Quantum mechanics II, Problems 7 : Perturbation Theory

Solutions

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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 $\hat{V}(\hat{x}) = F\hat{x}$.

1. Sketch the total potential experienced by the electron for $F > 0$.
   The total potential is an infinite barrier potential with a sloped bottom along a line with positive slope $F = -eE > 0$ (i.e. $E < 0$). This corresponds to the function
   $$V_{tot}(x) = \begin{cases} Fx & \text{if } |x| \leq L/2 \text{ ,} \\ \infty & \text{else.} \end{cases} \tag{1}$$
   (Notice that the force F acts along $-x$, i.e. $\mathbf{F} = -F\mathbf{e}_x$ as $\mathbf{F} = -\nabla V$.)
2. Provide the Hamiltonian $\hat{H}_0$. Recall the eigenenergies E_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.
   The perturbed system Hamiltonian is written :
   $$\hat{H} = \underbrace{\frac{\hat{p}^2}{2m} + V_0\left(\hat{x}\right)}_{=\hat{H}_0} + F\hat{x} \text{ ,} \tag{2}$$
   where $V_0(\hat{x})$ is the potential well. In the position space, it is given by
   $$V_0(x) = \begin{cases} 0 & \text{if } |x| \leq L/2 \text{ ,} \\ \infty & \text{else.} \end{cases} \tag{3}$$
   In the case where $F = 0$ the eigenenergies of the confined electron are
   $$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2}, \; n > 0 \tag{4}$$
   and the corresponding wavefunctions
   $$\varphi_n\left(x\right) = \begin{cases} \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi}{L}x\right), & \text{if } n \text{ is odd ,} \\ \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right), & \text{if } n \text{ is even} \end{cases} \tag{5}$$
   Recall that these results are obtained by solving Schrödinger equation of a free electron (i.e. with Hamiltonian $\frac{\hat{p}^2}{2m}$) inside the potential well. Then, the potential barrier implies $\phi_n(x) = 0$ for $|x| \geq L/2$. In particular, the wavefunctions inside the well must match the bound conditions i.e. $\phi_n(\pm L/2) = 0$ to avoid discontinuity. (see course or e.g. "Particle in a box - Wikipedia")

3. Calculate the first-order energy correction $E_1^{(1)}$ for the ground state in the case $F \neq 0$. What do you notice ?
   In the case where $F \neq 0$, the energy correction of the ground state is the average value of the perturbation operator on the unperturbed states, which is given by :
$$E_1^{(1)} = \int_{-L/2}^{+L/2} \varphi_1^*(x)\, Fx\varphi_1(x)\, dx = \frac{2F}{L} \int_{-L/2}^{+L/2} x\cos^2\left(\frac{\pi}{L}x\right) dx \tag{6}$$
   Directly by noticing that $x \mapsto x\cos^2(x)$ is odd, or by integrating by parts, we find $E_1^{(1)} = 0$.
4. Derive the first-order energy corrections $E_n^{(1)}$ for excited states with $n > 1$.
   The energy correction of the excited states is given by
$$E_n^{(1)} = \begin{cases} \frac{2F}{L} \int_{-L/2}^{+L/2} x\sin^2\left(\frac{n\pi}{L}x\right) dx, & \text{if } n \text{ is even ,} \\ \frac{2F}{L} \int_{-L/2}^{+L/2} x\cos^2\left(\frac{n\pi}{L}x\right) dx, & \text{if } n \text{ is odd ,} \end{cases} \tag{7}$$
   and also involve odd integrands for any n, so we simply have $E_n^{(1)} = 0$ for all n.
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.
   The energy correction $E_1^{(2)}$ of the ground state at order 2 involves non-zero matrix elements
$$V_{j1} = \frac{2F}{L} \int_{-L/2}^{+L/2} x\sin\left(\frac{j\pi}{L}x\right)\cos\left(\frac{\pi}{L}x\right) dx \tag{8}$$
   only if j is even. Indeed, in cases where j is odd, the elements are zero due to parity (i.e. as $x \mapsto x\cos\left(\frac{j\pi}{L}x\right)\cos\left(\frac{\pi}{L}x\right)$ is odd). If we consider only the coupling with the first excited level, namely $j = 2$, the correction to the ground state is simply
$$E_1^{(2)} = -\frac{V_{21}^* V_{21}}{E_2 - E_1} \tag{9}$$
   with
$$V_{21} = \frac{16}{9\pi^2} FL \tag{10}$$
   using the identity $\sin(a)\cos(b) = \frac{1}{2}(\sin(a+b) + \sin(a-b))$ and by integrating terms of the form $x\sin(wx)$ by part (notice that $x\sin(wx) = \frac{d}{dx}\left(\frac{\sin(wx) - wx\cos(wx)}{w^2}\right)$). And so finally
$$E_1^{(2)} = -\frac{256}{243\pi^4}\frac{F^2L^2}{E_1} \tag{11}$$
6. Intuitively and qualitatively depict the shape of the wavefunction of the ground state in the total potential.
   The wavefunction of the ground state becomes asymmetric and localizes where the potential is the weakest (i.e. on the left).

Problem 2 : Interacting particles in a potential well

We consider two indistinguishable (spinless) particles of mass m confined in a one-dimensional square potential well $V(x)$. We assume that the barrier height is such that only states associated with the wavefunctions $\varphi_1(x)$ and $\varphi_2(x)$ are confined in the well. The Hamiltonian of the system is given by :

$$\hat{H}^{(0)} = \hat{H}_1 + \hat{H}_2, \tag{12}$$

with

$$\hat{H}_1 = \frac{\hat{p}_1^2}{2m} + V(\hat{x}_1), \quad \hat{H}_2 = \frac{\hat{p}_2^2}{2m} + V(\hat{x}_2). \tag{13}$$

1. Suppose that the two-particle states are symmetric under permutations. Determine a basis of two-particle states, from the single particle states φ_1 and φ_2.
   This is similar to "Problem sheet 6 : Fermions and Bosons". The parity operator in basis $\{|\varphi_1\rangle|\varphi_1\rangle, |\varphi_1\rangle|\varphi_2\rangle, |\varphi_2\rangle|\varphi_1\rangle, |\varphi_2\rangle|\varphi_2\rangle\}$ can be diagonalised. Then, the eigenstates with eigenvalues $+1$ are

$$\begin{aligned} |\psi_1\rangle &= |\varphi_1\rangle|\varphi_1\rangle \qquad (14)\\ |\psi_2\rangle &= \frac{1}{\sqrt{2}}(|\varphi_1\rangle|\varphi_2\rangle + |\varphi_1\rangle|\varphi_2\rangle) \qquad (15)\\ |\psi_3\rangle &= |\varphi_2\rangle|\varphi_2\rangle\ , \qquad (16)\end{aligned}$$

   which forms a basis for the two-particle states that are symmetric under permutations.
   In the position representation, the associated wavefunctions are

$$\begin{aligned} \psi_1(x_1,x_2) &= \varphi_1(x_1)\varphi_1(x_2) \qquad (17)\\ \psi_2(x_1,x_2) &= [\varphi_1(x_1)\varphi_2(x_2) + \varphi_1(x_2)\varphi_2(x_1)]/\sqrt{2} \qquad (18)\\ \psi_3(x_1,x_2) &= \varphi_2(x_1)\varphi_2(x_2)\ . \qquad (19)\end{aligned}$$

2. Now assume that the particles can interact when they are precisely at the same location (contact interaction), which is represented by the perturbation $\hat{V}_{\text{int}} = V_0\delta(\hat{x}_1 - \hat{x}_2)$, where $\delta(\hat{x}_1 - \hat{x}_2)$ is the Dirac delta function. Calculate the first-order energy correction for each of the two-particle states established earlier. Discuss the relative values and signs of these corrections.
   The energy corrections at 1st order are

$$\Delta E_j^{(1)} = \langle\psi_j|\hat{V}_{\text{int}}|\psi_j\rangle \tag{20}$$

   And by using the definition of the delta function

$$\begin{aligned} \Delta E_1^{(1)} &= V_0\int|\varphi_1(x_1)|^4 dx_1 \qquad (21)\\ \Delta E_2^{(1)} &= 2V_0\int|\varphi_1(x_1)\varphi_2(x_1)|^2 dx_1 \qquad (22)\\ \Delta E_3^{(1)} &= V_0\int|\varphi_2(x_1)|^4 dx_1 \qquad (23)\end{aligned}$$

3. Repeat the previous calculations assuming the two-particle states are anti-symmetric under permutations. Compare the results obtained with the symmetric case and draw conclusions.
   Only one possible state in this case

$$\psi_1(x_1, x_2) = [\varphi_1(x_1)\varphi_2(x_2) - \varphi_1(x_2)\varphi_2(x_1)]/\sqrt{2} \tag{24}$$

   In this case the energy correction

$$\Delta E_1^{(1)} = V_0 \int [\varphi_1(x_1)\varphi_2(x_1) - \varphi_1(x_1)\varphi_2(x_1)]^2 \, dx_1 = 0 \tag{25}$$

   is null. This is predictable since the potential acts when the particles are at the same position, which is prohibited for an odd wavefunction.