiparticles with momentum $\mathbf{k}$ after inflation is calculated to be

$$
{}_{(0)}\langle 0|\hat{N}_{\mathbf{k}}^{(1)}|0\rangle_{(0)} = |\beta_k|^2 \ \rightarrow \ \frac{1}{2\pi|\mathcal{K}(k)\eta_1|^1}, \tag{8.7}
$$

as $\eta_1 \rightarrow 0$.

8.2 Relation to Lab-Frame Bogoliubov Excitations

In order to connect quantum physics in curved spacetime to the behavior of a realistic quantum fluid, Leonhardt *et al.* [104] investigated the Hawking effect within the Bogoliubov theory of the elementary excitations in BEC. A more detailed correspondence was discussed by Jain *et al.* [103], giving an analytical expression for the analogue cosmological particle creation spectrum in terms of the Bogoliubov mode functions in the case of a homogeneous BEC. Kurita *et al.* [95] demonstrated the equivalence of the two procedures in the long-wavelength acoustic limit. They showed that the number of quanta in analogue spacetime is different from that of Bogoliubov quasiparticles, unless the corresponding field is normalized correctly. Barceló *et al.* [96] consolidated the equivalence of the two approaches by generalizing the Klein-Gordon formalism beyond the limit of validity of the acoustic approximation. They showed that both formalism lead to the same concept of positive and negative solutions. This line of research allows us to establish a deep conceptual connection between the two formalisms, the first one being inherently nonrelativistic while the second is relativistic, up to corrections which are vanishingly small for long wavelengths. In the following, we discuss the measurement implications of the predictions of previous sections, based on a generalized version of the theory formulated in [96].

Under the scaling transformation (3.9) and the scaling conditions (3.11) and (3.12), the Heisenberg equation of motion for the field operator $\hat{\psi}(\mathbf{x}, \tau)$ reads

$$
i\hbar\partial_\tau\hat{\psi} = \left[-\frac{\hbar^2}{2m}\nabla_x^2 + f^2\frac{m}{2}\omega_0^2 x^2 + f^2\int d^2\mathbf{x}'\, V_{\text{int},0}^{\text{2D}}(\mathbf{x}-\mathbf{x}')\hat{\psi}^\dagger(\mathbf{x}')\hat{\psi}(\mathbf{x}')\right]\hat{\psi}. \tag{8.8}
$$

Expanding the field operator in canonical way, $\hat{\psi} = \psi_0 + \delta\hat{\psi}$, we obtain the GP equation

(4.1) for the order parameter ψ_0, and the Bogoliubov equation [105]

$$i\hbar\partial_\tau\delta\hat{\psi} = (\mathcal{H}+\mathcal{A})\delta\hat{\psi} + \mathcal{B}\delta\hat{\psi}^\dagger, \tag{8.9}$$

where

$$\begin{aligned}\mathcal{H} &= -\frac{\hbar^2}{2m}\nabla_x^2 + \frac{\hbar^2}{2m\sqrt{\rho_0}}\nabla_x^2\sqrt{\rho_0} - \frac{1}{2}mv_0^2 - \hbar\partial_\tau\phi_0, \\ \mathcal{A} &= f^2\psi_0(\mathbf{x})\int d^2\mathbf{x}'\, V^{\mathrm{2D}}_{\mathrm{int},0}(\mathbf{x}-\mathbf{x}')\psi_0^*(\mathbf{x}')\star(\mathbf{x}'), \\ \mathcal{B} &= f^2\psi_0(\mathbf{x})\int d^2\mathbf{x}'\, V^{\mathrm{2D}}_{\mathrm{int},0}(\mathbf{x}-\mathbf{x}')\psi_0(\mathbf{x}')\star(\mathbf{x}').\end{aligned} \tag{8.10}$$

In deriving (8.10), we have used (4.2). The $\star$ stands for the argument upon which $\mathcal{A}$ and $\mathcal{B}$ acts. Note that Eq. (8.9) is a complex equation and is nonlinear: If $\delta\psi$ is a solution, then $\alpha\delta\psi$ is not unless α is real. Therefore we cannot directly perform a mode expansion to find the general solution. In order to overcome this problem, we enlarge the space: We introduce the spinor field

$$\delta\underline{\Upsilon} = \begin{pmatrix}\delta\psi \\ \delta\bar{\psi}\end{pmatrix},$$

subject to the evolution equation

$$i\hbar\partial_\tau\delta\underline{\Upsilon} = \mathcal{M}\delta\underline{\Upsilon}, \qquad \mathcal{M} = \begin{pmatrix}\mathcal{H}+\mathcal{A} & \mathcal{B} \\ -\mathcal{B}^* & -\mathcal{H}-\mathcal{A}^*\end{pmatrix}. \tag{8.11}$$

This equation is now linear, and the solutions to the Bogoliubov equation (8.9) are obtained by restricting the solutions of (8.11) by the condition

$$\delta\bar{\psi} = \delta\psi^*, \quad \text{or} \quad \sigma_x\delta\underline{\Upsilon}^* = \delta\underline{\Upsilon}, \tag{8.12}$$

where $\sigma_{x,y,z}$ are the Pauli matrices. We introduce here a conserved "Bogoliubov" inner-product

$$\langle\delta\underline{\Upsilon}|\delta\underline{\Upsilon}'\rangle_{\mathrm{B}} = \int d^2\mathbf{x}'\,\delta\underline{\Upsilon}^\dagger\sigma_z\delta\underline{\Upsilon}'.$$

One can check that the operator $\mathcal{M}$ is self-adjoint with respect to this inner product

$$\langle\delta\underline{\Upsilon}|\mathcal{M}\delta\underline{\Upsilon}'\rangle_{\mathrm{B}} = \langle\mathcal{M}\delta\underline{\Upsilon}|\delta\underline{\Upsilon}'\rangle_{\mathrm{B}}.$$

This implies that the "Bogoliubov" inner product is conserved for solutions of (8.11). Note that this inner product is not positive definite, since it satisfies

$$\langle \sigma_x \delta\underline{\Upsilon}^* | \sigma_x \delta\underline{\Upsilon}'^* \rangle_{\mathrm{B}} = -\langle \delta\underline{\Upsilon}' | \delta\underline{\Upsilon} \rangle_{\mathrm{B}},$$

and so the physical solutions, i.e. those that satisfy $\sigma_x \delta\underline{\Upsilon}^* = \delta\underline{\Upsilon}$, have zero norm.

The evolution operator $\mathcal{M}$ is self-adjoint in a non-positive-definite inner product space, and therefore it may have complex eigenvalues. We will assume that the condensate is stable and $\mathcal{M}$ has complete othonormal set of eigenspinors with real eigenvalues [96]. One can easily check that $\sigma_x \mathcal{M} \sigma_x = -\mathcal{M}^*$ holds, and in view of this property, one can see that if

$$U_k = \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix}$$

is an eigenspinor of $\mathcal{M}$ with eigenvalue $\omega_{\mathbf{k}}$, then $V_{\mathbf{k}}^* = \sigma_x U_{\mathbf{k}}^*$ is another eigenspinor of $\mathcal{M}$ with eigenvalue $-\omega_{\mathbf{k}}$. Furthermore, the modes $U_{\mathbf{k}}$ and $V_{\mathbf{k}}^*$ are orthogonal and can be chosen orthonormal in the Bogoliubov inner product:

$$\langle U_{\mathbf{k}} | U_{\mathbf{l}} \rangle_{\mathrm{B}} = \delta^{(2)}_{\mathbf{k},\mathbf{l}}, \quad \langle U_{\mathbf{k}} | V_{\mathbf{l}}^* \rangle_{\mathrm{B}} = 0, \quad \langle V_{\mathbf{k}}^* | V_{\mathbf{l}}^* \rangle_{\mathrm{B}} = -\delta^{(2)}_{\mathbf{k},\mathbf{l}}.$$

Any spinor solution $\delta\underline{\Upsilon}$ of Eq. (8.11) can be expanded in this basis:

$$\delta\underline{\Upsilon} = \sum_{\mathbf{k}} b_{\mathbf{k}} U_{\mathbf{k}} + c_{\mathbf{k}}^* V_{\mathbf{k}}^*.$$

Note that the modes $U_{\mathbf{k}}$ and $V_{\mathbf{k}}^*$ themselves are not physical, while physical solutions are linear combinations of them.

Now the mode expansion for the physical spinor field becomes of the form

$$\delta\underline{\hat{\Upsilon}} = \sum_{\mathbf{k}} \underline{\hat{b}}_{\mathbf{k}} U_{\mathbf{k}} + \underline{\hat{b}}_{\mathbf{k}}^\dagger V_{\mathbf{k}}^*,$$

where $\underline{\hat{b}}_{\mathbf{k}}$ and $\underline{\hat{b}}_{\mathbf{k}}^\dagger$ are operators for Bogoliubov quasiparticles. The (physical or unphysical) spinor field $\delta\underline{\Upsilon}$ corresponds to (complexified) density and phase fluctuations by

$$\delta\rho = \sqrt{\rho_0}\big(e^{-i\phi_0}\delta\psi + e^{i\phi_0}\delta\bar{\psi}\big), \qquad \delta\phi = \frac{1}{2i\sqrt{\rho_0}}\big(e^{-i\phi_0}\delta\psi - e^{i\phi_0}\delta\bar{\psi}\big). \tag{8.13}$$

The condition (8.12) that $\delta\psi$ and $\delta\bar{\psi}$ represent physical solutions to the Bogoliubov equation (8.11) translates into reality conditions for $\delta\rho$ and $\delta\phi$. The density and current operators are then expanded as $\hat{\rho} = \hat{\psi}^\dagger\hat{\psi} = \rho_0 + \delta\hat{\rho}$ and $\hat{\mathbf{j}} = (\hbar/2mi)(\hat{\psi}^\dagger\nabla\hat{\psi} - \nabla\hat{\psi}^\dagger\hat{\psi}) = \rho_0\mathbf{v}_{\rm com} + \mathbf{v}_{\rm com}\delta\rho + (\rho_0\hbar/m)\nabla_x\delta\hat{\phi}$. In addition, from the Bosonic commutation relations $[\delta\hat{\psi}(\mathbf{x}), \delta\hat{\psi}^\dagger(\mathbf{x}')] = \delta^{(2)}(\mathbf{x}-\mathbf{x}')$ etc., one obtains $[\delta\hat{\rho}(\mathbf{x}), \delta\hat{\phi}(\mathbf{x}')] = i\delta^{(2)}(\mathbf{x}-\mathbf{x}')$, i.e., the density and phase fluctuations are canonically conjugate fields. By the relation (8.13), there is one-to-one correspondence between spinor fields $\delta\underline{\Upsilon}$ and complexified density and phase fluctuations $\delta\rho,\ \delta\phi$. Provided they are physical solutions, $\delta\rho$ and $\delta\phi$ are related by (4.10).

One can readily derive

$$\langle\delta\underline{\Upsilon}|\delta\underline{\Upsilon}'\rangle_{\rm B} = (\delta\tilde{\phi}, \delta\tilde{\phi}')_{\mathcal{W}\text{-KG}}, \tag{8.14}$$

where $\delta\tilde{\phi} = \Omega^{-1/2}\delta\phi$, and $\mathcal{W}$-KG inner product is as defined in (7.2). For a given set of mode functions $\{f_{\mathbf{k}}^{(\lambda)}\}$ for the field $\delta\tilde{\phi}$, which for example were obtained in (8.1) and (8.2), one can find corresponding mode functions $\{U_{\mathbf{k}}^{(\lambda)}\}$ for the spinor field by using (8.17) and (8.18), and this gives an exact relation between analogue cosmological particles $\hat{\tilde{a}}_{\mathbf{k}}^{(\lambda)}$ and Bogoliubov quasiparticles $\hat{\underline{b}}_{\mathbf{k}}^{(\lambda)}$:

$$\hat{\tilde{a}}_{\mathbf{k}}^{(\lambda)} = (f_{\mathbf{k}}^{(\lambda)}, \delta\hat{\tilde{\phi}})_{\mathcal{W}\text{-KG}} = \langle U_{\mathbf{k}}^{(\lambda)}|\delta\hat{\underline{\Upsilon}}\rangle_{\rm B} = \hat{\underline{b}}_{\mathbf{k}}^{(\lambda)}. \tag{8.15}$$

Therefore the number operator of cosmological particles is identical with that of Bogoliubov quasiparticles:

$$\hat{\tilde{a}}_{\mathbf{k}}^{(\lambda)\dagger}\hat{\tilde{a}}_{\mathbf{k}}^{(\lambda)} = \hat{\underline{b}}_{\mathbf{k}}^{(\lambda)\dagger}\hat{\underline{b}}_{\mathbf{k}}^{(\lambda)}. \tag{8.16}$$

We note here that the operators $\hat{\tilde{a}}_{\mathbf{k}}^{(\lambda)}$ and $\hat{\underline{b}}_{\mathbf{k}}^{(\lambda)}$ correspond to particles that are detected in the comoving frame (3.9). However, experiments obviously implement particle detection in the lab frame. Therefore, one more translation into the lab frame is needed, and is specified below.

8.3 Translation into Lab-Frame Variables

When a normalized mode function $\sqrt{\Omega} f_{\mathbf{k}}^{(\lambda)}$ for the field $\delta\phi = \sqrt{\Omega}\delta\tilde{\phi}$ is given, one can get a mode function for the field $\delta\rho$ by the relation

$$\delta\rho = -\frac{a^2\hbar}{g_0^{\text{eff}}}\mathcal{W}^{-1}\partial_\tau \delta\phi, \tag{8.17}$$

which is immediate from Eq. (4.6). Then one gets the mode functions for $\delta\underline{\Upsilon}$ via

$$\delta\underline{\Upsilon} = \begin{pmatrix} \delta\psi \\ \\ \delta\bar{\psi} \end{pmatrix} = \begin{pmatrix} e^{i\phi_0}\left[\frac{1}{2\sqrt{\rho_0}}\delta\rho + i\sqrt{\rho_0}\delta\phi\right] \\ \\ e^{-i\phi_0}\left[\frac{1}{2\sqrt{\rho_0}}\delta\rho - i\sqrt{\rho_0}\delta\phi\right] \end{pmatrix}, \tag{8.18}$$

which have already been normalized by (8.14). The perturbed field $\delta\psi$ of the scaled order parameter is related to that of the original Bose field in the lab frame by ($\Phi = mr^2\partial_t b/2\hbar b$)

$$\delta\Psi = \frac{e^{i\Phi}}{b}\delta\psi, \quad \delta\bar{\Psi} = \frac{e^{-i\Phi}}{b}\delta\bar{\psi}. \tag{8.19}$$

The normalization should however still be verified for this field: We form a spinor field

$$\delta\Upsilon = \begin{pmatrix} \delta\Psi \\ \delta\bar{\Psi} \end{pmatrix} = \frac{1}{b}\begin{pmatrix} e^{i\Phi}\delta\psi \\ e^{-i\Phi}\delta\bar{\psi} \end{pmatrix}, \tag{8.20}$$

and introduce the Bogoliubov inner product

$$\begin{aligned} \langle\delta\Upsilon|\delta\Upsilon'\rangle_{\text{B}} &= \int d^2\mathbf{r}\,\delta\Upsilon^\dagger\sigma_z\delta\Upsilon' = \int d^2\mathbf{x}\,\delta\underline{\Upsilon}^\dagger\sigma_z\delta\underline{\Upsilon}' \\ &= \langle\delta\underline{\Upsilon}|\delta\underline{\Upsilon}'\rangle_{\text{B}} = (\delta\tilde{\phi}, \delta\tilde{\phi}')_{\mathcal{W}\text{-KG}}. \end{aligned} \tag{8.21}$$

This implies that the cosmological particles are equivalent to the Bogoliubov quasiparticles observed in the lab frame provided the mode functions are chosen consistent with (8.17), (8.18), (8.19), and (8.20). It leads to the lab frame Bogoliubov quasiparticle operators when expansion stops, see above discussion between Eqs. (8.1) and (8.7), being given by $\hat{b}^{(1)}_{\mathbf{k}/b_1} = \hat{\tilde{a}}^{(1)}_{\mathbf{k}}$, where $b_1 \equiv b(t_1)$ is the final scale factor and $\hat{b}_{\mathbf{k}}$ are the annihilation operators associated to $\delta\Upsilon$.

Chapter 9

Pair Creation of Quasiparticles

9.1 A Practical Problem

We have developed in the preceding chapters the emergence of analogue spacetime in a dipolar Bose-Einstein condensate with time-varying trapping frequency and/or interaction coupling strengths. We have shown that the inflationary scenario can be simulated via the expansion of dipolar condensates. Especially, taking adventage of well developed microscopic theory of ultracold quantum gases, one can explore the influence of (analogue) trans-Planckian physics on the sub-Planckian physics of everyday life: There will be roton imprint in the matter distribution after the freezing process. With all these predictions, however, the theory is basically a zero temperature theory, in which the generation of unwanted, detrimental thermal excitations is ignored. In a real experiment, it obviously is impossible to avoid the thermal noise however low the temperature is, and this will dim us in observing the pure quantum effect of cosmological particle production by the inflation.

Let us recall the measurement available for ultracold quantum gases. One can take the *in situ* image of the atomic quantum gases, from which the density-density correlations and the static structure factor can be extracted [106]. In *in situ* imaging, one typically divides the density images into small unit cells or pixels and then evaluates the statistical correlation of the signals in the cells. If both the dimension of the cell and the imaging resolution are much smaller than the correlation length of the sample, the interpretation of the result is straightforward. Recently, it has been revealed that the density-density correlations are related to the quasiparticle quantum state, or the entanglement features displayed by the emitted phonons [107]. The detection of such entanglement would provide an ultimate proof of the quantum nature of the analogue cosmological particle production which thermal excitations do not possess.

In the following, we first characterize the influence of the initial thermal noise by comparing the correlation function with or without the initial thermal noise. And we cosider the entanglement measure by which one can quantify the degree of "quantumness". This will provide the ultimate proof for the quantum nature of cosmological particle production even in the presence of detrimental thermal noise. We also discuss the advantage that roton minimum provides for the experimental protocol suggested.

9.2 Bogoliubov-de Gennes Equation

The quantum nature of the system can clearly be seen when we take the Hamiltonian approach. By applying Legendre transform to the Lagrangian (3.14), one obtains the Hamiltonian of the system. The the Heisenberg equation of motion for the field operator reads

$$i\partial_\tau \hat{\psi} = \left[-\frac{1}{2m}\nabla^2_{\mathbf{x}} + f^2 \frac{1}{2} m\omega_0^2 x^2 + f^2 \int d^2\mathbf{x}'\, V^{\rm 2D}_{\rm int,0}(\mathbf{x}-\mathbf{x}')\hat{\psi}^\dagger(\mathbf{x}')\hat{\psi}(\mathbf{x}') \right] \hat{\psi}.$$

We expand the field operator by the form, $\hat{\psi} = \psi_0(1+\hat{\phi})$, where $|\psi_0(\mathbf{x},\tau)|^2 =: \rho_0$ represents the condensate density, and where $\hat{\phi}$ describes the perturbations (excitations) on top of the condensate. The Bogoliubov-de Gennes equation obeyed by the fluctuation field $\hat{\phi}$ reads [105]

$$i\partial_\tau \hat{\phi} = \mathcal{H}\hat{\phi} + \mathcal{A}(\hat{\phi} + \hat{\phi}^\dagger), \tag{9.1}$$

in which we define the two operators

$$\begin{aligned} \mathcal{H} &= -\frac{1}{2m}\nabla^2_{\mathbf{x}} - \frac{1}{m\sqrt{\rho_0}}(\nabla_{\mathbf{x}}\sqrt{\rho_0}) \cdot \nabla_{\mathbf{x}} - i\mathbf{v}_{\rm com} \cdot \nabla_{\mathbf{x}}, \\ \mathcal{A}F &= f^2 \int d^2\mathbf{x}'\, V^{\rm 2D}_{\rm int,0}(\mathbf{x}-\mathbf{x}')|\psi_0(\mathbf{x}')|^2 F(\mathbf{x}'), \end{aligned} \tag{9.2}$$

where $\mathcal{A}$ acts by convolution on an arbitrary function $F(\mathbf{x})$. Here $\mathbf{v}_{\rm com} = \frac{1}{m}\nabla_{\mathbf{x}}\theta_0$, where $\psi_0 = \sqrt{\rho_0}e^{i\theta_0}$, denotes the comoving frame velocity [73].

Assuming vanishingly small comoving velocity, $\mathbf{v}_{\rm com} = 0$, and quasi-homogeneity, $\nabla_{\mathbf{x}}\sqrt{\rho_0} \simeq \mathbf{0}$, then ρ_0 and θ_0 become independent of $\mathbf{x}$, and we obtain

$$i\partial_\tau \hat{\phi} = -\frac{1}{2m}\nabla^2_{\mathbf{x}}\hat{\phi} + f^2\rho_0 \int d^2\mathbf{x}'\, V^{\rm 2D}_{\rm int,0}(\mathbf{x}-\mathbf{x}')(\hat{\phi}(\mathbf{x}') + \hat{\phi}^\dagger(\mathbf{x}')).$$

In momentum space, we decompose the fluctuations into their Fourier components, $\hat{\phi}(\mathbf{x}) = (1/\sqrt{N})\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}\hat{\phi}_{\mathbf{k}}$, $\hat{\phi}_{\mathbf{k}} = \sqrt{N}\int d^2\mathbf{x}' e^{-i\mathbf{k}\cdot\mathbf{x}'}\hat{\phi}(\mathbf{x}')$ with N being the total number of atoms in the condensate. Here and in what follows, we set the (initial) normalization area of the plane to unity in the definition of Fourier transforms and their inverse, and $\mathbf{k}$ represents *comoving (scaling)* momentum, as we work in the scaling frame of reference. Now each terms become

$$
\begin{aligned}
i\partial_\tau \hat{\phi} &= \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} i\partial_\tau \hat{\phi}_{\mathbf{k}}, \\
-\frac{1}{2m}\nabla^2_{\mathbf{x}}\hat{\phi} &= -\frac{1}{2m}\frac{1}{\sqrt{N}}\sum_{\mathbf{k}} \hat{\phi}_{\mathbf{k}} \nabla^2_{\mathbf{x}} e^{i\mathbf{k}\cdot\mathbf{x}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} \left(\frac{k^2}{2m}\hat{\phi}_{\mathbf{k}}\right), \\
f^2\rho_0 \frac{1}{\sqrt{N}} &\sum_{\mathbf{k}} \int d^2\mathbf{x}'\, V^{2D}_{\text{int},0}(\mathbf{x}-\mathbf{x}') \left(e^{i\mathbf{k}\cdot\mathbf{x}'}\hat{\phi}_{\mathbf{k}} + e^{-i\mathbf{k}\cdot\mathbf{x}'}\hat{\phi}^\dagger_{\mathbf{k}}\right) \\
&= f^2\rho_0 \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \left\{ \hat{\phi}_{\mathbf{k}} \int d^x\mathbf{x}'' \left[V^{2D}_{\text{int},0}(\mathbf{x}'') e^{-i\mathbf{k}\cdot\mathbf{x}''}\right] e^{i\mathbf{k}\cdot\mathbf{x}} + (\text{h.c.}) \right\} \\
&= f^2\rho_0 \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \left\{ e^{i\mathbf{k}\cdot\mathbf{x}}\hat{\phi}_{\mathbf{k}} V^{2D}_{\text{int},0}(k) + \hat{\phi}^\dagger_{-\mathbf{k}} V^{2D}_{\text{int},0}(k) e^{i\mathbf{k}\cdot\mathbf{x}} \right\}.
\end{aligned}
$$

Reading the equality between Fourier components, we obtain the Fourier space Bogoliubov-de Gennes equation,

$$
\begin{aligned}
i\partial_\tau \hat{\phi}_{\mathbf{k}} &= \frac{k^2}{2m}\hat{\phi}_{\mathbf{k}} + f^2\rho_0 V^{2D}_{\text{int},0}(k)\hat{\phi}_{\mathbf{k}} + f^2\rho_0 V^{2D}_{\text{int},0}(k)\hat{\phi}^\dagger_{-\mathbf{k}} \\
-i\partial_\tau \hat{\phi}^\dagger_{-\mathbf{k}} &= \frac{k^2}{2m}\hat{\phi}^\dagger_{-\mathbf{k}} + f^2\rho_0 V^{2D}_{\text{int},0}(k)\hat{\phi}_{\mathbf{k}} + f^2\rho_0 V^{2D}_{\text{int},0}(k)\hat{\phi}^\dagger_{-\mathbf{k}}.
\end{aligned}
$$

Define $\mathcal{H}_{\mathbf{k}} \equiv k^2/2m$ and $\mathcal{A}_{\mathbf{k}} \equiv f^2\rho_0 V^{2D}_{\text{int},0}(k)$. Then the equation can be written in a matrix form,

$$
i\partial_\tau \begin{bmatrix} \hat{\phi}_{\mathbf{k}} \\ \hat{\phi}^\dagger_{-\mathbf{k}} \end{bmatrix} = \begin{bmatrix} \mathcal{H}_{\mathbf{k}} + \mathcal{A}_{\mathbf{k}} & \mathcal{A}_{\mathbf{k}} \\ -\mathcal{A}_{\mathbf{k}} & -(\mathcal{H}_{\mathbf{k}} + \mathcal{A}_{\mathbf{k}}) \end{bmatrix} \begin{bmatrix} \hat{\phi}_{\mathbf{k}} \\ \hat{\phi}^\dagger_{-\mathbf{k}} \end{bmatrix}. \tag{9.3}
$$

Note that the commutation relations of $\hat{\phi}_{\mathbf{k}}$ is inheritted from the Bosonic field operators:

$$
\begin{aligned}
[\hat{\phi}_{\mathbf{k}}, \hat{\phi}^\dagger_{\mathbf{k}'}] &= N \int d^2\mathbf{x} d^2\mathbf{x}'\, e^{-i\mathbf{k}'\cdot\mathbf{x}} e^{i\mathbf{k}'\cdot\mathbf{x}'} [\hat{\phi}(\mathbf{x}), \hat{\phi}^\dagger(\mathbf{x}')] \\
&= N \int d^2\mathbf{x} d^2\mathbf{x}'\, e^{-i\mathbf{k}'\cdot\mathbf{x}} e^{i\mathbf{k}'\cdot\mathbf{x}'} [\frac{1}{\psi_0(\mathbf{x})}\hat{\psi}(\mathbf{x}) - 1,\ \frac{1}{\psi_0^*(\mathbf{x})}\hat{\phi}^\dagger(bx') - 1] \\
&= \frac{N}{\rho_0} \int d^x\mathbf{x} d^2\mathbf{x}' e^{-i\mathbf{k}\cdot\mathbf{x} + i\mathbf{k}'\cdot\mathbf{x}'} \delta(\mathbf{x}-\mathbf{x}') = \delta_{\mathbf{k},\mathbf{k}'}.
\end{aligned}
$$

We use the notation $\hat{\phi}_{\mathbf{k}}$ for the original fluctuation operators and $\hat{\varphi}_{\mathbf{k}}$ for the Bogoliubov quasiparticle operators. To diagonalize (9.3), we thus apply a Bogoliubov transformation with coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ as follows:

$$\begin{bmatrix} \hat{\phi}_{\mathbf{k}} \\ \hat{\phi}^{\dagger}_{-\mathbf{k}} \end{bmatrix} = \begin{bmatrix} u_{\mathbf{k}} & v_{\mathbf{k}} \\ v_{\mathbf{k}} & u_{\mathbf{k}} \end{bmatrix} \begin{bmatrix} \hat{\varphi}_{\mathbf{k}} \\ \hat{\varphi}^{\dagger}_{-\mathbf{k}} \end{bmatrix}, \tag{9.4}$$

where imposing the Bosonic algebra for $\hat{\varphi}_{\mathbf{k}}$, we obtain a normalization condition for $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$,

$$1 = [\hat{\phi}_{\mathbf{k}}, \hat{\phi}^{\dagger}_{\mathbf{k}}] = [u_{\mathbf{k}}\hat{\varphi}_{\mathbf{k}} + v_{\mathbf{k}}\hat{\varphi}^{\dagger}_{-\mathbf{k}}, v_{\mathbf{k}}\hat{\varphi}_{-\mathbf{k}} + u_{\mathbf{k}}\hat{\varphi}^{\dagger}_{\mathbf{k}}] = u^2_{\mathbf{k}} - v^2_{\mathbf{k}}. \tag{9.5}$$

Thereby solving the eigenproblem of (9.3), we obtain

$$\begin{matrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{matrix} = \frac{\sqrt{\mathcal{H}_{\mathbf{k}}} \pm \sqrt{\mathcal{H}_{\mathbf{k}} + 2\mathcal{A}_{\mathbf{k}}}}{2(\mathcal{H}^2_{\mathbf{k}} + 2\mathcal{H}_{\mathbf{k}}\mathcal{A}_{\mathbf{k}})^{1/4}}, \tag{9.6}$$

where upper/lower sign refers to $u_{\mathbf{k}}$,$v_{\mathbf{k}}$, respectively. Then, $[u_{\mathbf{k}}\ v_{\mathbf{k}}]^T$ is the eigenvector with eigenvalue $\omega_{\mathbf{k}}(\tau)$, and $[v_{\mathbf{k}}\ u_{\mathbf{k}}]^T$ is the eigenvector with eigenvalue $-\omega_{\mathbf{k}}(\tau)$, where $\omega_{\mathbf{k}}$ is as defined in (9.8).

In general, the excitation frequencies are scaling time dependent, and Eq.(9.3) yields

$$i\partial_\tau \begin{bmatrix} \hat{\varphi}_{\mathbf{k}} \\ \hat{\varphi}^{\dagger}_{-\mathbf{k}} \end{bmatrix} = \begin{bmatrix} \omega_{\mathbf{k}} & i\partial_\tau\omega_{\mathbf{k}}/2\omega_{\mathbf{k}} \\ i\partial_\tau\omega_{\mathbf{k}}/2\omega_{\mathbf{k}} & -\omega_{\mathbf{k}} \end{bmatrix} \begin{bmatrix} \hat{\varphi}_{\mathbf{k}} \\ \hat{\varphi}^{\dagger}_{-\mathbf{k}} \end{bmatrix}, \tag{9.7}$$

where the excitation spectrum is given by

$$\omega_{\mathbf{k}}(\tau) = \sqrt{\mathcal{H}^2_{\mathbf{k}} + 2\mathcal{H}_k\mathcal{A}_{\mathbf{k}}(\tau)}. \tag{9.8}$$

Here we introduce the parameter,

$$c(\tau) = f(\tau)\sqrt{g^{\text{eff}}_0\rho_0/m} = f(\tau)c_0, \tag{9.9}$$

which is the (scaling time dependent) speed of sound. It is the slope of the linear, low-$\mathbf{k}$ part of the dispersion relation (9.8). We may also define, in addition to R in (3.17), anotion dimensionless parameter

$$A = \frac{mc^2_0}{\omega_{z,0}} = \frac{g^{\text{eff}}_0\rho_0}{\omega_{z,0}}, \tag{9.10}$$

representing an effective chemical potential as measured relative to the (initial) transverse trapping, linear in both the codensate density and the effective contact coupling defined in (3.16).

For a stationary state $f = 1$ $[c(\tau) = c_0]$, the healing length is given by

$$\xi_0 = 1/(mc_0). \tag{9.11}$$

The inverse of ξ_0, $k_{\text{P}l} \equiv 1/\xi_0$, is an anlogue “Planck scale.” Close to the roton minimum at $k\xi_0 \approx 0.9$, then, Lorentz invariance is strongly broken and a particular variant of *Planckian* ($k \sim k_{\text{P}l}$) physics can be simlated [73]. In Fig. 9.1, we plot the corresponding stationary state Bogoliubov excitation energy, from which we see that the spectrum in a strongly dipolar BEC develops a roton minimum for sufficiently large A. The system becomes unstable past the critical value $A = A_c = 3.4454$ (when $R = \sqrt{\pi/2}$ [63]). In the low-momentum corner, the spectrum is generally linear in momentum,

$$\omega_{\mathbf{k}} = c_0 k \qquad (k\xi_0 \ll 1), \tag{9.12}$$

implying the (pseudo-)Lorentz invariance of the system from which the effective metric concept for the propagating quantum field of phonons emerges [23].

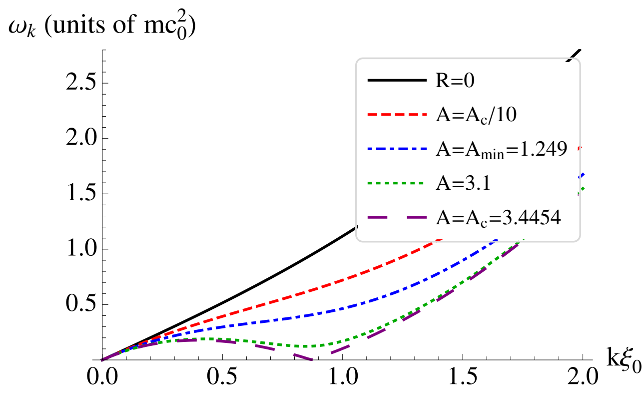


Figure 9.1: *Stationary state excitation spectrum.* Bogoliubov excitation energy in units of mc_0^2, for DDI dominance, $R = \sqrt{\pi/2}$. For $A > A_{\text{min}} = 1.249$, the spectrum develops a roton minimum and becomes unstable for $A > A_c = 3.4454$. $R = 0$ denotes the contact interaction case where the Bogoliubov excitation energy, when normalized to mc_0^2, as here, is independent of A. ξ_0 is healing length defined in (9.11).

For a stationary system, we find that the operators $\hat{\varphi}_{\mathbf{k}}$ and $\hat{\varphi}^{\dagger}_{-\mathbf{k}}$ decouple, and oscillate at constant frequencies $\pm\omega_{\mathbf{k}}$, where $\tau = t$ for the stationary case with $f = b = 1$ in (3.9),

$$\hat{\varphi}_{\mathbf{k}}(\tau) = \hat{b}_{\mathbf{k}}\, e^{-i\omega_{\mathbf{k}} t}, \qquad \hat{\varphi}^{\dagger}_{-\mathbf{k}}(\tau) = \hat{b}^{\dagger}_{-\mathbf{k}}\, e^{i\omega_{\mathbf{k}} t}. \tag{9.13}$$

Here $\hat{b}_{\mathbf{k}}$ and $\hat{b}^{\dagger}_{\mathbf{k}}$ are, respectively, annihilation and creation operators of collective excitations with momentum $\mathbf{k}$ above the stationary condensate.

9.3 Mode Mixing

As a result of a rapid temporal change of c^2, as defined in (9.9), and which is encoded in the scale factor f defined in (3.12), Eq. (9.7) engenders mode mixing between the quasiparticle modes of momenta $\mathbf{k}$ and $-\mathbf{k}$, which entails the amplification of quantum and thermal fluctuations. It is convenient to characterize the mode mixing by introducing the coefficients $\alpha_{\mathbf{k}}(\tau)$ and $\beta_{\mathbf{k}}(\tau)$ [108]:

$$\begin{aligned} \hat{\varphi}_{\mathbf{k}}(\tau) &= \left[\alpha_{\mathbf{k}}(\tau)\hat{b}^{\text{in}}_{\mathbf{k}} + \beta^{*}_{\mathbf{k}}(\tau)\hat{b}^{\text{in}\dagger}_{-\mathbf{k}}\right] \exp\left[-i\int^{\tau}\omega_{\mathbf{k}}(\tau')d\tau'\right], \\ \hat{\varphi}^{\dagger}_{-\mathbf{k}}(\tau) &= \left[\alpha^{*}_{\mathbf{k}}(\tau)\hat{b}^{\text{in}\dagger}_{-\mathbf{k}} + \beta_{\mathbf{k}}(\tau)\hat{b}^{\text{in}}_{\mathbf{k}}\right] \exp\left[i\int^{\tau}\omega_{\mathbf{k}}(\tau')d\tau'\right]. \end{aligned} \tag{9.14}$$

In the limit $\tau \to -\infty$, $\hat{b}^{\text{in}}_{\mathbf{k}}$ and $\hat{b}^{\text{in}\dagger}_{-\mathbf{k}}$ are defined such that $\hat{\varphi}_{\mathbf{k}}(\tau) \to \hat{b}^{\text{in}}_{\mathbf{k}}e^{-i\omega_{\mathbf{k}}\tau}$, $\hat{\varphi}^{\dagger}_{-\mathbf{k}}(\tau) \to \hat{b}^{\text{in}\dagger}_{-\mathbf{k}}e^{i\omega_{\mathbf{k}}\tau}$, or equivalently, $\alpha_{\mathbf{k}} \to 1$ and $\beta_{\mathbf{k}} \to 0$ as $\tau \to -\infty$. That is to say, the operators $\hat{b}^{\text{in}}_{\mathbf{k}}$ and $\hat{b}^{\text{in}\dagger}_{\mathbf{k}}$ are, respectively, the annihilation and creation operators of collective excitations with momentum $\mathbf{k}$ in the initial stationary state. From Eqs. (9.7) and (9.14), we find that the evolution of the operators $\hat{\varphi}_{\mathbf{k}}(\tau)$ and $\hat{\varphi}^{\dagger}_{-\mathbf{k}}(\tau)$ is completely determined by $\alpha_{\mathbf{k}}(\tau)$ and $\beta_{\mathbf{k}}(\tau)$, and the corresponding evolution equations of $\alpha_{\mathbf{k}}(\tau)$ and $\beta_{\mathbf{k}}(\tau)$ are:

$$\begin{aligned} \partial_\tau \alpha_{\mathbf{k}} &= \frac{\partial_\tau \omega_{\mathbf{k}}}{2\omega_{\mathbf{k}}} \exp\left(2i\int^{\tau}\omega_{\mathbf{k}}(\tau')d\tau'\right)\beta_{\mathbf{k}}, \\ \partial_\tau \beta_{\mathbf{k}} &= \frac{\partial_\tau \omega_{\mathbf{k}}}{2\omega_{\mathbf{k}}} \exp\left(-2i\int^{\tau}\omega_{\mathbf{k}}(\tau')d\tau'\right)\alpha_{\mathbf{k}}. \end{aligned} \tag{9.15}$$

Given the temporal change $c^2 = c^2(\tau)$, the above equations can be solved to obtain $\alpha_{\mathbf{k}}(\tau)$ and $\beta_{\mathbf{k}}(\tau)$, and hence $\hat{\varphi}_{\mathbf{k}}(\tau)$ and $\hat{\varphi}^{\dagger}_{-\mathbf{k}}(\tau)$.

The phase factors of $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$ in (9.15) determine the phase of the oscillations of the density-density correlation function (i.e., Eq. (11.3)) around its mean value. We note in this regard that a typo has occurred in Eqs. (21) and (26) of Ref. [37], where the sign "−" should be a "+". However, this sign has no effect on the minimal values of the density-density correlation amplitude one is interested in. To verify nonseparability and steerability for modes with a given momentum, one therefore seeks the minimal values reached by the Fourier space density-density correlation function during its oscillations, to determine whether they drop below the thresholds for nonseparability and steerability, see Eqs. (10.9) and (10.12) below, respectively [51].

Chapter 10

Measuring Quantum Correlation

A direct measurement performed on the Bose gas is for example a determination of the instantaneous atom density (locally within a given experimental resolution), in particular the fluctuations about its mean. The corresponding density-density correlations [106], are related to the quasiparticle quantum state [107]. We will now demonstrate how to use these correlations to measure nonseparability and steerability between the created quasiparticles with opposite momenta $\mathbf{k}$ and $-\mathbf{k}$, which are due to temporal variations of the condensate background. Below, we closely follow the density-density correlation-function based discussion of the criteria for nonseparability and steerability contained in Refs. [37, 51].

10.1 Density-Density Correlation Function

The total atom number density in the condensate is given in the fluctuations by

$$\hat{\rho}(\tau,\mathbf{x}) = \hat{\psi}^\dagger(\tau,\mathbf{x})\hat{\psi}(\tau,\mathbf{x}) \simeq \rho_0(1 + \hat{\phi}^\dagger(\tau,\mathbf{x}) + \hat{\phi}(\tau,\mathbf{x})), \tag{10.1}$$

to linear order. In a homogeneous system, the background density ρ_0 is constant, and the relative density fluctuation is

$$\frac{\delta\hat{\rho}(\tau,\mathbf{x})}{\rho_0} = \frac{\hat{\rho}(\tau,\mathbf{x}) - \rho_0}{\rho_0} = \hat{\phi}^\dagger(\tau,\mathbf{x}) + \hat{\phi}(\tau,\mathbf{x}). \tag{10.2}$$

We consider *in situ* measurements of $\delta\hat{\rho}(\tau,\mathbf{x})$ performed at some (scaling) measurement time $\tau = \tau_m$. From the equal-time commutators,

$$[\hat{\psi}(\tau,\mathbf{x}),\hat{\psi}(\tau,\mathbf{x}')] = 0, \qquad [\hat{\psi}(\tau,\mathbf{x}),\hat{\psi}^\dagger(\tau,\mathbf{x}')] = \delta(\mathbf{x}-\mathbf{x}'),$$

one can easily verify that $\delta\hat{\rho}(\tau,\mathbf{x})$ and $\delta\hat{\rho}(\tau,\mathbf{x}')$ commute with each other. In momentum space, where the Fourier transform is performed by

$$\hat{\phi}_\mathbf{k}(\tau) = \sqrt{N}\int d^2\mathbf{x}' e^{-i\mathbf{k}\cdot\mathbf{x}'}\hat{\phi}(\tau,\mathbf{x}'),$$

we express the relative density fluctuation (10.2) in terms of quasiparticle operators,

$$\frac{\delta\hat{\rho}_{\mathbf{k}}(\tau)}{\rho_0} = \hat{\phi}_{\mathbf{k}}(\tau) + \hat{\phi}^{\dagger}_{-\mathbf{k}}(\tau) = (u_{\mathbf{k}} + v_{\mathbf{k}})(\hat{\varphi}_{\mathbf{k}}(\tau) + \hat{\varphi}^{\dagger}_{-\mathbf{k}}(\tau)). \tag{10.3}$$

Note that taking the Hermitian conjugate of the operator (10.3) is equivalent to changing the sign of $\mathbf{k}$, as a consequence of the fact that the relative density fluctuation operator in (10.2) is itself a Hermitian operator and thus is an observable (the results of the corresponding measurement are real quantities). It is straightforward to show that this operator commutes with its Hermitian conjugate, and thus the following correlation function is well defined:

$$G_{2,\mathbf{k}}(\tau) = \frac{\langle|\delta\hat{\rho}_{\mathbf{k}}(\tau)|^2\rangle}{\rho_0^2} = (u_{\mathbf{k}} + v_{\mathbf{k}})^2(2n_{\mathbf{k}} + 1 + 2\Re[c_{\mathbf{k}}e^{-2i\omega_{\mathbf{k}}\tau}]), \tag{10.4}$$

where $n_{\mathbf{k}} = \langle\hat{b}^{\dagger}_{\mathbf{k}}\hat{b}_{\mathbf{k}}\rangle$ is mean occupation number, and $c_{\mathbf{k}} = \langle\hat{b}_{\mathbf{k}}\hat{b}_{-\mathbf{k}}\rangle$ is pair amplitude. To obtain the above relation, the relation $n_{\mathbf{k}} = n_{-\mathbf{k}}$ has been made. The equality holds when the background has reached a stationary state, so that the frequencies $\omega_{\mathbf{k}}$ become time-independent.

The mean occupation number $n_{\mathbf{k}}$ determines the time-averaged mean of $G_{2,\mathbf{k}}(\tau)$, while the magnitude and phase of the correlation $c_{\mathbf{k}}$ respectively determine the magnitude and phase of the oscillations of $G_{2,\mathbf{k}}(\tau)$ around its mean value. For the vacuum case, i.e., $n_{\mathbf{k}} = 0$ (and hence $c_{\mathbf{k}} = 0$), in the correlation function there is just one constant term (the "$+1$") left, which is also measurable as well and encodes the vacuum fluctuations of the quasiparticle field. This will become of importance later on.

For a thermal initial state with the equilibrium distribution $2n_{\mathbf{k}} + 1 = \coth\big(\omega_{\mathbf{k}}/2T\big)$, the term containing $c_{\mathbf{k}}$ vanishes and the correlation function in Eq. (10.4) reads

$$G_{2,\mathbf{k}} = \frac{k\xi_0/2}{\sqrt{\left(\frac{k\xi_0}{2}\right)^2 + 1 - \frac{3R}{2}k\xi_0\sqrt{A}w\left[\frac{k\xi_0}{\sqrt{2}}\sqrt{A}\right]}} \times \\ \coth\left[\frac{k\xi_0\sqrt{\left(\frac{k\xi_0}{2}\right)^2 + 1 - \frac{3R}{2}k\xi_0\sqrt{A}w\left[\frac{k\xi_0}{\sqrt{2}}\sqrt{A}\right]}}{2T/mc_0^2}\right]. \tag{10.5}$$

In Fig. 10.1, we plot the thermal density-density correlation function (10.5) of a dipolar BEC at various initial temperatures (in units of mc_0^2), and as a function of the nondi-

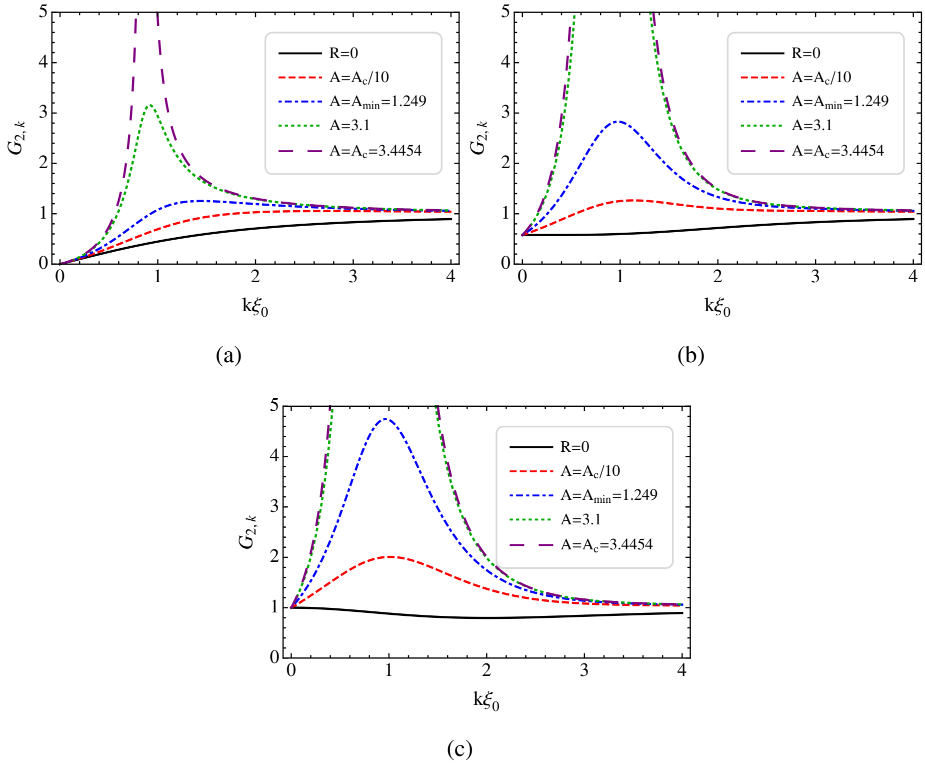


Figure 10.1: *Stationary state density-density correlations for increasing temperature (from left to right).* The density-density correlation function $G_{2,\mathbf{k}}$ in thermal and quasiparticle ground states. The initial temperatures are (a) $T/mc_0^2 = 0$, (b) $T/mc_0^2 = 1/\sqrt{3}$, and (c) $T/mc_0^2 = 1$. The black solid line corresponds to contact interaction, $R = 0$ ($A = A_c/10$). DDI dominated cases ($R = \sqrt{\pi/2}$) are shown by the remaining curves with A specified in the insets.

mensionalized momentum $k\xi_0$, with fixed A and R [109]. We see that the density-density correlation function is strongly modified near the roton minimum of the spectrum. In particular, when the roton minimum approaches zero (near criticality), the modification of the density-density correlation function relative to the pure contact case diverges.

We now discuss the high- and low-temperature limits of (10.5) separately. When $\omega_k/T \ll 1$, we have $2n_{\mathbf{k}} + 1 = \coth\left(\omega_{\mathbf{k}}/2T\right) \simeq 2T/\omega_{\mathbf{k}} + \omega_{\mathbf{k}}/6T$, so that Eq. (10.5) becomes in the low-momentum (phonon) limit, expanding to quadratic order in $k\xi_0$,

$$G_{2,\mathbf{k}} = \frac{T}{mc_0^2}\left[1 + \frac{3}{2}\sqrt{A}Rk\xi_0\right] - \left[\frac{T}{mc_0^2}\left(\frac{1}{4} + \frac{3AR}{\sqrt{2\pi}} + \frac{9AR^2}{4}\right) - \frac{mc_0^2}{12T}\right](k\xi_0)^2 + \mathcal{O}((k\xi_0)^3). \tag{10.6}$$

For the contact interaction, i.e., $R = 0$ case, we reproduce the result of Ref. [37]. On the other hand, we see that for finite relative strength R and density of dipoles encapsulated in A, both R and A enter the correlation function. For $k \to 0$, $G_{2,\mathbf{k}}$ simply approaches the dimensionless temperature T/mc_0^2; one can thus determine the temperature of the gas by examining the low-momentum density fluctuations.

When $\omega_{\mathbf{k}}/T \gg 1$, we have $\coth\big(\omega_{\mathbf{k}}/2T\big) \simeq 1$, so that Eq. (10.5) becomes

$$G_{2,\mathbf{k}} \simeq \frac{k\xi_0/2}{\sqrt{\left(\frac{k\xi_0}{2}\right)^2 + 1 - \frac{3R}{2}k\xi_0\sqrt{A}w\left[\frac{k\xi_0}{\sqrt{2}}\sqrt{A}\right]}}. \tag{10.7}$$

Again, the difference to the contact case $R = 0$ is manifest, because the relative strength and density of dipoles are explicitly involved via R and A, respectively. In the high-momentum limit of free particles $k\xi_0 \gg 1$, $G_{2,\mathbf{k}}$ approaches unity, regardless of temperature and interactions. The function $\zeta w[\zeta]$ occurring in $G_{2,\mathbf{k}}$ approaches a constant in this limit [63].

10.2 Criteria for Nonseparability and Steerability

Pair production in a time-dependent background can be caused by quasiparticles already present, e.g. in a thermal state, or emerge from quasiparticle quantum vacuum fluctuations. The created pairs possess opposite momenta $\mathbf{k}$ and $-\mathbf{k}$ and are correlated. To study the quantum correlation between the created pairs as a consequence of temporal variations of the condensate, we therefore restrict our considerations to a bipartite quantum state.

The bipartite Gaussian quantum state of quasiparticle pairs is called separable whenever the density matrix $\hat{\rho}_{\mathbf{k},-\mathbf{k}}$ can be written in the form [110, 111]

$$\hat{\rho}_{\mathbf{k},-\mathbf{k}} = \sum_a P_a \hat{\rho}^a_{\mathbf{k}} \otimes \hat{\rho}^a_{-\mathbf{k}}, \tag{10.8}$$

where $\hat{\rho}^a_j$ are density matrices pertaining to the subsystem $j = \pm\mathbf{k}$, which are in a set indexed by a, and P_a describes the probability for obtaining $\hat{\rho}^a_{\mathbf{k}} \otimes \hat{\rho}^a_{-\mathbf{k}}$ with $0 \leq P_a \leq 1$ and $\sum_a P_a = 1$. Conversely, if a bipartite state can not be written in the form of (10.8), such states are nonseparable, i.e., entanglement exists between the mode $\mathbf{k}$ and the mode $-\mathbf{k}$.

Criteria to assess the degrees of correlation between the created quasiparticles using density-density correlations have previously been analyzed in detail in Refs. [37, 51]. The generalized Peres-Horodecki (gPH) criterion is an algebraic condition on the covariance matrix of a two-mode system, and provides a criterion for the nonseparability of continuous variable bipartite systems, cf. ,e.g., [50,51,107]. It leads to the following sufficient condition for nonseparability in terms of density-density correlations [51]

$$G_{2,\mathbf{k}}(\tau) < G_{2,\mathbf{k}}^{\rm vac} = (u_{\mathbf{k}} + v_{\mathbf{k}})^2 \text{ for some } \mathbf{k} \quad \text{[Nonseparable].} \tag{10.9}$$

Here, $G_{2,\mathbf{k}}^{\rm vac}$ is the correlation due to quasiparticle vacuum fluctuations. Whenever $G_{2,\mathbf{k}}$ dips below its vacuum value for some times, the state is nonseparable.

One can, furthermore, investigate whether quantum steering of one quasiparticle mode by another mode with opposite momentum takes place. The primary idea behind steering is to infer the values of correlated quantities for one subsystem, e.g., mode $-\mathbf{k}$, as depending on the results that are obtained from the measurements performed on the other subsystem, e.g., mode $\mathbf{k}$. Steering is encapsulated in the inequality [17, 51]:

$$\Delta_{\rm inf} A_{-\mathbf{k}} \cdot \Delta_{\rm inf} B_{-\mathbf{k}} < \frac{1}{2} \left| \left\langle \left[\hat{A}_{-\mathbf{k}}, \hat{B}_{-\mathbf{k}} \right] \right\rangle \right|, \tag{10.10}$$

where $\hat{A}_{\mathbf{k}}$ and $\hat{B}_{\mathbf{k}}$ are *measurement operators*. The notation

$$\Delta_{\rm inf} A_{-\mathbf{k}} = \sqrt{\left\langle \left(\hat{A}_{-\mathbf{k}} - \bar{A}_{-\mathbf{k}}(A_{\mathbf{k}}) \right)^2 \right\rangle}$$

indicates the inferred standard deviation of $A_{-\mathbf{k}}$ on subsystem $-\mathbf{k}$ with the measurement $\hat{A}_{\mathbf{k}}$ having been made on subsystem $\mathbf{k}$. In these relations, $\bar{A}_{-\mathbf{k}}(A_{\mathbf{k}})$ is the conditional (mean) value of $\hat{A}_{-\mathbf{k}}$ given that measurement of $\hat{A}_{\mathbf{k}}$ on subsystem $\mathbf{k}$ yields the eigenvalue $A_{\mathbf{k}}$; a similar definition applies to $\Delta_{\rm inf} B_{-\mathbf{k}}$. Note that $\hat{A}_{\mathbf{k}}, \hat{B}_{\mathbf{k}}$ are required to be noncommuting, in distinction to the density operators contained in the definition of $G_{2,\mathbf{k}}$. For example, the measurement operators can be chosen to be quasiparticle quadratures [107],

$$\hat{X}_{\pm\mathbf{k}} = \frac{1}{\sqrt{2}}(\hat{\varphi}_{\pm\mathbf{k}} + \hat{\varphi}^{\dagger}_{\pm\mathbf{k}}), \qquad \hat{P}_{\pm\mathbf{k}} = \frac{i}{\sqrt{2}}(\hat{\varphi}^{\dagger}_{\pm\mathbf{k}} - \hat{\varphi}_{\pm\mathbf{k}}). \tag{10.11}$$

The product of standard deviations on the left side of inequality (10.10) would obey the Heisenberg uncertainty principle whenever *noninferred* variances are calculated: The left hand side would be *larger or equal* to the right hand side. The state is steerable, however, whenever the inferred standard deviations are violating the conventional Heisenberg uncertainty relation, i.e., when inequality (10.10) is satisfied due to the existence of strong correlations between the two subsystems labeled by $\pm\mathbf{k}$.

In Ref. [51], a sufficient condition for steerability in terms of the density-density correlations $G_{2,\mathbf{k}}(\tau)$ and $G_{2,\mathbf{k}}^{\mathrm{vac}}$ was stated

$$G_{2,\mathbf{k}}(\tau) < \frac{1}{2} G_{2,\mathbf{k}}^{\mathrm{vac}} \quad \text{[Steerable]}. \tag{10.12}$$

Note in this regard that although steerability is originally formulated in terms of inferred variances of noncommuting operators, Eq. (10.10), a sufficient criterion can be expressed in terms of variances of linear combinations of operators pertaining to the two subsystems, here the density fluctuation operators of (10.3), $\hat{\phi}_{\mathbf{k}}(\tau)$ and $\hat{\phi}^{\dagger}_{-\mathbf{k}}$ [51].

Compared with the nonseparability condition in (10.9), the criterion for steerability shown in (10.12) is more stringent due to the factor of 1/2 on the right hand side, again reflecting the fact that quasiparticle states exhibiting steering form a subset of nonseparable states. We also note that a concrete experimental protocol to assess quasiparticle entanglement by the covariance matrix of the quasiparticle quadratures was proposed in Ref. [107].

Chapter 11

Analogue Dynamical Casimir Effect

11.1 Rapid Changes of Sound Speed

In order to observe sizable dynamical Casimir effect (DCE), the cavity should be vibrating with speed comparable to the speed of light. It is demonstrated that the vibrating cavity can be replaced with the changing speed of light, since this will change the optical length between the wall. For analogue system, one needs to change the speed of sound [36, 40].

With this background, we now impose a time-dependent background by assuming that $c^2 = c^2(\tau)$ is of the form

$$\frac{c^2(\tau)}{c_f^2} = \frac{1}{2}\left(1 + \frac{c_i^2}{c_f^2}\right) + \frac{1}{2}\left(1 - \frac{c_i^2}{c_f^2}\right)\tanh(a\tau). \tag{11.1}$$

We choose this form of the quench of the sound speed for a direct comparison with the results of [37], and do indeed find that $R = 0$ reproduces the results of the latter reference. The above $c^2(\tau)$, in particular, implies two asymptotic values, $c_i^2 = c_0^2$ and c_f^2 which are obtained when $\tau \to -\infty$ and $\tau \to \infty$, respectively, and for which the gas and thus the quasiparticle vacuum become stationary. In the examples below, we quench the system to a larger sound speed $c_f > c_i$.

According to (3.12) and (9.9), for constant g_d and g_c, the scale factor is, given a prescribed form of $c^2(\tau)$ as in (11.1)

$$b(\tau) = \frac{1}{f^2(\tau)} = \frac{c_0^2}{c^2(\tau)}. \tag{11.2}$$

The gas, for $c_f > c_i$, therefore contracts, with $b(t_f) < b(t_i)$. We plot the scale factor $b(t)$ with respect to the lab time t in Fig. 11.1, for various quench rates a of the speed of sound in (11.1).

As a consequence of the temporal change of c^2, the quasiparticle state is probed by the operators $\hat{\varphi}_{\pm\mathbf{k}}(\tau)$ whose equation of motion is Eq. (9.7). From the time dependence of the excitation frequencies $\omega_{\mathbf{k}}(\tau)$, the Bogoliubov coefficients $\alpha_{\mathbf{k}}(\tau)$ and $\beta_{\mathbf{k}}(\tau)$ are func-

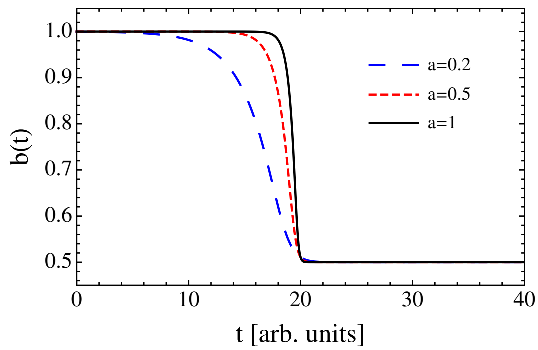


Figure 11.1: *Scale factor* $b(t)$. The scale factor b in (11.2) with respect to the real lab time t in (3.9), showing the compression of the condensate as a function of the speed of sound quench rate a (in arbitrary units of inverse time). Here we take $c_i^2/c_f^2 = 1/2$.

tions of scaling time τ as well, satisfying the evolution equations (9.15). The corresponding correlation function in the first line of Eq. (10.4) becomes

$$G_{2,\mathbf{k}}(\tau) = (u_\mathbf{k}(\tau) + v_\mathbf{k}(\tau))^2 \big[|\alpha_\mathbf{k}(\tau)|^2 + |\beta_\mathbf{k}(\tau)|^2 + 2\Re\big\{\alpha_\mathbf{k}(\tau)\beta^*_\mathbf{k}(\tau)e^{-2i\int^\tau \omega_\mathbf{k}(\tau')d\tau'}\big\}\big](2n^{\text{in}}_\mathbf{k} + 1). \quad (11.3)$$

We can rewrite Eq. (11.3) in the form of Eq. (10.4), with

$$\begin{aligned} 2n_\mathbf{k} + 1 &= (|\alpha_\mathbf{k}|^2 + |\beta_\mathbf{k}|^2)(2n^{\text{in}}_\mathbf{k} + 1), \\ c_\mathbf{k} &= \alpha_\mathbf{k}\beta^*_\mathbf{k}(2n^{\text{in}}_\mathbf{k} + 1). \end{aligned} \quad (11.4)$$

For adiabatic variations ($a \to 0$ in (11.1)), $\alpha_\mathbf{k}$ and $\beta_\mathbf{k}$ do essentially not change and remain very close to 1 and 0, respectively; $G_{2,\mathbf{k}}$ then varies in time only because $(u_\mathbf{k} + v_\mathbf{k})^2$ does so. However, when we are in a nonadiabatic regime, $\alpha_\mathbf{k}$ and $\beta_\mathbf{k}$ evolve in time, and the degree of nonadiabaticity is encoded in them. We conclude from Eq. (11.4) that initial thermal quasiparticle noise can enhance quasiparticle production because the quantities shown in (11.4), which occur in (10.4), are proportional to the initial thermal background multiplicative factor $2n^{\text{in}}_\mathbf{k} + 1$.

With the time evolution of $c^2(\tau)$ as prescribed in Eq. (11.1), we obtain the time-dependent $\omega_\mathbf{k}(\tau)$ in (9.8), and then can solve the coupled Eqs. (9.15) numerically. In Fig. 11.2 we show some examples of the evolution of the quasiparticle frequencies at fixed momentum (left panel), and the corresponding correlation function response in Eq. (11.3) to this evolution (right panel). In what follows, we will use the following definitions of healing length and effective chemical potential, respectively:

$$\xi_f = \frac{1}{mc_f}, \qquad \tilde{A} = \frac{mc_f^2}{\omega_{z,0}} = A\frac{c_f^2}{c_i^2}. \tag{11.5}$$

The quasiparticle frequencies approach two asymptotics because $c^2(\tau)$ approaches constants in the limits of $\tau \to -\infty$ and $\tau \to \infty$, respectively (left panel of Fig. 11.2). For $k\xi_f = 1$, when $\tilde{A} < 1.073$, the initial frequencies $\omega_{\mathbf{k}\,i} = \lim_{\tau\to-\infty}\omega_{\mathbf{k}}(\tau)$ are smaller than the final frequencies $\omega_{\mathbf{k}\,f} = \lim_{\tau\to\infty}\omega_{\mathbf{k}}(\tau)$. However, when $\tilde{A}$ is large (assuming DDI dominance, $R = \sqrt{\pi/2}$), i.e., $1.073 < \tilde{A} \leq 3.4454$ for $k\xi_f = 1$, the initial frequencies $\omega_{\mathbf{k}\,i} = \lim_{\tau\to-\infty}\omega_{\mathbf{k}}(\tau)$ are larger than the corresponding final ones, $\omega_{\mathbf{k}\,f} = \lim_{\tau\to\infty}\omega_{\mathbf{k}}(\tau)$. This implies that (a dominant) DDI and the density of the gas, parametrized by R and $\tilde{A}$, respectively, together affect the qualitative behavior of the quasiparticle spectra more deeply than contact interactions would. In the presence of a (sufficiently strong) DDI, a roton minimum appears. For increasing roton depth, finite-momentum excitation frequencies near the roton minimum are small; hence these modes are more sensitive to temporal changes of the background.

In the two asymptotical regimes, one has a well defined vacuum for the quasiparticles. These vacua are not necessarily equivalent to each other. The vacuum defined in the far-past region are seen as a two-mode squeezed state from the viewpoint of the observer in the far-future region. That is to say, although there are no quasiparticles at the beginning, due to an expansion or contraction of the condensate, excitations will be created from the quasiparticle vacuum.

The temporal behavior of the correlation function in Eq. (11.3) is strongly affected by the strength of the DDI and the gas density (see right panel of Fig. 11.2). When the variation in time of $\omega_{\mathbf{k}}$ is slow, i.e., when a is small, $G_{2,\mathbf{k}}(\tau)$ varies smoothly for small $\tilde{A}$ ($\tilde{A} < 1.073$ in Fig. 11.2). When the change of c^2 is sufficiently abrupt, the two-point density correlation function oscillates such that it can periodically dip below its vacuum value. For large $\tilde{A}$ ($\tilde{A} > 1.073$ in Fig. 11.2), the corresponding two-point density correlations oscillate with larger amplitude than for smaller $\tilde{A}$ (smaller chemical potential).

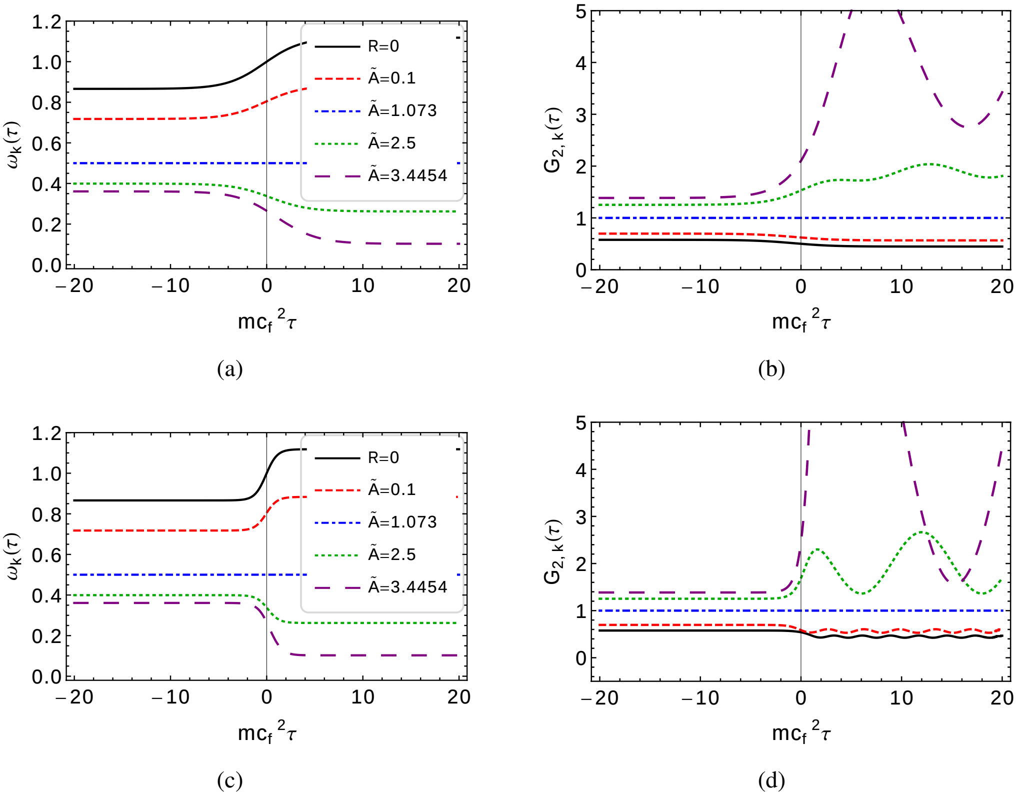


Figure 11.2: *Time-dependence of Bogoliubov excitation frequencies and density-density correlations.* The Bogoliubov excitation energy $\omega_{\mathbf{k}}$ (plots (a) and (c)) and the corresponding correlation function in Eq. (11.3) (plots (b) and (d)) for zero temperature as a function of the parametrized time $mc_f^2\tau$. Here we fix $k\xi_f := 1$, $c_i^2/c_f^2 = 1/2$. The rate of change in (11.1) is taken as $a/\omega_{\mathbf{k}i} = 0.3$ for plots (a) and (b), and $a/\omega_{\mathbf{k}i} = 1$ for plots (c) and (d). The black solid curves correspond to contact interaction, $R = 0$ ($\tilde{A} = 0.1$). The DDI dominated case ($R = \sqrt{\pi/2}$) with varying values of $\tilde{A}$, specified in the insets of (a) and (c), is represented by the other curves.

11.2 Quench Production of Entanglement

In an experiment, a measurement is performed on the condensate at some given time τ_{m}. To study quantum correlations between the produced quasiparticle modes, we are thus interested in the variation of the correlation function with momentum $k\xi_f$ at fixed time τ_m. As an example, we plot in Fig. 11.3 the variation of the correlation function in the momentum at fixed measurement time $\tau = \tau_m$. To examine nonseparability and steerability between the produced quasiparticles, we plot the normalized correlation function, i.e. the correlation function divided by its vacuum value

$$\tilde{G}_{2,\mathbf{k}}(\tau) := \frac{G_{2,k}}{G_{2,\mathbf{k}}^{\mathrm{vac}}} = \frac{G_{2,\mathbf{k}}}{(u_{\mathbf{k}} + v_{\mathbf{k}})^2}. \tag{11.6}$$

The nonseparability and steerability thresholds then occur according to Eqs. (10.9) and (10.12) at $\tilde{G}_{2,\mathbf{k}} = 1$ and $\tilde{G}_{2,\mathbf{k}} = 1/2$, respectively.

The normalized density-density correlation function periodically changes and potentially dips below unity. When the normalized density-density correlation function is smaller than 1 for some times, the final quasiparticle state is nonseparable. This implies that entanglement is created between quasiparticles with opposite momentum $\mathbf{k}$ and $-\mathbf{k}$ due to the nonadiabatic variation of the speed of sound of the condensate and the excitation of the condensate vacuum. Furthermore, even though initial thermal noise decreases the range of nonseparable $\mathbf{k}$'s (right panel of Fig. 11.3), a sufficiently dense dipolar gas close to criticality still creates entanglement (comparing (d) with (c) in Fig. 11.3). Specifically, the momentum which renders the final quasiparticle state nonseparable, that is which satisfies the inequality (10.9), is for the dipolar gas smaller than for contact interactions.

The quantum steering of the final quasiparticle state produced due to the nonadiabatic evolution of the condensate is enhanced in a dipolar gas. Although the sufficient condition (10.12) for steerability might not be satisfied for any value of $\mathbf{k}$ in the final quasiparticle state when only contact interactions are present, the DDI generically induces a state which does satisfy this criterion (see the green dotted and purple long-dashed curves in (c) of Fig.11.3). there might be no steering in the final quasiparticle state for any value of $\mathbf{k}$ when only contact interactions are present, the DDI induces the creation of steering between quasiparticles (see the green dotted and purple long-dashed curves in (c) of Fig. 11.3). As mentioned in the Introduction, steerability is a more stringent correlation property of quantum states than nonseparability is (however weaker than Bell nonlocality). Steering implies that the state is nonseparable but not vice versa, a fact which is readily confirmed with Figs. 11.3 and 11.4.

The time-dependent speed of sound as specified in (11.1) can, for example, be adjusted by the external potential trapping the condensate, according to the scaling equations (3.9) and (3.12). To determine how the quench rate and final sound speed squared, c_f^2, affect the creation of quasiparticle entanglement, we plot the normalized density-density correlation functions in Fig. 11.4. We conclude that quantum steering between quasiparticles

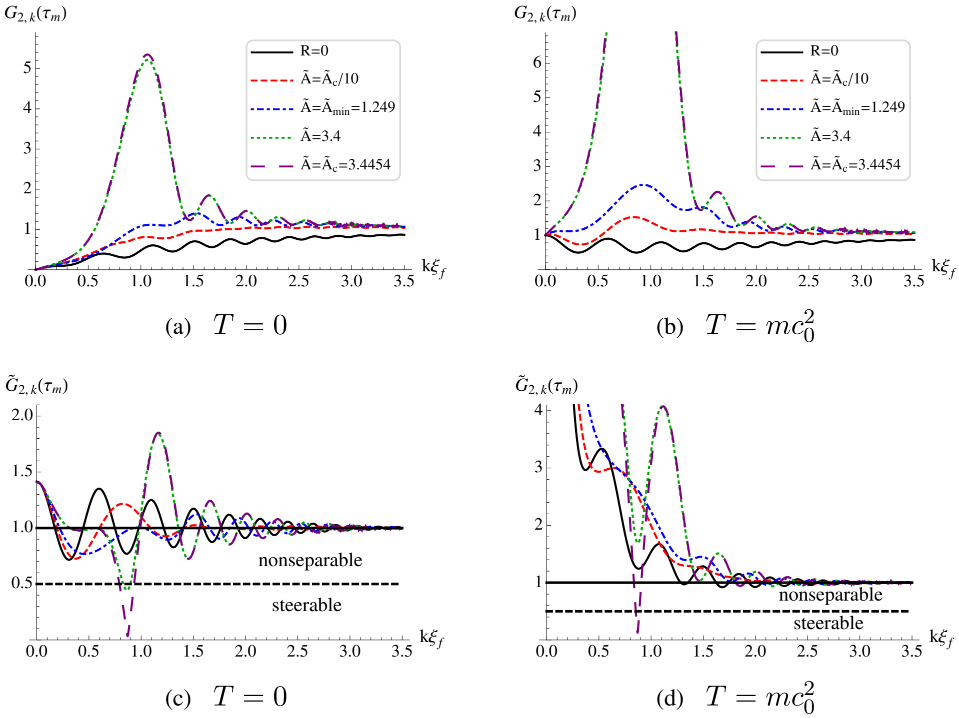
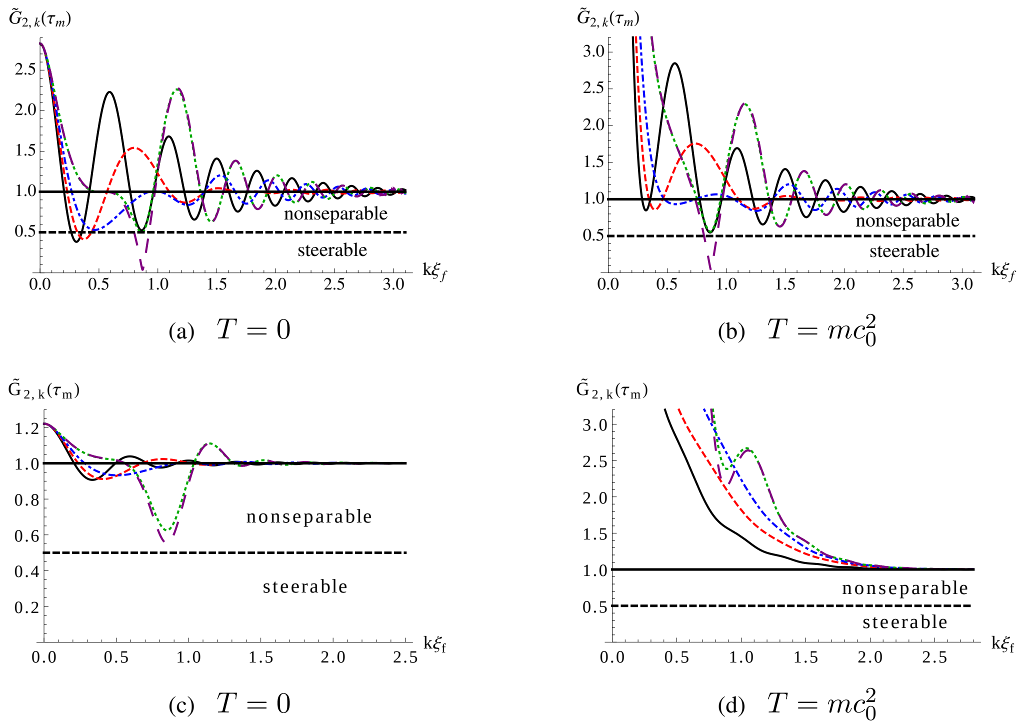


Figure 11.3: *Density-density correlations as a function of* $k\xi_f$ *at zero temperature (left) and finite temperature (right).* The measurement time is $\tau_{\rm m} = 5 \times (mc_f^2)^{-1}$. Here $c_i^2/c_f^2 = 1/2$, and the rate of change $a/\omega_{\mathbf{k}i} = 1 (k\xi_f = 3)$. The solid curve corresponds to contact interaction, $R = 0$ ($\tilde{A} = \tilde{A}_c/10$). DDI dominance ($R = \sqrt{\pi/2}$) for the other curves, with $\tilde{A}$ specified in the insets of (a) and (b). The lower plots show correlation functions normalized by $(u_{\mathbf{k}} + v_{\mathbf{k}})^2$, such that the nonseparability and steerability thresholds occur at 1 (thick black line) and $1/2$ (dashed thick black line), respectively.

is robustly obtained whenever we are near criticality $\tilde{A} \lesssim \tilde{A}_{\rm c}$. Furthermore, we observe that an increase of c_f^2 amplifies the fluctuations of the normalized density-density correlation functions around their mean values (comparing (a) in Fig. 11.4 with (c) in Fig. 11.3), and induces the creation of quasiparticle steering in a condensate with relatively low density ($\tilde{A} < \tilde{A}_{\rm min}$). On the other hand, smaller sweep rates $a/\omega_{\mathbf{k}i}$ decrease the amplitude of the fluctuations of the normalized density-density correlation functions (comparing (c) in Fig. 11.4 with (c) in Fig. 11.3); they however enhance the production of quasiparticle steering near criticality.

To show the domains of nonseparability and steerability more clearly, and make the comparison between the contact interaction case and the DDI case more readily accessible,



(a) $T = 0$ (b) $T = mc_0^2$

(c) $T = 0$ (d) $T = mc_0^2$

Figure 11.4: *Varying c_f^2 and sweep rate a for zero temperature (left) and finite temperature (right).* Shown is the variation of the normalized density-density correlation functions with $k\xi_f$ at fixed measurement time $\tau_{\rm m} = 5 \times (mc_f^2)^{-1}$. *(a) and (b)* Larger final sound speed $c_i^2/c_f^2 = 1/8$ than in Fig. 11.3 c) and (d), with identical rate of change $a/\omega_{\mathbf{k}i} = 1$ ($k\xi_f = 3$). *(c) and (d)* Smaller sweep rate than in Fig. 11.3 c) and (d), with identical $c_i^2/c_f^2 = 1/2$, and the rate of change $a/\omega_{\mathbf{k}i} = 0.05$ ($k\xi_f = 3$). The values of $\tilde{A}$ corresponding to the various curves are found in the insets of Fig. 11.3 (a) and (b).

in Fig. 11.5 we plot the envelopes for the contact interaction case and the DDI case with the critical value of $\tilde{A} = 3.4454$ shown in Figs. 11.3 and 11.4. It can be seen that the created quasiparticles with frequencies near the roton minimum are steerable, which does not occur for contact interactions. Therefore, we conclude that compared to a gas with repulsive contact interactions, the DDI Bose gas system displays an enhanced potential for the presence of steering in the bipartite quantum state of quasiparticle pairs resulting from the quench. In addition, this enhancement is robust against thermal noise, and variation of the difference between the initial and final speeds of sound as well as of the quench rate.

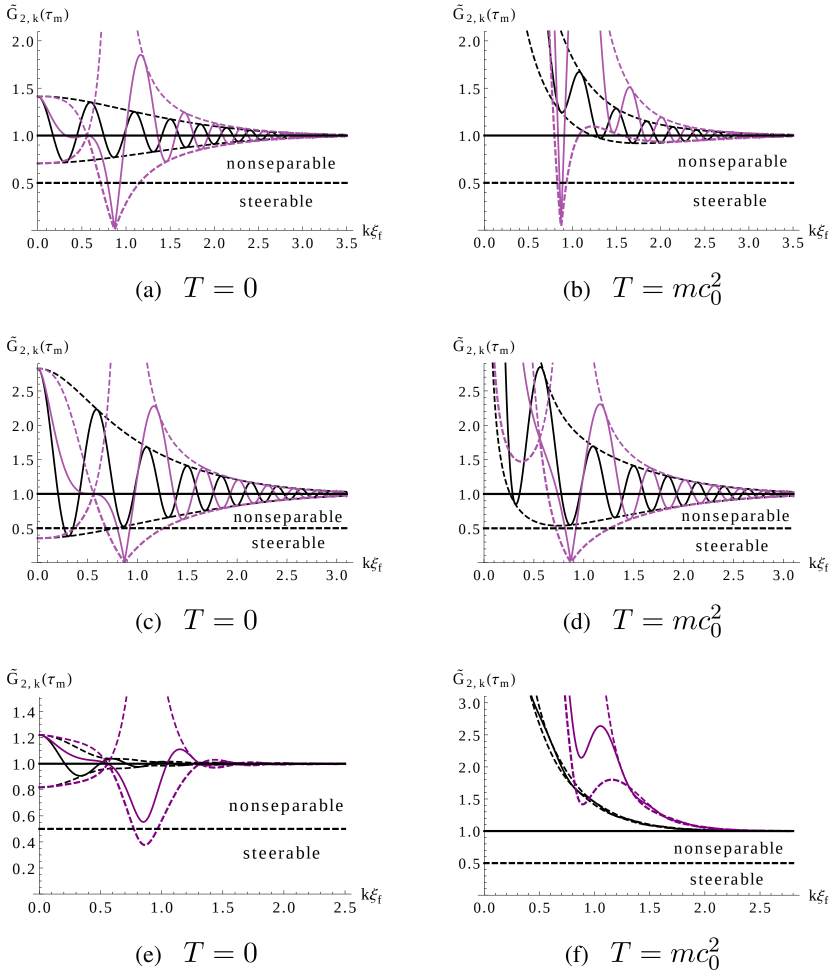


Figure 11.5: *Density-density correlations as a function of $k\xi_f$ at zero temperature (left) and finite temperature (right).* The measurement time is $\tau_\mathrm{m} = 5 \times (mc_f^2)^{-1}$. Here $c_i^2/c_f^2 = 1/2$, and the rate of change $a/\omega_{\mathbf{k}i} = 1(k\xi_f = 3)$ for (a) and (b); $c_i^2/c_f^2 = 1/8$, and the rate of change $a/\omega_{\mathbf{k}i} = 1(k\xi_f = 3)$ for (c) and (d); and $c_i^2/c_f^2 = 1/2$, and the rate of change $a/\omega_{\mathbf{k}i} = 0.05(k\xi_f = 3)$ for (e) and (f). The black solid curves corresponds to contact interaction, $R = 0$ ($\tilde{A} = \tilde{A}_c/10$). The solid purple curves are for the DDI-dominated case ($R = \sqrt{\pi/2}$) at criticality, $\tilde{A} = 3.4454$. The dashed lines are envelopes. Correlation functions are normalized by $(u_\mathbf{k} + v_\mathbf{k})^2$, such that the nonseparability and steerability thresholds occur at 1 (thick black line) and $1/2$ (dashed thick black line), respectively.

Chapter 12

Conclusion

We have found that when there are only contact interactions between particles, $R = 0$, SIPS is retained (in the limit of many e-folds), while there appear strong deviations from scale invariance in the presence of strong DDI (Fig. 7.3), due to an initially present roton minimum. Importantly, the influence of the trans-Planckian nonlinear dispersion is manifest even far from criticality at A_c. When a negative slope in the excitation spectrum occurs ($A > A_{\min}$ in Fig.4.2), the power spectrum shows a general tendency of increase at high momenta. On the other hand, for monotonically increasing spectrum, i.e. when $A \leq A_{\min}$, the power spectrum oscillates around the SIPS prediction.

The proposed experiment (or variants thereof, possibly with other engineered interaction potentials) adds a new example to analogue gravity program for exploring trans-Planckian backaction in quantum simulation of kinematical effects in curved spacetime. Hence the system will potentially lead to conclusions about the trans-Planckian physics of quantum fields in early cosmological stages.

We stress that the presence of a minimum in the spectrum does *not necessarily* imply violations of scale invariance: It is possible to construct an analytic solution to the full Bogoliubov equations for a spectrum with minimum, which displays SIPS (cf. Sec. 7.2). We also note in this regard that SIPS is a kinematical effect for quantum fields in de Sitter spacetime, in analogy to Hawking radiation from black holes [6], and therefore, like the latter, does not require the Einstein equations to hold.

We also have studied the production of quasiparticle pairs in a quasi-two-dimensional dipolar condensate undergoing a rapid temporal variation of its speed of sound, and focused on the density-density correlation function to determine the nonseparability and steerability of the final quasiparticle state. As demonstrated in Figs. 11.3, 11.4 and 11.5, the DDI between the gas particles significantly enhances the potential for the creation of entanglement and steering, being established between quasiparticle modes $\mathbf{k}$ and $-\mathbf{k}$. This will provide ease to detect the quantum correlations in the presence of finite temperature thermal noise.

Going beyond mean-field theory, future perspectives include to study the influence of strong quantum fluctuations of high density electrically dipolar gases [55], prevailing in an early, possibly pre-metric stage, onto the analogue cosmological evolution in the inflationary scenario.

APPENDICES

Chapter A

Cosmological Models of General Relativity

A.1 Conceptual Introduction to General Relativity

Despite the mathematical complexity, general relativity is at heart a highly intuitive theory. The most important concepts of the theory can be dealt without requiring mathematical sophistication, and we begin with these physical fundamentals. From the constancy of c, the speed of light, it is simple to show that the only possible linear transformation relating the coordinates measured by different observers is the Lorentz transformation:

$$\begin{aligned} dx' &= \gamma \left(dx - \frac{v}{c} cdt \right) \\ cdt' &= \gamma \left(cdt - \frac{v}{c} dx \right), \end{aligned} \tag{A.1}$$

where $\gamma = \frac{1}{\sqrt{1-(v/c)^2}} > 1$. We define a relativistic invariant, the proper time $d\tau$, by

$$c^2 d\tau^2 = c^2 dt^2 - dx^2 - dy^2 - dz^2. \tag{A.2}$$

Observe that the derivative of τ with respect to coordinate time t yields

$$c\frac{d\tau}{dt} = \sqrt{c^2 - v^2} \quad \Rightarrow \quad \frac{dt}{d\tau} = \frac{1}{\sqrt{1-(v/c)^2}} = \gamma,$$

in terms of which we find the 4-velocity $U^\mu = dx^\mu / d\tau$ is written as

$$U^\mu = \left(c\frac{dt}{d\tau}, \frac{d\mathbf{x}}{d\tau} \right) = \frac{dt}{d\tau}(c, \mathbf{v}) = \gamma(c, \mathbf{v}).$$

Defining the 4-momentum $P^\mu = m\, dx^\mu / d\tau$ allows an immediate relativistic generalization of conservation of mass and momentum; Newton's second law $\mathbf{F} = m\, d\mathbf{u}/dt$ is not a relation between the spatial components of two 4-vectors. The obvious way to define 4-force is

$$F^\mu = \frac{dP^\mu}{d\tau}. \tag{A.3}$$

But where does the 3-force $\mathbf{F}$ sit in F^μ? Force will still be defined as rate of change of momentum, $\mathbf{F} = d\mathbf{P}/dt$; the required components of F^μ are $F^\mu = \gamma(\partial_0 E, \mathbf{F})$, and the equation (A.3) yields the correct relativistic force-acceleration relation

$$\gamma\mathbf{F} = m\frac{d}{d\tau}(\gamma\mathbf{u}) = m\frac{dt}{d\tau}\frac{d}{dt}(\gamma\mathbf{u}) \quad \Rightarrow \quad \mathbf{F} = m\frac{d}{dt}(\gamma\mathbf{u}). \tag{A.4}$$

However, it turns out that, in curved spacetime, (A.3) cannot be a law of physics.

Consider how the components of dx^μ transform under the adoption of a new set of coordinates x'^μ, which are functions of x^ν:

$$dx'^\mu = \frac{\partial x'^\mu}{\partial x^\nu} dx^\nu. \tag{A.5}$$

This apparently trivial equation may be divided by $d\tau$ on either side to obtain a similar transformation law for 4-velocity U^μ:

$$U'^\mu = \frac{\partial x'^\mu}{\partial x^\nu} U^\nu, \tag{A.6}$$

and we conclude that U^μ is a general 4-vector. However, things unfortunately go wrong at the next level, when we try to differentiate this new equation to form the 4-acceleration $A^\mu = dU^\mu/d\tau$:

$$A'^\mu = \frac{d}{d\tau}U'^\mu = \frac{\partial x'^\mu}{\partial x^\nu} A^\nu + \frac{\partial^2 x'^\mu}{\partial\tau\partial x^\nu} U^\nu. \tag{A.7}$$

The second term on the right-hand side is zero only when the transformation coefficients are constants. This is so for the Lorentz transformation, but not in general. Hence A^μ is not a 4-vector, and the equation $F^\mu = dP^\mu/d\tau = m\, dU^\mu/d\tau = mA^\mu$ cannot be a law of physics, since mA^μ is not a general 4-vector.

The Equivalence Principle

The **weak equivalence principle** is a statement only about space and time. It says that in any gravitational field, however strong, a freely falling observer will experience no gravitational effects — with the important exception of tidal forces in non-uniform fields. The spacetime will be that of special relativity.

The **strong equivalence principle** takes this a stage further and asserts that not only is the spacetime as in special relativity, but all the laws of physics take the same form in the freely falling frame as they would in the absence of gravity. This form of the equivalence principle is crucial in that it will allow us to deduce the generally valid laws governing physics once the special-relativistic forms are known.

Many of the important features of general relativity can be obtained via rather simple arguments that use the equivalence principle. Consider an accelerating frame, which is conventionally a rocket of height h, with a clock mounted on the roof that regularly disgorges photons towards the floor. (Fig. A.1) If the rocket accelerates upwards at g, the floor acquires a speed $v = gh/c$ in the time taken for a photon to travel from roof to floor. There will thus be a blueshift in the frequency of received photons, given by $\Delta\nu/\nu = v/c = gh/c^2$, and it is easy to see that the rate of reception of photons will increase by the same factor.

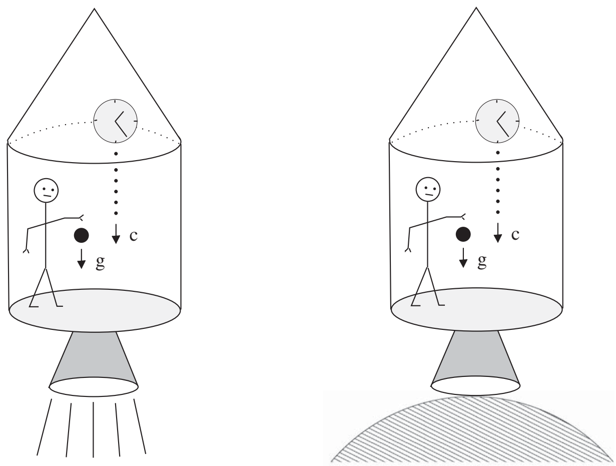


Figure A.1: If the box is made to accelerate 'upwards' and has a clock that emits a photon every second mounted on its roof, you will receive photons more rapidly. According to the equivalence principle, the situation is exactly equivalent to the second picture in which the box sits at rest on the surface of the Earth. Since there is nowhere for the excess photons to accumulate, the conclusion has to be that clocks above us in a gravitational field run fast.

The conclusion of an observer on the floor of the rocket is that in a real sense the clock on the roof is running fast. When the rocket stops accelerating, the clock on the roof will have gained a time Δt by comparison with an identical clock kept on the floor. The equivalence principle can be brought in to conclude that gravity must cause the same effect. Noting that $\Delta\phi = gh$ is the difference in potential between roof and floor, it is simple to generalize this to

$$\frac{\Delta t}{t} = \frac{\Delta \phi}{c^2}. \tag{A.8}$$

The same thought experiment can also be used to show that light must be deflected in a gravitational field: consider a ray that crosses the rocket cabin horizontally when stationary. This track will appear curved when the rocket accelerates.

The Equation of Motion

As mentioned above, the equivalence principle allows us to bootstrap our way from physics in Minkowski spacetime to general laws. Consider freely falling observers, who erect a special-relativity cordinate frame ξ^μ in their neighborhood. The equation of motion for nearby particles is simple:

$$\frac{d^2\xi^\mu}{d\tau^2} = 0; \qquad \xi^\mu = (ct,\, x,\, y,\, z), \tag{A.9}$$

i.e. they have zero acceleration, and we have Minkowski spacetime

$$c^2 d\tau^2 = (cdt)^2 - dx^2 - dy^2 - dz^2 = \eta_{\alpha\beta} d\xi^\alpha d\xi^\beta, \tag{A.10}$$

where $\eta_{\alpha\beta}$ is just a diagonal matrix $\eta_{\alpha\beta} = \mathrm{diag}(1, -1, -1, -1)$. Now suppose the observers make a transformation to some other set of coordinates x^μ. What results is the perfectly general relation

$$d\xi^\mu = \frac{\partial \xi^\mu}{\partial x^\nu} dx^\nu. \tag{A.11}$$

Since $(\partial\xi^\nu/\partial x^\mu)(\partial x^\mu/\partial\xi^\gamma) = \partial\xi^\nu/\partial\xi^\gamma = \delta^\nu_\gamma$, $\partial x^\mu/\partial\xi^\gamma$ is the inverse of $\partial\xi^\nu/\partial x^\mu$. Therefore, substituting (A.11) into (A.9) leads to

$$0 = \frac{d}{d\tau}\left(\frac{\partial\xi^\mu}{\partial x^\nu}\frac{dx^\nu}{d\tau}\right) = \frac{\partial^2\xi^\mu}{\partial x^\rho \partial x^\nu}\frac{dx^\rho}{d\tau}\frac{dx^\nu}{d\tau} + \frac{\partial\xi^\mu}{\partial x^\nu}\frac{d^2x^\nu}{d\tau^2}$$
$$\Rightarrow \quad \frac{d^2x^\nu}{d\tau^2} + \frac{\partial x^\nu}{\partial\xi^\mu}\frac{\partial^2\xi^\mu}{\partial x^\rho\partial x^\nu}\frac{dx^\rho}{d\tau}\frac{dx^\nu}{d\tau} = 0 \quad \Rightarrow \quad \frac{d^2x^\mu}{d\tau^2} + \Gamma^\mu_{\alpha\beta}\frac{dx^\alpha}{d\tau}\frac{dx^\beta}{d\tau} = 0, \tag{A.12}$$

and the metric (A.10) becomes

$$c^2 d\tau^2 = \eta_{\alpha\beta}\frac{\partial\xi^\alpha}{\partial x^\mu}\frac{\partial\xi^\beta}{\partial x^\nu}dx^\mu dx^\nu = g_{\mu\nu}dx^\mu dx^\nu.$$

At this stage, the new quantities appearing in these equations are defined only in terms of our transformation coefficients:

$$\Gamma^{\mu}_{\alpha\beta} = \frac{\partial x^{\mu}}{\partial \xi^{\nu}} \frac{\partial^2 \xi^{\nu}}{\partial x^{\alpha} \partial x^{\beta}} \tag{A.13}$$

$$g_{\mu\nu} = \eta_{\alpha\beta} \frac{\partial \xi^{\alpha}}{\partial x^{\mu}} \frac{\partial \xi^{\beta}}{\partial x^{\nu}}. \tag{A.14}$$

Coordinate Transformations

What is the physical meaning of this analysis? We have taken the special relativity equations for motion and the structure of spacetime and looked at the effects of a general coordinate transformation. A general transformation could be one to the frame of an accelerating observer, but the transformation might have no direct physical interpretation at all. It is important to realize that general relativity makes no distinction between coordinate transformations associated with motion of the observer and a simple change of variable. This flexibility of the theory is something of a problem: it can sometimes be hard to see when some feature of a problem is 'real', or just an artifact of the coordinate adopted. A common term for the latter class is **gauge transformation**. The term gauge always refers to some freedom within a theory that has no observable consequence (e.g. the arbitrary value of $\nabla \cdot \mathbf{A}$, where $\mathbf{A}$ is the vector potential in electrodynamics).

Connection

What is the meaning of the coefficients $\Gamma^{\mu}_{\alpha\beta}$? These are known as components of the **affine connection** or as **Christoffel symbols**. These quantities obviously correspond roughly to the gravitational force — but what determines whether such a force exists? The answer is that gravitational acceleration depends on spatial change in the metric. We can differentiate the equation for $g_{\mu\nu}$, eq.(A.14), to get

$$\begin{aligned}
\frac{\partial g_{\mu\nu}}{\partial x^{\lambda}} &= \eta_{\alpha\beta} \frac{\partial^2 \xi^{\alpha}}{\partial x^{\lambda} \partial x^{\mu}} \frac{\partial \xi^{\beta}}{\partial x^{\nu}} + \eta_{\alpha\beta} \frac{\partial \xi^{\alpha}}{\partial x^{\mu}} \frac{\partial^2 \xi^{\beta}}{\partial x^{\lambda} \partial x^{\nu}} \\
&= \eta_{\alpha\beta} \frac{\partial^2 \xi^{\gamma}}{\partial x^{\lambda} \partial x^{\mu}} \frac{\partial \xi^{\alpha}}{\partial \xi^{\beta}} \frac{\partial \xi^{\beta}}{\partial x^{\nu}} + \eta_{\alpha\beta} \frac{\partial^2 \xi^{\gamma}}{\partial x^{\lambda} \partial x^{\nu}} \frac{\xi^{\beta}}{\xi^{\gamma}} \frac{\partial \xi^{\alpha}}{\partial x^{\mu}} \\
&= \left(\frac{\partial^2 \xi^{\gamma}}{\partial x^{\lambda} \partial x^{\mu}} \frac{\partial x^{\sigma}}{\partial \xi^{\gamma}} \right) \eta_{\alpha\beta} \frac{\partial \xi^{\alpha}}{\partial x^{\sigma}} \frac{\partial \xi^{\beta}}{\partial x^{\nu}} + \left(\frac{\partial^2 \xi^{\gamma}}{\partial x^{\lambda} \partial x^{\nu}} \frac{\partial x^{\sigma}}{\partial \xi^{\gamma}} \right) \eta_{\alpha\beta} \frac{\partial \xi^{\beta}}{\partial x^{\sigma}} \frac{\partial \xi^{\alpha}}{\partial x^{\mu}} \\
&= \Gamma^{\sigma}_{\lambda\mu} g_{\sigma\nu} + \Gamma^{\sigma}_{\lambda\nu} g_{\sigma\mu}.
\end{aligned}$$

Therefore we obtain

$$
\begin{aligned}
(i) \quad & \frac{\partial g_{\mu\nu}}{\partial x^{\lambda}} = \Gamma^{\alpha}_{\lambda\mu} g_{\alpha\nu} + \Gamma^{\beta}_{\lambda\nu} g_{\beta\mu} \\
(ii) \quad & \frac{\partial g_{\lambda\nu}}{\partial x^{\mu}} = \Gamma^{\alpha}_{\lambda\mu} g_{\alpha\nu} + \Gamma^{\beta}_{\mu\nu} g_{\beta\lambda} \qquad (\mu \leftrightarrow \lambda) \\
(iii) \quad & \frac{\partial g_{\mu\lambda}}{\partial x^{\nu}} = \Gamma^{\alpha}_{\nu\mu} g_{\alpha\lambda} + \Gamma^{\beta}_{\lambda\nu} g_{\beta\mu} \qquad (\nu \leftrightarrow \lambda)
\end{aligned}
$$

Taking $(i) + (ii) - (iii)$, we obtain

$$\Gamma^{\alpha}_{\lambda\mu} = \frac{1}{2} g^{\alpha\nu} \left(\partial_{\lambda} g_{\mu\nu} + \partial_{\mu} g_{\lambda\nu} - \partial_{\nu} g_{\mu\lambda} \right).$$

A.2 Tensors and Relativity

One can only construct an invariant quantity in general relativity (i.e. one that is the same for all observers) by **contracting** vector or tensor indices in pairs: $A^{\mu} A_{\mu}$ is the invariant 'size' or **norm** of the vector A^{μ}. Suppose we are given an equation such as $A^{\mu} B_{\mu} = 1$, and that A^{μ} is known to be a 4-vector. Clearly, the right-hand side of the equation is invariant, and so the only way in which this can happen in general is if B_{μ} is also a 4-vector. This trick of deducing the nature of quantities in a relativistic equation is called the principle of **manifest covariance**.

For example, in special relativity, the 4-derivatives are given by

$$
\begin{aligned}
\partial_{\mu} &= \left(\frac{\partial}{\partial ct}, \nabla \right) \\
\partial^{\mu} &= \left(\frac{\partial}{\partial ct}, -\nabla \right).
\end{aligned}
\tag{A.15}
$$

Manifest covariance allows quantities like the **4-current** $J^{\mu} = (c\rho, \mathbf{j})$ to be recognized as 4-vectors, since they allow the conservation law to be written relativistically: $\partial^{\mu} J_{\mu} = \partial_t \rho + \nabla \cdot \mathbf{j} = 0$.

Pseudotensors and Tensor Densities

We can take the determinant of the metric:

$$g = \det(g_{\mu\nu}).$$

This is not an invariant scalar: thinking of tensor transformations in matrix terms,

$$g'_{\mu\nu} = \frac{\partial x^\alpha}{\partial x'^\mu}\frac{\partial x^\beta}{\partial x'^\nu} g_{\alpha\beta} \quad \Leftrightarrow \quad G' = \Lambda^T G \Lambda, \qquad \Lambda_{ab} = \frac{\partial x^a}{\partial x'^b}, \quad G_{ab} = g_{ab},$$

shows that g' depends on the Jacobian of the coordinate transformation:

$$g' = (\det \Lambda)^2 g = \left| \frac{\partial x'^\alpha}{\partial x^\beta} \right|^{-2} g. \tag{A.16}$$

On the other hand, under a general coordinate transformation, the hypervolume element behaves as

$$d^4x' = \left| \frac{\partial x'^\alpha}{\partial x^\beta} \right| d^4x,$$

so that we find the invariant volume element to be

$$\sqrt{-g'} d^4x' = \left| \frac{\partial x'^\alpha}{\partial x^\beta} \right|^{-1} \sqrt{-g} \left| \frac{\partial x'^\alpha}{\partial x^\beta} \right| d^4x = \sqrt{-g} d^4x.$$

We say that an object formed from a tensor and n powers of $\left| \partial x'^\alpha / \partial x^\beta \right|^{-1}$ is called a **tensor density** of weight n.

Proper and Improper Transformations

It is usual to distinguish between different classes of Lorentz transformations according to the sign of their corresponding Jacobians: **proper Lorentz transformations** have $J > 0$, whereas those with negative Jacobians are termed **improper**.

In special relativity, where $g = -1$ always, seeing (A.16), there are two possibilities: $J = \pm 1$. Thus, a tensor density will in special relativity transform like a tensor if we restrict ourselves to proper transformations. However, on spatial inversion, densities of odd weight will change sign. Such quantities are referred to as **pseudotensors** (or, in special cases pseudovectors or pseudoscalars). The mose famous example of this is the totally antisymmetric **Levi-Civita pseudotensor** $\epsilon^{\alpha\beta\gamma\delta}$, which has components $+1$ when $\alpha\beta\gamma\delta$ is an even permutation of 0123, -1 for odd permutations and zero otherwise. This frame-independent component definition implies that this is a tensor density of weight -1:

$$\epsilon'^{\alpha\beta\gamma\delta} = \frac{\partial x'^\alpha}{\partial x^\mu}\frac{\partial x'^\beta}{\partial x^\nu}\frac{\partial x'^\gamma}{\partial x^\rho}\frac{\partial x'^\delta}{\partial x^\sigma} \epsilon^{\mu\nu\rho\sigma} = \left| \frac{\partial x'^\mu}{\partial x^\nu} \right| \epsilon^{\alpha\beta\gamma\delta}.$$

Lowering indices with the metric tensor produces

$$\epsilon_{\alpha\beta\gamma\delta} = g_{\alpha\mu}g_{\beta\nu}g_{\gamma\rho}g_{\delta\sigma}\epsilon^{\mu\nu\rho\sigma} = g\epsilon^{\alpha\beta\gamma\delta}. \tag{A.17}$$

In special relativity, $\epsilon^{\alpha\beta\gamma\delta}$ is therefore of opposite sign to $\epsilon_{\alpha\beta\gamma\delta}$.

Physics in General Relativity

So far, we have dealt with gravitational dynamics only. How are other parts of physics incorporated into general relativity? A hint at the answer is obtained by looking again at the equation of motion (A.12), $d^2x^\mu/d\tau^2 + \Gamma^\mu_{\alpha\beta}(dx^\alpha/d\tau)(dx^\beta/d\tau) = 0$. Remembering that $d^2x^\mu/d\tau^2$ is not a general 4-vector, we see that the addition of the term containing the affine connection has made the equation **gauge invariant**. The term 'gauge' means that there are hidden degrees of freedom (coordinate transformations in this case) that do not affect physical observables. We introduce the **covariant derivative**:

$$DA^\mu \equiv dA^\mu + \Gamma^\mu_{\alpha\beta}A^\alpha dx^\beta. \tag{A.18}$$

Then the equation of motion under gravity is then most simply expressed by saying that the covariant derivative of 4-velocity vanishes: $DU^\mu/d\tau = 0$. By using the manifest covariance, it is easy to see that covariant derivative transforms as a 4-vector: the form of DU^μ was deduced by transforming the relation $dU^\mu/d\tau = 0$ from the local freely falling frame to a general frame. If $DU^\mu/d\tau$ vanishes in all frames, it must be a general 4-vector.

In the presence of non-gravitational forces, the equation of motion for a particle become

$$m\frac{DU^\mu}{d\tau} = F^\mu. \tag{A.19}$$

We impose that the covariant derivative of a scalar field is the same as the ordinary derivative, and that the Leibniz rule is satisfied by the covariant derivative. Then the derivatives of covariant vectors can be derived:

$$\begin{aligned} & d(A^\mu B_\mu) = D(A^\mu B_\mu) = (DA^\mu)B_\mu + A^\mu(DB_\mu) \\ \Rightarrow \quad & A^\mu(DB_\mu) = d(A^\mu B_\mu) - (DA^\mu)B_\mu = A^\mu dB_\mu - \left(\Gamma^\mu_{\alpha\beta}A^\alpha dx^\beta\right)B_\mu \\ & \qquad = A^\mu\left(dB_\mu - \Gamma^\alpha_{\mu\beta}B_\alpha dx^\beta\right) \end{aligned}$$

$$\Rightarrow \qquad DB_\mu = dB_\mu - \Gamma^\alpha_{\mu\beta} B_\alpha dx^\beta.$$

We remark here that the following relation holds.

$$\frac{DA^\mu}{dx^\nu} = \nabla_\nu A^\mu = \partial_\nu A^\mu + \Gamma^\mu_{\nu\rho} A^\rho.$$

Geodesics

It is easy to see that the variation $x^\mu \to x^\mu + \delta x^\mu$ applied to

$$\delta \int g_{\mu\nu} U^\mu U^\nu d\tau = 0$$

yields the correct equation of motion:

$$\begin{aligned}
&\frac{d}{d\tau}\left(2g_{\mu\nu}U^\nu\right) - U^\alpha U^\beta \frac{\partial g_{\alpha\beta}}{\partial x^\mu} = 0 \\
\Rightarrow \quad & 2\frac{\partial g_{\mu\nu}}{\partial x^\alpha} U^\alpha U^\nu + 2g_{\mu\nu}\frac{d^2x^\nu}{d\tau^2} - U^\alpha U^\beta \frac{\partial g_{\alpha\beta}}{\partial x^\mu} = 0 \\
\Rightarrow \quad & \frac{d^2x^\nu}{d\tau^2} = -\frac{1}{2} g^{\nu\mu}\left(-\frac{\partial g_{\alpha\beta}}{\partial x^\mu} + \frac{\partial g_{\alpha\mu}}{\partial x^\beta} + \frac{\partial g_{\mu\beta}}{\partial x^\alpha}\right) U^\alpha U^\beta = -\Gamma^\nu_{\alpha\beta} U^\alpha U^\beta. \qquad \text{(A.20)}
\end{aligned}$$

Energy-Momentum Tensor

The Einstein's equation, which will be discussed in the following section, relates the distribution of matter with the metric and its derivatives. We model the matter content not by a collection of point particles but by a fluid, a continuum characterized by macroscopic quantities such as density, pressure, entropy, viscosity, and so on. A single momentum four-vector field, e.g. the 4-current $J^\mu = (c\rho, \mathbf{j})$, is insufficient to describe the energy momentum of a fluid. We thus introduce the energy-momentum tensor $T^{\mu\nu}$ which is symmetric $(2, 0)$ tensor. In the Minkowski spacetime, it is easy to state the physical meaning of each components of energy-momentum tensor $T^{\mu\nu}$: "the flux of four momentum p^ν across a surface of constant x^μ."

In many cosmologically interesting cases, relativists usually consider a special type of fluid of matter, the **perfect fluid**, which is defined by, in the Minkowski spacetime,

$$T^{\mu\nu} = (\rho + p/c^2) U^\mu U^\nu - p\eta^{\mu\nu}, \qquad \text{(A.21)}$$

where ρ is the rest frame mass density, p is an isotropic pressure, and U^μ is the (constant) 4-velocity field of the fluid. The rest frame $T^{\mu\nu}$ is given by just $\mathrm{diag}(\rho c^2, p, p, p)$.

One reason for considering such an exotic energy-momentum tensor is that the conservation law $\partial_\mu T^{\mu\nu} = 0$ reduces, in the non-relativistic limit, to the continuity equation and the Euler equation of fluid dynamics: for the perfect fluid (A.21),

$$0 = \partial_\mu T^{\mu\nu} = \partial_\mu(\rho + p/c^2)U^\mu U^\nu + (\rho + p/c^2)(U^\nu \partial_\mu U^\mu + U^\mu \partial_\mu U^\nu) - \partial^\nu p. \quad \text{(A.22)}$$

To analyze what this equation means, it is helpful to consider separately what happens when we project it into pieces along and orthogonal to the 4-velocity field U^μ. To project (A.22) along the 4-velocity, we simply contract it with U_ν:

$$0 = U_\nu \partial_\mu T^{\mu\nu} = c^2 \partial_\mu(\rho U^\mu) + p \partial_\mu U^\mu, \quad \text{(A.23)}$$

where we used the normalization $U_\nu U^\nu = c^2$ and its implication $U_\nu \partial_\mu U^\nu = \frac{1}{2}\partial_\mu(U_\nu U^\nu) = 0$. Now we take the non-relativistic limit, in which

$$\rho c^2 \gg p, \qquad U^\mu = (c, \mathbf{u}), \qquad c \gg u. \quad \text{(A.24)}$$

Then the result (A.23) becomes

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0,$$

which is the continuity equation for mass density.

We next consider the part of (A.22) that is orthogonal to U^μ. For that purpose we multiply it by the projection tensor

$$P^\sigma{}_\nu = \delta^\sigma_\nu - U^\sigma U_\nu / c^2.$$

Observe that the projection operator annihilates any vector proportional to U^ν, and preserves the orthogonal one. When applied to $\partial_\mu T^{\mu\nu}$, we obtain

$$P^\sigma{}_\nu \partial_\mu T^{\mu\nu} = (\rho + p/c^2) U^\mu \partial_\mu U^\sigma - \partial^\sigma p + U^\sigma U^\mu \partial_\mu p / c^2.$$

In the non-relativistic limit (A.24), setting the spatial components of this expression equal to zero yields $\rho\,[\partial_t + \mathbf{u}\cdot\nabla]\,\mathbf{u} + \nabla p + \mathbf{u}(\partial_t p + \mathbf{u}\cdot\nabla p)/c^2 = 0$. Here we may neglect the third term in the limit (A.24) and obtain

$$\partial_t\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\frac{1}{\rho}\nabla p,$$

which is the Euler equation familiar in fluid mechanics.

The following expression is clearly a tensor and reduces to the rest-frame Minkowski expression (A.21):

$$T^{\mu\nu} = (\rho + p/c^2)U^\mu U^\nu - p g^{\mu\nu};$$

thus it must be the general expression for the energy-momentum tensor of a perfect fluid by the technique of manifest covariance.

Field Equations

The only ingredient now missing from a classical theory of relativistic gravitation is a field equation: the presence of mass must determine the gravitational field. The existence of a general metric says that spacetime is curved in a way that is revealed by non-zero second derivatives of $g^{\mu\nu}$. There has to be some covariant description of this curvature, and this is exactly what the **Riemann tensor** provides:

$$R^\mu{}_{\alpha\beta\gamma} = \Gamma^\mu_{\alpha\gamma,\beta} - \Gamma^\mu_{\alpha\beta,\gamma} + \Gamma^\mu_{\sigma\beta}\Gamma^\sigma_{\gamma\alpha} - \Gamma^\mu_{\sigma\gamma}\Gamma^\sigma_{\beta\alpha}.$$

The Riemann tensor is contracted to the Ricci tensor $R^{\mu\nu}$ and further to the curvature scalar R:

$$R_{\alpha\beta} = R^\mu_{\alpha\beta\mu}, \qquad R = R^\mu_\mu = g^{\mu\nu}R_{\mu\nu}.$$

Unfortunately, these definitions are not universally agreed, and different signs can arise in the final equations according to which convention is adopted. All authors, however, agree on the definition of the Einstein tensor $G^{\mu\nu}$:

$$G^{\mu\nu} = R^{\mu\nu} - \frac{1}{2}g^{\mu\nu}R.$$

This tensor has zero covariant divergence: $G^{\mu\nu}_{;\nu} = \partial_\nu G^{\mu\nu} + \Gamma^\mu_{\alpha\nu}G^{\alpha\nu} + G^\nu_{\alpha\nu}G^{\mu\alpha} = 0$. Since $T^{\mu\nu}$ also has zero covariant divergence by virtue of the conservation laws it expresses, it therefore seems reasonable to guess that the two are proportional:

$$G^{\mu\nu} = kT^{\mu\nu}. \tag{A.25}$$

The correct constant of proportionality will be obtained below by considering the weak-field limit, where Einstein's theory must go over to Newtonian gravity.

Sign Conventions

Incidentally, we mention that there are few universal conventions in general relativity. The distinctions that exist were analysed into three signs by Misner, Thorne & Wheeler (1973):

$$\begin{aligned} \eta^{\mu\nu} &= [S1] \times \mathrm{diag}(-1,\ +1,\ +1,\ +1) \\ R^{\mu}{}_{\alpha\beta\gamma} &= [S2] \times \left(\Gamma^{\mu}_{\alpha\gamma,\beta} - \Gamma^{\mu}_{\alpha\beta,\gamma} + \Gamma^{\mu}_{\sigma\beta}\Gamma^{\sigma}_{\gamma\alpha} - \Gamma^{\mu}_{\sigma\gamma}\Gamma^{\sigma}_{\beta\alpha}\right) \\ G_{\mu\nu} &= [S3] \times \frac{8\pi G}{c^4} T_{\mu\nu}. \end{aligned}$$

The third sign above is related to the choice of convention for the Ricci tensor:

$$R_{\mu\nu} = [S2] \times [S3] \times R^{\alpha}_{\mu\alpha\nu}.$$

With these definitions, Misnoer, Thorne & Wheeler classify themselves as $(+++)$, whereas Weinberg (1972) is $(+--)$, Peebles (1980, 1993) and Efstathiou (1990) are $(-++)$. This review is $(-+-)$, as are Rindler (1977), Atwater (1974), Narlikar & Padmanabhan (1986), Collins, Martin & Squires (1989), and Peacock (1999).

Newtonian Limit

To obtain the correct proportionality constant in the eq. (A.25), we consider the limit of a *stationary particle* in a *stationary* (i.e. time-independent) *weak field*. To first order in the field, we can replace τ by t, and the spatial part of the geodesic equation (A.20) is then

$$\ddot{x}^i + c^2\Gamma^i_{00} = 0,$$

where $\Gamma^i_{00} = -\frac{1}{2}g^{ij}\partial_j g_{00} = \frac{1}{2}\partial_i g_{00}$. Thus we have

$$\ddot{\mathbf{x}} = -\frac{c^2}{2}\nabla g_{00} \equiv -\nabla\phi,$$

where we obtained a expression for Newtonian potential $\phi = \frac{c^2}{2}g_{00}$ in the stationary, weak-field limit. In the Newtonian mechanics, the Newtonian potential is supposed to satisfy the Poisson equation $\nabla^2\phi = 4\pi G\rho$. Thus we have

$$\Gamma^i_{00,i} = \frac{1}{2}\nabla^2 g_{00} = \frac{1}{c^2}\nabla^2\phi = \frac{4\pi G}{c^2}\rho. \tag{A.26}$$

Considering a classical source of gravity, with $p \ll \rho c^2$, so that the only non-zero component of $T^{\mu\nu}$ is $T^{00} = c^2\rho$, the spatial parts of $R^{\mu\nu}$ must be given by

$$\begin{aligned} R^{ij} = \frac{1}{2}g^{ij}R \quad &\Rightarrow \quad R^i{}_\nu = \frac{1}{2}g^i{}_\nu R = \frac{1}{2}\delta^i{}_\nu R \quad \Rightarrow \quad R^i{}_i = \frac{1}{2}\delta^i{}_i R = \frac{3}{2}R \\ &\Rightarrow \quad R - R^0{}_0 = \frac{3}{2}R \quad \Rightarrow \quad R - g_{0\nu}R^{00} = \frac{3}{2}R \\ &\Rightarrow \quad R = -2R^{00}. \end{aligned}$$

And hence

$$G^{00} = G_{00} = 2R_{00}. \tag{A.27}$$

Discarding nonlinear (2nd order) terms in the definition of the Riemann tensor leaves

$$R_{\alpha\beta} = \Gamma^\mu_{\alpha\mu,\beta} - \Gamma^\mu_{\alpha\beta,\mu} \quad \Rightarrow \quad R_{00} = -\Gamma^i_{00,i} \tag{A.28}$$

for the case of a stationary field.

Combining eqs. (A.26), (A.27) and (A.28), we find

$$G^{00} = 2R_{00} = -2\Gamma^i_{00,i} = -\frac{8\pi G}{c^2}\rho = -\frac{8\pi G}{c^4}T^{00},$$

and we obtain the field equations with correct constant of proportionallity:

$$G^{\mu\nu} = -\frac{8\pi G}{c^4}T^{\mu\nu}. \tag{A.29}$$

Pressure as a Source of Gravity

Newtonian gravitation is modified in the case of a relativistic fluid (i.e. where we cannot assume $p \ll \rho c^2$). We recast the field equations by contracting the equation to obtain $R = (8\pi G/c^4)T$. This allows us to write an equation for $R^{\mu\nu}$:

$$R^{\mu\nu} = -\frac{8\pi G}{c^4}(T^{\mu\nu} - \frac{1}{2}g^{\mu\nu}T).$$

Since $T = c^2\rho - 3p$, we get a modified Poisson equation:

$$\begin{aligned}
&\Rightarrow R^{00} = -\frac{8\pi G}{c^4}(T^{00} - \frac{1}{2}(c^2\rho - 3p)) \\
&\Rightarrow -\frac{4\pi G}{c^2}\rho = -\frac{4\pi G}{c^2}(\rho + 3p/c^2) \\
&\Rightarrow \nabla^2\phi = 4\pi G(\rho + 3p/c^2).
\end{aligned}$$

Energy Density of Vacuum

One consequence of the gravitational effects of pressure that may seem of mathematical interest only is that a negative-pressure equation of state that achieved $\rho c^2 + 3p < 0$ would produce gravitational *repulsion*.

When Einstein was first thinking about the cosmological consequences of general relativity, he believed the universe to be static. It should be obvious, even in the context of Newtonian gravity, that such a universe is not stable: the mutual attraction of all particles would cause the distribution of mass to undergo a global contraction. This could be prevented only by either postulating an expanding universe (which idea Einstein unfortunately discarded at that time), or by interfering with the long-range properties of gravity.

Einstein was loath to complicate the beautiful simplicity of the field equations, and there seemed only one way out. He introduced the energy-momentum tensor of the vacuum:

$$T^{\mu\nu}_{\text{vac}} = \frac{\Lambda c^4}{8\pi G}g^{\mu\nu},$$

and then the field equation has the form

$$G^{\mu\nu} + \Lambda g^{\mu\nu} = -\frac{8\pi G}{c^4}T^{\mu\nu}.$$

How can a vacuum have a non-zero energy density and pressure? It is well known hard to predict what the properties of the vacuum should be. Assuming the energy and pressure of the vacuum to be apart from zero, the energy momentum tensor of the vacuum $T^{\mu\nu}_{\rm vac}$ must be proportional to the metric tensor in order for being unaltered by Lorentz transformations. Therefore, it is inevitable that the vacuum (at least in special relativity) will have a negative-pressure equation of state:

$$p_{\rm vac} = -\rho_{\rm vac} c^2, \qquad \rho_{\rm vac} = \frac{\Lambda c^2}{8\pi G}.$$

In this case, $\rho c^2 + 3p$ is indeed negative: a positive Λ will act to cause a large-scale repulsion.

Since the vacuum energy is a constant, independent of time, there might seem to be a problem with conservation of energy in an expanding universe. However, since the pressure is negative, the work done by the pressure is negative, and this becomes a source of energy, which can supply as much as is required to inflate a given region to any required size at constant energy density. This supply of energy is what is used in 'inflationary' theories of cosmology to create the whole universe out of almost nothing.

A.3 Maximally Symmetric Spacetime

Noether theorem of field theory in flat spacetime states that "symmetry of the spacetime implies a conserved quantity." In the context of general relativity, in which the background geometry is generally curved, there arises the need for rigorous charaterization of concepts of symmetry and conserved quantity.

Symmetries of a manifold are related to a special kind of transformations (isometries) defined on the manifold. Actually, we need a continuous family of transformations to characterize a symmetry of the manifold. And it can be shown that these continuous families of transformations, each of which corresponds to a symmetry of the manifold, are in one-to-one correspondence with vector fields, the Killing vector fields, which will be defined soon.

It is easy to figure out a condition for a vector field to imply a symmetry of the spacetime and a conserved quantity. Suppose that a particle (massive or massless) is moving along a geodesic in a given spacetime. Let's denote the 4-momentm of a massive particle by a product of its rest mass and its 4-velocity, $p^\mu = mU^\mu$. Here, the 4-velocity is the derivative of the spacetime position of the particle with repect to the proper time, $U^\mu = dx^\mu/d\tau$.

For the case of massless particles, the affine parameter λ is chosen so that the tangent vector $dx^\mu/d\lambda$ gives the 4-momentum of the particle, $p^\mu = dx^\mu/d\lambda$, since the proper time for a massless particle is identically zero ($d\tau = 0$, null geodesic). By definition, the geodesic is a parametrized curve which parallel transports its tangent vector (and its scalar multiples of course) along the trajectory. Thus $p^\mu \nabla_\mu p^\nu = 0$ holds. Now, consider a vector field K^ν which is defined over the spacetime. The quantity we want to secure its constancy is $K^\nu p_\nu = K_\nu p^\nu$, namely we want to show

$$p^\mu \nabla_\mu (K_\nu p^\nu) = 0.$$

By expanding the left hand side, we obtain,

$$\begin{aligned} p^\mu \nabla (K_\nu p^\nu) &= p^\nu p^\mu \nabla_\mu K_\nu + K_\nu p^\mu \nabla_\mu p^\nu \\ &= p^\mu p^\nu \nabla_{(\mu} K_{\nu)}. \end{aligned}$$

For this to vanish for any 4-momentum p^μ, it is necessary and sufficient that the condition,

$$\nabla_{(\mu} K_{\nu)} = 0$$

hold. This equation is known as **Killing's equation** and the vector fields satisfying this equation are called the **Killing vector fields**. If the metric is independent of some coordinate $x^{\sigma *}$, the vector field $K = \partial_{\sigma *}$ can be an easy example of Killing vector field, i.e., a vector field satisfying the Killing's equation : $K^\nu = (\partial_{\sigma *})^\nu = \delta^\nu_{\sigma *},\ K_\nu = K^\mu g_{\mu\nu} = \delta^\mu{}_{\sigma^*} g_{\mu\nu}$,

$$\begin{aligned} \nabla_{(\mu} K_{\nu)} &= \frac{1}{2} \left(\nabla_\mu (g_{\alpha\nu} \delta^\alpha{}_{\sigma^*}) + \nabla_\nu (g_{\alpha\mu} \delta^\alpha{}_{\sigma^*}) \right) = \frac{1}{2} \left(g_{\alpha\nu} \Gamma^\alpha_{\mu\sigma^*} + g_{\alpha\mu} \Gamma^\alpha_{\nu\sigma^*} \right) \\ &= \frac{1}{2} \Big(\delta^\beta{}_\nu (\partial_\mu g_{\beta\sigma^*} + \partial_{\sigma^*} g_{\beta\mu} - \partial_\beta g_{\mu\sigma^*}) + \delta^\beta{}_\mu (\partial_n u g_{\beta\sigma^*} + \partial_{\sigma^*} g_{\beta\nu} - \partial_\beta g_{\nu\sigma^*}) \Big) \\ &= \partial_{\sigma^*} (g_{\mu\nu}) \\ &= 0. \end{aligned}$$

The conserved quantity along the geodesic, in this case, is the component of the 4-momentum in $\partial_{\sigma *}$ direction : $K^\nu p_\nu = p_{\sigma *}$.

Although, for each Killing vector field, there is a coordinate system in which a coordinate vector coincides with the Killing vector field, there is in general no coordinate system in which more than one cordinate vectors are the same as given Killing vectors. This is partly because Killing vectors don't need to be linearly independent, and partly because there can be more than n independent Killing vector fields in an n-dimensional manifold.

But there is a highest possible number of Killing vectors in an n-dimensional manifold. For counting, let us focus on a neighborhood of a point p in an n-dimensional manifold. Since any sufficiently small neighborhood resembles $\mathbb{R}^n$ with canonical metric, we count the number of possible isometries by counting those of $\mathbb{R}^n$. First, there are n independent translations. And there are rotations around the point p. We can count the number of rotations by counting the number of 2 dimensional subspaces of $\mathbb{R}^n$, which is ${}_nC_2 = n(n-1)/2$. If the metric signiture were not Euclidean, some of the rotations will actually be boosts, but again the counting will be the same. Therefore, the total number of independent isometries of $\mathbb{R}^n$ is

$$n + \frac{1}{2}n(n-1) = \frac{1}{2}n(n+1).$$

Since our counting argument only refers to the behavior of the symmetry in a neighborhood of p, even in the presence of curvature the counting should be the same. We refer to an n-dimensional manifold with $\frac{1}{2}n(n+1)$ Killing vectors as a **maximally symmetric space**.

If a manifold is maximally symmetric, the curvature is the same everywhere and the same in every direction. This idea ends up with an equation true in any maximally symmetric spaces, at any point, in any coordinate system:

$$R_{\rho\sigma\mu\nu} = \frac{R}{n(n-1)}(g_{\rho\mu}g_{\sigma\nu} - g_{\rho\nu}g_{\sigma\mu}), \tag{A.30}$$

where the Ricci scalar R is constant over the manifold. Convince yourself that the indices in the RHS have the symmetric properties of Riemann tensor. Conversely, if the Riemann tensor satisfies this condition (A.30) (with R a constant over the manifold), the metric will be maximally symmetric. We omit the proof.

Since the magnitude of the Ricci scalar R can be absorbed to the metric, we can classify the maximally symmetric spaces according to the sign of R. For Euclidean signitures, the flat maximally symmetric spaces are planes or appropriate higher-dimensional generalizations, while the positively curved ones are spheres, and negatively curved ones are hyperboloids, denoted H^n.

A.4 de Sitter Universe

The Copernican principle is related to two mathematically precise properties that a manifold might have : isotropy and homogeniety. Isotropy applies at some specific point in the manifold, and states that the space looks the same no matter in which direction we look. More formally, a manifold $\mathcal{M}$ is **isotropic** around a point p if, for any two vectors V and W in $T_p\mathcal{M}$, there is an isometry of $\mathcal{M}$ such that the pushforward of W under the isometry is parallel with V (not pushed forward). **Homogeniety** is the statement that the metric is the same throughout the manifold. In other words, given any two points p and q in $\mathcal{M}$, there is an isometry that takes p into q.

An extreme application of the Copernican principle would be to insist that spacetime is maximally symmetric. But, in fact, observationally we know that the universe is homogeneous and isotropic in *space*, but not at all of *spacetime*. However, it would be interesting to begin by considering spacetimes that are maximally symmetric, the de Sitter and anti-de Sitter spacetime. We mentioned in section A.3 that the Riemann tensor for a maximally symmetric n-dimensional manifold with metric $g_{\mu\nu}$ can be written as

$$R_{\rho\sigma\mu\nu} = \kappa(g_{\rho\mu}g_{\sigma\nu} - g_{\rho\nu}g_{\sigma\mu}),$$

where κ is a normalized measure of the Ricci curvature

$$\kappa = \frac{R}{n(n-1)}$$

and the Ricci scalar R will be a constant over the manifold. For vanishing curvature ($\kappa = 0$), a possible maximally symmetric spacetime is the well known Minkowski spacetime.

Maximally Symmetric Spacetime with Positive Curvature

The maximally symmetric spacetime with positive curvature ($\kappa > 0$) is called **de Sitter spacetime**. Consider a five-dimensional Minkowski space with metric $ds_5^2 = du^2 - dx^2 - dy^2 - dz^2 + d\omega^2$, and embed a hyperboloid given by

$$-u^2 + x^2 + y^2 + z^2 + \omega^2 = \alpha^2.$$

Now introduce coordinates $\{t, \chi, \theta, \phi\}$ on the hyperboloid via

$$
\begin{aligned}
u &= \alpha \sinh(t/\alpha) \\
\omega &= \alpha \cosh(t/\alpha) \cos\chi \\
x &= \alpha \cosh(t/\alpha) \sin\chi \cos\theta \\
y &= \alpha \cosh(t/\alpha) \sin\chi \sin\theta \cos\phi \\
z &= \alpha \cosh(t/\alpha) \sin\chi \sin\theta \sin\phi
\end{aligned}
$$

with ranges $-\infty < t < \infty,\ 0 < \chi < \pi,\ 0 < \theta < \pi,$ and $0 < \phi < 2\pi$. The metric on the hyperboloid becomes

$$ds^2 = dt^2 - \alpha^2 \cosh^2(t/\alpha)\Big[d\chi^2 + \sin^2\chi(d\theta^2 + \sin^2\theta d\phi^2)\Big] \tag{A.31}$$

Now we perform a clever coordinate transformation to obtain conformal diagram of de Sitter space. Consider the transformation from t to t' via

$$\cosh(t/\alpha) = \frac{1}{\cos(t')}$$

where t' assumes $-\frac{\pi}{2} < t' < \frac{\pi}{2}$. Then the metric (A.31) becomes

$$
\begin{aligned}
& \frac{1}{\alpha}\sinh(t/\alpha)dt = \frac{\sin(t')}{\cos^2(t')}dt' \\
\Rightarrow\quad & \frac{1}{\alpha^2}\Big(\cosh^2(t/\alpha) - 1\Big)dt^2 = \frac{\sin^2(t')}{\cos^4(t')}dt'^2 = \frac{1}{\cos^2(t')}\Big(\frac{1}{\cos^2(t') - 1}\Big)dt'^2 \\
\Rightarrow\quad & dt^2 = \frac{\alpha^2}{\cos^2(t')}dt'^2 \\
\Rightarrow\quad & ds^2 = \frac{\alpha^2}{\cos^2(t')}\Big((dt')^2 - d\chi^2 - \sin^2\chi d\Omega_2^2\Big).
\end{aligned}
$$

Recall that the ranges are $-\frac{\pi}{2} < t' < \frac{\pi}{2}$ and $0 < \chi < \pi$. So the conformal diagram is just a square. (Fig. A.2)

One special feature that de Sitter spacetime has is that two points can have future (or past) light cones that are completely disconnected; this reflects the fact that the spherical spatial sections are expanding so rapidly that light from one point can never come into contact with light from the other.

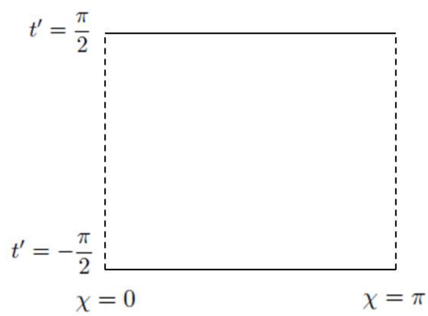


Figure A.2: Conformal diagram for de Sitter spacetime

If we introduce

$$\begin{aligned} u &= \frac{2c}{H}\sinh(Ht/2) + Hr'^2 e^{Ht/2}/4c \\ \omega &= \frac{2c}{H}\cosh(Ht/2) - Hr'^2 e^{Ht/2}/4c \\ x &= e^{Ht/2}x' \\ y &= e^{Ht/2}y' \\ z &= e^{Ht/2}z', \end{aligned}$$

where $r'^2 = x'^2 + y'^2 + z'^2$, them the metric becomes

$$ds^2 = c^2dt^2 - e^{Ht}d\mathbf{r}'^2.$$

This is called the flat slicing of de Sitter spacetime, which is used to model the accelerated expansion of the universe.

Maximally Symmetric Spacetime with Negative Curvature

Now let us consider the negative curvature case of maximally symmetric spacetime, known as **anti-de Sitter spacetime**. Begin with a fictitious five-dimensional flat manifold with metric $ds_5^2 = du^2 + dv^2 - dx^2 - dy^2 - dz^2$, and embed a hyperboloid given by

$$-u^2 - v^2 + x^2 + y^2 + z^2 = -\alpha^2.$$

We introduce coordinates $\{t', \rho.\theta, \phi\}$ on the hyperboloid via

$$\begin{aligned} u &= \alpha \sin(t') \cosh(\rho) \\ v &= \alpha \cos(t') \cosh(\rho) \\ x &= \alpha \sinh(\rho) \cos\theta \\ y &= \alpha \sinh(\rho) \sin\theta \cos\phi \\ z &= \alpha \sinh(\rho) \sin\theta \sin\phi \end{aligned} \tag{A.32}$$

with ranges $-\infty < t' < \infty,\ 0 < \rho < \infty,\ 0 < \theta < \pi,$ and $0 < \phi < 2\pi$. Actually, there is redundancy in the range of t'. The range $0 < t' < 2\pi$ is enough, and it is not legitimate to extend this interval because it will break the injectiveness of the chart. By allowing t' to range from $-\infty$ to ∞, we actually are considering the "covering space" of the embeded hyperboloid, which we will take as the definition of anti-de Sitter space. The metric in terms of these new coordinates becomes

$$ds^2 = \alpha^2\Big(\cosh^2(\rho)(dt')^2 - d\rho^2 - \sinh^2(\rho)d\Omega_2^2\Big).$$

Now we perform coordinate transformations to derive the conformal diagram. Define a new coordinate χ by

$$\cosh(\rho) = \frac{1}{\cos\chi}$$

with $0 < \chi < \frac{\pi}{2}$, so that

$$\begin{aligned} ds^2 &= \alpha^2\left(\frac{1}{\cos^2\chi}(dt')^2 - \frac{\sin^2\chi}{\cos^4\chi}\frac{\cos^2\chi}{\sin^2\chi}d\chi^2 - \frac{\sin^2\chi}{\cos^2\chi}d\Omega_2^2\right) \\ &= \frac{\alpha^2}{\cos^2\chi}\Big((dt')^2 - d\chi^2 - \sin^2\chi d\Omega_2^2\Big) \\ &= \frac{\alpha^2}{\cos^2\chi}d\bar{s}^2 \end{aligned}$$

where $d\bar{s}^2$ represents the metric on the Einstein static universe.

The conformal diagram is shown in Fig. A.3, which illustrates a few representative timelike and spacelike geodesics passing through the point $t' = 0, \chi = 0$.

So we have three spacetimes of maximal symmetry: Minkowski ($\kappa = 0$), de Sitter ($\kappa > 0$), and anti-de Sitter ($\kappa < 0$). We can ask, at this point, whether any one of these

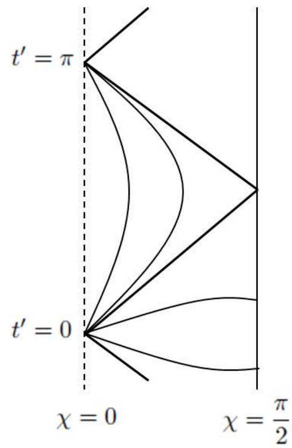


Figure A.3: Conformal diagram for anti-de Siter spacetime

spaces model the real world.

Unfortunately, the maximally symmetric spacetimes are not reasonable models of the universe, which will be explained in detail later. Until now, there was no restriction on introducing spacetime and its metric. But, in fact, not all of these spacetimes are physically meaningful. Then what will be physically meaningful spacetime?

A.5 FRW Universe

Just as Einstein aimed to write down the simplest possible relativistic generalization of the laws of gravity, so cosmological investigation began by considering the simplest possible mass distribution: one whose properties are homogeneous (constant density) and isotropic (the same in all directions).

Isotropy Implies Homogeneity

Consider an observer who is surrounded by a matter distribution that is perceived to be **isotropic**. Most scientists believe that it is not reasonable to adopt a cosmological model in which humans are privileged observers. This attitude is called the **Copernican principle**. It is therefore a reasonable supposition that, if the universe appears isotropic about our position, it would also appear isotropic to observers in other galaxies; the term ‘isotropic’ is therefore often employed in cosmology as a shorthand for ‘isotropic about all locations’. This is a crucial shift in meaning, for the properties of such a universe are highly restricted.

In fact, given only two points (A and B) from which conditions appear isotropic, we can prove that they must be homogeneous everywhere. (See Fig.A.4.)

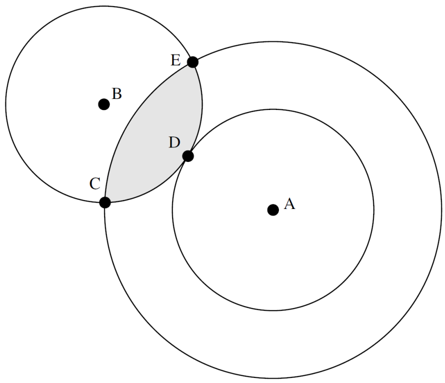


Figure A.4: Isotropy about two points A and B shows that the universe is homogeneous. From isotropy about B, the density is the same at each of C, D, E. By constructing spheres of different radii about A, the shaded zone is swept out and shown to be homogeneous. By using large enough shells, this argument extends to the entire universe.

Having chosen a model mass distribution, the next step is to solve the field equations to find the correponding metric. Since our model is a particularly symmetric one, many of the features of the metric can be deduced from symmetry alone. These general arguments were put forward independently by H.P. Robertson and A.G. Walker in 1936.

Cosmological Time and Foliation of Spacelike Slices

The first point to note is that a universal time exists in an isotropic universe. Consider a set of observers in different locations, all of whom are at rest with respect to the matter in their vicinity (these characters are usually termed **fundamental observers**). We can define a global time coordinate t, which is the time measured by the clocks of these observers – i.e. t is the proper time measured by an observer at rest with respect to the local matter distribution. The coordinate is useful globally as well as locally because the clocks can be synchronized by the exchange of light signals between observers, who agree to set their clocks to a standard time when, e.g., the universal homogeneous density reaches some given value.

It turns out to be straightforward, and consistent with observation, to posit that the universe is spatially homogeneous and isotropic, but evolving in time. In general relativity this translates into the statement that the universe can be foliated into spacelike slices such that each three-dimensional slice is maximally symmetric. We therefore consider our spacetime to be $\mathbb{R} \times \Sigma$, where $\mathbb{R}$ represents the cosmological time direction and Σ is a maximally symmetric three-manifold. The spacetime metric thus takes the form

$$c^2 d\tau^2 = c^2 dt^2 - R^2(t) d\sigma^2$$

Here, we have used the equivalence principle to say that the proper time interval between two distant events would look locally like special relativity to a fundamental observer on the spot: for them, $c^2 d\tau^2 = c^2 dt^2 - dx'^2 - dy'^2 - dz'^2$, and the coefficient of dt^2 should be constant(c^2), not a function of r. $R(t)$ is a function known as the **scale factor**, and $d\sigma^2$ is the metric on Σ, which can be expressed as

$$d\sigma^2 = \gamma_{ij}(x) dx^i dx^j,$$

where (x^1, x^2, x^3) are coordinates on Σ and γ_{ij} is a maximally symmetric three dimensional metric. The coordinates used here, in which the metric is free of cross terms $dtdx^i$ and coefficient of dt^2 is independent of x^i, are known as **comoving coordinates**. An observer who stays at constant x^i is also called "comoving."

Robertson-Walker Metrics

Our interest is in maximally symmetric Euclidean three-metrics γ_{ij}. We know that maximally symmetric metrics obey

$${}^{(3)}R_{ijkl} = k(\gamma_{il}\gamma_{jk} - \gamma_{ik}\gamma_{jl}),$$

where for future convenience we have introduced

$$k = {}^{(3)}R/6,$$

and we put a superscript ${}^{(3)}$ on the Riemann tensor to remind that it is associated with the three-metric γ_{ij}, not the metric of the entire spacetime. The Ricci tensor is then

$${}^{(3)}R_{jk} = 2k\gamma_{jk}. \tag{A.33}$$

If the space is to be maximally symmetric, then it will certainly be spherically symmetric. One requirement to preserve spherical symmetry is that we maintain the form of $d\Omega^2$, that is, if we want our spheres to be perfectrly round, the coefficient of the $d\phi^2$ term should be $\sin^2\theta$ times that of the $d\theta^2$ term. But we are otherwise free to multiply all of the terms by separate coefficients, so long as they are only functions of the radial coordinate r:

$$d\sigma^2 = e^{2\beta(r)}dr^2 + e^{2\gamma(r)}r^2 d\Omega^2. \tag{A.34}$$

We've expressed our functions as exponentials so that the signature of the metric doesn't change.

Unlike other theories of physics, in general relativity we simultaneously define coordinates and the metric as a function of those coordinates. In other words, we don't know ahead of time what, for example, the radial coordiante r really is; we can only interpret it once the solution is in our hands. Let us therefore imagine defining a new coordinate $\bar{r}$ via

$$\bar{r} = e^{\gamma(r)}r,$$

with an associated basis one-form

$$d\bar{r} = \left(1 + r\frac{d\gamma}{dr}\right)e^{\gamma}dr.$$

In terms of this new variable, the metric (A.34) becomes

$$d\sigma^2 = \left(1 + r\frac{d\gamma}{dr}\right)^{-2} e^{2\beta(r)-2\gamma(r)}d\bar{r}^2 + \bar{r}^2 d\Omega^2, \tag{A.35}$$

where each function of r is a function of $\bar{r}$ in the obvious way. Now let us make the following relabelings:

$$\bar{r} \rightarrow r, \qquad \left(1 + r\frac{d\gamma}{dr}\right)^{-2} e^{2\beta(r)-2\gamma(r)} \rightarrow e^{2\beta}$$

Then our metric (A.35) becomes

$$d\sigma^2 = e^{2\beta(r)}dr^2 + r^2 d\Omega^2. \tag{A.36}$$

We have simply chosen a special coordinate system. Thus, (A.36) is precisely as general as (A.34).

The components of the Ricci tensor for such a metric can be obtained, and we will have

$$^{(3)}R_{11} = \frac{2}{r}\partial_r\beta, \quad ^{(3)}R_{22} = e^{-2\beta}(r\partial_r\beta - 1), \quad ^{(3)}R_{33} = [e^{-2\beta}(r\partial_r\beta - 1) + 1]\sin^2\theta.$$

We set these proportional to the metric using (A.33), and can solve for $\beta(r)$:

$$\beta = -\frac{1}{2}\ln(1 - kr^2),$$

which yields the metric on the three-surface Σ,

$$d\sigma^2 = \frac{dr^2}{1 - kr^2} + r^2 d\Omega^2.$$

It is common to normalize the value of k, which sets the curvature, so that $k \in \{+1,\ 0,\ -1\}$, and absorb the physical size of the manifold into the scale factor $R(t)$. Now the metric of the *spacetime* is written

$$c^2 d\tau^2 = c^2 dt^2 - R^2(t)\left(\frac{dr^2}{1 - kr^2} + r^2 d\Omega^2\right) \tag{A.37}$$

This is the **Robertson-Walker (RW) metric**. We have not yet made use of Einstein's equation; that will determine the behavior of the scale factor $R(t)$.

The most compact form of RW metric can be obtained by applying to (A.37) a transformation

$$d\tilde{r} = \frac{R_0 dr}{\sqrt{1 - kr^2}},$$

and defining

$$S_k(\tilde{r}) = \begin{cases} R_0 \sin\left(\frac{\tilde{r}}{R_0}\right) & (k = +1) \\ R_0 \sinh\left(\frac{\tilde{r}}{R_0}\right) & (k = -1) \\ \tilde{r} & (k = 0), \end{cases}$$

where R_0 is the crrent value of $R(t)$, $R_0 = R(t = 0)$. One can make the scale factor dimensionless, defining $a(t) \equiv R(t)/R_0$, so that $a = 1$ at the present.

The metric can now be written in the preferred form that we shall use throughout:

$$c^2 d\tau^2 = c^2 dt^2 - a^2(t)\left[dr^2 + S_k^2(r) d\Omega^2\right], \tag{A.38}$$

where we replaced $\tilde{r}$ with r. Cosmologists generally use the metric in the form of (A.37) or of (A.38) with **comoving distance** r whose value depends on which metric is being used in the context. We will use the metric (A.38) unless there is any notice.

It is also important to note that cosmologists tend to use the term 'distance' as meaning comoving distance unless otherwise specified, usually in units of Mpc.

Hubble's Law

The physical separation $r_{\rm ph}$ between two points with dimensionlesss comoving distance r is $r_{\rm ph} = a(t)r$, and therefore, the relative velocity between them can be written as $v_{\rm ph} \equiv dr_{\rm ph}/dt = \dot{a}r = Hr_{\rm ph}$, where

$$H = \frac{\dot{a}}{a},$$

and the Hubble's Law reads $v_{\rm ph} = Hr_{\rm ph}$.

Conformal Time

There is another modification of some importance; this is to define the **conformal time**

$$\eta = \int^t \frac{cdt'}{a(t')}, \tag{A.39}$$

which allows a factor of a^2 to be taken out of the metric

$$c^2 d\tau^2 = a^2(t)\left[d\eta^2 - dr^2 - S_k^2(r)\Omega^2\right]$$

This is a special case of a conformal transformation in general relativity, such transformations correspond to $g^{\mu\nu} \to fg^{\mu\nu}$, where f is some arbitrary spacetime function. The universe with $k = 0$, although certainly possessing spacetime curvature, is obviously directly related to Minkowski spacetime via a conformal transformation, and so tends to be loosely known as the 'flat' model. If we denote the begining of the conformal time by η_i, the maximal distance that light could propagate in the past is

$$r_p = \eta - \eta_i = \int_{t_i}^t \frac{cdt'}{a(t')}.$$

We call r_p the dimensionless comoving particle horizon, and corresponding distance ar_p is called the **particle horizon**. Points far from each other by r_p cannot be causally connected in the past times.

On the other hand, if we denote the ending of the conformal time by $\eta_{\max}$, the maximal distance that light can propagate in the future is

$$r_e = \eta_{\max} - \eta = \int_t^{\infty} \frac{cdt'}{a(t')}.$$

We call r_e the dimensionless comoving event horizon, and corresponding distance ar_e is called the **event horizon**.

The Redshift

Since photons travel on null geodesics of zero proper time, we see directly from the metric (A.38) that

$$r = \int_{t_{\text{emit}}}^{t_{\text{obs}}} \frac{cdt}{a(t)}.$$

The comoving distance between two fundamental observer is constant, whereas the domain of integration in time extends from t_{emit} to t_{obs}; these are the times of emission and reception of a photon. Photons that are emitted at later times $t_{\text{emit}} + dt_{\text{emit}}$ will be received at later times $t_{\text{obs}} + dt_{\text{obs}}$, but these changes in t_{emit} and t_{obs} cannot alter the integral, since r is a comoving quantity. This requires the condition $dt_{\text{emit}}/a(t_{\text{emit}}) = dt_{\text{obs}}/a(t_{\text{obs}})$, or

$$\frac{dt_{\text{emit}}}{dt_{\text{obs}}} = \frac{a(t_{\text{emit}})}{a(t_{\text{obs}})},$$

which means that events on distant galaxies time-dilate according to how much the universe has expanded since the photons we see now were emitted. We therefore get

$$\frac{\nu_{\text{emit}}}{\nu_{\text{obs}}} = \frac{R(t_{\text{obs}})}{R(t_{\text{emit}})}.$$

Cosmologists like to speak of this in terms of the **redshift** z between the two events, defined by the fractional change in wavelength:

$$z \equiv \frac{\lambda_{\text{obs}} - \lambda_{\text{emit}}}{\lambda_{\text{emit}}} \quad \Rightarrow \quad 1 + z \equiv \frac{\nu_{\text{emit}}}{\nu_{\text{obs}}} = \frac{a(t_{\text{obs}})}{a(t_{\text{emit}})}.$$

In terms of the normalized scale factor $a(t)$ we have simply $a(t) = (1 + z)^{-1}$. Photon wavelengths therefore stretch with the universe.

This is the only correct interpretation of the redshift at large distances; it is common but misleading to convert a large redshift to a recession velocity using the special-relativistic formula $1 + z = [(1 + v/c)/(1 - v/c)]^{1/2}$. Any such temptation should be avoided.

Causal Structure and Conservation Laws

For general RW universe spatial slices are curved. Here we consider flat RW universe. The spacetime is provided with the metric

$$ds^2 = c^2dt^2 - a^2(t)[dx^2 + dy^2 + dz^2] \tag{A.40}$$

This describes a universe for which "space at a fixed moment of time" is a flat three dimensional Euclidean space, which is expanding as a function of time.

Worldlines that remain at constant spatial coordinates x^i are said to be **comoving**; similarly, we denote a region of space that expands along with boundaries defined by fixed spatial coordinates as a "comoving volume." Since the metric describes $(\text{distance})^2$, the relative distance between comoving points is growing as $a(t)$ in this spacetime; the function a is called the **scale factor**.

For this metric to model the physical universe, we assume the scale factor $a(t)$ to satisfy

(i) $a(t) > 0$,

(ii) $\lim_{t\to 0} a(t) = 0$,

(iii) $\lim_{t\to 0} \dfrac{t}{a(t)} < \infty$.

The first condition is needed to maintain the Lorentzian signiture of the metric. The second and third conditions will be derived from the Einstein's equation, the dynamical equation that determines the metric from given energy-momentum tensor.

Note that there is a crucial difference between this metric and that of Minkowski space; this metric has a singularity at $t = 0$, which restricts the range of our coordinate:

$$0 < t < \infty.$$

This is a coordinate-dependent statement, and in principle there might be another coordinate system in which everything looks finite; in this case, however, $t = 0$ represents a true singularity of the geometry (the "Big Bang"), and should be excluded from the manifold.

Let's first look at the causal structure of the flat RW universe. We put the metric in polar coordinates on space,

$$ds^2 = dt^2 - a^2(t)[dr^2 + r^2 d\Omega^2].$$

Because of the condition (iii) on the scale factor, the integral $\eta = \int_0^t \frac{cdt}{a(t)}$ gives finite value. The range of conformal time is thus $0 < \eta < \infty$ and, by definition,

$$a(\eta)d\eta = cdt,$$

where $a(\eta) = a(t(\eta))$, which can be obtained by inverting (A.39) to obtain $t(\eta)$ and by substituing this into $a(t)$. Now the metric becomes

$$\begin{aligned} ds^2 &= a^2(\eta)d\eta^2 - a^2(\eta)[dr^2 + r^2 d\Omega^2] \\ &= a^2(\eta)\big(d\eta^2 - dr^2 - r^2 d\Omega^2\big) \end{aligned}$$

Now that we have our expanding-universe metric in the form of a conformal factor times Minkowski metric, we can perform the same sequence of coordinate transformations as in the derivation of the conformal diagram for Minkowski spacetime. Define $u := \eta - r$ and $v := \eta + r$, with corresponding ranges given by $-\infty < u < \infty,\ 0 < v < \infty$ and $|u| \leq v$. Then the metric becomes

$$ds^2 = a^2(u,v)\Big(\frac{1}{2}(dudv + dvdu) - \frac{1}{4}(v-u)^2 d\Omega^2\Big).$$

Now let $U := \arctan u$ and $V := \arctan v$, with ranges $-\frac{\pi}{2} < U < \frac{\pi}{2},\ 0 < v < \frac{\pi}{2}$ and $|U| \leq V$. Then we have

$$ds^2 = \frac{a^2(U,V)}{4\cos^2 U \cos^2 V}\Big[2(dUdV + dVdU) - \sin^2(V-U)d\Omega^2\Big].$$

Finally we introduce $T := V + U$ and $R = V - U$, with ranges $0 \leq R < \pi,\ 0 \leq T < \pi$ and $|T| + R < \pi$. The metric becomes

$$ds^2 = \omega^{-2}(T,R)\Big(dT^2 - dR^2 - \sin^2 R d\Omega^2\Big),$$

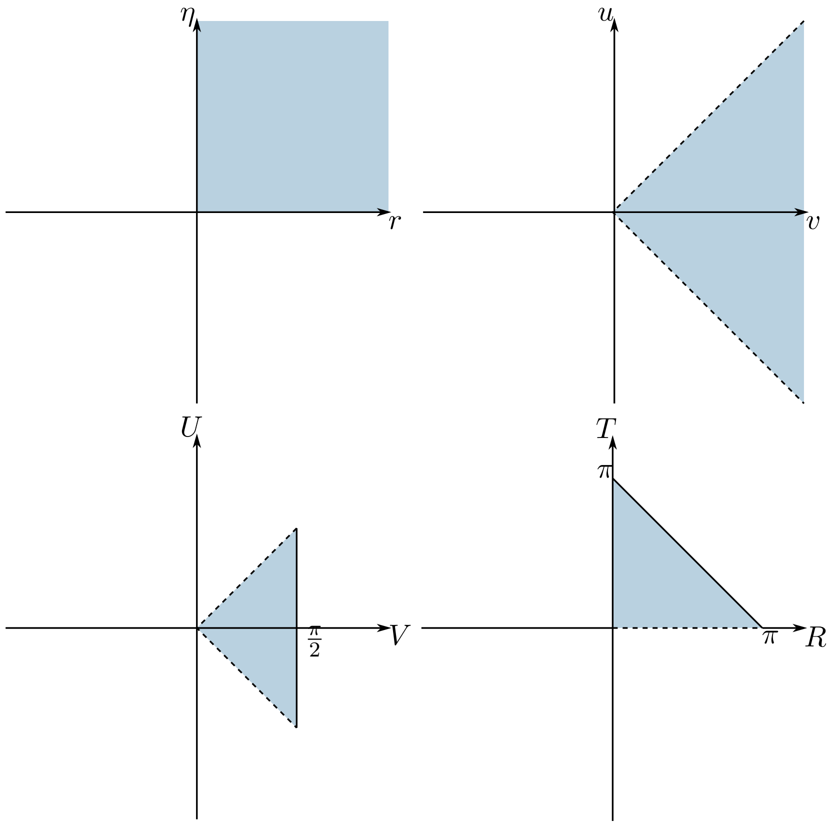


Figure A.5: Ranges of variables

where $\omega^{-2}(T, R)$ is unimportant conformal factor. The ranges can be easily traced by looking at the region depicted in Fig. A.5.

We obtain the conformal diagram for a flat Robertson-Walker metric.(Fig. A.6) The important distinction between this case and that of flat spacetime is that timelike coordinate ends at the singularity $T = 0$; otherwise the spacetime diagram is identical to that of Minkowski spacetime. The light cones appear at $45°$. It is straightforward to choose two events in the spacetime with the property that their past light cones will hit the singularity before they intersect(while future light cones will always overlap).

Having understood the causal structure of the flat RW spacetime, let us investigate the implications of the energy-momentum conservation. In the Minkowski spacetime, it is stated as $\partial_\mu T^{\mu\nu} = 0$. But in general curved spacetime, this statment is coordinate dependent and so cannot have physical meaning. As we will discuss more detail in the next chapter, a simple rule of thumb is simply to replace all partial derivatives by covariant derivatives,

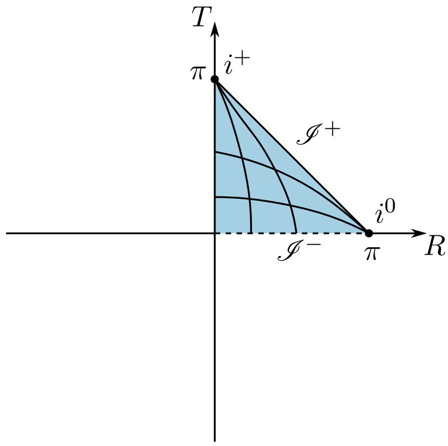


Figure A.6: Conformal diagram for flat Robertson-Walker universe

and all appearance of the flat spacetime metric $\eta_{\mu\nu}$ by the curved metric $g_{\mu\nu}$. Thus the energy-momentum conservation equation becomes

$$\nabla_\mu T^{\mu\nu} = 0, \tag{A.41}$$

or

$$\nabla_\mu T^{\mu\nu} = \partial_\mu T^{\mu\nu} + \Gamma^\mu_{\mu\lambda} T^{\lambda\nu} + \Gamma^\nu_{\mu\lambda} T^{\mu\lambda} = 0. \tag{A.42}$$

Now we find the Christoffel symbols of the metric (A.40). Consider the functional

$$I = \frac{1}{2}\int \left(\frac{cdt}{d\tau}\right)^2 - a^2(t)\left[\left(\frac{dx}{d\tau}\right)^2 + \left(\frac{dy}{d\tau}\right)^2 + \left(\frac{dz}{d\tau}\right)^2\right] d\tau.$$

Let's start with $t \to t + \delta t$. We have

$$\begin{aligned}\delta I &= \frac{1}{2}\int 2\frac{cdt}{d\tau}\frac{cd\delta t}{d\tau} - 2a\dot{a}\left[\left(\frac{dx}{d\tau}\right)^2 + \left(\frac{dy}{d\tau}\right)^2 + \left(\frac{dz}{d\tau}\right)^2\right]\delta t \, d\tau \\ &= \int \left\{-\frac{c^2 d^2 t}{d\tau^2} - a\dot{a}\left[\left(\frac{dx}{d\tau}\right)^2 + \left(\frac{dy}{d\tau}\right)^2 + \left(\frac{dz}{d\tau}\right)^2\right]\right\}\delta t \, d\tau,\end{aligned}$$

from which we have

$$\Gamma^0_{00} = 0, \qquad \Gamma^0_{i0} = \Gamma^0_{0i} = 0, \qquad \Gamma^0_{ij} = \delta_{ij}\frac{a\dot{a}}{c}.$$

Next we consider $x \to x + \delta x$, which yields

$$\delta I = \frac{1}{2}\int 2a^2 \frac{dx}{d\tau}\frac{d\delta x}{d\tau}\, d\tau = \int \Big(\frac{2a\dot{a}}{c}\frac{dx}{d\tau}\frac{cdt}{d\tau} + a^2\frac{d^2x}{d\tau^2}\Big)\delta x\, d\tau.$$

Since the spatial part is isotropic, we would get the same result for y and z coordinates. Thus we obtain

$$\Gamma^i_{00} = 0, \qquad \Gamma^i_{j0} = \Gamma^i_{0j} = \frac{\dot{a}}{ca}\delta^i_j, \qquad \Gamma^i_{jk} = 0.$$

Now that everything is prepared, let's face the equation (A.41). In cosmology, physicists typically model the matter filling the universe as a perfect fluid; the corresponding energy-momentum tensor comes from generalizing (A.21) to curved spacetime,

$$T^{\mu\nu} = (\rho + p/c^2)U^\mu U^\nu - pg^{\mu\nu}.$$

Recall that ρ is the energy density, p is the pressure, and U^μ is the constant four-velocity of the fluid. For metric (A.40), the components of inverse metric are

$$g^{\mu\nu} = \begin{bmatrix} 1 & & & \\ & -a^{-2} & & \\ & & -a^{-2} & \\ & & & -a^{-2} \end{bmatrix}$$

The energy-momentum tensor is a kind of source for the metric of the spacetime. So it is clear that, if a fluid that is isotropic in some frame leads to a metric that is isotropic in the same frame. That is, the fluid will be at rest in comoving coordinates, in which the metric looks like (A.40). The four-velocity is then

$$U^\mu = (c, 0, 0, 0),$$

and the energy-momentum tensor $T^{\mu\nu} = (\rho + p/c^2)U^\mu U^\nu - pg^{\mu\nu}$ becomes

$$T^{\mu\nu} = \begin{bmatrix} \rho c^2 & & & \\ & a^{-2}p & & \\ & & a^{-2}p & \\ & & & a^{-2}p \end{bmatrix}.$$

The equation (A.42) has four components, one for each μ, although the three $\mu = i \in \{1, 2, 3\}$ are equivalent. Let's first look at the $\nu = 0$ component, piece by piece. The first term is straightforward,

$$\partial_\mu T^{\mu 0} = \partial_0 T^{00} = \dot{\rho} c.$$

The second term is

$$\Gamma^\mu_{\mu\lambda} T^{\lambda 0} = \Gamma^\mu_{\mu 0} T^{00} = 3\frac{\dot{a}}{a}\rho c,$$

and the third term is

$$\Gamma^0_{\mu\lambda} T^{\mu\lambda} = \Gamma^0_{00} T^{00} + \Gamma^0_{11} T^{11} + \Gamma^0_{22} T^{22} + \Gamma^0_{33} T^{33} = 3\frac{\dot{a}}{ca} p.$$

altogether, then, we find

$$\dot{\rho} c = -3\frac{\dot{a}}{ca}(\rho c^2 + p). \tag{A.43}$$

Now let's look at one of the spatial components, choosing $\nu = 1$ for definiteness. Once again working piece by piece, we have for the first term in (A.42),

$$\partial_\mu T^{\mu 1} = \partial_1 T^{11} = a^{-2} \partial_x p.$$

The second and third terms are

$$\Gamma^\mu_{\mu\lambda} T^{\lambda 1} = \Gamma^\mu_{\mu 1} T^{11} = 0, \qquad \Gamma^1_{\mu\lambda} T^{\mu\lambda} = \Gamma^1_{00} T^{00} + \Gamma^1_{11} T^{11} + \Gamma^1_{22} T^{22} + \Gamma^1_{33} T^{33} = 0.$$

Equivalent results will hold for $\nu = 2$ and $\nu = 3$. So the spatial components of the energy-momentum conservation equation simply amount to

$$\partial_i p = 0.$$

This does not involve any effect from the scale factor, thus there is no effect of curvature on the spatial components.

Often the perfect fluids relevant to cosmology obey the simple equation of state,

$$p = \omega \rho c^2,$$

where ω is some constant independent of time. Then the (A.43) becomes $\dot{\rho}/\rho = -3(1 +$

$\omega)(\dot{a}/a)$, which can be solved to yield

$$\rho \propto a^{-3(1+\omega)}.$$

Further investigation neccessarily stimulates the issue of what physically meaningful space-time is. At this moment, we have to verify the value of ω and the behavior of the scale factor $a(t)$. The former is determined by 'energy conditions', and the later is determined by the Einstein's equation. Therfore, in the following sections, we move to the discussion of Einstein's equation and the energy conditions.

Dynamics of RW Universe

Consider a sphere about some arbitrary point, and let the radius be $a(t)r$, where r is arbitrary. The motion of a point at the edge of the sphere will, in Newtonian gravity, be influenced only by the interior mass. We can therefore write down immediately a differential equation (**Friedmann's equation**) that expresses conservation of energy:

$$\frac{(\dot{a}r)^2}{2} - \frac{GM}{ar} = \text{const.} \tag{A.44}$$

In fact, the result that the gravitational field inside a uniform shell is zero does hold in general relativity, and is known as **Birkhoff's theorem**. General relativity becomes even more vital in giving us the constant of integration in Friedmann's equation. To this end, we investigate the Einstein's equation with the Robertson Walker metric (A.37):

$$g_{\mu\nu} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -\frac{R^2}{1-kr^2} & 0 & 0 \\ 0 & 0 & -R^2r^2 & 0 \\ 0 & 0 & 0 & -R^2r^2\sin^2\theta \end{bmatrix}.$$

Corresponding Christoffel symbols are calculated as

$$\Gamma^{ct} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{R\dot{R}}{(1-kr^2)c} & 0 & 0 \\ 0 & 0 & \frac{R\dot{R}r^2}{c} & 0 \\ 0 & 0 & 0 & \frac{R\dot{R}r^2\sin^2\theta}{c} \end{bmatrix},$$

$$\Gamma^\theta = \begin{bmatrix} 0 & 0 & \frac{\dot{R}}{Rc} & 0 \\ 0 & 0 & \frac{1}{r} & 0 \\ \frac{\dot{R}}{R} & \frac{1}{r} & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sin 2\theta}{2} \end{bmatrix}, \quad \Gamma^\phi = \begin{bmatrix} 0 & 0 & 0 & \frac{\dot{R}}{Rc} \\ 0 & 0 & 0 & \frac{1}{r} \\ 0 & 0 & 0 & \cot\theta \\ \frac{\dot{R}}{Rc} & \frac{1}{r} & \cot\theta & 0 \end{bmatrix},$$

$$\Gamma^r = \begin{bmatrix} 0 & \frac{\dot{R}}{Rc} & 0 & 0 \\ \frac{\dot{R}}{Rc} & \frac{kr}{1-kr^2} & 0 & 0 \\ 0 & 0 & -(1-kr^2)r & 0 \\ 0 & 0 & 0 & -(1-kr^2)r\sin^2\theta \end{bmatrix},$$

and the non-vanishing Riemann tensors are

$$R_{0r0r} = \frac{R\ddot{R}}{(1-kr^2)c^2} \qquad R_{0\theta0\theta} = \frac{rR\ddot{R}}{c^2}$$

$$R_{0\phi0\phi} = \frac{R\ddot{R}r^2}{c^2}\sin^2\theta \qquad R_{r\theta r\theta} = -\frac{R^2r^2(\dot{R}^2/c^2+k)}{1-kr^2}$$

$$R_{r\phi r\phi} = -\frac{R^2r^2(\dot{R}^2/c^2+k)}{1-kr^2}\sin^2\theta \qquad R_{\theta\phi\theta\phi} = -R^2r^4(\dot{R}^2/c^2+k)\sin^2\theta.$$

The Ricci tensors are

$$R_{00} = 3\frac{\ddot{R}}{Rc^2} \qquad R_{rr} = -\frac{R\ddot{R}/c^2 + 2(\dot{R}^2/c^2+k)}{1-kr^2}$$

$$R_{\theta\theta} = -r^2\left(\frac{R\ddot{R}}{c^2} + 2\frac{\dot{R}^2}{c^2} + 2k\right) \qquad R_{\phi\phi} = -r^2\sin^2\theta\left(\frac{R\ddot{R}}{c^2} + 2\frac{\dot{R}^2}{c^2} + 2k\right),$$

and the Ricci scalar is

$$R = 6\left\{\frac{\ddot{R}}{Rc^2} + \left(\frac{\dot{R}}{cR}\right)^2 + \frac{k}{R^2}\right\}.$$

(Be careful not to confuse the Ricci scalar R on the l.h.s. with the scale factor $R(t)$.) The energy momentum tensor, $T_{\mu\nu} = (\rho + p/c^2)U_\mu U_\nu - pg_{\mu\nu}$, observed in a rest frame in which $U^\mu = (c, \mathbf{0})$, reads

$$T_{\mu\nu} = \mathrm{diag}\left(\rho c^2,\ \frac{pR^2}{1-kr^2},\ pR^2r^2,\ pR^2r^2\sin\theta\right).$$

Now, the 00-component of the Einstein's equation yields

$$R_{00} - \frac{1}{2}g_{00}R = -\frac{8\pi G}{c^4}T_{00} \quad \Rightarrow \quad \left(\frac{\dot{R}}{R}\right)^2 = \frac{8\pi G}{3}\rho - \frac{c^2 k}{R^2}, \tag{A.45}$$

which is the celerbrated **Friedmann's equation** (cf. (A.44)). Looking at the trace of the Einstein's equation, we obtain

$$-R = -\frac{8\pi G}{c^4}T \quad \Rightarrow \quad \ddot{R} = -\frac{4\pi G}{3}R(\rho + 3p/c^2), \tag{A.46}$$

from which one can show that the change of entropy of the universe during its evolution is zero:

$$TdS = dE + pdV \propto d(\rho c^2 R) + pd(R^3) = 0.$$

(A.46) is sometimes called the second Friedmann equation.

Note that the equation (A.45) covers all contributions to ρ, i.e. those from matter, radiation and vacuum; it is independent of the equation of state. The Friedmann equation is so named because Friedmann was the first to appreciate, in 1922, that Einstein's equations admitted cosmological solutions containing matter only. The term Friedmann model is therefore often used to indicate a matter-only cosmology, even though his equation includes contributions from all equations of state. A common shorthand for relativistic cosmological models, which are described by the Robertson-Walker metric and which obey the Friedmann equation, is called **FRW universe**.

Chapter B

Cosmological Particle Production

Identifying particle concept in a curved spacetime is controversial in that it depends on the state of motion of the observer. Even in flat Minkowski spacetime, an accelerated detector will register quanta from the vacuum state in the point of view of inertial observers. A special feature of Minkowski spacetime is that there exists an agreed vacuum for all inertial observers throughout the spacetime. This is because the agreed vacuum is invariant under Poincaré group.

In some restricted situations, we can secure the particle concept even in the presence of spacetime curvature. In many problems of interest, the spacetime can be treated as asymptotically Minkowskian in the remote past and/or future. We will refer to the remote past and futre as *in* and *out* regions, respectively. Under these circumstances, the absence of particles according to inertial observers in the asymptotic region can be taken to be the commonly accepted idea of a vacuum in that region.

If we work in the Heisenberg picture, a chosen vacuum state in the remote past will remain in that state during its subsequent evolution. However, that state may not coincide with the vacuum state in the remote future. In that case, an inertial observer in the future region will detect the presence of particles. We can therefore say that particles have been 'created' by the time-dependent external gravitational field. This is a remarkable prediction in that a galaxy can be created out of vacuum soley from the expansion of the universe.

B.1 Scalar Field Residing on a Flat FRW Universe

Suppose we are given a spacetime with metric

$$ds^2 = c^2 dt^2 - a(t)^2 (dx^2 + dy^2 + dz^2). \tag{B.1}$$

We assume that the manifold is a simple product of temporal part and spatial part: the temporal part is $\mathbb{R}$ and the spatial part is a cube of finite volume V such that the faces standing opposite are identified (3-torus). This spacetime is called spatially flat Friedmann-

Robertson-Walker universe. Define conformal time $\eta(t)$ by

$$\eta(t) \equiv \int_0^t \frac{cdt}{a(t)}.$$

We assume $a(t) > 0$ so that $\eta(t)$ is a strictly increasing function. In terms of conformal time, the metric (B.1) becomes

$$ds^2 = a(\eta)^2 \left[d\eta^2 - dx^2 - dy^2 - dz^2\right] = a(\eta)^2 \eta_{\mu\nu} dx^\mu dx^\nu,$$

where $a(\eta) = a(t(\eta))$, $\eta_{\mu\nu} = \text{diag}(1, -1, -1, -1)$, and $x^0 = \eta$. Setting $g_{\mu\nu} = a^2\eta_{\mu\nu}$, we have $g^{\mu\nu} = a^{-2}\eta^{\mu\nu}$ and $g = \det(g_{\mu\nu}) = -a^8$. Note that (η, x, y, z) is also a coordinate chart for the manifold. By the general covariance, the action for a real minimally coupled massive scalar field $\phi(x)$ becomes

$$\begin{aligned} S &= \frac{1}{2} \int d^4x \sqrt{-g} \left[g^{\mu\nu} \partial_\mu \phi \partial_\nu \phi - m^2 \phi^2\right] \\ &= \frac{1}{2} \int d^4\phi \, a^2 \left[\dot{\phi}^2 - (\nabla\phi)^2 - m^2 a^2 \phi^2\right], \end{aligned} \tag{B.2}$$

where $\dot{\phi} = \partial\phi/\partial\eta$.

We introduce an auxiliary field $\chi(\eta, \mathbf{x}) \equiv a(\eta)\phi(\eta, \mathbf{x})$. Then the action can be rewritten in terms of χ as

$$\begin{aligned} S &= \frac{1}{2} \int d^4x \, a^2 \left[\left(\frac{1}{a}\dot{\chi} - \frac{\dot{a}}{a^2}\chi\right)^2 - \left(\frac{1}{a}\nabla\chi\right)^2 - m^2\chi^2\right] \\ &= \frac{1}{2} \int d^4x \left[\dot{\chi}^2 - \frac{\dot{a}}{a}\dot{\chi}\chi - \frac{\dot{a}}{a}\chi\dot{\chi} + \frac{\dot{a}^2}{a^2}\chi^2 - (\nabla\chi)^2 - m^2 a^2 \chi^2\right]. \end{aligned} \tag{B.3}$$

Substituting $-\frac{\dot{a}}{a}\chi\dot{\chi} = -\frac{\partial}{\partial\eta}\left(\frac{\dot{a}}{a}\chi\chi\right) + \frac{\partial}{\partial\eta}\left(\frac{\dot{a}}{a}\chi\right)\chi$, and discarding the boundary term (which is constant), we obtain

$$S[\chi] = \frac{1}{2} \int d^4x \left[\dot{\chi}^2 - (\nabla\chi)^2 - \left(m^2 a^2 - \frac{\ddot{a}}{a}\right)\chi^2\right]. \tag{B.4}$$

By taking Euler-Lagrange equation for χ yields,

$$\ddot{\chi} - \nabla^2\chi + m_{\text{eff}}^2\chi = 0, \tag{B.5}$$

where $m_{\text{eff}}^2(\eta) \equiv m^2a^2 - \frac{\ddot{a}}{a}$. We remark here that the field χ is a classical field and all the derivations above are classical. We continue the classical analysis.

Expanding the field χ in Fourier modes (this is possible because the given metric (B.1) is spatially flat), we have

$$\chi(\eta, \mathbf{x}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \chi_{\mathbf{k}}(\eta) e^{i\mathbf{k}\cdot\mathbf{x}}, \qquad \pi(\eta, \mathbf{x}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \pi_{\mathbf{k}}(\eta) e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{B.6}$$

where $\pi(\eta, \mathbf{x})$ is the conjugate momentum of $\chi(\eta, \mathbf{x})$, $\pi(\eta, \mathbf{x}) = \partial_0 \chi(\eta, \mathbf{x})$. For Fourier coefficients, we have $\pi_{\mathbf{k}}(\eta) = \dot{\chi}_{\mathbf{k}}(\eta)$. Substituting this expansion into (B.5), we find

$$\ddot{\chi}_{\mathbf{k}} + \omega^2(\eta)\chi_{\mathbf{k}} = 0, \tag{B.7}$$

where $\omega_{\mathbf{k}}(\eta) \equiv \sqrt{k^2 + m_{\text{eff}}(\eta)}$. This is a second order homogeneous linear ODE. Therefore, if we found two linearly independent solutions, then we can express the general solutions as a linear combination of them.

B.2 Mode Expansion

Let $v_k(\eta)$ be a solution for (B.7). Since ω_k depends only on the magnitude $k = |\mathbf{k}|$, $v_k(\eta)$ is a solution for any $\mathbf{k}$ with $|\mathbf{k}| = k$. Observe that v_k^* is also a solution for (B.7). Observe also that

$$\begin{aligned}
v_k \text{ and } v_k^* \text{ are linearly independent.} \;&\Leftrightarrow\; l_1 v_k + l_2 v_k^* = 0 \text{ implies } l_1 = l_2 = 0. \\
&\Leftrightarrow\; \begin{bmatrix} v_k & v_k^* \\ \dot{v}_k & \dot{v}_k^* \end{bmatrix} \begin{bmatrix} l_1 \\ l_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \text{ implies } l_1 = l_2 = 0. \\
&\Leftrightarrow\; W[v_k, v_k^*] = \det \begin{bmatrix} v_k & v_k^* \\ \dot{v}_k & \dot{v}_k^* \end{bmatrix} \neq 0.
\end{aligned}$$

Given a specific $\omega_k(\eta)$, we can find v_k with non-zero Wronskian $W[v_k, v_k^*]$. It is easy to see the following properties of the Wronskian $W[v_k, v_k^*]$.

(i) $\frac{d}{d\eta} W[v_k, v_k^*] = 0$.

(ii) $W[v_k, v_k^*]^* = -W[v_k, v_k^*]$.

(iii) $W[\lambda v_k, (\lambda v_k)^*] = |\lambda|^2 W[v_k, v_k^*]$ for any $\lambda \in \mathbb{C}$.

First two properties imply that the Wronskian $W[v_k, v_k^*]$ is a pure imaginary constant. The third property implies that we may assume that $W[v_k, v_k^*] = -2i$ or $W[v_k^*, v_k] = 2i$ hold, by multiplying appropriate constant. We choose such v_k and v_k^* as two linearly independent solutions for (B.7).

Define a sesqui-linear form (f, g), for functions $f(\eta)$ and $g(\eta)$, by

$$(f, g) \equiv \frac{1}{2i} W[f^*, g] = \frac{1}{2i}(f^* \dot{g} - \dot{f}^* g).$$

Then $(g, f) = (f, g)^*$ and $(f, g)^* = -(f^*, g^*)$ hold. Since the solutions v_k and v_k^* satisfy $W[v_k^*, v_k] = 2i$, we see that $(v_k, v_k) = \frac{1}{2i} W[v_k^*, v_k] = 1$. Summarizing the results,

$$(v_k, v_k) = 1, \qquad (v_k^*, v_k^*) = -1, \qquad (v_k, v_k^*) = (v_k^*, v_k) = 0. \tag{B.8}$$

Now the general solution for (B.7) can be written as a linear combination of v_k and v_k^*:

$$\chi_{\mathbf{k}}(\eta) = \frac{1}{\sqrt{2}} \left(a_{\mathbf{k}} v_k^*(\eta) + b_{\mathbf{k}} v_k(\eta) \right), \tag{B.9}$$

where the prefactor $1/\sqrt{2}$ is introduced for convenience. For $\chi(\eta, \mathbf{x})$ in (B.5) to be real, $\chi_{\mathbf{k}}(\eta)$ must satisfy $\chi_{\mathbf{k}}^* = \chi_{-\mathbf{k}}$. We now have

$$a_{\mathbf{k}}^* v_k + b_{\mathbf{k}}^* v_k^* = a_{-\mathbf{k}} v_k^* + b_{-\mathbf{k}} v_k.$$

By taking inner-product with v_k on the left, and using (B.8), we obtain $a_{\mathbf{k}}^* = b_{-\mathbf{k}}$ or $b_{\mathbf{k}} = a_{-\mathbf{k}}^*$. We get the same result by taking inner-product with v_k^*. Now the solution (B.9) becomes

$$\chi_{\mathbf{k}}(\eta) = \frac{1}{\sqrt{2}} \left(a_{\mathbf{k}} v_k^*(\eta) + a_{-\mathbf{k}}^* v_k(\eta) \right). \tag{B.10}$$

We can invert this relations to obtain expressions for $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^\dagger$ in terms of $\chi_{\mathbf{k}}$ and $\pi_{\mathbf{k}}$:

$$a_{\mathbf{k}} = -\sqrt{2}(v_k^*, \chi_{\mathbf{k}}) = -\frac{\sqrt{2}}{2i}(v_k \dot{\chi}_{\mathbf{k}} - \dot{v}_k \chi_{\mathbf{k}}) = -\frac{1}{\sqrt{2}i}(v_k \pi_{\mathbf{k}} - \dot{v}_k \chi_{\mathbf{k}})$$
$$a_{\mathbf{k}}^* = \sqrt{2}(v_k, \chi_{-\mathbf{k}}) = \frac{\sqrt{2}}{2i}(v_k^* \dot{\chi}_{-\mathbf{k}} - \dot{v}_k^* \chi_{-\mathbf{k}}) = \frac{1}{\sqrt{2}i}(v_k^* \pi_{-\mathbf{k}} - \dot{v}_k^* \chi_{-\mathbf{k}}).$$

Substituting (B.10) into (B.5), we find

$$\begin{aligned}\chi(\eta,\mathbf{x}) &= \frac{1}{\sqrt{2V}}\sum_{\mathbf{k}}\left(a_{\mathbf{k}}v_k^*(\eta)+a_{-\mathbf{k}}^*v_k(\eta)\right)e^{i\mathbf{k}\cdot\mathbf{x}} \\ &= \frac{1}{\sqrt{2V}}\sum_{\mathbf{k}} a_{\mathbf{k}}v_k^*(\eta)e^{i\mathbf{k}\cdot\mathbf{x}}+a_{\mathbf{k}}^*v_k(\eta)e^{-i\mathbf{k}\cdot\mathbf{x}}, \\ \pi(\eta,\mathbf{x}) &= \frac{1}{\sqrt{2V}}\sum_{\mathbf{k}} a_{\mathbf{k}}\dot{v}_k^*(\eta)e^{i\mathbf{k}\cdot\mathbf{x}}+a_{\mathbf{k}}^*\dot{v}_k(\eta)e^{-i\mathbf{k}\cdot\mathbf{x}},\end{aligned} \tag{B.11}$$

where in the second term the summation variable $\mathbf{k}$ was changed from $\mathbf{k}$ to $-\mathbf{k}$.

B.3 Canonical Quantization

We regard $\chi(\eta,\mathbf{x})$ and its conjugate momentum $\pi(\eta,\mathbf{x})$ as Hermitian operators in the Heisenberg picture. The field operator $\hat{\chi}$'s being Hermitian is equivalent to say that $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^*$ are operators and are Hermitian conjugate to each other. We designate $a_{\mathbf{k}}$ as $\hat{a}_{\mathbf{k}}$, and $a_{\mathbf{k}}^*$ as $\hat{a}_{\mathbf{k}}^\dagger$. Now the field operators becomes

$$\begin{aligned}\hat{\chi}(\eta,\mathbf{x}) &= \frac{1}{\sqrt{2V}}\sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}v_k^*(\eta)e^{i\mathbf{k}\cdot\mathbf{x}}+\hat{a}_{\mathbf{k}}^\dagger v_k(\eta)e^{-i\mathbf{k}\cdot\mathbf{x}}, \\ \hat{\pi}(\eta,\mathbf{x}) &= \frac{1}{\sqrt{2V}}\sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}\dot{v}_k^*(\eta)e^{i\mathbf{k}\cdot\mathbf{x}}+\hat{a}_{\mathbf{k}}^\dagger \dot{v}_k(\eta)e^{-i\mathbf{k}\cdot\mathbf{x}}.\end{aligned} \tag{B.12}$$

We impose the equal time commutation relations:

$$[\hat{\chi}(\eta,\mathbf{x}),\hat{\pi}(\eta,\mathbf{y})] = i\delta^{(3)}(\mathbf{x}-\mathbf{y}), \quad [\hat{\chi}(\eta,\mathbf{x}),\hat{\chi}(\eta,\mathbf{y})] = [\hat{\pi}(\eta,\mathbf{x}),\hat{\pi}(\eta,\mathbf{y})] = 0. \tag{B.13}$$

These are equivalent to the commutation relations for the Fourier components:

$$\begin{aligned}&[\hat{\chi}_{\mathbf{k}}(\eta),\hat{\pi}_{\mathbf{l}}(\eta)] = \int d^3\mathbf{x}d^3\mathbf{y}e^{-i\mathbf{k}\cdot\mathbf{x}}e^{-\mathbf{l}\cdot\mathbf{y}}[\hat{\chi}(\eta,\mathbf{x}),\hat{\pi}(\eta,\mathbf{y})] = i\delta_{\mathbf{k},-\mathbf{l}}, \\ &[\hat{\chi}_{\mathbf{k}}(\eta),\hat{\chi}_{\mathbf{l}}(\eta)] = \hat{\pi}_{\mathbf{k}}(\eta),\hat{\pi}_{\mathbf{l}}(\eta)] = 0.\end{aligned} \tag{B.14}$$

These again are equivalent to the commutation relations for $\hat{a}_{\mathbf{k}}$ and $\hat{a}_{\mathbf{k}}^\dagger$:

$$\begin{aligned}[\hat{a}_{\mathbf{k}},\hat{a}_{\mathbf{l}}^\dagger] &= \frac{1}{2}[v_k\hat{\pi}_{\mathbf{k}}(\eta)-\dot{v}_k\hat{\chi}_{\mathbf{k}}(\eta), v_k^*\hat{\pi}_{-\mathbf{l}}(\eta)-\dot{v}_k^*\hat{\chi}_{-\mathbf{l}}(\eta)] \\ &= \frac{1}{2i}(v_k^*\dot{v}_k-\dot{v}_k^*v_k)\delta_{\mathbf{k},\mathbf{l}} = \frac{1}{2i}2i(v_k,v_k)\delta_{\mathbf{k},\mathbf{l}} = \delta_{\mathbf{k},\mathbf{l}}\end{aligned}$$

$$[\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{l}}] = [\hat{a}_{\mathbf{k}}^{\dagger}, \hat{a}_{\mathbf{l}}^{\dagger}] = 0,$$

which implies that $\hat{a}_{\mathbf{k}}^{\dagger}$ and $\hat{a}_{\mathbf{k}}$ are Bosonic creation/annihilation operators.

B.4 Bogoliubov Transformation

Consider functions defined by the expression

$$u_k(\eta) = \alpha_k v_k(\eta) + \beta_k v_k^*(\eta), \tag{B.15}$$

where α_k and β_k are time-dependent constants satisfying

$$|\alpha_k|^2 - |\beta_k|^2 = 1.$$

Then $u_k(\eta)$ and $u_k^*(\eta)$ are also solutions of (B.7) and satisfy

$$(u_k, u_k) = 1, \qquad (u_k^*, u_k^*) = -1, \qquad (u_k, u_k^*) = (u_k^*, u_k) = 0.$$

If we define $\hat{b}_{\mathbf{k}}$ and $\hat{b}_{\mathbf{k}}^{\dagger}$ by

$$\hat{b}_{\mathbf{k}} \equiv -\sqrt{2}(u_k^*, \hat{\chi}_{\mathbf{k}}(\eta)), \qquad \hat{b}_{\mathbf{k}}^{\dagger} \equiv \sqrt{2}(u_k, \hat{\chi}_{-\mathbf{k}}(\eta)), \tag{B.16}$$

we obtain

$$\hat{\chi}_{\mathbf{k}}(\eta) = \frac{1}{\sqrt{2}} \left(\hat{b}_{\mathbf{k}} u_k^*(\eta) + \hat{b}_{-\mathbf{k}}^{\dagger} u_k(\eta) \right)$$

and

$$\hat{\chi}(\eta, \mathbf{x}) = \frac{1}{\sqrt{2V}} \sum_{\mathbf{k}} \hat{b}_{\mathbf{k}} u_k^*(\eta) e^{i\mathbf{k}\cdot\mathbf{x}} + \hat{b}_{\mathbf{k}}^{\dagger} u_k(\eta) e^{-i\mathbf{k}\cdot\mathbf{x}}$$
$$\hat{\pi}(\eta, \mathbf{x}) = \frac{1}{\sqrt{2V}} \sum_{\mathbf{k}} \hat{b}_{\mathbf{k}} \dot{u}_k^*(\eta) e^{i\mathbf{k}\cdot\mathbf{x}} + \hat{b}_{\mathbf{k}}^{\dagger} \dot{u}_k(\eta) e^{-i\mathbf{k}\cdot\mathbf{x}}.$$

From this we can deduce that the canonical commutation relation (B.15) implies the followings hold.

$$[\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{l}}^{\dagger}] = \delta_{\mathbf{k},\mathbf{l}}, \qquad [\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{l}}] = [\hat{b}_{\mathbf{k}}^{\dagger}, \hat{b}_{\mathbf{l}}^{\dagger}] = 0.$$

Observe how the operators $\hat{b}_{\mathbf{k}}$, $\hat{b}^\dagger_{\mathbf{k}}$ are related to $\hat{a}_{\mathbf{k}}$, $\hat{a}^\dagger_{\mathbf{k}}$. From the definition (B.16) we have

$$\begin{aligned} \hat{b}_{\mathbf{k}} &= -\sqrt{2}(u_k^*, \hat{\chi}_{\mathbf{k}}(\eta)) = -(\alpha_k^* v_k^* + \beta_k^* v_k, \hat{a}_{\mathbf{k}} v_k^* + \hat{a}^\dagger_{-\mathbf{k}} v_k) = \alpha_k \hat{a}_{\mathbf{k}} - \beta_k^* \hat{a}^\dagger_{-\mathbf{k}}, \\ \hat{b}^\dagger_{\mathbf{k}} &= \alpha_k^* \hat{a}^\dagger_{\mathbf{k}} - \beta_k \hat{a}_{-\mathbf{k}}. \end{aligned} \tag{B.17}$$

The coefficients α_k and β_k are called the **Bogoliubov coefficients**.

Both sets of operators, $\{\hat{a}_{\mathbf{k}}, \hat{a}^\dagger_{\mathbf{k}}\}$ and $\{\hat{b}_{\mathbf{k}}, \hat{b}^\dagger_{\mathbf{k}}\}$ can be used to build a basis for the Fock space relevant to the system. There are two different vacuum states $|0_a\rangle$, $|0_b\rangle$ defined by

$$\hat{a}_{\mathbf{k}}|0_a\rangle = 0, \quad \hat{b}_{\mathbf{k}}|0_b\rangle = 0 \ \text{ for all } \mathbf{k}.$$

We call them "a-vacuum" and "b-vacuum" respectively. If $\beta_k \neq 0$, then the a-vacuum contains "b-particles". To verify this statement, we calculate the expectation value of b-particle number operator $\hat{N}^{(b)}_{\mathbf{k}} = \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}}$ in the state $|0_a\rangle$. Using (B.17), we obtain

$$\begin{aligned} \langle 0_a|\hat{N}^{(b)}_{\mathbf{k}}|0_a\rangle &= \langle 0_a|(\alpha_k^* \hat{a}^\dagger_{\mathbf{k}} - \beta_k \hat{a}_{-\mathbf{k}})(\alpha_k \hat{a}_{\mathbf{k}} - \beta_k^* \hat{a}^\dagger_{-\mathbf{k}})|0_a\rangle \\ &= |\beta_k|^2 \langle 0_a|\hat{a}_{-\mathbf{k}} \hat{a}^\dagger_{-\mathbf{k}}|0_a\rangle \\ &= |\beta_k|^2 \neq 0. \end{aligned}$$

We conclude that the particle interpretation depends on the choice of mode functions. If their were no rules in choosing mode functions, the particle concept becomes obsolete.

Suppose that the spacetime is flat in the remote past $(t < -T)$ and remote future $(t > T)$. Then we can secure an acceptable particle interpretation. Suppose that the scale factor $a(t)$ in the metric (B.1) satisfies

$$a(t) = \begin{cases} a_1 & \text{for } t < -T, \\ a_2 & \text{for } t > T. \end{cases}$$

Since the conformal time η is an increasing function of t, the effective mass $m^2_{\text{eff}}(\eta) = m^2 a^2 - \ddot{a}/a$ and the frequency $\omega_k^2(\eta) = k^2 + m^2_{\text{eff}}(\eta)$ satisfy similar conditions,

$$\omega_k(\eta) = \begin{cases} \omega_k^{\text{in}} & \text{for } \eta < -T', \\ \omega_k^{\text{out}} & \text{for } \eta > T', \end{cases}$$

where $\pm T' = \eta(\pm T)$. In these asymptotic regions, the equation (B.7) becomes the equation for a simple harmonic oscillator. Thus we may choose mode functions u_k and v_k such that

$$\begin{aligned} u_k(\eta) &\propto e^{i\omega_k^{\rm in}}\eta \quad \text{for } \eta < -T', \\ v_k(\eta) &\propto e^{i\omega_k^{\rm out}}\eta \quad \text{for } \eta > T', \end{aligned}$$

which becomes the initial condition for the second order ODE (B.7). If the solutions were found, they can be related each other by the Bogoliubov coefficients,

$$u_k(\eta) = \alpha_k v_k(\eta) + \beta_k v_k^*(\eta).$$

The coefficients are determined by

$$\alpha_k(v_k, u_k), \qquad \beta_k = -(v_k^*, u_k).$$

Let $\hat{a}_{\mathbf{k}}$ and $\hat{b}_{\mathbf{k}}$ be the annihilation operators corresponding to the mode functions $u_k(\eta)$ and $v_k(\eta)$, respectively. The field operator can be written in two different ways:

$$\begin{aligned} \hat{\chi}(\eta, \mathbf{x}) &= \frac{1}{\sqrt{2V}} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} u_k^* e^{i\mathbf{k}\cdot\mathbf{x}} + \hat{a}_{\mathbf{k}}^\dagger u_k e^{-i\mathbf{k}\cdot\mathbf{x}}, \\ \hat{\chi}(\eta, \mathbf{x}) &= \frac{1}{\sqrt{2V}} \sum_{\mathbf{k}} \hat{b}_{\mathbf{k}} v_k^* e^{i\mathbf{k}\cdot\mathbf{x}} + \hat{b}_{\mathbf{k}}^\dagger v_k e^{-i\mathbf{k}\cdot\mathbf{x}}. \end{aligned}$$

These expressions are the expansions of the field operator $\hat{\chi}$ in terms of the particle operators of *in* region and of *out* region, respectively. The initial and final vacuums, $|0_a\rangle$ and $|0_b\rangle$, have physical meaning in that they are the agreed vacuum identified by the inertial observers in the corresponding asymptotic regions. Since we are working in Heisenberg picture, the initial vacuum state $|0_a\rangle$ remains unchanged. Thus the result $\langle 0_a|\hat{N}_{\mathbf{k}}^{(b)}|0_a\rangle = |\beta_k|^2 \neq 0$ implies that the expectation value of number of particles in the initial vacuum can become nonzero in the remote future. Particles can be created by time-dependent gravitational background.

Chapter C

Quantum Many-Body Physics

C.1 Fock Space

Let $\mathcal{H}$ be a Hilbert space to which the single particle state vectors $|\psi\rangle$ belong. To construct a mathematical architecture that models physical quantum system consisting of many particles, we are to consider N-fold tensor product of $\mathcal{H}$:

$$\mathcal{H}^N \equiv \mathcal{H} \otimes \cdots \otimes \mathcal{H} = \bigotimes_{i=1}^{N} \mathcal{H}$$

A quick and dirty way to define the tensor product is to pick a basis $\{|\lambda\rangle : \lambda \in I\}$ for $\mathcal{H}$, e.g. the collection of eigenvectors corresponding to a Hermitian operator on $\mathcal{H}$. Then $\mathcal{H}^N$ is the vector space whose basis is given by all expressions of the form $|\lambda_1\rangle \otimes \cdots \otimes |\lambda_N\rangle,\ \lambda_k \in I$. Thus a general element of $\mathcal{H}^N$ can be expressed as

$$\sum_{\lambda_1 \cdots \lambda_N \in I} C_{\lambda_1 \cdots \lambda_N} |\lambda_1\rangle \otimes \cdots \otimes |\lambda_N\rangle$$

where each λ_i runs over the whole index set I. The dimension of $\mathcal{H}^N$ is, if $\dim \mathcal{H}$ were finite, is equal to $(\dim \mathcal{H})^N$. The innerproduct of $\mathcal{H}^N$ is defined by

$$\big(\langle\lambda_1| \otimes \cdots \otimes \langle\lambda_N|\big)\big(|\lambda_1'\rangle \otimes \cdots \otimes |\lambda_N'\rangle\big) \equiv \langle\lambda_1 \,|\, \lambda_1'\rangle \cdots \langle\lambda_N \,|\, \lambda_N'\rangle$$

for basis vectors. For general vectors, the innerproduct is defined by linear extension.

According to the basic postulates of quantum mechanics, physical quantum many-body systems are divided into two classes referred to as Bosonic and Fermionic system, repectively. And the constituents of each system are called as Bosons and Fermions. We are to construct mathematical architecture to describe these systems. It is very rare to consider a mixture of Bosons and Fermions. For such cases, we can describe the system as a statistical ensemble of quantum states, which cannot be described by a single (many-body) wavefunction.

Consider an observable A and its corresponding eigenstates which constitutes a basis $\{|\lambda\rangle \ : \ \lambda \in I\}$. And consider the corresponding basis for $\mathcal{H}^N$, $\{|\lambda_1\rangle \otimes \cdots \otimes |\lambda_N\rangle \ : \ \lambda_k \in I, \ k = 1, \cdots, N\}$. Let us denote the symmetric group of N integers (the set of all permutations defined on $\{1, \cdots, N\}$) by S_N. For each $\sigma \in S_N$, define an operator $\mathcal{P}_\sigma : \mathcal{H}^N \to \mathcal{H}^N$ by

$$\mathcal{P}_\sigma\big(|\lambda_1\rangle \otimes \cdots \otimes |\lambda_N\rangle\big) = |\lambda_{\sigma(1)}\rangle \otimes \cdots \otimes |\lambda_{\sigma(N)}\rangle.$$

It is well known that a linear operator is determined if its images for basis vectors are specified. If we act $\mathcal{P}_\sigma$ to a generic vector, we obtain

$$\begin{aligned}\mathcal{P}_\sigma\Big(\sum_{\lambda_1\cdots\lambda_N} C_{\lambda_1\cdots\lambda_N}|\lambda_1\rangle \otimes \cdots \otimes |\lambda_N\rangle\Big) &= \sum_{\lambda_1\cdots\lambda_N} C_{\lambda_1\cdots\lambda_N}\mathcal{P}_\sigma\big(|\lambda_1\rangle \otimes \cdots \otimes |\lambda_N\rangle\big)\\ &= \sum_{\lambda_1\cdots\lambda_N} C_{\lambda_1\cdots\lambda_N}|\lambda_{\sigma(1)}\rangle \otimes \cdots \otimes |\lambda_{\sigma(N)}\rangle.\end{aligned}$$

Now consider special subspaces of $\mathcal{H}^N$ defined by

$$\begin{aligned}\mathcal{F}_B^N &\equiv \Big\{|\Psi\rangle \in \mathcal{H}^N \ : \ \mathcal{P}_\sigma|\Psi\rangle = |\Psi\rangle \ \text{ for all } \sigma \in S_N\Big\}\\ \mathcal{F}_F^N &\equiv \Big\{|\Psi\rangle \in \mathcal{H}^M \ : \ \mathcal{P}_\sigma|\Psi\rangle = \mathrm{sgn}(\sigma)|\Psi\rangle \ \text{ for all } \sigma \in S_N\Big\}\end{aligned}$$

$\mathcal{F}_B^N$ and $\mathcal{F}_F^N$ are called Bosonic and Fermionic subspace, repetively. It can easily be shown that these form subspaces of $\mathcal{H}^N$. For example,

$$\begin{aligned}&|\Psi\rangle, |\Phi\rangle \in \mathcal{F}_F^N, \quad \alpha, \beta \in \mathbb{C},\\ &\Rightarrow \mathcal{P}_\sigma\big(\alpha|\Psi\rangle + \beta|\Phi\rangle\big) = \alpha\mathcal{P}_\sigma|\Psi\rangle + \beta\mathcal{P}_\sigma|\Phi\rangle = \mathrm{sgn}(\sigma)\big(\alpha|\Psi\rangle + \beta|\Phi\rangle\big)\\ &\Rightarrow \alpha|\Psi\rangle + \beta|\Phi\rangle \in \mathcal{F}_F^N.\end{aligned}$$

Thus we conclude that $\mathcal{F}_F^N$ is a subspace of $\mathcal{H}^N$.

To construct a basis for $\mathcal{F}_\zeta^N$, we consider the vectors of the form

$$|\lambda_1 \cdots \lambda_N\rangle_\zeta \equiv \frac{1}{\sqrt{N!\prod_\lambda n_\lambda!}} \sum_{\sigma \in S_N} \zeta^{(1-\mathrm{sgn}\sigma)/2}|\lambda_{\sigma(1)}\rangle \otimes \cdots \otimes |\lambda_{\sigma(N)}\rangle \tag{C.1}$$

where $\zeta = 1$ for Bosons and $\zeta = -1$ for Fermions. Note that $\zeta^{(1-\mathrm{sgn}\sigma)/2} = 1$ for Bosons and $\zeta^{(1-\mathrm{sgn}\sigma)/2} = \mathrm{sgn}(\sigma)$ for Fermions. One can check that $|\lambda_1 \cdots \lambda_N\rangle_\zeta$ is an element of $\mathcal{F}_\zeta^N$. For the case of fermions ($\zeta = -1$),

$$\begin{aligned}
&\mathcal{P}_\sigma\big(|\lambda_1 \cdots \lambda_N\rangle_\zeta\big) \\
&= \mathcal{P}_\sigma\Big(\frac{1}{\sqrt{N!\prod_\lambda n_\lambda!}} \sum_{\tau \in S_N} \mathrm{sgn}(\tau)|\lambda_{\tau(1)}\rangle \otimes \cdots \otimes |\lambda_{\tau(N)}\rangle\Big) \\
&= \frac{1}{\sqrt{N!\prod_\lambda n_\lambda!}} \sum_{\tau \in S_N} \mathrm{sgn}(\tau)|\lambda_{\tau(\sigma(1))}\rangle \otimes \cdots \otimes |\lambda_{\tau(\sigma(N))}\rangle \\
&= \frac{1}{\sqrt{N!\prod_\lambda n_\lambda!}}\mathrm{sgn}(\sigma) \sum_{\tau \in S_N} \mathrm{sgn}(\tau\circ\sigma)|\lambda_{\tau\circ\sigma(1)}\rangle \otimes \cdots \otimes |\lambda_{\tau\circ\sigma(N)}\rangle \\
&= \mathrm{sgn}(\sigma)|\lambda_1 \cdots \lambda_N\rangle_\zeta \\
&\Rightarrow |\lambda_1 \cdots \lambda_N\rangle_\zeta \in \mathcal{F}_F^N.
\end{aligned}$$

Observe that, for some $\tau \in S_N$,

$$\begin{aligned}
&|\lambda_{\tau(1)} \cdots \lambda_{\tau(N)}\rangle_\zeta \\
&= \frac{1}{\sqrt{N!\prod_\lambda n_\lambda!}} \sum_{\sigma \in S_N} \zeta^{(1-\mathrm{sgn}\sigma)/2}|\lambda_{\sigma(\tau(1))}\rangle \otimes \cdots \otimes |\lambda_{\sigma(\tau(N))}\rangle \\
&= \begin{cases}
\frac{1}{\sqrt{N!\prod_\lambda n_\lambda!}} \sum_{\sigma \in S_N} |\lambda_{\sigma(\tau(1))}\rangle \otimes \cdots \otimes |\lambda_{\sigma(\tau(N))}\rangle & \text{(Boson)} \\
\frac{1}{\sqrt{N!\prod_\lambda n_\lambda!}} \sum_{\sigma \in S_N} \mathrm{sgn}(\sigma)|\lambda_{\sigma(\tau(1))}\rangle \otimes \cdots \otimes |\lambda_{\sigma(\tau(N))}\rangle & \text{(Fermion).}
\end{cases}
\end{aligned}$$

Since $\sum_{\sigma \in S_N} f(\sigma\circ\tau) = \sum_{\sigma \in S_N} f(\sigma)$, we have

$$\begin{aligned}
&= \begin{cases}
\frac{1}{\sqrt{N!\prod_\lambda n_\lambda!}} \sum_{\sigma \in S_N} |\lambda_{\sigma(1)}\rangle \otimes \cdots \otimes |\lambda_{\sigma(N)}\rangle & \text{(Boson)} \\
\frac{1}{\sqrt{N!\prod_\lambda n_\lambda!}} \sum_{\sigma \in S_N} \mathrm{sgn}(\sigma\circ\tau^{-1})|\lambda_{\sigma(1)}\rangle \otimes \cdots \otimes |\lambda_{\sigma(N)}\rangle & \text{(fermion)}
\end{cases} \\
&= \zeta^{(1-\mathrm{sgn}\tau)/2}|\lambda_1 \cdots \lambda_N\rangle_\zeta.
\end{aligned}$$

Thus, we may switch the position of $\lambda_1, \cdots, \lambda_N$ at the cost of, at most, a change of sign. From now on, we assume that whenever we use expressions like (C.1), $\lambda_1, \cdots, \lambda_N$ are arranged according to a certain ordering. If we rename λ's by its ordering label, in the case of discrete λ, λ's would take values $1, 2, 3, \cdots \in \mathbb{N}$.

We see that, if the set $\{\lambda_1, \cdots, \lambda_N\}$ and $\{\lambda'_1, \cdots, \lambda'_N\}$ are not identical, $|\lambda_1 \cdots \lambda_N\rangle_\zeta$ and $|\lambda'_1 \cdots \lambda'_N\rangle_\zeta$ must be orthogonal, since every term in the innerproduct of them must contain a factor $\langle \lambda \,|\, \lambda' \rangle$ with $\lambda \neq \lambda'$, which is zero. This condition for orthogonality can be even neater. We have introduced a certain ordering on $\lambda_1, \cdots, \lambda_N$. So we can assert that $|\lambda_1 \cdots \lambda_N\rangle_\zeta$ and $|\lambda'_1 \cdots \lambda'_N\rangle_\zeta$ are orthogonal if $\lambda_i \neq \lambda'_i$ for some i. As a conclusion, a collection of vectors of the form $|\lambda_1 \cdots \lambda_N\rangle_\zeta$ with n-tuples $(\lambda_1, \cdots, \lambda_N)$'s being all distinct is linearly independent.

We have checked that $|\lambda_1 \cdots \lambda_N\rangle_\zeta$ belongs to $\mathcal{F}_\zeta^N$ and that these vectors are linearly independent. Although we did not checked whether they can span $\mathcal{F}_\zeta^N$, it is known that $|\lambda_1 \cdots \lambda_N\rangle_\zeta$ forms a basis for $\mathcal{F}_\zeta^N$, whose proof we omit here. Therefore any Bosonic or Fermionic state vectors can be expressed uniquely as a linear combination of $|\lambda_1 \cdots \lambda_N\rangle_\zeta$'s:

$$|\Psi\rangle = \sum_{\lambda_1 \leq \cdots \leq \lambda_N} C_{\lambda_1 \cdots \lambda_N} \, |\lambda_1 \cdots \lambda_N\rangle_\zeta, \tag{C.2}$$

where $\lambda_1 \leq \cdots \leq \lambda_N$ means that one must sum over arranged tuples $(\lambda_1, \cdots, \lambda_N)$ only.

The prefactor in the definition (C.1) was needed to secure the normalization condition.

$$\begin{aligned}
&{}_\zeta\langle \lambda_1 \cdots \lambda_N | \lambda_1 \cdots \lambda_N \rangle_\zeta \\
&= \frac{1}{N! \prod_\lambda (n_\lambda !)} \left(\sum_{\sigma \in S_N} \zeta^{(1-\mathrm{sgn}\sigma)/2} \langle \lambda_{\sigma(1)} | \otimes \cdots \otimes \langle \lambda_{\sigma(N)} | \right) \\
&\qquad\qquad\qquad\qquad \times \left(\sum_{\tau \in S_N} \zeta^{(1-\mathrm{sgn}\tau)/2} |\lambda_{\tau(1)}\rangle \otimes \cdots \otimes |\lambda_{\tau(N)}\rangle \right) \\
&= \frac{1}{N! \prod_\lambda (n_\lambda !)} \sum_{\sigma, \tau \in S_N} \zeta^{(1-\mathrm{sgn}\sigma)/2} \zeta^{(1-\mathrm{sgn}\tau)/2} \langle \lambda_{\sigma(1)} \,|\, \lambda_{\tau(1)} \rangle \cdots \langle \lambda_{\sigma(N)} \,|\, \lambda_{\tau(N)} \rangle.
\end{aligned}$$

For Fermions, $n_\lambda ! = 1$ for all λ. Thus

$$\begin{aligned}
{}_\zeta\langle \lambda_1 \cdots \lambda_N \,|\, \lambda_1 \cdots \lambda_N \rangle_\zeta &= \frac{1}{N!} \sum_{\sigma, \tau \in S_N} \mathrm{sgn}(\sigma)\mathrm{sgn}(\tau) \langle \lambda_{\sigma(1)} \,|\, \lambda_{\tau(1)} \rangle \cdots \langle \lambda_{\sigma(N)} \,|\, \lambda_{\tau(N)} \rangle \\
&= \frac{1}{N!} \sum_\sigma \mathrm{sgn}(\sigma)^2 \sum_\tau \mathrm{sgn}(\tau) \langle \lambda_1 \,|\, \lambda_{\tau(1)} \rangle \cdots \langle \lambda_N \,|\, \lambda_{\tau(N)} \rangle \\
&= \sum_\tau \mathrm{sgn}(\tau) \langle \lambda_1 \,|\, \lambda_{\tau(1)} \rangle \cdots \langle \lambda_N \,|\, \lambda_{\tau(N)} \rangle \\
&= 1.
\end{aligned}$$

For Bosons,

$$ {}_\zeta\langle\lambda_1\cdots\lambda_N\,|\,\lambda_1\cdots\lambda_N\rangle_\zeta = \frac{1}{N!\prod_\lambda(n_\lambda!)}\sum_{\sigma,\tau}\langle\lambda_{\sigma(1)}\,|\,\lambda_{\tau(1)}\rangle\cdots\langle\lambda_{\sigma(N)}\,|\,\lambda_{\tau(N)}\rangle. $$

For fixed σ, among $N!$ τ's, only $\prod_\lambda(n_\lambda!)$ of them make the same arrangements as $\sigma(1),\cdots,$ $\sigma(N)$. Thus

$$ \begin{aligned} &= \frac{1}{N!}\sum_\sigma\langle\lambda_{\sigma(1)}\,|\,\lambda_{\sigma(1)}\rangle\cdots\langle\lambda_{\sigma(N)}\,|\,\lambda_{\sigma(N)}\rangle \\ &= 1. \end{aligned} $$

Thus we conclude that $|\lambda_1\cdots\lambda_N\rangle_\zeta$ is normalized. Let us omit the subscript ζ if there is no confusion about which species we are considering.

After we respect the ordering, we can uniquely write $|\lambda_1\cdots\lambda_N\rangle$ as $|n_1n_2\cdots\rangle$. For example, we can denote $|111122333466\cdots\rangle$ simply by $|423102\cdots\rangle$. We call this kind of representation as the **occupation number representation**. Now (C.2) can be written as

$$ |\Psi\rangle = \sum_{\substack{n_1n_2\cdots \\ \sum n_i=N}} C_{n_1n_2\cdots}\,|n_1n_2\cdots\rangle. \tag{C.3} $$

Although we changed our notation, the vectors $|n_1n_2\cdots\rangle$ still are the basis vectors for $\mathcal{F}^N$ given by (C.1).

If the eigenvalue λ can take M values (i.e. if the dimension of the Hilbert space $\mathcal{H}$ were M), we can explicitly count the dimension of $\mathcal{F}^N$:

$$ \dim\mathcal{F}^N = \begin{cases} \frac{M!}{N!(M-N)!} & \text{(Fermions)} \qquad \leftarrow \text{Choose } N \text{ states to occupy among } M \text{ states.} \\ \frac{(N+M-1)!}{N!(M-1)!} & \text{(Bosons)} \qquad \leftarrow \text{Distribute } N \text{ balls into } M \text{ baskets.} \end{cases} $$

Altough we considered $N \geq 1$ only, we add an artificial case $N = 0$. $\mathcal{F}^0$ is an 1-dimensional space with a basis vector $|0\rangle$ which is called the **vacuum state**. Now we form a direct sum,

$$ \mathcal{F} \equiv \bigoplus_{N=0}^{\infty}\mathcal{F}^N. $$

Direct sum $V \oplus W$ of vector spaces $V,\ W$ is defined by, for $(v_1, w_1),\ (v_2, w_2) \in V \oplus W$

and $\alpha \in \mathbb{C}$,

$$(v_1, w_1) + (v_2, w_2) = (v_1 + v_2, w_1 + w_2); \qquad \alpha(v_1, w_1) = (\alpha v_1, \alpha w_1).$$

If $\{v_1, \cdots, v_n\}$ were a basis for V and $\{w_1, \cdots, w_m\}$ were a basis for W, $\big\{(v_1, 0), \cdots, (v_n, 0), (0, w_1), \cdots, (0, w_m)\big\}$ is a basis for $V \oplus W$. Thus $\dim(V \oplus W) = \dim V + \dim W$. If we identify $(v_i, 0)$ with v_i and $(0, w_i)$ with w_i, the direct sum $V \oplus W$ is just a vector space with basis $v_1, \cdots, v_n, w_1, \cdots, w_m$.

We have shown that $\mathcal{F}^N$ has $|n_1 n_2 \cdots\rangle$ $(n_1 + n_2 + \cdots = N)$ as its basis. Thus the direct sum $\bigoplus_{N=0}^{\infty} \mathcal{F}^N$ has $|n_1 n_2 \cdots\rangle$ as its basis with no restriction on the total number $\sum_i n_i$. The space $\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{F}^N$ is called the **Fock space**. A general vector in $\mathcal{F}$ can be written as

$$|\Psi\rangle = \sum_{n_1 n_2 \cdots} C_{n_1 n_2 \cdots} |n_1 n_2 \cdots\rangle.$$

This differs from (C.3) in that it does not have any restriction on the total number of particles.

C.2 Creation and Annihilation Operators

Having defined the space where many-body state vectors live, we move onto the discussion of operators defined on the Fock space. Let $\mathcal{H}$ be a Hilbert space, A be a Hermitian operator defined on $\mathcal{H}$, and $|\lambda\rangle$ be the corresponding eigenstates. And let $\mathcal{F}$ be the Fock space constructed from $\mathcal{H}$. We define a special operators $a_i^\dagger : \mathcal{F} \to \mathcal{F}$ by

$$a_i^\dagger |n_1 n_2 \cdots\rangle \equiv \sqrt{n_i + 1}\zeta^{s_i} |n_1 \cdots n_i + 1 \cdots\rangle \tag{C.4}$$

where $s_i = \sum_{j=1}^{i-1} n_j$. In Fermionic case, the prefactor $n_i + 1$ has to be understood mod 2, i.e., $1 + 1 = 0$ mod 2.

Observe that, for any $M \in \mathbb{N}$,

$$\begin{aligned}\prod_{i=1}^{M} \frac{1}{\sqrt{n_i!}} (a_i^\dagger)^{n_i} |0\rangle &= \frac{1}{\sqrt{n_1!}} (a_1^\dagger)^{n_1} \cdots \frac{1}{\sqrt{n_{M-1}!}} (a_{M-1}^\dagger)^{n_{M-1}} \frac{1}{\sqrt{n_M!}} (a_M^\dagger)^{n_M} |0\rangle \\ &= |n_1 \cdots n_M\rangle.\end{aligned}$$

Thus we obtain,

$$|n_1 n_2 \cdots\rangle = \prod_{i=1}^{\infty} \frac{1}{\sqrt{n_i!}} (a_i^\dagger)^{n_i} |0\rangle. \tag{C.5}$$

It would be instructive to recall that $|n_1 n_2 \cdots\rangle$ was originally,

$$\begin{aligned} |n_1 n_2 \cdots\rangle &= |\lambda_1 \cdots \lambda_N\rangle_\zeta \\ &= \frac{1}{\sqrt{N! \prod_\lambda (n_\lambda !)}} \sum_{\sigma \in S_N} \zeta^{(1-\mathrm{sgn}\sigma)/2} |\lambda_{\sigma(1)}\rangle \otimes \cdots \otimes |\lambda_{\sigma(N)}\rangle. \end{aligned} \tag{C.6}$$

Comparing (C.5) and (C.6), we see that (C.5) is easier to notice. In (C.5), N-fold application of $a^\dagger$ generates N-particle state. So $a^\dagger$ are commonly called the **creation operators**.

Using the definition (C.4), we can show that, for $i \neq j$,

$$\begin{aligned} & a_i^\dagger a_j^\dagger |n_1 n_2 \cdots\rangle \\ &= \sqrt{n_j + 1} \zeta^{\sum_{k=1}^{j-1} n_k} a_i^\dagger |n_1 \cdots n_j + 1 \cdots\rangle \\ &= \begin{cases} \sqrt{n_j + 1}\sqrt{n_i + 1} \zeta^{\sum_{k=1}^{j-1} n_k} \zeta^{\sum_{k=1}^{i-1} n_k} |n_1 \cdots n_i + 1 \cdots n_j + 1 \cdots\rangle & (i < j) \\ \sqrt{n_j + 1}\sqrt{n_i + 1} \zeta^{\sum_{k=1}^{j-1} n_k} \zeta^{\sum_{k=1}^{i-1} n_k + 1} |n_1 \cdots n_j + 1 \cdots n_i + 1 \cdots\rangle & (i > j) \end{cases} \end{aligned}$$

$$\begin{aligned} & a_j^\dagger a_i^\dagger |n_1 n_2 \cdots\rangle \\ &= \begin{cases} \sqrt{n_j + 1}\sqrt{n_i + 1} \zeta^{\sum_{k=1}^{i-1} n_k} \zeta^{\sum_{k=1}^{j-1} n_k + 1} |n_1 \cdots n_i + 1 \cdots n_j + 1 \cdots\rangle & (i < j) \\ \sqrt{n_j + 1}\sqrt{n_i + 1} \zeta^{\sum_{k=1}^{i-1} n_k} \zeta^{\sum_{k=1}^{j-1} n_k} |n_1 \cdots n_j + 1 \cdots n_i + 1 \cdots\rangle & (i > j). \end{cases} \end{aligned}$$

Thus we obtain

$$(a_i^\dagger a_j^\dagger - \zeta a_j^\dagger a_i^\dagger)|n_1 n_2 \cdots\rangle = 0 \quad \Rightarrow \quad [a_i^\dagger, a_j^\dagger]_\zeta := a_i^\dagger a_j^\dagger - \zeta a_j^\dagger a_i^\dagger = 0.$$

In the case of $i = j$, for Bosons, obviously $[a_i^\dagger, a_i^\dagger]_{+1} = a_i^\dagger a_i^\dagger - a_i^\dagger a_i^\dagger = 0$. For Fermions we can show as above that $(a_i^\dagger)^2 = 0$ using the fact that $1 + 1 = 0 \bmod 2$. Thus we get $[a_i^\dagger, a_i^\dagger]_{-1} = 0$. $(a_i^\dagger)^2 = 0$ says that two-fold application of $a_i^\dagger$ to any state leads to its annihilation. Actually, although not intuitively straightforward, this is a formal statement of the Pauli exclusion principle.

Now we consider the Hermitian conjugate of $a_i^\dagger$ denoted by $(a_i^\dagger)^\dagger = a_i$.

$$a_i|n_1 n_2 \cdots\rangle = \sum_{n'_1 n'_2 \cdots} C_{n'_1 n'_2 \cdots} |n'_1 n'_2 \cdots\rangle$$
$$\Rightarrow C_{n'_1 n'_2 \cdots} = \langle n'_1 n'_2 \cdots |a_i| n_1 n_2 \cdots\rangle = \langle n_1 n_2 \cdots |a_i^\dagger| n'_1 n'_2 \cdots\rangle^*$$
$$= \sqrt{n'_i + 1}\zeta^{\sum_{j=1}^{i-1} n'_j} \delta_{n_1 n'_1} \cdots \delta_{n_i n'_i + 1} \cdots$$
$$\Rightarrow a_i|n_1 n_2 \cdots\rangle = \sum_{n'_1 n'_2 \cdots} \sqrt{n'_i + 1}\zeta^{\sum_{j=1}^{i=1} n_j} \delta_{n_1 n'_1} \cdots \delta_{n_i, n'_i + 1} \cdots |n'_1 n'_2 \cdots\rangle$$
$$\Rightarrow a_i|n_1 n_2 \cdots\rangle = \sqrt{n_i}\zeta^{s_i} |n_1 \cdots n_i - 1 \cdots\rangle. \tag{C.7}$$

The operators a are commonly called the **annihilation operators**.

Using (C.4) and (C.7), a straightforward calculation shows that

$$[a_i, a_j^\dagger]_\zeta = \delta_{ij}, \quad \text{and} \quad [a_i, a_j]_\zeta = [a_i^\dagger, a_j^\dagger]_\zeta = 0. \tag{C.8}$$

People use the following notation

$$[A, B]_- = AB - BA, \qquad [A, B]_+ = AB + BA.$$

Thus, for Bosons, the commutation relation between the creation/annihilation operators can be written as

$$[a_i, a_j^\dagger]_- = \delta_{ij}, \quad \text{and} \quad [a_i, a_j]_- = [a_i^\dagger, a_j^\dagger]_- = 0.$$

Incidentally, it can be shown that the algebra (C.8) fully characterizes the operator action so that we can find a unique (up to unitary equivalence) representation of these operators and a unique state $|0\rangle$ from which all other states can be reached by repeated application of $a_i^\dagger$. This is the statement of the Stone-von Neumann theorem (For more precise statement, see [112, pp. 45-46].)

We define an operator $\hat{n}_i \equiv a_i^\dagger a_i$ which is called an **occupation number operator**. It can be shown that $\hat{n}_i|n_1 n_2 \cdots\rangle = n_i|n_1 n_2 \cdots\rangle$. So far, we succeeded to express the state vectors in Fock space using creation and annihilation operators. Now we seek for an expression for observables in terms of these operators.

C.3 One-Body and Two-Body Operators

Let $\mathcal{H}$ be a Hilbert space. Consider an observable A and its corresponding eigenstates $|\lambda\rangle,\ \lambda \in I$. And consider another observable B and its eigenstates $|\tilde{\lambda}\rangle,\ \tilde{\lambda} \in \tilde{I}$. By definition, $a^\dagger_\lambda|0\rangle = |0\cdots 1\cdots\rangle = |\lambda\rangle$ and $a^\dagger_{\tilde{\lambda}}|0\rangle = |0\cdots 1\cdots\rangle = |\tilde{\lambda}\rangle$ hold. Thus we obtain

$$a^\dagger_{\tilde{\lambda}}|0\rangle = |\tilde{\lambda}\rangle = \sum_\lambda \langle\lambda\,|\,\tilde{\lambda}\rangle|\lambda\rangle = \sum_\lambda \langle\lambda\,|\,\tilde{\lambda}\rangle a^\dagger_\lambda|0\rangle.$$

In general it is known that

$$a^\dagger_{\tilde{\lambda}} = \sum_\lambda \langle\lambda\,|\,\tilde{\lambda}\rangle a^\dagger_\lambda, \tag{C.9}$$

i.e., creation operators transform covariantly under basis change. By taking Hermitian conjugate of (C.9), we get

$$a_{\tilde{\lambda}} = \sum_\lambda \langle\tilde{\lambda}\,|\,\lambda\rangle a_\lambda, \tag{C.10}$$

i.e., annihilation operators transform contravariantly under basis change.

Let $\hat{o}$ be a Hermitian operator defined on a Hilbert space. **One-body operator** $\hat{\mathcal{O}}_1$ corresponding to $\hat{o}$ is an operator acting on N-particle Fock space $\mathcal{F}^N$ and is defined by

$$\hat{\mathcal{O}}_1 \equiv \sum_{n=1}^N \hat{o}_n, \quad \hat{o_n} = 1\otimes\cdots\otimes\hat{o}\otimes\cdots\otimes 1$$

where $\hat{o}$ is an ordinary single particle operator and 1 is the identity operator. Here, $\hat{o}_n$ is an operator that applies $\hat{o}$ only to the n-th particle while all the other particles remain unchanged. A typical example of single-particle operator would be the kinetic energy operator $\hat{T} = \sum_n \frac{\mathbf{p}_n^2}{2m}$.

Let $|\lambda\rangle$ be the eigenstates of $\hat{o}$ and we introduce the occupation number representation corresponding to these eigenstates. Then

$$\hat{\mathcal{O}}_1|n_1 n_2\cdots\rangle = \frac{1}{\sqrt{N!\prod_\lambda(n_\lambda!)}}\sum_{\sigma\in S_N}\zeta^{(1-\mathrm{sgn}\sigma)/2}\sum_{n=1}^N \hat{o}_n|\lambda_{\sigma(1)}\rangle\otimes\cdots\otimes|\lambda_{\sigma(N)}\rangle.$$

One may notice here that

$$\sum_{n=1}^N \hat{o}_n|\lambda_{\sigma(1)}\rangle\otimes\cdots\otimes|\lambda_{\sigma(N)}\rangle = \Big(\sum_\lambda \lambda n_\lambda\Big)|\lambda_{\sigma(1)}\rangle\otimes\cdots\otimes|\lambda_{\sigma(N)}\rangle$$

holds. Therefore we obtain

$$\hat{\mathcal{O}}_1|n_1n_2\cdots\rangle = \Big(\sum_\lambda \lambda n_\lambda\Big)|n_1n_2\cdots\rangle = \Big(\sum_\lambda \lambda \hat{n}_\lambda\Big)|n_1n_2\cdots\rangle.$$

We finally get an expression for the single-particle operator $\hat{\mathcal{O}}_1$ in terms of creation/annihilation operators:

$$\hat{\mathcal{O}}_1 = \sum_{\lambda\in I}\lambda\hat{n}_\lambda = \sum_{\lambda,\lambda'\in I}\langle\lambda|\hat{o}|\lambda'\rangle a^\dagger_\lambda a_{\lambda'}.$$

Let $\{|\mu\rangle : \mu\in J\}$ and $\{|\nu\rangle : \nu\in K\}$ be complete set of eigenstates corresponding to some other observables. Then,

$$\begin{aligned}
&= \sum_{\substack{\lambda,\lambda'\in I\\ \mu\in J,\nu\in K}} \langle\lambda\mid\mu\rangle\langle\mu|\hat{o}|\nu\rangle\langle\nu\mid\lambda'\rangle a^\dagger_\lambda a_{\lambda'}\\
&= \sum_{\mu\in J,\nu\in K}\langle\mu|\hat{o}|\nu\rangle\Big(\sum_{\lambda\in I}\langle\lambda\mid\mu\rangle a^\dagger_\lambda\Big)\Big(\sum_{\lambda'\in I}\langle\nu\mid\lambda'\rangle a_{\lambda'}\Big) = \sum_{\mu,\nu}\langle\mu|\hat{o}|\nu\rangle a^\dagger_\mu a_\nu.
\end{aligned}$$

Thus we conclude that

$$\hat{\mathcal{O}}_1 = \sum_{\mu,\nu}\langle\mu|\hat{o}|\nu\rangle a^\dagger_\mu a_\nu. \tag{C.11}$$

The representation of an operator in terms of creation/annihilation operators is usually called a **second quantized form** .

At this point, it would be instructive to look upon an example. Consider a single particle Hamiltonian $\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{x}})$. Using (C.11), single-particle operator corresponding to the Hamiltonian $\hat{H}$ can be represented by (we use the same symbol for single-particle operator)

$$\begin{aligned}
\hat{H} &= \int d\mathbf{r}d\mathbf{r}'\ \langle\mathbf{r}|\frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{x}})|\mathbf{r}'\rangle a^\dagger(\mathbf{r})a(\mathbf{r}')\\
&= \int d\mathbf{r}d\mathbf{r}'\ \Big(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\Big)\delta^3(\mathbf{r}-\mathbf{r}')a^\dagger(\mathbf{r})a(\mathbf{r}')\\
&= \int d\mathbf{r}d\mathbf{r}'\ \Big(-\frac{\hbar^2}{2m}\nabla'^2 + V(\mathbf{r})\Big)\delta^3(\mathbf{r}-\mathbf{r}')a^\dagger(\mathbf{r})a(\mathbf{r}')\\
&= \int d\mathbf{r}\ a^\dagger(\mathbf{r})\Big(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\Big)a(\mathbf{r}).
\end{aligned}$$

In this example, we applied the results we derived for discrete eigenvalues to a continuous eigenvalues (position). This will be justified in the following section.

Now we move onto the two-body operators, which are needed to describe pairwise interactions. Let $\hat{o}$ be an Hermitian operator defined on a product space $\mathcal{H}^2 = \mathcal{H} \otimes \mathcal{H}$, i.e., $\hat{o}$ acts on a state vector representing a system of two particles. Let $|\mu\rangle$ $(\mu \in I)$ be eigenstates of an observable $\hat{A}$ defined on the single particle Hilbert space $\mathcal{H}$. We assume that $\hat{o}$ is a function of $\hat{A}_1$ and $\hat{A}_2$, where $\hat{A}_i$ is just the observable $\hat{A}$ defined on i-th Hilbert space $\mathcal{H}$:

$$\hat{o} = o(\hat{A}_1, \hat{A}_2). \tag{C.12}$$

If we act $\hat{o}$ to a vector $|\mu\rangle|\nu\rangle \in \mathcal{H} \otimes \mathcal{H}$ (here we omitted $\otimes$ between $|\mu\rangle$ and $|\nu\rangle$), we obtain

$$\hat{o}|\mu\rangle|\nu\rangle = o(\hat{A}_1, \hat{A}_2)|\mu\rangle|\nu\rangle = o(\mu,\nu)|\mu\rangle|\nu\rangle.$$

We assume further that the function $o(\mu,\nu)$ is symmetric, i.e.,

$$o(\mu,\nu) = o(\nu,\mu). \tag{C.13}$$

The conditions (C.12) and (C.13) are usual properties of operators describing pairwise interactions, which we will see later.

The **two-body operator** $\hat{\mathcal{O}}_2$ corresponding to $\hat{o} = o(\hat{A}_1, \hat{A}_2)$ is an operator acting on $\mathcal{F}^N$ defined by

$$\hat{\mathcal{O}}_2|\lambda_1\rangle\cdots|\lambda_N\rangle = \sum_{1\le i<j\le N} o(\lambda_i,\lambda_j)|\lambda_1\rangle\cdots|\lambda_N\rangle,$$

which means, we pick all possible pairs of two vectors $|\lambda_i\rangle,\ |\lambda_j\rangle$, among $|\lambda_1\rangle,\cdots,|\lambda_N\rangle$, and act $\hat{o} = o(\hat{A}_1, \hat{A}_2)$ to obtain $\hat{o}|\lambda_i\rangle|\lambda_j\rangle = o(\lambda_i,\lambda_j)|\lambda_i\rangle|\lambda_j\rangle$, and put these vectors at the original position. A typical example of two-body operator is the coulomb potential $V(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{|\hat{\mathbf{r}}_1 - \hat{\mathbf{r}}_2|}$.

Now we claim that the second quantized form of the two-body operator $\hat{\mathcal{O}}_2$ is

$$\begin{aligned}\hat{\mathcal{O}}_2 &= \frac{1}{2}\sum_{\mu\nu\mu'\nu'} a^\dagger_\mu a^\dagger_\nu \langle\mu|\langle\nu|\hat{o}|\mu'\rangle|\nu'\rangle a_{\nu'} a_{\mu'} \qquad \text{(C.14)}\\ &= \frac{1}{2}\sum_{\mu\nu\mu'\nu'} a^\dagger_\mu a^\dagger_\nu\, o(\mu',\nu')\,\delta_{\mu\mu'}\delta_{\nu\nu'} a_{\nu'} a_{\mu'} = \frac{1}{2}\sum_{\mu\nu} a^\dagger_\mu a^\dagger_\nu\, o(\mu,\nu)\, a_\nu a_\mu.\end{aligned}$$

Here, the second and third lines are used more frequently in practical discussion.

Let's prove the claim. To this end, recall that

$$|\lambda_1 \cdots \lambda_N\rangle_\zeta \equiv \frac{1}{\sqrt{N! \prod_\lambda n_\lambda!}} \sum_{\sigma \in S_N} \zeta^{(1-\mathrm{sgn}\sigma)/2} |\lambda_{\sigma(1)}\rangle \otimes \cdots \otimes |\lambda_{\sigma(N)}\rangle \tag{C.15}$$

$$= \frac{1}{\sqrt{\prod_\lambda n_\lambda!}} a^\dagger_{\lambda_1} \cdots a^\dagger_{\lambda_N} |0\rangle \tag{C.16}$$

holds. Now we prove (C.14) as follows.

$$\hat{\mathcal{O}}_2 |\lambda_1 \cdots \lambda_N\rangle_\zeta = \sum_{\sigma \in S_N} \frac{\zeta^{(1-\mathrm{sgn}\sigma)/2}}{\sqrt{N! \prod_\lambda (n_\lambda!)}} \sum_{1 \le i < j \le N} o(\lambda_{\sigma(i)}, \lambda_{\sigma(j)}) |\lambda_{\sigma(1)}\rangle \cdots |\lambda_{\sigma(N)}\rangle.$$

Here, the factor $\sum_{1 \le i < j \le N} o(\lambda_{\sigma(i)}, \lambda_{\sigma(j)})$ can be separated from other parts of the above expression. For fixed σ, the pairs $(\lambda_{\sigma(i)}, \lambda_{\sigma(j)}),\ 1 \le i < j \le N$ sweeps every pairs $(\lambda_{i'}, \lambda_{j'})$, possibly $i' > j'$. But, by the symmetric property (C.13), it doesn't matter. Thus we have

$$\sum_{1 \le i < j \le N} o(\lambda_{\sigma(i)}, \lambda_{\sigma(j)}) = \sum_{1 \le i < j \le N} o(\lambda_i, \lambda_j),$$

and thus

$$\begin{aligned}
&\hat{\mathcal{O}}_2 |\lambda_1 \cdots \lambda_N\rangle_\zeta \\
&= \sum_{\sigma \in S_N} \frac{\zeta^{(1-\mathrm{sgn}\sigma)/2}}{\sqrt{N! \prod_\lambda (n_\lambda!)}} \sum_{1 \le i < j \le N} o(\lambda_i, \lambda_j) |\lambda_{\sigma(1)}\rangle \cdots |\lambda_{\sigma(N)}\rangle \frac{1}{\sqrt{N! \prod_\lambda (n_\lambda!)}} \\
&= \sum_{1 \le i < j \le N} o(\lambda_i, \lambda_j) |\lambda_1 \cdots \lambda_N\rangle_\zeta.
\end{aligned}$$

From (C.16), we have

$$\begin{aligned}
&= \sum_{1 \le i < j \le N} \frac{o(\lambda_j, \lambda_i)}{\sqrt{\prod_\lambda n_\lambda!}} a^\dagger_{\lambda_1} \cdots a^\dagger_{\lambda_N} |0\rangle \\
&= \sum_{\substack{1 \le i < j \le N \\ \sigma \in S_2}} \frac{\zeta^{(1-\mathrm{sgn}\sigma)/2}}{2\sqrt{\prod_\lambda n_\lambda!}} o\big(\sigma(\lambda_j), \sigma(\lambda_i)\big) a^\dagger_{\lambda_1} \cdots a^\dagger_{\sigma(\lambda_i)} \cdots a^\dagger_{\sigma(\lambda_j)} \cdots a^\dagger_{\lambda_N} |0\rangle \\
&= \sum_{\substack{1 \le i < j \le \le N \\ \sigma \in S_2 \\ \mu, \nu}} \frac{\zeta^{(1-\mathrm{sgn}\sigma)/2}}{2\sqrt{\prod_\lambda n_\lambda!}} o(\mu, \nu) \delta_{\mu\sigma(\lambda_j)} \delta_{\nu\sigma(\lambda_i)} \zeta^{i+j} a^\dagger_\mu a^\dagger_\nu a^\dagger_{\lambda_1} \cdots \widehat{a^\dagger_{\lambda_i}} \cdots \widehat{a^\dagger_{\lambda_j}} \cdots a^\dagger_{\lambda_N} |0\rangle.
\end{aligned}$$

Here, the wide hat implies its absence.

$$= \frac{1}{2\sqrt{\prod_\lambda n_\lambda!}} \sum_{\substack{\mu,\nu \\ \mu',\nu'}} o(\mu,\nu)\delta_{\mu\mu'}\delta_{\nu\nu'} a_\mu^\dagger a_\nu^\dagger \sum_{\substack{1\le i<j\le N \\ \sigma\in S_2}} \zeta^{i+j}\zeta^{(1-\mathrm{sgn}\sigma)/2}\delta_{\mu'\sigma(\lambda_j)}\delta_{\nu'\sigma(\lambda_i)}$$
$$\cdot a_{\lambda_1}^\dagger \cdots \widehat{a_{\lambda_i}^\dagger} \cdots \widehat{a_{\lambda_j}^\dagger} \cdots a_{\lambda_N}^\dagger |0\rangle$$
$$= \frac{1}{2\sqrt{\prod_\lambda n_\lambda!}} \sum_{\substack{\mu,\nu \\ \mu',\nu'}} a_\mu^\dagger a_\nu^\dagger \langle\mu|\langle\nu|\hat{o}|\mu'\rangle|\nu'\rangle \left[\sum_{\substack{1\le i<j\le N \\ \sigma\in S_2}} \zeta^{i+j}\zeta^{(1-\mathrm{sgn}\sigma)/2}\delta_{\mu'\sigma(\lambda_j)}\delta_{\nu'\sigma(\lambda_i)} \right.$$
$$\left. \cdot a_{\lambda_1}^\dagger \cdots \widehat{a_{\lambda_i}^\dagger} \cdots \widehat{a_{\lambda_j}^\dagger} \cdots a_{\lambda_N}^\dagger |0\rangle \right].$$

We claim that the factor in the square bracket can be written as $a_{\nu'}a_{\mu'}a_{\lambda_1}^\dagger \cdots a_{\lambda_N}^\dagger|0\rangle$. This can be shown as follows.

Imagine that we proceed $a_{\nu'}$ and $a_{\mu'}$ in $a_{\nu'}a_{\mu'}a_{\lambda_1}^\dagger \cdots a_{\lambda_N}^\dagger|0\rangle$ to the vacuum state vector $|0\rangle$ using commutation relations. Then it will have the form

$$a_{\nu'}a_{\mu'}a_{\lambda_1}^\dagger \cdots a_{\lambda_N}^\dagger|0\rangle = \sum_{1\le i<j\le N}\sum_{\sigma\in S_2} C_{ij\sigma}\delta_{\mu'\sigma(\lambda_j)}\delta_{\nu'\sigma(\lambda_i)} a_{\lambda_1}^\dagger \cdots \widehat{a_{\lambda_i}^\dagger} \cdots \widehat{a_{\lambda_j}^\dagger} \cdots a_{\lambda_N}^\dagger |0\rangle$$

where $C_{ij\sigma}$ are coefficients to be determined. Observe that

$$\begin{aligned}
&a_{\nu'}a_{\mu'}a_{\lambda_1}^\dagger \cdots a_{\lambda_N}^\dagger|0\rangle \\
&= a_{\nu'}a_{\mu'}\zeta^{(j-1)+(i-1)} a_{\lambda_j}^\dagger a_{\lambda_i}^\dagger a_{\lambda_1}^\dagger \cdots \widehat{a_{\lambda_i}^\dagger} \cdots \widehat{a_{\lambda_j}^\dagger} \cdots a_{\lambda_N}^\dagger |0\rangle \\
&= \zeta^{i+j}\zeta^{(1-\mathrm{sgn}\sigma)/2} a_{\nu'}a_{\mu'} a_{\sigma(\lambda_j)}^\dagger a_{\sigma(\lambda_i)}^\dagger a_{\lambda_1}^\dagger \cdots \widehat{a_{\lambda_i}^\dagger} \cdots \widehat{a_{\lambda_j}^\dagger} \cdots a_{\lambda_N}^\dagger |0\rangle \\
&= \zeta^{i+j}\zeta^{(1-\mathrm{sgn}\sigma)/2}\delta_{\mu'\sigma(\lambda_j)}\delta_{\nu'\sigma(\lambda_i)} a_{\lambda_1}^\dagger \cdots \widehat{a_{\lambda_i}^\dagger} \cdots \widehat{a_{\lambda_j}^\dagger} \cdots a_{\lambda_N}^\dagger |0\rangle + \cdots . \qquad \text{(C.17)}
\end{aligned}$$

Since $a_{\lambda_1}^\dagger \cdots \widehat{a_{\lambda_i}^\dagger} \cdots \widehat{a_{\lambda_j}^\dagger} \cdots a_{\lambda_N}^\dagger |0\rangle$'s are linearly independent for each $1 \le i < j \le N$, we can obtain the coefficient $C_{ij\sigma} = \zeta^{i+j}\zeta^{(1-\mathrm{sgn}\sigma)/2}$. Thus we have proved the claim,

$$\begin{aligned}
&a_{\nu'}a_{\mu'}a_{\lambda_1}^\dagger \cdots a_{\lambda_N}^\dagger|0\rangle \\
&\qquad = \sum_{1\le i<j\le N}\sum_{\sigma\in S_2} \zeta^{i+j+(1-\mathrm{sgn}\sigma)/2}\delta_{\mu'\sigma(\lambda_j)}\delta_{\nu'\sigma(\lambda_i)} a_{\lambda_1}^\dagger \cdots \widehat{a_{\lambda_i}^\dagger} \cdots \widehat{a_{\lambda_j}^\dagger} \cdots a_{\lambda_N}^\dagger |0\rangle.
\end{aligned}$$

Now we get

$$\begin{aligned}\hat{\mathcal{O}}_2|\lambda_1\cdots\lambda_N\rangle_\zeta &= \frac{1}{2\sqrt{\prod_\lambda n_\lambda!}}\sum_{\substack{\mu,\nu\\ \mu',\nu'}} a^\dagger_\mu a^\dagger_\nu \langle\mu|\langle\nu|\hat{o}|\mu'\rangle|\nu'\rangle a_{\nu'}a_{\mu'}a^\dagger_{\lambda_1}\cdots a^\dagger_{\lambda_N}|0\rangle \\ &= \frac{1}{2}\sum_{\substack{\mu,\nu\\ \mu',\nu'}} a^\dagger_\mu a^\dagger_\nu \langle\mu|\langle\nu|\hat{o}|\mu'\rangle|\nu'\rangle a_{\nu'}a_{\mu'}|\lambda_1\cdots\lambda_N\rangle_\zeta\end{aligned}$$

by (C.16). Therefore we conclude that the second quantized form of the two-body operator $\hat{\mathcal{O}}_2$ is as in (C.14).

Let's look upon an example. The coulomb interaction between electrons can be represented as second quantized form by using (C.14):

$$\begin{aligned}\hat{V} &= \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'d\mathbf{r}''d\mathbf{r}'''a^\dagger_\sigma(\mathbf{r})a^\dagger_{\sigma'}(\mathbf{r}')\langle\mathbf{r}\sigma|\langle\mathbf{r}'\sigma'|\frac{1}{4\pi\varepsilon_0}\frac{e^2}{|\hat{\mathbf{x}}_1-\hat{\mathbf{x}}_2|}|\mathbf{r}''\sigma''\rangle|\mathbf{r}'''\sigma'''\rangle a_{\sigma'''}(\mathbf{r}''')a_{\sigma''}(\mathbf{r}'') \\ &= \frac{e^2}{8\pi\varepsilon_0}\int d\mathbf{r}d\mathbf{r}'d\mathbf{r}''d\mathbf{r}'''a^\dagger_\sigma(\mathbf{r})a^\dagger_{\sigma'}(\mathbf{r}')\frac{\delta_{\sigma\sigma''}\delta_{\sigma'\sigma'''}}{|\mathbf{r}-\mathbf{r}'|}\delta^3(\mathbf{r}-\mathbf{r}'')\delta^3(\mathbf{r}'-\mathbf{r}''')a_{\sigma'''}(\mathbf{r}''')a_{\sigma''}(\mathbf{r}'') \\ &= \frac{e^2}{8\pi\varepsilon_0}\int d\mathbf{r}d\mathbf{r}'a^\dagger_\sigma(\mathbf{r})a^\dagger_{\sigma'}(\mathbf{r}')\frac{1}{|\mathbf{r}-\mathbf{r}'|}a_{\sigma'}(\mathbf{r}')a_\sigma(\mathbf{r}),\end{aligned}$$

where summation on spin indices $\sigma = \pm\frac{1}{2}$ is assumed.

For many cases, we need to express a two-body operator by another basis, e.g., by the energy eigenstates of the system, rather than by the position eigenstates as in the example above. We must apply a change of basis in eq.(C.14). In another basis, the two-body operator still have the same form as before, while $|\mu\rangle,\ |\nu\rangle$ are not the eigenstates of $\hat{o}$ (of $\hat{A}$, more precisely) anymore.

We are relatively familiar with manipulations and interpretations of the (many particle) Schrödinger equation. The concepts and structures we have developed so far seems first somewhat abstract and impractical. And it is hard to see the connection between the many-body wave functions and the abstract Fock space state vectors. In the following sections, we are going to introduce a non-linear wave equation from the Fock space formalism. And we will clarify the relation between the Fock space state vectors and the many-body wave functions which are somewhat more tractable.

C.4 Ordering of Eigenvalues

Let $\mathcal{H}$ be a Hilbert space and consider a complete set of eigenstates $\{|\lambda\rangle : \lambda \in I\}$. We can construct a basis $\{|\lambda_1\rangle \otimes \cdots \otimes |\lambda_n\rangle : \lambda_k \in I,\ k = 1, \cdots, n\}$ for the n-fold tensor product space $\mathcal{H}^n$.

Let σ be an element of symmetric group S_n. If we define an operator $\mathcal{P}_\sigma : \mathcal{H}^n \to \mathcal{H}^n$ by $\mathcal{P}_\sigma(|\lambda_1\rangle\otimes\cdots\otimes|\lambda_n\rangle) = |\lambda_{\sigma(1)}\rangle\otimes\cdots\otimes|\lambda_{\sigma(n)}\rangle$, we can characterize the Bosonic/fermionic subspaces by

$$\mathcal{F}^n_\zeta \equiv \left\{|\varphi\rangle \in \mathcal{H}^n : \mathcal{P}_\sigma|\varphi\rangle = \zeta^{(1-\mathrm{sgn}\sigma)/2}|\varphi\rangle \text{ for all } \sigma \in S_n\right\}$$

where $\zeta = +1$ for Bosons and $\zeta = -1$ for fermions. Consider vectors of the form

$$|\lambda_1 \cdots \lambda_n\rangle_\zeta \equiv \frac{1}{\sqrt{n!\prod_\lambda n_\lambda!}} \sum_{\sigma\in S_n} \zeta^{(1-\mathrm{sgn}\sigma)/2}|\lambda_{\sigma(1)}\rangle \otimes \cdots \otimes |\lambda_{\sigma(n)}\rangle \tag{C.18}$$

where, in the prefactor, n_λ are nothing but the number of occurance of each eigenvalues in $\lambda_1, \cdots, \lambda_n$. Since we may switch the position of $\lambda_1, \cdots, \lambda_n$ at the cost of a change of sign, we introduce an ordering to fix the representation of the vector (C.18). In the previous sections, we saw that these vectors form an orthonormal basis for $\mathcal{F}^n_\zeta$.

After we respect the ordering of eigenvalues, we can write $|\lambda_1 \cdots \lambda_n\rangle_\zeta$ as $|n_1 n_2 \cdots\rangle$ uniquely. For example, we can denote $|1111223334667\cdots\rangle_\zeta$ simply by $|423102\cdots\rangle$. We call this kind of representation as occupation number representation. Now, an arbitrary vector $|\varphi\rangle \in \mathcal{F}^n_\zeta$ can be expressed as a linear combination of $|n_1 n_2 \cdots\rangle$'s.

$$|\varphi\rangle = \sum_{\substack{n_1 n_2 \cdots \\ \sum n_i = n}} C_{n_1 n_2 \cdots}|n_1 n_2 \cdots\rangle. \tag{C.19}$$

After we construct the Fock space $\mathcal{F}_\zeta \equiv \bigoplus_{n=0}^\infty \mathcal{F}^n_\zeta$, we define operators $a_i^\dagger$ and a_i by

$$a_i^\dagger|n_1 n_2 \cdots\rangle \equiv \sqrt{n_i + 1}\zeta^{s_i}|n_1 \cdots n_i + 1 \cdots\rangle$$
$$a_i|n_1 n_2 \cdots\rangle \equiv \sqrt{n_i}\zeta^{s_i}|n_1 \cdots n_i - 1 \cdots\rangle$$

where $s_i = \sum_{j=1}^{i-1} n_j$. From this definitions we can obtain the commutation relations.

$$[a_i, a_j^\dagger]_\pm = \delta_{ij}, \qquad [a_i, a_j]_\pm = [a_i^\dagger, a_j^\dagger]_\pm = 0$$

where upper signs are for fermions and lower signs are for Bosons. In terms of these creation/annihilation operators, we can express the basis vectors $|n_1 n_2 \cdots\rangle$ by

$$|n_1 n_2 \cdots\rangle = \prod_{i=1}^{\infty} \frac{1}{\sqrt{n_i!}} (a_i^\dagger)^{n_i} |0\rangle. \tag{C.20}$$

Although the occupation number representation (C.20) is a great simplification of the complicated notation (C.18), it still has several defects. One thing is that we have to define an ordering on the eigenvalues to arrange occupation numbers in unique way. The other defect is that, in the case of continuous eigenvalues, we have to introduce continuously many occupation numbers, which cannot be listed as before. To overcome these defects, we try to express a state vector not by a summation over occupation numbers (C.19), but by a summation over *eigenvalues*.

Let $|\varphi\rangle \in \mathcal{F}_\zeta^n$ be an arbitrary n-particle state vector. This vector can be expressed as a linear combination of $|n_1 n_2 \cdots\rangle$. Since each $|n_1 n_2 \cdots\rangle$ can be obtained by applying creation operators to the vacuum state for n times, we may express the generic state vector $|\varphi\rangle$ by

$$|\varphi\rangle = \sum_{\nu_1, \cdots, \nu_n} C_{\nu_1 \cdots \nu_n} \frac{1}{\sqrt{n!}} a_{\nu_1}^\dagger \cdots a_{\nu_n}^\dagger |0\rangle. \tag{C.21}$$

Note that (C.21) involves a summation over eigenvalues while (C.19) involves a summation over occupation numbers. The factor $\frac{1}{\sqrt{n!}}$ is conventional. Note also that there is no symmetric property on the indices of $C_{\nu_1 \cdots \nu_n}$ *yet*. But, by using the property $a_{\nu_{\sigma(1)}}^\dagger \cdots a_{\nu_{\sigma(n)}}^\dagger |0\rangle = \zeta^{(1-\mathrm{sgn}\sigma)/2} a_{\nu_1}^\dagger \cdots a_{\nu_n}^\dagger |0\rangle$, we can symmetrize/antisymmetrize the indices:

$$\begin{aligned}
|\varphi\rangle &= \sum_{\nu_1, \cdots, \nu_n} C_{\nu_1 \cdots \nu_n} \frac{1}{\sqrt{n!}} a_{\nu_1}^\dagger \cdots a_{\nu_n}^\dagger |0\rangle \\
&= \frac{1}{n!} \sum_{\sigma \in S_n} \zeta^{(1-\mathrm{sgn}\sigma)/2} \sum_{\nu_1, \cdots, \nu_n} C_{\nu_1 \cdots \nu_n} \frac{1}{\sqrt{n!}} a_{\nu_{\sigma(1)}}^\dagger \cdots a_{\nu_{\sigma(n)}}^\dagger |0\rangle.
\end{aligned}$$

For fixed $\sigma \in S_n$, define $\omega_i \equiv \nu_{\sigma(i)}$. Then

$$= \frac{1}{n!} \sum_{\sigma \in S_n} \zeta^{(1-\mathrm{sgn}\sigma)/2} \sum_{\nu_1, \cdots, \nu_n} C_{\omega_{\sigma^{-1}(1)} \cdots \omega_{\sigma^{-1}(n)}} \frac{1}{\sqrt{n!}} a_{\omega_1}^\dagger \cdots a_{\omega_n}^\dagger |0\rangle.$$

Since $(\nu_1, \cdots, \nu_n) \mapsto (\omega_1, \cdots, \omega_n) = (\nu_{\sigma(1)}, \cdots, \nu_{\sigma(n)})$ is bijective,

$$= \frac{1}{n!} \sum_{\sigma \in S_n} \zeta^{(1-\mathrm{sgn}\sigma)/2} \sum_{\omega_1, \cdots, \omega_n} C_{\omega_{\sigma^{-1}(1)} \cdots \omega_{\sigma^{-1}(n)}} \frac{1}{\sqrt{n!}} a^\dagger_{\omega_1} \cdots a^\dagger_{\omega_n} |0\rangle$$
$$= \sum_{\omega_1, \cdots, \omega_n} \left(\frac{1}{n!} \sum_{\sigma \in S_n} \zeta^{(1-\mathrm{sgn}\sigma)/2} C_{\omega_{\sigma(1)} \cdots \omega_{\sigma(n)}} \right) \frac{1}{\sqrt{n!}} a^\dagger_{\omega_1} \cdots a^\dagger_{\omega_n} |0\rangle.$$

If we define $\tilde{C}_{\omega_1 \cdots \omega_n} \equiv \frac{1}{n!} \sum_{\sigma \in S_n} \zeta^{(1-\mathrm{sgn}\sigma)/2} C_{\omega_{\sigma(1)} \cdots \omega_{\sigma(n)}}$, then the indices of $\tilde{C}_{\omega_1 \cdots, \omega_n}$ have desired symmetric/antisymmetric property, i.e., $\tilde{C}_{\omega_{\sigma(1)} \cdots \omega_{\sigma(n)}} = \zeta^{(1-\mathrm{sgn}\sigma)/2} \tilde{C}_{\omega_1 \cdots \omega_n}$. We finally obtain eq.(C.21) with $C_{\nu_1 \cdots \nu_n}$ having symmetric/antisymmetric property.

Now we determine the coefficients $C_{\omega_1 \cdots \omega_n}$. To this end, we calculate

$$\frac{1}{\sqrt{N!}} \langle 0 | a_{\nu'_N} \cdots a_{\nu'_1} a^\dagger_{\nu_1} \cdots a^\dagger_{\nu_N} |0\rangle \frac{1}{\sqrt{N!}}.$$

Imagine that $a_{\nu'_1}, \cdots, a^\dagger_{\nu'_N}$ are prodeeding to $|0\rangle$ by commuting with creation operators. Each $a_{\nu'_i}$ will meet $a^\dagger_{\nu_j}$ to give $\delta_{\nu'_i \nu_j}$. Thus it will become

$$\frac{1}{\sqrt{N!}} \langle 0 | a_{\nu'_N} \cdots a_{\nu'_1} a_{\nu_1} \cdots a_{\nu_N} |0\rangle \frac{1}{\sqrt{N!}} = \frac{1}{N!} \sum_{\sigma \in S_N} C_\sigma \delta_{\nu'_1 \nu_{\sigma(1)}} \cdots \delta_{\nu'_N \nu_{\sigma(N)}}$$

where C_σ are coefficient we cannot specify yet.

To determine C_σ, observe that

$$\frac{1}{\sqrt{N!}} \langle 0 | a_{\nu'_N} \cdots a_{\nu'_1} a^\dagger_{\nu_1} \cdots a^\dagger_{\nu_N} |0\rangle \frac{1}{\sqrt{N!}} = \frac{1}{N!} \zeta^{(1-\mathrm{sgn}\sigma)/2} \langle 0 | a_{\nu'_N} \cdots a_{\nu'_1} a^\dagger_{\nu_{\sigma(1)}} \cdots a^\dagger_{\nu_{\sigma(N)}} |0\rangle$$
$$= \frac{1}{N!} \zeta^{(1-\mathrm{sgn}\sigma)/2} \delta_{\nu'_1 \nu_{\sigma(1)}} \cdots \delta_{\nu'_N \nu_{\sigma(N)}} + \cdots .$$

We don't need to calculate the other terms. We see that $C_\sigma = \zeta^{(1-\mathrm{sgn}\sigma)/2}$. Therefore we conclude that

$$\frac{1}{\sqrt{N!}} \langle 0 | a_{\nu'_N} \cdots a_{\nu'_1} a_{\nu_1} \cdots a_{\nu_N} |0\rangle \frac{1}{\sqrt{N!}} = \frac{1}{N!} \sum_{\sigma \in S_N} \zeta^{(1-\mathrm{sgn}\sigma)/2} \delta_{\nu'_1 \nu_{\sigma(1)}} \cdots \delta_{\nu'_N \nu_{\sigma(N)}}. \tag{C.22}$$

Now, by applying $\frac{1}{\sqrt{N!}}\langle 0|a_{\nu'_N}\cdots a_{\nu'_1}$ to (C.21), we obtain

$$\begin{aligned}
\frac{1}{\sqrt{N!}}\langle 0|a_{\nu'_N}\cdots a_{\nu'_1}|\varphi\rangle &= \sum_{\nu_1\cdots\nu_N} C_{\nu_1\cdots\nu_N}\frac{1}{N!}\langle 0|a_{\nu'_N}\cdots a_{\nu'_1}a_{\nu_1}\cdots a_{\nu_N}|0\rangle \\
&= \sum_{\nu_1\cdots\nu_N} C_{\nu_1\cdots\nu_N}\frac{1}{N!}\sum_{\sigma\in S_N}\zeta^{(1-\mathrm{sgn}\sigma)/2}\delta_{\nu'_1\nu_{\sigma(1)}}\cdots\delta_{\nu'_N\nu_{\sigma(N)}} \\
&= \frac{1}{N!}\sum_{\sigma\in S_N}\zeta^{(1-\mathrm{sgn}\sigma)/2}C_{\nu'_{\sigma(1)}\cdots\nu'_{\sigma(N)}} = \frac{1}{N!}\sum_{\sigma\in S_N}C_{\nu'_1\cdots\nu'_N} \\
&= C_{\nu'_1\cdots\nu'_N}
\end{aligned}$$

Therefore, we finally get

$$|\varphi\rangle = \sum_{\nu_1\cdots\nu_N}\frac{1}{\sqrt{N!}}\langle 0|a_{\nu_N}\cdots a_{\nu_1}|\varphi\rangle\frac{1}{\sqrt{N!}}a^\dagger_{\nu_1}\cdots a^\dagger_{\nu_N}|0\rangle. \tag{C.23}$$

Eq.(C.23) involves summation over eigenvalues while eq.(C.19) involves summation over occupation numbers. This expression is convenient because we don't need to concern the ordering of eigenvalues. We will see how this is convenient.

C.5 Field Operators and Wavefunctions

It is desirable to see the connection between the many-body wavefunctions, which is more tractable, and the abstract Fock space vectors. To this end, we introduce field operators.

Let $\hat{A}$ be an observable and $\{|\nu\rangle\}$ be the corresponding eigenbasis. We can construct the creation/annihilation operators corresponding to the observable $\hat{A}$. We have the commutation relations,

$$[\hat{a}_\nu, \hat{a}^\dagger_{\nu'}]_\pm = \delta_{\nu\nu'}, \qquad [\hat{a}_\nu, \hat{a}_{\nu'}]_\pm = [\hat{a}^\dagger_\nu, \hat{a}^\dagger_{\nu'}]_\pm = 0, \tag{C.24}$$

where we revived the 'hat's to indicate that they are operators. Here '$+$' is for Fermions and '$-$' is for Bosons.

Now we define the **field operators** $\hat{\psi}(\mathbf{x})$ and $\hat{\psi}^\dagger(\mathbf{x})$ by

$$\hat{\psi}(\mathbf{x}) \equiv \sum_\nu u_\nu(\mathbf{x})\hat{a}_\nu, \qquad \hat{\psi}^\dagger(\mathbf{x}) = \sum_\nu u^*_\nu(\mathbf{x})\hat{a}^\dagger_\nu, \tag{C.25}$$

where $u_\nu(\mathbf{x}) = \langle \mathbf{x} \,|\, \nu \rangle$. We used special observable $\hat{A}$ and its eigenstates to define the field operators. For the field operators to be a natural concept, we have to show that the definition (C.25) does not depend on such choices.

Let $\hat{B}$ be another observable, $\{v_\mu(\mathbf{x})\}$ be the eigenfunctions of $\hat{B}$, and $\hat{b}_\mu^\dagger,\ \hat{b}_\mu$ be the creation/annihilation operators corresponding to $\hat{B}$. Then, by the transformation rule for creation/annihilation operators (C.9), we obtain

$$\sum_\nu u_\nu(\mathbf{x})\hat{a}_\nu = \sum_{\mu,\nu} \langle \mathbf{x} \,|\, \nu \rangle \langle \nu \,|\, \mu \rangle \hat{b}_\mu = \sum_\mu \langle \mathbf{x} \,|\, \mu \rangle \hat{b}_\mu = \sum_\mu v_\mu(\mathbf{x})\hat{b}_\mu.$$

Therefore the definition (C.25) does not depend on the choice of eigenbasis.

By using the commutation relations (C.24), we can show that

$$[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x})]_\pm = \delta(\mathbf{x} - \mathbf{x}'), \qquad [\hat{\psi}(\mathbf{x}), \hat{\psi}(\mathbf{x}')]_\pm = [\hat{\psi}^\dagger(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')]_\pm = 0. \tag{C.26}$$

For example,

$$[\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')]_\pm = \sum_{\nu,\nu'} u_\nu(\mathbf{x}) u_{\nu'}^*(\mathbf{x}')[\hat{a}_\nu, \hat{a}_{\nu'}^\dagger]_\pm = \sum_\nu \langle \mathbf{x} \,|\, \nu \rangle \langle \nu \,|\, \mathbf{x}' \rangle = \delta(\mathbf{x} - \mathbf{x}').$$

We may inverse the definition (C.25) by using orthogonality of $\{u_\nu(\mathbf{x})\}$ to obtain expressions for $\hat{a}_\nu$ and $\hat{a}_\nu^\dagger$ in terms of the field operators.

$$\hat{a}_\nu = \int d\mathbf{x}\, u_\nu^*(\mathbf{x})\hat{\psi}(\mathbf{x}), \qquad \hat{a}_\nu^\dagger = \int d\mathbf{x}\, u_\nu(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}). \tag{C.27}$$

For example,

$$\int d\mathbf{x}\, u_\nu^*(\mathbf{x})\hat{\psi}(\mathbf{x}) = \int d\mathbf{x}\, u_\nu^*(\mathbf{x}) \sum_{\nu'} u_{\nu'}(\mathbf{x})\hat{a}_{\nu'} = \sum_{\nu'} \delta_{\nu\nu'}\hat{a}_{\nu'} = \hat{a}_\nu.$$

Substituing (C.27) to (C.23), we obtain

$$\begin{aligned} |\varphi\rangle = \sum_{\nu_1,\cdots,\nu_N} \int & d\mathbf{x}_1 \cdots d\mathbf{x}'_N\, u_{\nu_N}^*(\mathbf{x}_N) \cdots u_{\nu_1}^*(\mathbf{x}_1) u_{\nu_1}(\mathbf{x}'_1) \cdots u_{\nu_N}(\mathbf{x}'_N) \\ & \cdot \frac{1}{\sqrt{N!}} \langle 0 | \hat{\psi}(\mathbf{x}_N) \cdots \hat{\psi}(\mathbf{x}_1) | \varphi \rangle \cdot \frac{1}{\sqrt{N!}} \hat{\psi}^\dagger(\mathbf{x}'_1) \cdots \hat{\psi}^\dagger(\mathbf{x}'_N) | 0 \rangle \\ = \int & d\mathbf{x}_1 \cdots d\mathbf{x}_N\, \frac{1}{\sqrt{N!}} \langle 0 | \hat{\psi}(\mathbf{x}_N) \cdots \hat{\psi}(\mathbf{x}_1) | \varphi \rangle \cdot \frac{1}{\sqrt{N!}} \hat{\psi}^\dagger(\mathbf{x}_1) \cdots \hat{\psi}^\dagger(\mathbf{x}_N) | 0 \rangle. \end{aligned} \tag{C.28}$$

This is the expression for a generic N-particle many-body state vector in terms of field operators. Eq.(C.28) shows that the collection $\left\{\frac{1}{\sqrt{N!}}\hat{\psi}^\dagger(\mathbf{x}_1)\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle \,:\, \mathbf{x}_i \in \mathbb{R}^3\right\}$ spans the space $\mathcal{F}_\zeta^N$. Furthermore, we see that the operator

$$1_N = \int d\mathbf{x}_1 \cdots d\mathbf{x}_N \, \frac{1}{\sqrt{N!}}\hat{\psi}^\dagger(\mathbf{x}_1)\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle\langle 0|\hat{\psi}(\mathbf{x}_N)\cdots\hat{\psi}(\mathbf{x}_1)\frac{1}{\sqrt{N!}}$$

can be regarded as the identity operator if it acts on N particle Fock space states. If it acts on a state with different number of particles, it gives zero.

Now we can reveal the connection between the Fock space vector $|\varphi\rangle$ and the tractable many-body wavefunction. Before revealing the connection, let us recall what we meant by saying many-body wavefunction $\varphi(\mathbf{x}_1, \cdots, \mathbf{x}_N)$. Consider a set of orthonormal wavefunctions $\{w_\nu(\mathbf{x})\}$. These are the single particle wavefunctions that we regard to be relevant to the system of concern. In case of hydrogenic atoms, these are products of the spherical harmonics and the radial wavefunctions. The many-body wavefunction with n_i particles being in $w_{\nu_i}(\mathbf{x})$ state is written as

$$\varphi(\mathbf{x}_1, \cdots, \mathbf{x}_N) = \frac{1}{\sqrt{N!\prod_\lambda n_\lambda!}} \sum_{\sigma \in S_N} \zeta^{(1-\mathrm{sgn}\sigma)/2} w_{\nu_{\sigma(1)}}(\mathbf{x}_1)\cdots w_{\nu_{\sigma(N)}}(\mathbf{x}_N). \qquad \text{(C.29)}$$

This is a usual quantum mechanical argument.

We define operators on the Fock space by

$$c_\nu \equiv \int d\mathbf{x}\, w_\nu^*(\mathbf{x})\hat{\psi}(\mathbf{x}) \qquad \text{and} \qquad c_\nu^\dagger \equiv \int d\mathbf{x}\, w_\nu(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}). \qquad \text{(C.30)}$$

Then the commutation relations (C.26) implies

$$[c_\nu, c_{\nu'}^\dagger]_\pm = \delta_{\nu\nu'}, \qquad [c_\nu, c_{\nu'}]_\pm = [c_\nu^\dagger, c_{\nu'}^\dagger]_\pm = 0.$$

And by inverting (C.30), we get $\hat{\psi}(\mathbf{x}) = \sum_\nu w_\nu(\mathbf{x})c_\nu$ and $\hat{\psi}^\dagger(\mathbf{x}) = \sum_\nu w_\nu^*(\mathbf{x})c_\nu^\dagger$.

Until this point, it is not clear why we introduced $c_\nu^\dagger$ and c_ν. We assert that the Fock space state vector $|\varphi\rangle$ that models a system with n_i particles being in $w_{\nu_i}(\mathbf{x})$ state is

$$|\varphi\rangle = \frac{1}{\sqrt{\prod_\lambda n_\lambda!}} c_{\nu_1}^\dagger \cdots c_{\nu_N}^\dagger |0\rangle.$$

And we claim that

$$\varphi(\mathbf{x}_1, \cdots, \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \langle 0|\hat{\psi}(\mathbf{x}_N)\cdots\hat{\psi}(\mathbf{x}_1)|\varphi\rangle \tag{C.31}$$

holds. This is the relation between the wavefunction and the field operators. The proof goes as follows.

$$\varphi(\mathbf{x}_1, \cdots, \mathbf{x}_N) \tag{C.32}$$

$$= \frac{1}{\sqrt{N! \prod_\lambda n_\lambda!}} \sum_{\sigma \in S_N} \zeta^{(1-\mathrm{sgn}\sigma)/2} w_{\nu_{\sigma(1)}}(\mathbf{x}_1) \cdots w_{\nu_{\sigma(N)}}(\mathbf{x}_N) \tag{C.33}$$

$$= \frac{1}{\sqrt{N!}} \sum_{\nu'_1 \cdots \nu'_N} w_{\nu'_1}(\mathbf{x}_1) \cdots w_{\nu'_N}(\mathbf{x}_N) \frac{1}{\sqrt{\prod_\lambda n_\lambda!}} \sum_{\sigma \in S_N} \zeta^{(1-\mathrm{sgn}\sigma)/2} \delta_{\nu_{\sigma(1)}\nu'_1} \cdots \delta_{\nu_{\sigma(N)}\nu'_N}.$$

Recalling the identity, $\langle 0|c_{\nu'_N} \cdots c_{\nu'_1} c^\dagger_{\nu_1} \cdots c^\dagger_{\nu_N}|0\rangle = \sum_{\sigma \in S_N} \zeta^{(1-\mathrm{sgn}\sigma)/2} \delta_{\nu_{\sigma(1)}\nu'_1} \cdots \delta_{\nu_{\sigma(N)}\nu'_N}$, we get

$$= \frac{1}{\sqrt{N!}} \sum_{\nu'_1 \cdots \nu'_N} w_{\nu'_1}(\mathbf{x}_1) \ldots w_{\nu'_N}(\mathbf{x}_N) \frac{1}{\sqrt{\prod_\lambda n_\lambda!}} \langle 0|c_{\nu'_N} \cdots c_{\nu'_1} c^\dagger_{\nu_1} \cdots c^\dagger_{\nu_N}|0\rangle$$

$$= \frac{1}{\sqrt{N!}} \langle 0|\hat{\psi}_N(\mathbf{x}_N) \cdots \hat{\psi}_1(\mathbf{x}_1) \frac{1}{\sqrt{\prod_\lambda n_\lambda!}} c^\dagger_{\nu_1} \cdots c^\dagger_{\nu_N}|0\rangle$$

$$= \frac{1}{\sqrt{N!}} \langle 0|\hat{\psi}_N(\mathbf{x}_N) \cdots \hat{\psi}_1(\mathbf{x}_1)|\varphi\rangle. \tag{C.34}$$

The claim (C.31) is proved.

By putting (C.31) into (C.28), we obtain the following expression for the state vector $|\varphi\rangle$:

$$|\varphi\rangle = \int d\mathbf{x}_1 \cdots d\mathbf{x}_N \, \varphi(\mathbf{x}_1, \cdots, \mathbf{x}_N) \frac{1}{\sqrt{N!}} \hat{\psi}^\dagger(\mathbf{x}_1) \cdots \hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle, \tag{C.35}$$

where $\varphi(\mathbf{x}_1, \cdots, \mathbf{x}_N) = \frac{1}{\sqrt{N!}} \langle 0|\hat{\psi}(\mathbf{x}_N) \cdots \hat{\psi}(\mathbf{x}_1)|\varphi\rangle$ is the tractable many-body wavefunction corresponding to the state vector $|\varphi\rangle$.

C.6 Density Operators

Density operators are fundamental objects in statistical mechanics in that they represent the ensemble itself and are the only things we need to know to calculate macroscopic observable quantities. Bose-Einstein condensation(BEC) is one of the most interesting many particle phenomenon and so it must be characterized (defined) in terms of density operator representing the system. In subsequent sections, we will discuss the definition of BEC and one of its sufficient condition, the celebrated concept of 'Off-Diagonal Long-Range Order (ODLRO)'. To this end, we develop here the theory of density operators.

Mathematically, **density operator** is a positive Hermitian operator with unit trace. Most easy but practical construction of a density operator for given system is to use all the possible states of the system. Suppose that an ensemble of systems can occupy states $|\Phi_i\rangle,\ i = 1, \cdots, M$. $|\Phi_i\rangle$ can be a state vector in a single particle Hilbert space $\mathcal{H}$ or a many particle state belonging to a Fock space. Suppose we also know the probability $p_i\ (0 \le p_i \le 1,\ \sum_i p_i = 1)$ that a system in the ensemble is in the state $|\Phi_i\rangle$. p_i is just the number of systems occupying state $|\Phi_i\rangle$ divided by the total number of systems in the ensemble. Now we represent the ensemble by a single mathematical object, the density operator:

$$\hat{\rho} = \sum_{i=1}^{M} p_i |\Phi_i\rangle\langle\Phi_i|. \tag{C.36}$$

The density operator $\hat{\rho}$ given by above equation is positive because

$$\langle\Psi|\hat{\rho}|\Psi\rangle = \sum_{i=1}^{M} p_i |\langle\Psi \mid \Phi_i\rangle|^2 \ge 0 \quad \text{for any } |\Psi\rangle.$$

$\hat{\rho}$ is Hermitian because

$$\hat{\rho}^\dagger = \sum_{i=1}^{M} p_i \big(|\Phi_i\rangle\langle\Phi_i|\big)^\dagger = \sum_{i=1}^{M} p_i |\Phi_i\rangle\langle\Phi_i| = \hat{\rho}.$$

Here we used $(|a\rangle\langle b|)^\dagger = |b\rangle\langle a|$. This can be proved easily:

$$\begin{aligned}\langle\varphi|(|a\rangle\langle b|)^\dagger|\psi\rangle &= \Big(\langle\psi|(|a\rangle\langle b|)|\varphi\rangle\Big)^* = \langle\varphi \mid b\rangle\langle a \mid \psi\rangle \\ &= \langle\varphi|(|b\rangle\langle a|)|\psi\rangle \quad \text{for all } |\psi\rangle, |\varphi\rangle \qquad \Rightarrow (|a\rangle\langle b|)^\dagger = |b\rangle\langle a|.\end{aligned}$$

$\hat{\rho}$ has unit trace. To see this, let's introduce a complete orthonormal basis $\{|\nu\rangle : \nu \in I\}$. Then we see that

$$\mathrm{Tr}(\hat{\rho}) = \sum_{\nu} \langle\nu|\hat{\rho}|\nu\rangle = \sum_{i=1}^{M} p_i \sum_{\nu} \langle\nu \mid \Phi_i\rangle\langle\Phi_i \mid \nu\rangle = \sum_{i=1}^{M} p_i \langle\Phi_i \mid \Phi_i\rangle = \sum_{i=1}^{M} p_i = 1.$$

Therefore the operator $\hat{\rho}$ defined in (C.36) is indeed a positive Hermitian operator with unit trace.

An ensemble is called in **pure state** if its density operator *can* be expressed by a single term, $\hat{\rho} = |\Phi\rangle\langle\Phi|$. If this is impossible, the ensemble is called in **mixed state**. This kind of terminology is well-defined because of a property of tensor product space : If a tensor $T \in V \otimes W$ can be expressed by

$$T = v_1 \otimes w_1 + \cdots + v_M \otimes w_M \tag{C.37}$$

with linearly independent $v_1, \cdots, v_M \in V$ and linearly independent $w_1, \cdots, w_M \in W$, then T cannot be manipulated to yield an expression having fewer terms, i.e., (C.37) is the shortest expression.

The expression (C.36) for a density operator $\hat{\rho}$ is the shortest expression if and only if $|\Phi_i\rangle$'s are linearly independent. Thus, if a density operator is expressed as $\frac{1}{2}|\Phi_1\rangle\langle\Phi_1| + \frac{1}{2}|\Phi_2\rangle\langle\Phi_2|$ and $|\Phi_1\rangle, |\Phi_2\rangle$ are linearly independent, then this represents a mixed state.

Now, let's consider a system of N particles. It is very rare to consider a mixture of Bosons and Fermions. It is difficult to describe such system, because the constituent particles are neither completely identical nor completely distinguishable. Let's restrict our consideration to a system of N Bosons or a system of N Fermions. This kind of systems can assume a state in $\mathcal{F}_\zeta^N$.

Obviously we cannot know the state of the system comletely. We usually have some partial information about the system, e.g., the temperature T, volume V, and the number of particles N of the system. To analyze this system, we have to introduce an ensemble of systems which assume a number of different states but all have the same macroscopic quantities T, V, N.

Let $\hat{\rho}$ be the density operator for the N particle system. To calcuate the expectation value of an observable $\hat{A}$, we have to take the **ensemble average** of this observable, which is defined by

$$\langle \hat{A} \rangle \equiv \mathrm{Tr}(\hat{\rho}\hat{A}).$$

Here, the meaning of trace is the obvious one:

$$\mathrm{Tr}(\hat{A}) = \sum_{\substack{\{n_\lambda\} \\ \sum_\lambda n_\lambda = N}} \big\langle \{n_\lambda\} \big| \hat{A} \big| \{n_\lambda\} \big\rangle,$$

where $\{n_\lambda\}$ represents the number distribution of particles over the eigenstates and

$$\big|\{n_\lambda\}\big\rangle = \prod_\lambda \frac{(a_\lambda^\dagger)^{n_\lambda}}{\sqrt{n_\lambda!}}|0\rangle = \frac{1}{\sqrt{\prod_\lambda n_\lambda!}} a_{\lambda_1}^\dagger \cdots a_{\lambda_N}^\dagger |0\rangle.$$

Here we assume $\lambda_1, \cdots, \lambda_N$ are arranged according to a certain ordering. Now, in favor of position variables, we replace $a_{\lambda_i}^\dagger$ with the field operator $\hat{\psi}^\dagger(\mathbf{x})$ by using $a_{\lambda_i}^\dagger = \int d\mathbf{x}\, u_{\lambda_i}(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})$, where $u_{\lambda_i}(\mathbf{x})$ is the eigenfunction $\langle \mathbf{x} \mid \lambda_i \rangle$. Then we obtain

$$\begin{aligned}
\mathrm{Tr}\hat{A} &= \sum_{\substack{\{n_\lambda\} \\ \sum_\lambda n_\lambda = N}} \frac{1}{\prod_\lambda n_\lambda!} \langle 0| a_{\lambda_N} \cdots a_{\lambda_1} \hat{A} a_{\lambda_1}^\dagger \cdots a_{\lambda_N}^\dagger |0\rangle \\
&= \sum_{\substack{\{n_\lambda\} \\ \sum_\lambda n_\lambda = N}} \frac{1}{\prod_\lambda n_\lambda!} \int d\mathbf{y}_1 \cdots d\mathbf{y}_N d\mathbf{x}_1 \cdots d\mathbf{x}_N u_{\lambda_N}^*(\mathbf{y}_N) \cdots u_{\lambda_1}^*(\mathbf{y}_1) u_{\lambda_1}(\mathbf{x}_1) \cdots u_{\lambda_N}(\mathbf{x}_N) \\
&\qquad \cdot \langle 0| \hat{\psi}(\mathbf{y}_N) \cdots \hat{\psi}(\mathbf{y}_1) \hat{A} \hat{\psi}^\dagger(\mathbf{x}_1) \cdots \hat{\psi}^\dagger(\mathbf{x}_N) |0\rangle
\end{aligned}$$

The summation over the number distribution $\{n_\lambda\}$, $\sum_\lambda n_\lambda = N$ is the same as the summation over N-tuple of eigenbalues $\lambda_1 \le \cdots \le \lambda_N$. Thus

$$= \sum_{\lambda_1 \le \cdots \le \lambda_N} \frac{1}{\prod_\lambda n_\lambda!} \int d\mathbf{y}_1 \cdots d\mathbf{y}_N d\mathbf{x}_1 \cdots d\mathbf{x}_N u_{\lambda_N}^*(\mathbf{y}_N) \cdots u_{\lambda_1}^*(\mathbf{y}_1) u_{\lambda_1}(\mathbf{x}_1) \cdots u_{\lambda_N}(\mathbf{x}_N).$$

Since $\mathbf{y}_1, \cdots, \mathbf{x}_N$ are just the integration variables,

$$\begin{aligned}
&= \sum_{\lambda_1 \le \cdots \le \lambda_N} \frac{1}{\prod_\lambda n_\lambda!} \frac{1}{N!} \sum_{\sigma \in S_N} \int d\mathbf{y}_1 \cdots d\mathbf{y}_N d\mathbf{x}_1 \cdots d\mathbf{x}_N u_{\lambda_N}^*(\mathbf{y}_{\sigma(N)}) \cdots u_{\lambda_1}^*(\mathbf{y}_{\sigma(1)}) \\
&\quad \times u_{\lambda_1}(\mathbf{x}_{\sigma(1)}) \cdots u_{\lambda_N}(\mathbf{x}_{\sigma(N)}) \cdot \langle 0| \hat{\psi}(\mathbf{y}_{\sigma(N)}) \cdots \hat{\psi}(\mathbf{y}_{\sigma(1)}) \hat{A} \hat{\psi}^\dagger(\mathbf{x}_{\sigma(1)}) \cdots \hat{\psi}^\dagger(\mathbf{x}_{\sigma(N)}) |0\rangle \\
&= \sum_{\lambda_1 \le \cdots \le \lambda_N} \frac{1}{\prod_\lambda n_\lambda!} \frac{1}{N!} \sum_{\sigma \in S_N} \int d\mathbf{y}_1 \cdots d\mathbf{y}_N d\mathbf{x}_1 \cdots d\mathbf{x}_N u_{\lambda_{\sigma(N)}}^*(\mathbf{y}_N) \cdots u_{\lambda_{\sigma(1)}}^*(\mathbf{y}_1) \\
&\quad \times u_{\lambda_{\sigma(1)}}(\mathbf{x}_1) \cdots u_{\lambda_{\sigma(N)}}(\mathbf{x}_N) \cdot \langle 0| \hat{\psi}(\mathbf{y}_N) \cdots \hat{\psi}(\mathbf{y}_1) \hat{A} \hat{\psi}^\dagger(\mathbf{x}_1) \cdots \hat{\psi}^\dagger(\mathbf{x}_N) |0\rangle.
\end{aligned}$$

Now, we apply the following replacement

$$\sum_{\lambda_1 \le \cdots \le \lambda_N} \frac{1}{\prod_\lambda n_\lambda!} \sum_{\sigma \in S_N} = \sum_{\lambda_1, \cdots, \lambda_N \in I}.$$

This is true since the set $\{(\lambda_1, \cdots, \lambda_N) : \lambda_i \in I\}$ is the same as $\{(\lambda_{\sigma(1)}, \cdots, \lambda_{\sigma(N)}) :$

$\lambda_1 \leq \cdots \leq \lambda_N,\ \sigma \in S_N\}$ except the redundance $\prod_\lambda n_\lambda!$ in the later. Therefore we obtain

$$\begin{aligned}\mathrm{Tr}\hat{A} &= \frac{1}{N!}\int d\mathbf{y}_1 \cdots d\mathbf{y}_N d\mathbf{x}_1 \cdots d\mathbf{x}_N \delta(\mathbf{x}_1 - \mathbf{y}_1)\cdots\delta(\mathbf{x}_N - \mathbf{y}_N)\\ &\qquad \cdot \langle 0|\hat{\psi}(\mathbf{y}_N)\cdots\hat{\psi}(\mathbf{y}_1)\hat{A}\hat{\psi}^\dagger(\mathbf{x}_1)\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle\\ &= \frac{1}{N!}\int d\mathbf{x}_1\cdots d\mathbf{x}_N \langle 0|\hat{\psi}(\mathbf{x}_N)\cdots\hat{\psi}(\mathbf{x}_1)\hat{A}\hat{\psi}^\dagger(\mathbf{x}_1)\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle\\ \Rightarrow \mathrm{Tr}\hat{A} &= \int d\mathbf{x}_1\cdots d\mathbf{x}_N \frac{1}{\sqrt{N!}}\langle 0|\hat{\psi}(\mathbf{x}_N)\cdots\hat{\psi}(\mathbf{x}_1)\hat{A}\hat{\psi}^\dagger(\mathbf{x}_1)\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle\frac{1}{\sqrt{N!}}. \qquad (C.38)\end{aligned}$$

The notions used to analyze a given system usually involves single particle : It is easier to understand a function of single position (e.g. density of particles) then a function of N positions. Thus we need to extract information from $\hat{\rho}$ so that we can describe the behavior of a single constituent particle among N identical particles in the system. For this usage, we introduce the **reduced single-particle density operator**:

$$\begin{aligned}&\hat{\rho}_1 \equiv \mathrm{Tr}_{2,3,\cdots,N}\hat{\rho}\\ &= \frac{1}{N!}\int d\mathbf{z}d\mathbf{y}|\mathbf{z}\rangle\int d\mathbf{x}_2\cdots d\mathbf{x}_N\langle 0|\hat{\psi}(\mathbf{x}_N)\cdots\hat{\psi}(\mathbf{x}_2)\hat{\psi}(\mathbf{z})\hat{\rho}\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}^\dagger(\mathbf{x}_2)\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle\langle\mathbf{y}|.\end{aligned}$$

We need reduced single-particle density operator when we calculate the expectation value of an observable related to a single particle $\langle\hat{A}\rangle_1 \equiv \mathrm{Tr}_1(\hat{\rho}_1\hat{A})$, where the subscript 1 at the trace means that we should use single particle states to evaluate the trace. $\hat{\rho}_1$ is conceptually closer to our analytic notions. However, it is cumbersome to derive $\hat{\rho}_1$ everytime we calculate the expectation values of 1-body observables. We claim here a convenient formula:

$$\mathrm{Tr}_1(\hat{\rho}_1\hat{A}) = \frac{1}{N}\mathrm{Tr}(\hat{\rho}\hat{A}). \qquad (C.39)$$

The proof is as follows.

$$\begin{aligned}\mathrm{Tr}(\hat{\rho}\hat{A}) &= \int d\mathbf{x}_1\cdots\mathbf{x}_N\frac{1}{\sqrt{N!}}\langle 0|\hat{\psi}(\mathbf{x}_N)\cdots\hat{\psi}(\mathbf{x}_1)\hat{\rho}\hat{A}\hat{\psi}^\dagger(\mathbf{x}_1)\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle\frac{1}{\sqrt{N!}}\\ &= \int d\mathbf{y}d\mathbf{z}\langle\mathbf{y}|A|\mathbf{z}\rangle\int d\mathbf{x}_1\cdots d\mathbf{x}_N\frac{1}{\sqrt{N!}}\langle 0|\hat{\psi}(\mathbf{x}_N)\cdots\hat{\psi}(\mathbf{x}_1)\hat{\rho}\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{z})\\ &\qquad\cdot\hat{\psi}^\dagger(\mathbf{x}_1)\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle\frac{1}{\sqrt{N!}}\end{aligned}$$

$$\mathrm{Tr}(\hat{\rho}\hat{A}) = \int d\mathbf{y}d\mathbf{z}\langle\mathbf{y}|A|\mathbf{z}\rangle \int d\mathbf{x}_1\cdots d\mathbf{x}_N \sum_{i=1}^{N}\delta(\mathbf{x}_i - \mathbf{z})$$
$$\cdot \frac{1}{N!}\langle 0|\hat{\psi}(\mathbf{x}_N)\cdots\widehat{\hat{\psi}(\mathbf{x}_i)}\cdots\hat{\psi}(\mathbf{x}_1)\hat{\psi}(\mathbf{x}_i)\hat{\rho}\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}^\dagger(\mathbf{x}_1)\cdots\widehat{\hat{\psi}^\dagger(\mathbf{x}_i)}\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle$$

By renaming the integration variables,

$$= \int d\mathbf{y}d\mathbf{z}\langle\mathbf{y}|A|\mathbf{z}\rangle\frac{N}{N!}\int d\mathbf{x}_1\cdots d\mathbf{x}_{N-1}\langle 0|\hat{\psi}(\mathbf{x}_{N-1})\cdots\hat{\psi}(\mathbf{x}_1)\hat{\psi}(\mathbf{z})\hat{\rho}\hat{\psi}^\dagger(\mathbf{y})$$
$$\cdot\hat{\psi}^\dagger(\mathbf{x}_1)\cdots\hat{\psi}^\dagger(\mathbf{x}_{N-1})|0\rangle$$
$$= N\int d\mathbf{z}\langle\mathbf{z}|\hat{\rho}_1\hat{A}|\mathbf{z}\rangle = N\cdot\mathrm{Tr}_1(\hat{\rho}\hat{A}).$$

The criterion for 'Off-Diagonal Long-Range Order' will be stated in terms of the matrix elements of $\hat{\rho}_1$ in position basis, the single particle reduced density *matrix* $\rho_1(\mathbf{r},\mathbf{r}') \equiv \langle\mathbf{r}'|\hat{\rho}_1|\mathbf{r}\rangle$. It is easy to see that $\rho_1(\mathbf{r},\mathbf{r}) = \rho(\mathbf{r})$ is the particle density:

$$\hat{\rho}_1 = \sum_i p_i|i\rangle\langle i| \quad\Rightarrow\quad \hat{\rho}_1(\mathbf{r},\mathbf{r}) = \langle\mathbf{r}|\hat{\rho}_1|\mathbf{r}\rangle = \sum_i p_i|\langle\mathbf{r}\mid i\rangle|^2 = \rho(\mathbf{r}).$$

In the literature, people define the reduced single-particle density matrix $\rho_1(\mathbf{r},\mathbf{r}')$ by the identity

$$\rho_1(\mathbf{r},\mathbf{r}') = \langle\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}')\rangle_1 = \frac{1}{N}\langle\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}')\rangle, \tag{C.40}$$

where the second identity came from eq.(C.39). We show the first identity here. Let's prove more general assertions: Let A be some Hermitian operator on the Hilbert space $\mathcal{H}$, $\{|\mu\rangle : \mu\in I\}$ be complete eigenbasis of A, and $a_\nu, a_\nu^\dagger$ be creation/annihilation operators corresponding to A. We claim that the matrix element $\rho_1(\mu,\mu') \equiv \langle\mu'|\hat{\rho}_1|\mu\rangle$ is given by

$$\rho_1(\mu,\mu') = \langle a_\mu^\dagger a_{\mu'}\rangle_1 = \frac{1}{N}\langle a_\mu^\dagger a_{\mu'}\rangle,$$

where the second identity again came from (C.39). The first identity can be shown as follows.

$$\langle a_\mu^\dagger a_{\mu'}\rangle_1 = \mathrm{Tr}_1(\hat{\rho}_1 a_\mu^\dagger a_{\mu'}) = \sum_\nu\langle\nu|\hat{\rho}_1 a_\mu^\dagger a_{\mu'}|\nu\rangle = \sum_\nu\langle\nu|\hat{\rho}_1 a_\mu^\dagger a_{\mu'}a_\nu^\dagger|0\rangle$$
$$= \sum_\nu\langle\nu|\hat{\rho}_1 a_\mu^\dagger(a_\nu^\dagger a_{\mu'} + \delta_{\mu'\nu})|0\rangle = 0 + \langle\mu'|\hat{\rho}_1 a_\mu^\dagger|0\rangle = \langle\mu'|\hat{\rho}_1|\mu\rangle = \rho_1(\mu,\mu').$$

By choosing position basis, we get (C.40). In short, we don't need to derive ρ_1 when we calculate reduced single-particle density matrix $\rho_1(\mu, \mu')$.

If the many body state of the whole system were $\hat{\rho} = \sum_{\{n\}} \rho_{\{n\}} \big|\{n\}\big\rangle\big\langle\{n\}\big|$, then

$$\rho_1(\mu, \mu') = \langle a^\dagger_\mu a_{\mu'} \rangle_1 = \frac{1}{N} \langle a^\dagger_\mu a_{\mu'} \rangle = \frac{1}{N} \sum_{\{n\}} \rho_{\{n\}} \big\langle \{n\} \big| a^\dagger_\mu a_{\mu'} \big| \{n\} \big\rangle.$$

Especially, if the many-body state were pure, $\rho = |\Phi\rangle\langle\Phi|$, then

$$\rho_1(\mu, \mu') = \frac{1}{N} \langle \Phi | a^\dagger_\mu a_{\mu'} | \Phi \rangle.$$

We can introduce reduced density operators $\hat{\rho}_n$ involving n $(\leq N)$ particles in the system. C. N. Yang [79] provided clear criterion for the existence of OLDRO in terms of these operators. In the following, we observe the definition and properties of $\hat{\rho}_2$ from which we can infer how the other reduced density operators will look like. The 2-particle reduced density operator is defined by

$$\begin{aligned}
&\hat{\rho}_2 \equiv \mathrm{Tr}_{3,\cdots,N} \hat{\rho} \\
&= \int d\mathbf{z}_1 d\mathbf{z}_2 d\mathbf{y}_1 d\mathbf{y}_2 \hat{\psi}^\dagger(\mathbf{z}_1) \hat{\psi}^\dagger(\mathbf{z}_2) |0\rangle \left[\int d\mathbf{x}_3 \cdots \mathbf{x}_N \langle 0 | \hat{\psi}(\mathbf{x}_N) \cdots \hat{\psi}(\mathbf{x}_3) \hat{\psi}(\mathbf{z}_2) \hat{\psi}(\mathbf{z}_1) \hat{\rho} \right. \\
&\left. \cdot\, \hat{\psi}^\dagger(\mathbf{y}_1) \hat{\psi}^\dagger(\mathbf{y}_2) \hat{\psi}^\dagger(\mathbf{x}_3) \cdots \hat{\psi}^\dagger(\mathbf{x}_N) |0\rangle \right] \langle 0 | \hat{\psi}(\mathbf{y}_2) \hat{\psi}(\mathbf{y}_1) \frac{1}{2! N!},
\end{aligned}$$

from which we can show that

$$\begin{aligned}
&\frac{1}{\sqrt{2!}} \langle 0 | \hat{\psi}(\mathbf{z}_1) \hat{\psi}(\mathbf{z}_2) \hat{\rho}_2 \hat{\psi}^\dagger(\mathbf{y}_1) \hat{\psi}^\dagger(\mathbf{y}_2) |0\rangle \frac{1}{\sqrt{2!}} \\
&= \frac{1}{N!} \int d\mathbf{x}_3 \cdots d\mathbf{x}_N \langle 0 | \hat{\psi}(\mathbf{x}_N) \cdots \hat{\psi}(\mathbf{x}_3) \hat{\psi}(\mathbf{z}_2) \hat{\psi}(\mathbf{z}_1) \hat{\rho} \hat{\psi}^\dagger(\mathbf{y}_1) \hat{\psi}^\dagger(\mathbf{y}_2) \hat{\psi}^\dagger(\mathbf{x}_3) \cdots \hat{\psi}^\dagger(\mathbf{x}_N) |0\rangle.
\end{aligned} \tag{C.41}$$

Let $\hat{A}$ be a 2-body operator (C.14):

$$\hat{A} = \frac{1}{2} \int d\mathbf{y}_1 d\mathbf{y}_2 d\mathbf{z}_1 d\mathbf{z}_2 \hat{\psi}^\dagger(\mathbf{y}_1) \hat{\psi}^\dagger(\mathbf{y}_2) \langle \mathbf{y}_1 | \langle \mathbf{y}_2 | A | \mathbf{z}_2 \rangle | \mathbf{z}_1 \rangle \hat{\psi}(\mathbf{z}_2) \hat{\psi}(\mathbf{z}_1). \tag{C.42}$$

We are going to prove the trace formula analogous to (C.39),

$$\mathrm{Tr}_2(\hat{\rho}_2 \hat{A}) = \frac{2!(N-2)!}{N!} \mathrm{Tr}(\hat{\rho} \hat{A}),$$

which allows us to calculate the expectation value of a 2-body operator $\hat{A}$ not knowing $\hat{\rho}_2$. The proof goes as follows.

For convenience, let us denote $\frac{1}{\sqrt{N!}}\hat{\psi}^\dagger(\mathbf{x}_1)\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle \equiv |\mathbf{x}_1\cdots\mathbf{x}_N\rangle_F$, where F is from Fock space.

$$
\begin{aligned}
&\mathrm{Tr}(\hat{\rho}\hat{A}) = \int d\mathbf{x}_1\cdots d\mathbf{x}_N\ {}_F\langle\mathbf{x}_1\cdots\mathbf{x}_N|\hat{\rho}\hat{A}|\mathbf{x}_1\cdots\mathbf{x}_N\rangle_F \\
&= \frac{1}{2}\int d\mathbf{y}_1 d\mathbf{y}_2 d\mathbf{z}_1 d\mathbf{z}_2 \langle\mathbf{y}_1|\langle\mathbf{y}_2|A|\mathbf{z}_2\rangle|\mathbf{z}_1\rangle \\
&\quad\cdot\int d\mathbf{x}_1\cdots d\mathbf{x}_N\ {}_F\langle\mathbf{x}_1\cdots\mathbf{x}_N|\hat{\rho}\hat{\psi}^\dagger(\mathbf{y}_1)\hat{\psi}^\dagger(\mathbf{y}_2)\underbrace{\hat{\psi}(\mathbf{z}_2)\hat{\psi}(\mathbf{z}_1)\hat{\psi}^\dagger(\mathbf{x}_1)\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle}_{(*)}\frac{1}{\sqrt{N!}}.
\end{aligned}
$$

The factor $(*)$ can be calculated easily. We proceed $\hat{\psi}(\mathbf{z}_2)\hat{\psi}(\mathbf{z}_1)$ to the vacuum state. Then the result will be

$$
\sum_{\substack{1\le i<j\le N\\ \sigma\in S_2}} C_{ij\sigma}\delta(\mathbf{x}_i-\mathbf{z}_{\sigma(1)})\delta(\mathbf{x}_j-\mathbf{z}_{\sigma(2)})\hat{\psi}^\dagger(\mathbf{x}_1)\cdots\widehat{\hat{\psi}^\dagger(\mathbf{x}_i)}\cdots\widehat{\hat{\psi}^\dagger(\mathbf{x}_j)}\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle,
$$

where the coefficients $C_{ij\sigma}$ need to be determined. To do this, observe that, for fixed $1 \le i < j \le N$,

$$
\begin{aligned}
&\hat{\psi}(\mathbf{z}_2)\hat{\psi}(\mathbf{z}_1)\hat{\psi}^\dagger(\mathbf{x}_1)\cdots\hat{\psi}^\dagger(\mathbf{x}_i)\cdots\hat{\psi}^\dagger(\mathbf{x}_j)\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle \\
&= \zeta^{(1-\mathrm{sgn}\sigma)/2}\hat{\psi}(\mathbf{z}_{\sigma(2)})\hat{\psi}(\mathbf{z}_{\sigma(1)})\hat{\psi}^\dagger(\mathbf{x}_1)\cdots\hat{\psi}^\dagger(\mathbf{x}_i)\cdots\hat{\psi}^\dagger(\mathbf{x}_j)\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle \\
&= \zeta^{(1-\mathrm{sgn}\sigma)/2}\zeta^{1+i}\zeta^{1+j}\delta(\mathbf{x}_i-\mathbf{z}_{\sigma(1)})\delta(\mathbf{x}_j-\mathbf{z}_{\sigma(2)})\hat{\psi}^\dagger(\mathbf{x}_1)\cdots\widehat{\hat{\psi}^\dagger(\mathbf{x}_i)}\cdots\widehat{\hat{\psi}^\dagger(\mathbf{x}_j)}\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle \\
&\quad+\cdots.
\end{aligned}
$$

Thus $C_{ij\sigma} = \zeta^{i+j}\zeta^{(1-\mathrm{sgn}\sigma)/2}$. Now we have

$$
\begin{aligned}
&\mathrm{Tr}(\hat{\rho}\hat{A}) \\
&= \frac{1}{2}\int d\mathbf{y}_1 d\mathbf{y}_2 d\mathbf{z}_2 d\mathbf{z}_1 \langle\mathbf{y}_1|\langle\mathbf{y}_2|A|\mathbf{z}_2\rangle|\mathbf{z}_1\rangle\Bigg[\int d\mathbf{x}_1\cdots d\mathbf{x}_N{}_F\langle\mathbf{x}_1\cdots\mathbf{x}_N|\hat{\rho}\hat{\psi}^\dagger(\mathbf{y}_1)\hat{\psi}^\dagger(\mathbf{y}_2) \\
&\quad\cdot\sum_{\substack{1\le i<j\le N\\ \sigma\in S_2}}\zeta^{i+j}\zeta^{(1-\mathrm{sgn}\sigma)/2}\delta(\mathbf{x}_i-\mathbf{z}_{\sigma(1)})\delta(\mathbf{x}_j-\mathbf{z}_{\sigma(2)}) \\
&\qquad\qquad\cdot\hat{\psi}^\dagger(\mathbf{x}_1)\cdots\widehat{\hat{\psi}^\dagger(\mathbf{x}_i)}\cdots\widehat{\hat{\psi}^\dagger(\mathbf{x}_j)}\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle\frac{1}{\sqrt{N!}}\Bigg].
\end{aligned}
$$

The terms in the bracket become

$$\int d\mathbf{x}_1 \cdots d\mathbf{x}_N {}_F\langle \mathbf{x}_1 \cdots \mathbf{x}_N|\hat{\rho} \sum_{\substack{1\le i<j\le N \\ \sigma\in S_2}} \zeta^{i+j}\zeta^{j-1}\zeta^{i-1}\zeta^{(1-\mathrm{sgn}\sigma)/2}\delta(\mathbf{x}_i - \mathbf{z}_{\sigma(1)})\delta(\mathbf{x}_j - \mathbf{z}_{\sigma(2)})$$

$$\cdot \hat{\psi}^\dagger(\mathbf{x}_1)\cdots\hat{\psi}^\dagger(\mathbf{y}_2)\cdots\hat{\psi}^\dagger(\mathbf{y}_1)\cdots\hat{\psi}^\dagger(\mathbf{x}_N)|0\rangle\frac{1}{\sqrt{N!}}$$

$$= \sum_{\substack{1\le i<j\le N \\ \sigma\in S_2}} \zeta^{(1-\mathrm{sgn}\sigma)/2}\int d\mathbf{x}_3\cdots d\mathbf{x}_N {}_F\langle \mathbf{z}_{\sigma(1)}\mathbf{z}_{\sigma(2)}\mathbf{x}_3\cdots\mathbf{x}_N|\hat{\rho}|\mathbf{y}_1\mathbf{y}_2\mathbf{x}_3\cdots\mathbf{x}_N\rangle_F$$

$$= \frac{N!}{(N-2)!} {}_F\langle \mathbf{z}_1\mathbf{z}_2|\hat{\rho}_2|\mathbf{y}_1\mathbf{y}_2\rangle_F,$$

where the last equality came from eq.(C.41). Now we get

$$\mathrm{Tr}(\hat{\rho}\hat{A}) = \frac{1}{2}\int d\mathbf{y}_1 d\mathbf{y}_2 d\mathbf{z}_1 d\mathbf{z}_2 \langle \mathbf{y}_1|\langle \mathbf{y}_2|A|\mathbf{z}_2\rangle|\mathbf{z}_1\rangle \frac{N!}{(N-2)!} {}_F\langle \mathbf{z}_1\mathbf{z}_2|\hat{\rho}_2|\mathbf{y}_1\mathbf{y}_2\rangle_F$$

Since $\mathbf{y}_1, \mathbf{y}_2, \mathbf{z}_1, \mathbf{z}_2$ are just integration variables, we have

$$= \int d\mathbf{y}_1 d\mathbf{y}_2 d\mathbf{z}_1 d\mathbf{z}_2 \sum_{\sigma,\tau\in S_2} \frac{N!\langle \mathbf{y}_{\tau(1)}|\langle \mathbf{y}_{\tau(2)}|A|\mathbf{z}_{\sigma(2)}\rangle|\mathbf{z}_{\sigma(2)}\rangle}{8(N-2)!} {}_F\langle \mathbf{z}_{\sigma(1)}\mathbf{z}_{\sigma(2)}|\hat{\rho}_2|\mathbf{y}_{\sigma(1)}\mathbf{y}_{\sigma(2)}\rangle_F$$

$$= \frac{1}{2}\int d\mathbf{y}_1 d\mathbf{y}_2 d\mathbf{z}_1 d\mathbf{z}_2 \left[\frac{1}{4}\sum_{\sigma,\tau\in S_2} \zeta^{(1-\mathrm{sgn}\sigma)/2}\zeta^{(1-\mathrm{sgn}\tau)/2}\langle \mathbf{y}_{\tau(1)}|\langle \mathbf{y}_{\tau(2)}|A|\mathbf{z}_{\sigma(1)}\rangle|\mathbf{z}_{\sigma(2)}\rangle\right]$$

$$\cdot \frac{N!}{(N-2)!} {}_F\langle \mathbf{z}_1\mathbf{z}_2|\hat{\rho}|\mathbf{y}_1\mathbf{y}_2\rangle_F.$$

The factor in the square bracket is equal to

$$\frac{1}{4}\sum_{\sigma,\tau\in S_2} \zeta^{(1-\mathrm{sgn}\sigma)/2}\zeta^{(1-\mathrm{sgn}\tau)/2}\langle \mathbf{y}_{\tau(1)}|\langle \mathbf{y}_{\tau(2)}|A|\mathbf{z}_{\sigma(2)}\rangle|\mathbf{z}_{\sigma(1)}\rangle$$

$$= \frac{1}{2}\int d\mathbf{y}_1' d\mathbf{y}_2' d\mathbf{z}_1' d\mathbf{z}_2' \frac{1}{\sqrt{2}}\langle 0| \left(\sum_{\tau\in S_2}\zeta^{(1-\mathrm{sgn}\tau)/2}\delta(\mathbf{y}_1' - \mathbf{y}_{\tau(1)})\delta(\mathbf{y}_2' - \mathbf{y}_{\tau(2)})\right)$$

$$\cdot \langle \mathbf{y}_1'|\langle \mathbf{y}_2'|A|\mathbf{z}_1'\rangle|\mathbf{z}_2'\rangle \left(\sum_{\sigma\in S_2}\zeta^{(1-\mathrm{sgn}\sigma)/2}\delta(\mathbf{z}_1' - \mathbf{z}_{\sigma(1)})\delta(\mathbf{z}_2' - \mathbf{z}_{\sigma(2)})\right)|0\rangle\frac{1}{\sqrt{2}}$$

$$= {}_F\langle \mathbf{y}_1\mathbf{y}_2|\hat{A}|\mathbf{z}_1\mathbf{z}_2\rangle_F.$$

Now we conclude that

$$\begin{aligned}\mathrm{Tr}(\hat{\rho}\hat{A}) &= \frac{1}{2}\int d\mathbf{y}_1 d\mathbf{y}_2 d\mathbf{z}_1 d\mathbf{z}_2 \;{}_F\langle \mathbf{y}_1\mathbf{y}_2|\hat{A}|\mathbf{z}_1\mathbf{z}_2\rangle_F \frac{N!}{(N-2)!}\,{}_F\langle \mathbf{z}_1\mathbf{z}_2|\hat{\rho}_2|\mathbf{y}_1\mathbf{y}_2\rangle_F \\ &= \frac{N!}{2!(N-2)!}\mathrm{Tr}_2(\hat{\rho}_2\hat{A}).\end{aligned}$$

Therefore, the proof is done.

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국 문 초 록

본 연구는 의사 2차원 쌍극자 보스-아인슈타인 응축체 (quasi-two-dimensional dipolar Bose-Einstein condensates) 내에 형성되는 유효 굽은 시공간(effective curved spacetime)을 다루고 있다. 굽은 시공간의 시간에 따른 변화는 우주론적 입자생성(cosmological particle production)을 일으키며, 이는 실험실에서 관측할 수 있 보골류보프 의사 입자들(Bogoliubov quasiparticle excitations)로 나타나게 된다. 쌍극자 상호작용의 비등방적 성질은 생성된 보골류보프 의사 입자들의 분산관계(dispersion relation)에 깊은 로톤 극소점(roton minimum)을 만들어내게 되는데, 본 연구는 이 로톤 극소점의 세기에 따라서 어떠한 측정 가능한 효과가 나타나는지를 다루고 있다.

본 연구는 크게 두 부분으로 나뉘어질 수 있다. 첫째로, 본 연구는 팽창하는 쌍극자 보스-아인슈타인 응축체 속에 형성된 유추 드지터 공간(analogue de Sitter spacetime)을 다루었다. 여기서는 인플레이션 우주론의 주요 결과인 규모 불변적 물질 분포(scale invariant power spectrum)가 인플레이션 발생 초기에 로톤 극소점이 존재하는 경우 큰 변형을 겪게 됨을 보였다. 이 결과는 쌍극자 보스-아인슈타인 응축체가 조작이 용이한 실험 도구로서 초 플랑크 영역의 물리학(trans-Planckian physics)이 로렌츠 불변적인 저에너지 물리학에 주는 영향을 연구하는데 사용될 수 있음을 예시한 것으로, 특히 인플레이션 우주론의 주요 결과가 위반될 수 있음을 보인 것이다.

둘째로, 본 연구는 쌍극자 보스-아인슈타인 응축체 내에서 음속(speed of sound)을 급격히 변화시킬 때 발생하는 유추 동적 카시미르 효과(analogue dynamical Casimir effect)를 다루었다. 여기서는 서로 반대 방향의 운동량을 갖는 의사 입자의 쌍들 사이에 존재하는 얽힘(entanglement)이 쌍극자 상호작용의 세기에 따라 크게 강화될 수 있음을 절대 영도와 유한한 온도의 환경에서 각기 보였다. 그 결과 서로 얽힌 의사 입자들의 쌍들이 가지는 양자역학적 상관 관계(quantum correlation)가 입자들 사이에 접촉 상호작용만 존재할 때보다 쌍극자 상호작용까지 존재할때 더욱 강화되며, 특히 로톤 극소점 근처의 운동량을 가지는 입자 쌍들의 얽힘이 밀도-밀도 상관함수(density-density correlation function)에 의하여 실험적으로 측정 가능함을 보였다.

주요어 : 보스-아인슈타인 응축, 쌍극자 상호작용, 인플레이션, 동적 카시미르 효과, 초 플랑크 영역 물리, 중력 유추, 로톤 극소점

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감사의 글

이 논문은 2012년 지금의 연구실에 들어온 때로부터 5년, 그리고 2015년 박사과정을 수료한 전일제 연구생이 된 때로부터 2년 만에 마무리된 연구의 결과물입니다. 문득 새삼스레 중학생 시절을 되새겨 보니, 당시의 저는 무슨 뜻인지도 모르는 양자역학이나 상대성 이론을 연구하고 싶다는 막연한 꿈을 가지고 있었습니다. 그래서인지 오늘에 이르러 참 오래도록 바라던 일이 이루어진 것 같아 기쁘고 벅찬 감정을 숨기기가 어렵습니다. 이미 많은 분들께서 졸업을 축하해 주셔서 마음이 한껏 고양되었지만, 한편으로는 저의 능력 이상의 큰 축하와 격려를 받았다는 생각에 더 부단히 노력해야 한다는 큰 책임감을 느낍니다. 부족한 부분을 숨길 수 없어 적나라하게 드러나 보임에도 불구하고 저를 축하해 주시고 응원해 주시는 분들에게 깊은 감사의 마음을 지울수가 없습니다. 아래에는 특히 이 논문을 쓰기까지 저를 도와주신 분들을 위한 짤막한 감사의 인사를 적습니다.

먼저 저를 지도해주신 피셔 교수님(Prof. Uwe R. Fischer)께 감사의 말씀을 전합니다. 저의 논문 제목은 5년 전 교수님께서 처음 정해주신 제목과 크게 다르지 않습니다. 교수님께서는 저에게 나아갈 방향을 제시해 주셨고, 자유로운 연구 활동을 지지해 주셨으며, 저의 부족한 지식을 채워 주셨습니다. 이 논문에서 아름다운 표현이나 새로운 내용이 있다면 그것은 모두 피셔교수님에게서 나온 것임을 이곳에 밝힙니다. 한편, 논문을 직접적으로 함께 완성했던 티안 박사님(Dr. Zehua Tian)께도 감사의 말씀을 전합니다. 티안 박사님은 동적 카시미르 효과와 양자 얽힘에 관련된 후반 부분을 전적으로 완성하셨고, 저의 편협한 지식을 넓혀주셨습니다.

저의 대학 생활의 시작과 끝에는 이준규 교수님이 계셨습니다. 2006년 서울대학교 물리학부 정시면접장에서는 저의 심사위원이셨으며, 2018년 서울대학교 물리천문학부 대학원 박사논문 심사에서는 저의 논문 심사 위원이 되어주셨습니다. 일찍이 저의 게으르고 둔함을 꿰뚫어 보시고 채찍질 하셨으며, 동시에 제가 자신감을 갖도록 작은 성취도 크게 칭찬하시며 북돋우어 주셨습니다. 이준규 교수님과 함께 박사논문 심사를 맡아주셨던 정현석 교수님, 신용일 교수님, 한정훈 교수님께도 이 자리를 빌려 감사의 말씀을 전합니다.

다른 연구실 소속이지만 같은 오피스인 56동 520호에서 오랜 기간 함께 지내온 최동진에게도 감사의 말을 남깁니다. 동진이는 훌륭한 능력에도 불구하고 언제나 겸손하며 저의 모자란 질문에도 기대 이상의 답을 들려주었습니다. 나이는 저보다 한 살 어리지만 물리 뿐만 아니라 삶의 여러 부분에서도 배울점이 많은 친구였습니다. 그동안 같은 오피

스에 머물렀던 이강수, 강명균 선배님, 연구실 후배인 박상신, 박재균 에게도 이 자리를 빌려 감사의 말을 전합니다. 특히 우리 연구실의 후배들에게는 앞의 두 선배들이 저에게 해준 만큼의 든든한 버팀목 역할을 못해준것 같아 미안한 마음이 듭니다. 연구실을 위해서 나름대로 많은 노력을 기울였지만 사람들을 이끄는 능력의 부족을 끝내 채우지 못하고 먼저 졸업을 합니다. 하지만 연구가 막힐때나 인생의 앞날이 보이지 않을 때 저에게 언제든 연락해도 좋으니, 시작한 연구를 포기하지 말고 멋지게 마무리하여 훌륭한 박사 졸업생이 되기를 기원합니다.

저희 연구실의 로고를 만들어준 서울대학교 미술대학의 조현지와 저의 연구를 과학동아에 실어주신 우아영 기자님께도 감사 인사를 전합니다. 교수님의 복지와 연말정산 등을 관리해주신 김현정 선생님, 교수님의 물건 구입과 까다로운 요구사항을 들어주신 오선근 선생님, 연구비를 관리해주신 홍지선 선생님, 컴퓨터 관련 기술적인 도움을 주신 박용호 선생님, 그리고 주말도 없이 수업과 학사일정 관련 행정업무를 돌봐주신 김영희 선생님 감사합니다. 지금은 안계시지만 제가 아르바이트로 일하기도 했었던 BK행정실의 장혜인, 김다솜 선생님, 그리고 물리학과 독서실의 길효정 선생님께도 감사의 말씀을 남깁니다.

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