Problem Set 11

Phys 342

Due April 24

Exercises, Due Friday, April 24
Email your homework to me at larkoski@reed.edu

1. It's useful to see how our quantum perturbation theory works in a case that we can solve exactly. Let's consider a two-state system in which the Hamiltonian is

$$\hat{H}_0 = \left(\begin{array}{cc} E_0 & 0 \\ 0 & E_1 \end{array} \right) , \tag{1}$$

for energies $E_0 \leq E_1$. Now, let's consider adding a small perturbation to this Hamiltonian:

$$\hat{H}' = \left(\begin{array}{cc} \epsilon & \epsilon \\ \epsilon & \epsilon \end{array} \right) , \tag{2}$$

for some $\epsilon > 0$. The complete Hamiltonian of our system we are considering is $\hat{H} = \hat{H}_0 + \hat{H}'$.

   (a) First, calculate the exact energy eigenstates and eigenvalues of the complete Hamiltonian. From your complete result, Taylor expand it to first order in ϵ.

   (b) Now, use our formulation of quantum perturbation theory to calculate the first corrections to the energy eigenstates and eigenvalues. Do these corrections agree with the explicit expansion from part (a)?

   (c) From the Taylor expansion in part (a), for what range of ϵ does the Taylor expansion converge?

2. Let's see how the variational method works in another application. Let's assume we didn't know the ground state energy of the quantum harmonic oscillator and use the variational method to determine it. First, the Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 . \tag{3}$$

Note that this potential is symmetric about $x = 0$ and position extends over the entire real line: $x \in (-\infty, \infty)$. This motivates the guess for the ground state wavefunction

$$\psi(x; a) = N(a^2 - x^2) , \tag{4}$$

for a normalization constant N and a is the parameter that we will minimize over. Now, this wavefunction is only defined on $x \in [-a, a]$.

(a) Let's first calculate the normalization factor N, as a function of a.

(b) Now, calculate the expectation value of the Hamiltonian on this state, $\langle\psi|\hat{H}|\psi\rangle$, as a function of the parameter a.

(c) Finally, minimize the expectation value over a to provide an upper bound on the ground state energy, E_0. How does this estimate compare to the known, exact value?

3. Let's now study the power method for estimating the ground state energy, applied to the quantum harmonic oscillator. For this problem, we will work with the Hamiltonian

$$\hat{H} = \hbar\omega(1 + a^\dagger a)\,, \tag{5}$$

where a and $a^\dagger$ are the familiar lowering and raising operators, respectively. Note the slight difference between this Hamiltonian and what we would typically think of as the harmonic oscillator: all we've done here is shift the potential up by an amount $\hbar\omega/2$ which will make some of the mathematical manipulations simpler later. Importantly, this constant shift does not affect the eigenstates of the Hamiltonian, it just shifts the eigenvalues up by that same amount.

(a) Let's first calculate the inverse of this Hamiltonian, $\hat{H}^{-1}$. One answer is, of course, simply

$$\hat{H}^{-1} = \frac{1}{\hbar\omega}\frac{1}{1 + a^\dagger a}\,. \tag{6}$$

However, this isn't so useful for determining how this operator acts on states. Instead, we can express the inverse Hamiltonian as a sum over products of a and $a^\dagger$:

$$\hat{H}^{-1} = \sum_{n=0} \beta_0\, (a^\dagger)^n a^n\,, \tag{7}$$

for some coefficients β_n. Determine the coefficients β_n and thus the inverse Hamiltonian $\hat{H}^{-1}$ by demanding that $\hat{H}\hat{H}^{-1} = 1$.

Nota Bene: By the way this way of ordering the terms in $\hat{H}^{-1}$ is called **normal order**: all raising operators $a^\dagger$ are to the left of all lowering operators a in each term in the sum.

(b) Let's use this inverse Hamiltonian to estimate the ground state energy of the harmonic oscillator in which we start with a coherent state $|\chi\rangle$. Recall that $|\chi\rangle$ satisfies

$$a|\chi\rangle = \lambda|\chi\rangle\,, \tag{8}$$

for some complex number λ. From this coherent state, what is the expectation value of the Hamiltonian, $\langle\chi|\hat{H}|\chi\rangle$?

(c) Now, let's use the inverse Hamiltonian to improve our estimate of the ground state energy. What is your new estimate of the ground state after one application of $\hat{H}^{-1}$ on the coherent state? Recall that this estimate is

$$E_0 \simeq \frac{\langle\chi|\hat{H}^{-1}\hat{H}\hat{H}^{-1}|\chi\rangle}{\langle\chi|\hat{H}^{-1}\hat{H}^{-1}|\chi\rangle}\,. \tag{9}$$

You should ultimately find

$$E_0 \simeq \frac{\langle\chi|\hat{H}^{-1}\hat{H}\hat{H}^{-1}|\chi\rangle}{\langle\chi|\hat{H}^{-1}\hat{H}^{-1}|\chi\rangle} = \hbar\omega\,\frac{e^{|\lambda|^2}-1}{\int_0^{|\lambda|^2} dx\,\frac{e^x-1}{x}}\,. \tag{10}$$

The integral that remains can't be expressed in terms of elementary functions. *Hint*: Remember, $\hat{H}\hat{H}^{-1} = 1$. For the denominator factor, it might help to slide "1" in between the two inverse Hamiltonians, where

$$1 = \sum_{n=0}^{\infty} |\psi_n\rangle\langle\psi_n|\,, \tag{11}$$

where $|\psi_n\rangle$ is the nth energy eigenstate, and recall the definition of the normalized coherent state from Homework 6.

(d) Now, just to get a sense of this approximation, verify that you get the exact result for the ground state energy if $\lambda \to 0$. Also, evaluate the approximation of part (c) for $\lambda = 1$. The remaining integral evaluates to

$$\int_0^1 dx\,\frac{e^x-1}{x} = 1.31790215\ldots\,. \tag{12}$$

How does this result compare to the initial estimate of part (b)?