Energy Corrections in a Perturbed Infinite Well Activity

Phase I. Construct your own pictures

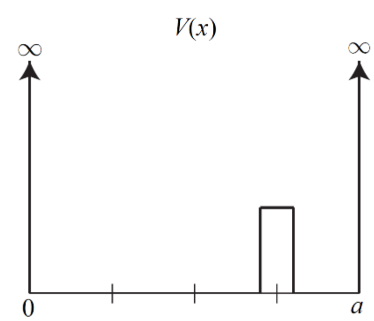
As presented in lecture, an important result from time-independent perturbation theory is that the first-order correction to the n^{th} energy eigenvalue is given by $E_n^{(1)} = \left\langle \psi_n^{(0)} \middle| \hat{V} \middle| \psi_n^{(0)} \right\rangle$, where $V(x)$ is the perturbation. Note all energy corrections in this activity are first-order.

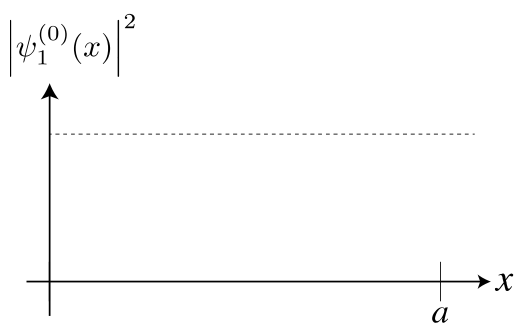
1. Rewrite the expression for $E_n^{(1)}$ as an integral. (Do not write out $\psi_n^{(0)}(x)$ or $V(x)$ in terms of x or evaluate the integral.)

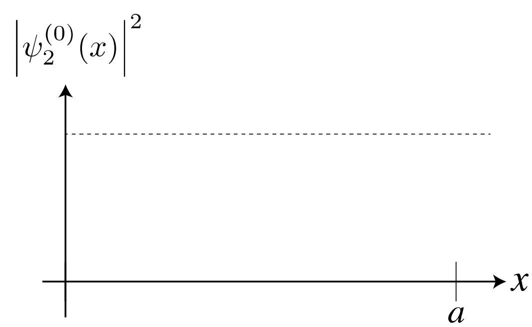
   Assume $\hat{V}$ is just a function of position, $V(x)$. Write the integral expression for the energy correction $E_n^{(1)}$ in terms of $V(x)$ and the probability density $\left|\psi_n^{(0)}(x)\right|^2$. Explain why you can re-order the integrand in this case.

2. Consider an infinite square well of width a, shown at right. A perturbation is added to this potential that is zero everywhere except within a small region, centered at $3a/4$, at which it takes a (small) uniform value.

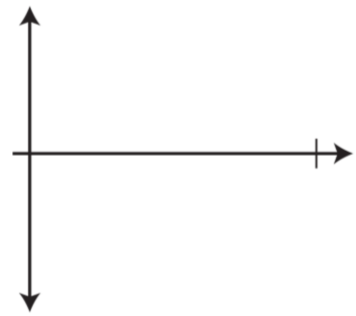
   a. In the spaces below, draw the **probability densities** for the **unperturbed** ground state (n = 1) and **unperturbed** first excited state (n = 2). Draw each graph using the same vertical scale.







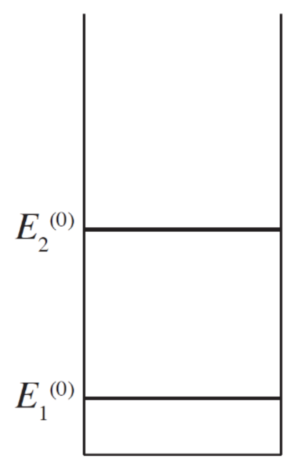
b. For the **ground state** of the system above, determine whether the first-order correction to the energy $E_1^{(1)}$ is *positive*, *negative*, or *zero*. Explain your answer...

<table>
<tr><td>i) by writing down the integral expression for the energy correction and considering the sign of the integrand.</td><td>ii) by sketching the integrand $V(x)\left|\psi_1^{(0)}(x)\right|^2$ and considering the integral as an area under a curve. Label the axes of your graph.</td></tr>
<tr><td></td><td></td></tr>
<tr><td colspan="2">Explain how the integral expression in part i) and the graph in part ii) are related.</td></tr>
</table>

c. For the **first-excited state** of the system above, determine whether the first-order correction to the energy is *positive*, *negative*, or *zero*. Explain your answer.

d. For which of the above states is the magnitude of the first-order correction to the energy larger? Explain your answer.

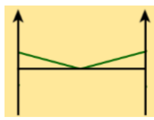
e. On the energy level diagram provided at right, qualitatively draw the locations of the
(i) perturbed energy levels, and
(ii) the first order energy corrections for the ground state and the first excited state.

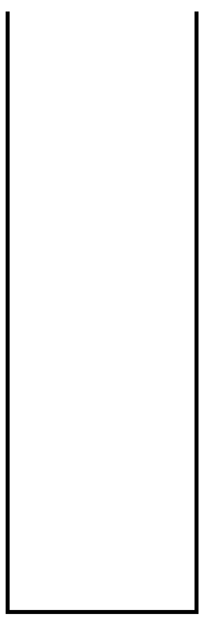
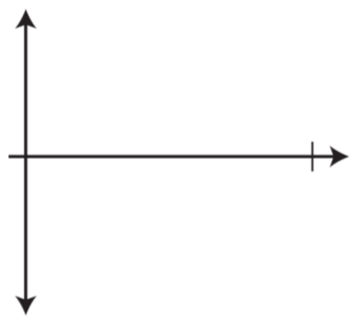
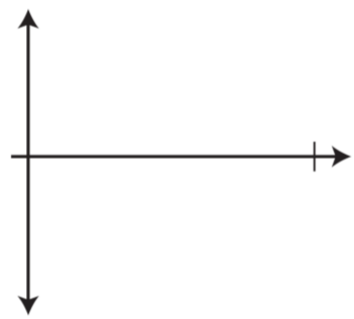
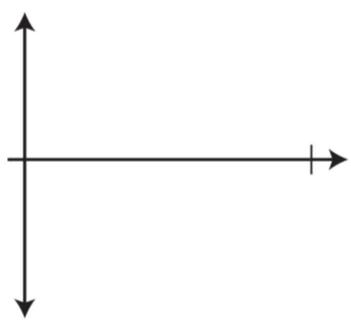


Phase II. Connect the simulation with your pictures and explore further

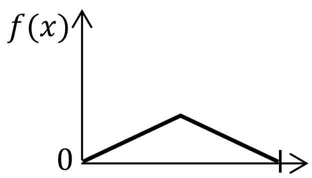
3. a. Play with the simulation found at tinyurl.com/pertgame for a few minutes before continuing. Note that all energy corrections in the simulation and the questions below are assumed to be first order. Feel free to revisit the simulation while answering the questions.

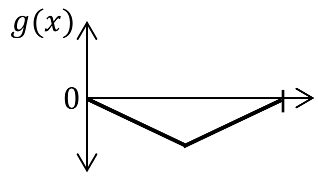
   b. Note three things about the energy corrections that you have found out from the simulation.

4. Consider the perturbation  with **a positive slider value** and the perturbed **ground state** of the infinite well.

<table>
<tr><td>a) i) Sketch the unperturbed and perturbed ground state energies as shown in the left-hand energy level diagram.</td><td>ii) Sketch the right-hand graphs of V, $|\psi_1|^2$ and the product curve $V|\psi_1|^2$ shown in the simulation. Label the axes of your graphs.</td></tr>
<tr><td></td><td>  </td></tr>
<tr><td colspan="2">b. On the left-hand and right-hand sketches above, indicate how you can see the sign of the energy correction.</td></tr>
<tr><td colspan="2">c. Using your left-hand energy level sketch, explain the difference between $E_1^{(0)}, E_1^{(1)}$ and $E_1^{(0)} + E_1^{(1)}$.</td></tr>
</table>

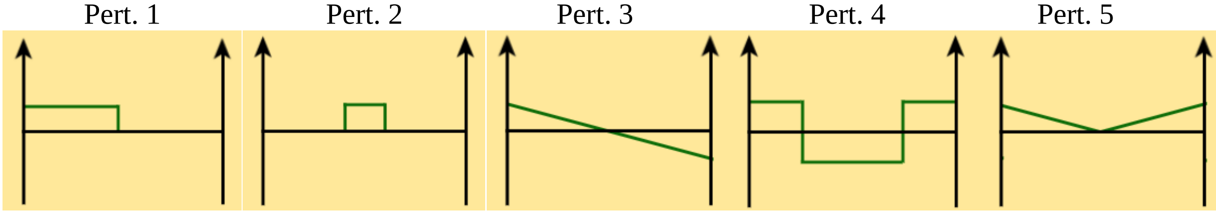
5. Thinking about the area under the $V|\psi_n|^2$ product graph can be a quick way to determine the sign and relative magnitude of energy corrections.
Consider the functions $f(x)$ and $g(x)$ below. Sketch the *product* curve $f(x)g(x)$ (*not the sum*!) and explain the shape of your curve (is it linear, parabolic, etc.). Explain how the product curve is obtained. Would the inner product $\langle f|g\rangle$ be *positive*, *negative* or *zero*?





The simulation has five different perturbations, pictured below:

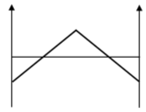
Pert. 1 Pert. 2 Pert. 3 Pert. 4 Pert. 5



For the following questions, consider these five perturbations each with a **positive slider value**.

6. Which, if any, of the perturbations 1 to 5 have a zero energy correction for ALL energy eigenfunctions? Explain your reasoning.

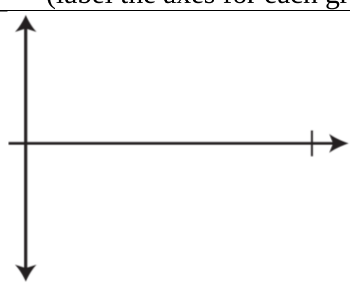
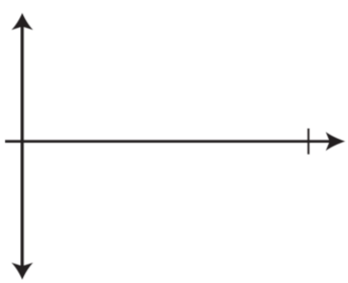
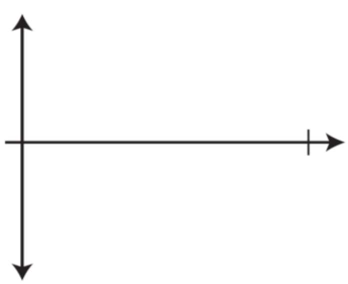
Sketch a perturbation different to the ones shown in the simulation (this includes negative slider values) that would have zero energy correction for all energy eigenfunctions. Explain your reasoning.

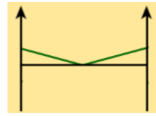
7. Two students are discussing the following perturbation  (**not** shown in the simulation). Just like perturbation 3, this perturbation has equal areas above and below the x-axis.

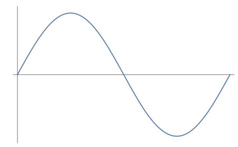
   Student A: *"V has equal areas above and below the x-axis. This implies that all energy corrections will be zero just like for perturbation 3, as the average value of V is zero. The symmetry of V plays no role."*

   Student B: *"But isn't the formula $E_n^{(1)} = \int_0^L V\,|\psi_n|^2\,dx$, so that we need to consider the product of V and $|\psi_n|^2$? For the ground state, the probability density is greater in the middle than at the edges, so the product graph won't average to zero."*

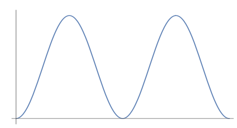
Use the space on the left to draw graphs in order to determine which student is correct. Label your graphs. Use the space on the right to correct the incorrect student's statements.

Sketches for the ground state (label the axes for each graph)	Correct the incorrect student's statements
   **Sign (or value if zero) of $E_1^{(1)}$:**	

8. Two students are discussing perturbation 5  with **a positive slider value**, and the **sign of the first-order correction to the first-excited state**.
Point out any errors in the students' reasoning and correct them.



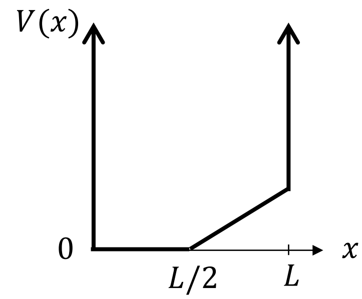
Student A: *"The formula* $E_2^{(1)} = \langle \psi_2^{(0)} | \hat{V} | \psi_2^{(0)} \rangle$ *shows that we need to apply the perturbation* $\hat{V}$ *to* ψ_2*. The graph of the first excited state* ψ_2 *(see figure) is antisymmetric and the perturbation is symmetric. Thus, the two halves will cancel out in the integral and the first-order energy correction* $E_2^{(1)}$ *is zero."*



Student B: "*Your symmetry reasoning is correct but inconsistent with the formula. I think it would be far better if you drew* $|\psi_2|^2$ *(see figure) instead of* ψ_2*. As* $E_2^{(1)} = \langle \psi_2^{(0)} | \hat{V} | \psi_2^{(0)} \rangle = \int_0^L V\, |\psi_2|^2\, dx$*, the integrand is the product of the probability density and the perturbation, not the wave function and the perturbation. You can see from the sketches that* $|\psi_2|^2$ *and* V *are both positive (and the product of two positive values is again positive), so the energy correction* $E_2^{(1)}$ *as the area under the product curve is positive."*

Do you agree with student B that "it would be far better if you drew $|\psi_2|^2$ instead of ψ_2"? Explain why.

9. a. Consider the perturbed infinite square well shown in the figure. Would the first-order energy correction for the first-excited state be *greater than*, *less than*, or *equal to* the correction for the ground state?
Show your reasoning.



b. Sketch a perturbation V different to the ones shown in the simulation and this activity for which the energy correction for the **first excited state** is **greater than** the energy correction for the ground state.
i) For which the perturbation $V(x) \geq 0$ for all x;
ii) For which the perturbation $V(x)$ has both positive and negative values.
Briefly explain your sketches.