Quantum Mechanics

Homework 6: Time-Independent Approximation Methods

1. Time-independent non-degenerate perturbation theory assumes that the stationary states and eigen-energies of a time-independent system can be expanded in convergent power series in a perturbation parameter about, respectively:

   a) the stationary states and eigen-energies of another system.
   b) the eigen-energies and stationary states of a time-dependent system.   c) the origin.
   d) the center.   e) infinity.

2. The zeroth order perturbation of a system is:

   a) the most strongly perturbed system.   b) the mostest strongly perturbed system.
   c) the deeply disturbed system.   d) the negatively perturbed system
   e) the unperturbed system.

3. The formula

$$E_n^{\text{1st}} = E_n^{(0)} + \lambda \langle \psi_n^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle$$

   is a:

   a) 0th order perturbed energy.   b) 1st order perturbed energy.
   c) 2nd order perturbed energy.   d) 1st order perturbed state.   e) 2nd order perturbed state.

4. The formula

$$|\psi_n^{\text{1st}}\rangle = |\psi_n^{(0)}\rangle + \lambda \sum_{\text{all } k, \text{ except } k \neq n} \frac{\langle \psi_k^{(0)} | H^{(1)} | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_k^{(0)}} |\psi_k^{(0)}\rangle$$

   is a:

   a) 0th order perturbed energy.   b) 1st order perturbed energy.
   c) 2nd order perturbed energy.   d) 1st order perturbed state.   e) 2nd order perturbed state.

5. "Let's play *Jeopardy*! For $100, the answer is: A common cause for the failure of time-independent perturbation theory—but failure can be recovered from with diagonalization."

   What is _____, Alex?

   a) degeneracy   b) tarnation   c) subversion   d) lunacy   e) regency

6. "Let's play *Jeopardy*! For $100, the answer is: A standard, non-perturbative approximate method of solving for the eigen-energies and stationary states of a system. If the system is in a finite Hilbert space (i.e., a finite function space), the method can be done for an exact solution."

   What is _____, Alex?

   a) perturbation theory   b) divagation   c) strangulation   d) triangulation
   e) diagonalization

7. Say you have a 1-dimensional infinite square well with

$$V(x) = \begin{cases} 0 & \text{for the } x \text{ range 0 to } a; \\ \infty & \text{otherwise.} \end{cases}$$

   a) Solve for the eigen-states (i.e., stationary states) and eigen-energies from the time-independent Schrödinger equation. You must properly normalize the eigen-states states to answer part (b) correctly.

   b) Say we add the Dirac delta function perturbation Hamiltonian

$$H^{(1)} = c\delta(x - a/2) .$$

   What is the general expression for this perturbation for the first order perturbation energy correction for all eigen-states? Simplify the formula as much as possible.

8. Say you have a 1-dimensional infinite square well with

$$V(x) = \begin{cases} 0 & \text{for the } x \text{ range 0 to } a; \\ \infty & \text{otherwise.} \end{cases}$$

The stationary states are

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin(k_n x) \ ,$$

where

$$k_n a = n\pi \qquad \text{and} \qquad k_n = \frac{n\pi}{a}$$

with $n = 1, 2, 3, \ldots$ as allowed quantum numbers. The eigen-energies are

$$E_n^{\{0\}} = \frac{\hbar^2}{2m} \left(\frac{\pi}{a}\right)^2 n^2 = E_1^{\{0\}} n^2 \ .$$

We now add the Dirac delta function perturbation Hamiltonian

$$H^{(1)} = c\delta(x - a/2) \ .$$

a) Can we use non-degenerate perturbation theory for the infinite square well? Why or why not?

b) What is the general formula for the perturbation for the 1st order perturbation energy correction for all eigen-states? Simplify the formula as much as possible.

c) Now evaluate a general matrix element for the perturbation

$$\langle \psi_m | H^{(1)} | \psi_n \rangle \ .$$

d) Simplify the general matrix element by inventing two simple functions of integer ℓ. The first is zero for ℓ even and 1 for ℓ odd. The second is 1 for k odd and -1 for k even where odd $\ell = 2k + 1$ and k runs through all positive integers: i.e., $0, 1, 2, 3, \ldots$. **HINT:** If you this can't get this part, go on since the later parts don't require it.

e) Write out the 1st order perturbation correction formula for a general state n in as explicit and as simplified a form as reasonably possible. Note the correction is wanted, not the full 2nd order corrected state. **HINT:** Just leave the unperturbed states in the ket form $|\psi_n^0\rangle$. For compactness, one doesn't want to be explicit about them.

f) Write out the 2nd order perturbation correction formula for a general eigen-energy n in as explicit and as simplified a form as reasonably possible. Note the correction is wanted, not the full 2nd order corrected eigen-energy.

9. The single-particle stationary states and eigen-energies for a 1-dimensional infinite square well for region $[0, a]$ are, respectively,

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \qquad \text{and} \qquad E_n = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 n^2 \ .$$

a) What is the expression for elementary 2-particle stationary states for **DISTINCT** spinless particles of the same mass? Label the particles 1 and 2 for convenience. Label the states n and n' for convenience too. What is the general expression for the energy of such 2-particle states? What are all the possible reduced energies $n^2 + n'^2$ up to 100? These energies can be called energy levels: the levels may correspond to more than one state. What are are degeneracies of the energy levels? Remember the particles are **DISTINCT**. **HINT:** You are permitted to use a computer program to generate energy levels and degeneracies. But you can find them by hand too—a little tedious, but not hard if you go at it systematically.

b) Now suppose we turn on a perturbation potential for the non-identical particles of the form

$$H^{(1)} = V(x_1, x_2) = aV_0\delta(x_1 - x_2) \ .$$

What is the expression for the diagonal matrix element

$$H_{(nn')(nn')} = \langle \psi_{nn'}(x_1, x_2) | H^{(1)} | \psi_{nn'}(x_1, x_2) \rangle \ ?$$

If you expand sine functions in exponentials evaluating, the matrix element is pretty easy, but you do have to treat the cases where $n \neq n'$ and $n = n'$ a bit differently.

Can you do perturbation theory on all the 2-particle states?

c) What is the expression for elementary 2-particle stationary states if we replace the distinct particles by identical spinless bosons? What is the general expression for the energy of such 2-particle states? (we have turned off the perturbation potential.) What are all the possible reduced energies $n^2 + n'^2$ up to 100? These energies can be called energy levels: the levels may correspond to more than one state. What are are degeneracies of the energy levels? **HINT:** You don't have to do part (a) all over again, just *mutatis mutandis* it.)

d) Now suppose we turn on a perturbation potential of part (b) for the identical bosons. What is the expression for the diagonal matrix element

$$H_{(nn')(nn')} = \langle \psi_{nn'}(x_1, x_2) | H^{(1)} | \psi_{nn'}(x_1, x_2) \rangle \ ?$$

If you expand sine functions exponentials evaluating, the matrix element is pretty easy, but you do have to treat the cases where $n \neq n'$ and $n = n'$ a bit differently. Note the perturbation correction is a bit different from the distinct particle case. Why?

Can you do perturbation theory on all the 2-particle states?

e) What is the expression for elementary 2-particle stationary states if the 2 particles identical fermions with the same spin coordinate. Since the spin coordinates are identical, the spin part of the single-particle states are symmetrical. Don't bother writing down spinors or such. What is the general expression for the energy of such 2-particle states? What are all the possible reduced energies $n^2 + n'^2$ up to 100? **HINT:** You don't have to do part (a) all over again, just *mutatis mutandis* it.)

f) Now suppose we turn on a perturbation potential of part (b) for the identical fermions. What is the expression for the diagonal matrix element

$$H_{(nn')(nn')} = \langle \psi_{nn'}(x_a, x_b) | H^{(1)} | \psi_{nn'}(x_a, x_b) \rangle \ .$$

Don't whine: this is easy if you see the trick. Why do you get the simple result you get?

Can you do perturbation theory on all the 2-particle states?

g) What does the Dirac delta potential

$$V(x_a - x_b) = aV_0(x_a - x_b)$$

imply or do physically?

10. You are given a zeroth order Hamiltonian matrix

$$H^{(0)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

a) Solve for the eigenvalues and normalized eigenvectors by inspection. You should label the states 1, 2, 3, and 4 for convenience. Is there any degeneracy and if so what are the degenerate states?

b) The evil wizard of physics now turns on a perturbation and the Hamiltonian becomes

$$H = \begin{pmatrix} 1 & \epsilon & 0 & 0 \\ \epsilon & 1 & 0 & 0 \\ 0 & 0 & 1 & \epsilon \\ 0 & 0 & \epsilon & -1 \end{pmatrix},$$

where ϵ is a small quantity. Solve for the exact eigenvalues and normalized eigenvectors in this case: i.e., diagonalize the perturbed Hamiltonian matrix. Is there any degeneracy now? **HINT:** Is

there any reason why the two 2×2 blocks in the matrix cannot be treated as separate eigenvalue problems and the two-component eigenvectors extended trivially for the 4×4 problem?

c) Do non-degenerate perturbation theory to solve for the energy to 2nd order for those initial eigenstates which are **NOT** degenerate. **HINT:** All the perturbation matrix elements can be found in the part (b) **QUESTION**.

11. Consider quantum system of 3 dimensions with initial Hamiltonian

$$H^{(0)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

and perturbed Hamiltonian

$$H = \begin{pmatrix} 1-\epsilon & 0 & 0 \\ 0 & 1 & \epsilon \\ 0 & \epsilon & 2 \end{pmatrix}.$$

Note we assume $\epsilon \ll 1$. Also note that $H^{(0)}$ and H are matrix Hamiltonians: i.e., Hamiltonians in a particular representation. The matrix elements are $\langle \phi_i | H_{\mathrm{op}}^{(0)} | \phi_k \rangle$. $\langle \phi_i | H_{\mathrm{op}} | \phi_k \rangle$, respectively, where $H_{\mathrm{op}}^{(0)}$ and H_{op} are operator versions of the Hamiltonian and the set $\{|\phi_i\rangle\}$ is an orthonormal basis. Usually we drop the "op" subscript and allow context to tell whether the Hamiltonian is in matrix or operator representation.

a) Solve by inspection for the eigen-energies and eigenvectors of the initial unperturbed Hamiltonian. To help with the rest of the problem label the states 1, 2, and 3 in some sensible order.

b) Solve for the exact eigen-energies and normalized eigenvectors of the perturbed Hamiltonian: i.e., diagonalize the perturbed Hamiltonian matrix. **HINTS:** It's not so hard—if you don't make a mistake in the first step.

c) Expand the exact eigen-energies and eigenvectors (where applicable) to 2nd order in small ϵ. (Note I mean Taylor expansion, not perturbation series expansion although the two expansion are closely related in this case.) Simplify the eigenvectors to nice forms so that it is easy to see which perturbed vector grew out of which unperturbed vector as ϵ grew from 0.

d) Determine from (weak-coupling) perturbation theory the energies to 2nd order and the eigenvectors to 1st order of the perturbed Hamiltonian. How do these results compare with those of the part (c) answer? **HINT:** Perturbation theory can be applied to the degenerate states in this case because they are completely uncoupled.

e) Now use the truncated Hamiltonian matrix method (or linear variational method if you know it) to find approximate eigen-energies and eigenvectors for the two initially degenerate eigen-energy states. To what order goodness in small ϵ are the results? Why the are results for one perturbed state exact and for the other rather poor compared to the exact results?