Quantum mechanics II, Problems 13 : Time-independent Perturbation Theory and Variational Principle

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Problem 1 : Confined quantum Stark effect

We consider an electron of mass m in a one-dimensional potential well of width L, whose infinite barriers are located at $x = \pm L/2$, described by the Hamiltonian $\hat{H}_0$. A constant electric field of intensity E is applied to the system, which subjects the electron to the Coulomb force $F = -eE$, resulting in a perturbation $\hat{V} = F\hat{x}$.

1. Sketch the total potential experienced by the electron for $F > 0$ (i.e. $E < 0$).
2. Provide the Hamiltonian $\hat{H}_0$. Recall the eigenenergies ϵ_n and wavefunctions $\varphi_n(x)$ $(n = 1, 2, \ldots)$ of the unperturbed electron, i.e., when $F = 0$, distinguishing between even and odd n cases.
3. Calculate the first-order energy correction $E_1^{(1)}$ for the ground state in the case $F \neq 0$. What do you notice ?
4. Derive the first-order energy corrections $E_n^{(1)}$ for excited states with $n > 1$.
5. Now calculate the second-order energy correction $E_1^{(2)}$ for the ground state (exploit the wavefunction parity). For the sums over intermediate states, consider only the states $\varphi_1(x)$ and $\varphi_2(x)$, and denote by V_{21} the matrix element of the perturbation, computed between these two states.
6. Intuitively and qualitatively depict the shape of the wavefunction of the ground state in the total potential.

Problem 2 : Degenerate Perturbation Theory for a 3-State System

We consider the following Hamiltonian acting on a spin 1 :

$$\hat{H} = -D\hat{S}_z^2 + \lambda B\hat{S}_x \tag{1}$$

This is a model that can be realistic in certain materials. The first term represents an anisotropy, and the second a magnetic field along the x direction. We propose to diagonalize this Hamiltonian by considering the term $\lambda B\hat{S}_x$ as a perturbation. Subsequently, we assume that B and D are non-zero. *Reminder from "quantum physics 1" course :* For a spins s, we have $\hat{S}_z |s, m\rangle = \hbar m |s, m\rangle$ with $-s \leq m \leq s$. And the raising/lowering operators $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$ acting on these eigenvectors gives $\hat{S}_\pm |s, m\rangle = \sqrt{s(s+1) - m(m \pm 1)}\, |s, m \pm 1\rangle$.

1. Under what condition does the Hamiltonian commute with $\hat{S}_z$? In this case, give the eigenvalues and eigenvectors of $\hat{H}$.
2. Subsequently, we consider $\lambda \neq 0$. Write down the matrix of the Hamiltonian in the basis of eigenstates of $\hat{S}_z$. Using second order perturbation theory, compute the energy correction for the state $|m = 0\rangle$. Calculate the correction to the associated eigenvector, to first order in perturbation theory.

3. To calculate the effect of the perturbation on the other two states, it is necessary to use degenerate perturbation theory. What is the matrix of the operator $\hat{S}_x$ in the degenerate subspace ? Deduce that the first-order correction is zero.

Problem 3 : Potential well

Summary The aim of this exercise is to understand the principle of the variational method.
We consider the problem of an infinite 1D potential well, defined by :

$$V(x) = \begin{cases} 0 & \text{if} \quad |x| < a \\ +\infty & \text{if} \quad |x| \geq a \end{cases}$$

where the ground state is given by :

$$E_0 = \frac{\hbar^2}{2m}\frac{\pi^2}{4a^2} \tag{2}$$

We propose to seek an approximate value of the ground state energy by the variational method. To this end, we consider the functions :

$$\psi_\lambda(x) = \begin{cases} a^\lambda - |x|^\lambda & \text{if} \quad |x| < a \\ 0 & \text{if} \quad |x| \geq a \end{cases} \tag{3}$$

We recall that the condition $\lambda > 1$ is imposed because the derivative of a wavefunction is generally continuous at all points where the potential is continuous (or has only a finite jump).

1. Calculate $\langle\psi_\lambda|\psi_\lambda\rangle$.
2. Determine the value of λ that minimizes the energy. Compare with the exact ground state energy and deduce the relative error.