Lecture 20. Perturbation Theory: Examples

* The tilted potential well

  $\Rightarrow$ The quantum-confined Stark effect

* Degenerate perturbation theory

  $\Rightarrow$ Two-dimensional quantum well

The Tilted Potential Well

• **Previously we discussed an APPROXIMATE approach to determine the energy eigenvalues and eigenfunctions of a PERTURBED system in terms of those of an EXACT system**

$$E_n = \varepsilon_n + V_{nn} + \sum_{k,k\neq n} \frac{V_{nk}^* V_{nk}}{\varepsilon_n - \varepsilon_k} + \dots \qquad (19.23)$$

$$\psi_n = \varphi_n + \sum_{k,k\neq n} \frac{V_{nk}^*}{\varepsilon_n - \varepsilon_k}\varphi_k + \dots \qquad (19.24)$$

*** In these equations ε_n and φ_n are the energy eigenvalues and eigenfunctions of the exact system while E_n and ψ_n are those of the perturbed system**

*** Today we discuss some illustrative APPLICATIONS of this PERTURBATION THEORY**

⇒ We begin by considering the case of an electron that moves in a TILTED potential well that results when a uniform electric field is applied to the system

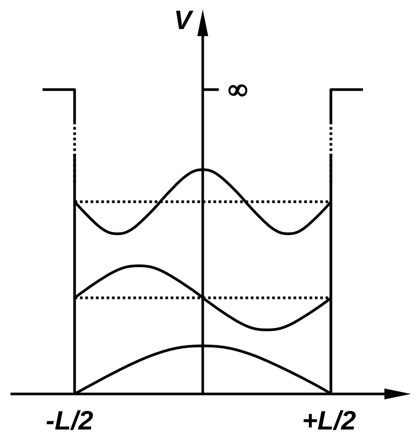
The Tilted Potential Well

• The **UNPERTURBED** system that here is taken to be an **INFINITE** potential well centered on the origin $x = 0$

* The energy **EIGENVALUES** for this system were computed previously

$$\varepsilon_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2}, \quad n = 1, 2, 3, \ldots$$

* With the well centered on the origin it is easy to show that the **EIGENFUNCTIONS** of the Hamiltonian exhibit either **EVEN** or **ODD** symmetry and take the form



$$\varphi_{n_{even}}(x) = \sqrt{\frac{2}{L}} \cos\left[\frac{n\pi}{L} x\right], \quad n = 1, 3, 5, \ldots \qquad (20.1)$$

$$\varphi_{n_{odd}}(x) = \sqrt{\frac{2}{L}} \sin\left[\frac{n\pi}{L} x\right], \quad n = 2, 4, 6, \ldots \qquad (20.2)$$

The Tilted Potential Well

• **For the PERTURBED system we wish to consider how the GROUND-STATE energy is modified by the application of the electric field**

*** The perturbation to the exact Hamiltonian due to the application of the electric field is**

$$V = eEx \qquad (20.3)$$

*** The FIRST-ORDER correction to the ground-state energy depends on the matrix element V_{11} and VANISHES due to the antisymmetry of the integrand**

$$E_1^{(1)} = V_{11} = \frac{2}{L} eE \int_{-L/2}^{L/2} x \cos^2\left[\frac{\pi}{L} x\right] dx = 0 \qquad (20.4)$$

$\Rightarrow$ **This result is true for ALL eigenvalues of the potential well whose first-order corrections all vanish due to antisymmetry**

$\Rightarrow$ **This is REASSURING since the correction to the energy should NOT depend on the direction of the electric field**

The Tilted Potential Well

• The **SECOND-ORDER** correction to the energy depends on matrix elements of the form

$$V_{1k} = \frac{2}{L} eE \int_{-L/2}^{L/2} \sin\left[\frac{k\pi}{L}x\right] x \cos\left[\frac{\pi}{L}x\right] dx\,, \quad k = 2, 4, 6, \ldots \qquad (20.5)$$

*** Here we have exploited the fact that the function *x* is antisymmetric while cos[*πx/L*] is symmetric so that the only matrix elements that do not vanish are those involving EVEN values of *k* whose wavefunctions are ANTISYMMETRIC**

⇒ **The second-order energy correction to the ground-state eigenvalue is therefore**

$$E_1^{(2)} = -\sum_{k=1}^{\infty} \frac{V_{2k,1}^{*} V_{2k,1}}{\varepsilon_{2k} - \varepsilon_1}\,, \quad k = 1, 2, 3 \ldots \qquad (20.6)$$

⇒ **As discussed previously we see that the energy is LOWERED due to the presence of the perturbation**

The Tilted Potential Well

• **For a LOWER-BOUND on the second-order energy correction $E_1^{(2)}$ we consider the FIRST term of Eq. 20.6 alone (V_{21})**

$$V_{21} = \frac{2}{L} eE \int_{-L/2}^{L/2} \sin\left[\frac{2\pi}{L} x\right] x \cos\left[\frac{\pi}{L} x\right] dx = \frac{16}{9\pi^2} eEL \qquad (20.7)$$

*** Substituting this result into Eq. 20.6 we may therefore write**

$$E_1^{(2)} = -\frac{V_{21}^* V_{21}}{\varepsilon_2 - \varepsilon_1} = -\frac{V_{21}^* V_{21}}{3\varepsilon_1} = -\frac{256}{243\pi^4} \frac{e^2 E^2 L^2}{\varepsilon_1} \qquad (20.8)$$

⇒ **Note here that we have exploited the fact that for the infinite well $\varepsilon_2 = 4\varepsilon_1$**

⇒ **In order for this result to be valid we require the energy shift $E_1^{(2)}$ be SMALLER than the inter-level separation $\sim\varepsilon_1$**

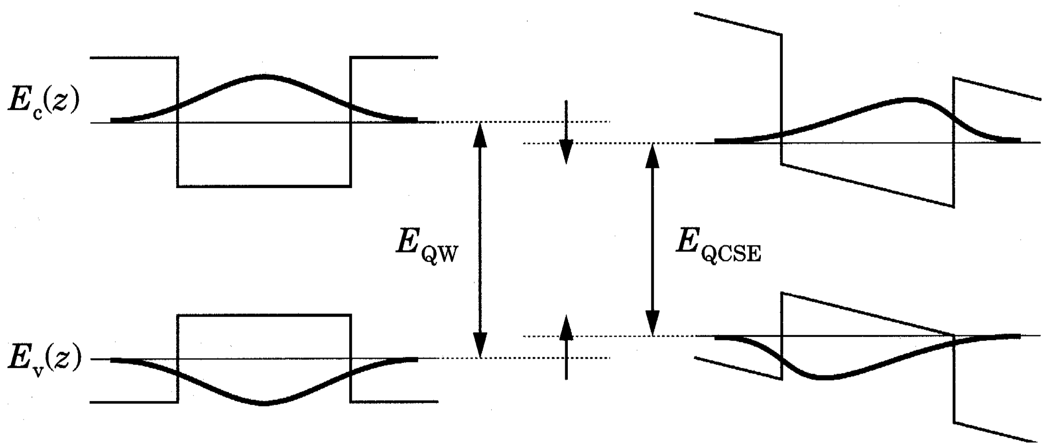
The Tilted Potential Well

• While we have only considered the LOWEST matrix element V_{21} in our calculation of $E_1^{(2)}$ the calculation CAN be extended to higher order elements $V_{2k,1}$

* An analytical solution is actually possible in this case but yields a result that differs by only 0.1% from Eq. 20.8

* An important result of our analysis is that in a quantum well formed between different semiconductors an electric field REDUCES the energy gap for electron-hole pair creation

⇒ This is referred to as the QUANTUM-CONFINED STARK EFFECT



• SHOWN LEFT IS THE POTENTIAL WELL IN THE ABSENCE OF THE ELECTRIC FIELD WHILE THE WELL IN THE APPLIED FIELD IS SHOWN RIGHT

• NOTE HOW THE ENERGY GAP FOR ELECTRON EXCITATION TO THE CONDUCTION BAND IS REDUCED IN THE PRESENCE OF THE ELECTRIC FIELD

• THIS SHIFTS THE ABSORPTION THRESHOLD OF THE QUANTUM WELL TO LOWER FREQUENCIES

Example

- * A particle of mass *m* is confined in an infinite potential well of length *L*. If this potential is now subject to a δ-function perturbation of the form $V(x) = L\omega_o\delta(x-L/2)$ estimate the resulting modifications to the energy levels of the well

$$\varphi_n(x) = \sqrt{\frac{2}{L}}\sin\left[\frac{n\pi}{L}x\right], \quad n = 1, 2, 3, \ldots$$

$$\therefore \quad E_n^{(1)} = \frac{2}{L}\int_0^L \sin^2\frac{n\pi x}{L} L\omega_o\delta(x - L/2)dx = \begin{cases} 2\omega_o, & n\ odd \\ 0, & n\ even \end{cases}$$

⇒ **The ODD energy levels are all RAISED by the SAME amount $2\omega_o$**

⇒ **The EVEN energy levels are UNAFFECTED by the perturbation to first order however since their wavefunctions all VANISH at the position where the delta-function perturbation is located**

Degenerate Perturbation Theory

• **The perturbation theory that we have developed thus far can FAIL if two or more levels of the system under study are degenerate since the perturbation expansion then DIVERGES**

$$E_n = \varepsilon_n + V_{nn} + \sum_{k,k\neq n} \frac{V_{nk}^* V_{nk}}{\varepsilon_n - \varepsilon_k} + \ldots \quad \infty \qquad (19.23)$$

*** A NEW approach is needed here and to develop this we note that since the degenerate levels lead to divergence this suggests that we FOCUS on the effects of these levels**

*** To develop this degenerate perturbation theory we consider the specific problem of a TWO-DIMENSIONAL infinite square well of side length *a* in the *x*-*y* plane**

⇒ It is relatively straightforward to show that the quantized energies of such a well are given by

$$\varepsilon_{p,q} = \frac{\pi^2 \hbar^2}{2ma^2}(p^2 + q^2), \quad p, q = 1, 2, 3, \ldots \qquad (20.9)$$

Degenerate Perturbation Theory

• **The GROUND-STATE of the well is found by taking *p* = *q* = 1 and is therefore NON-DEGENERATE**

  *** The next energy level is DOUBLY DEGENERATE however**

$$\varepsilon \equiv \varepsilon_{1,2} = \frac{\pi^2\hbar^2}{2ma^2}(1^2+2^2) = \frac{\pi^2\hbar^2}{2ma^2}(2^2+1^2) \qquad (20.10)$$

  *** It is straightforward to show that the wavefunctions associated with these two degenerate levels are**

$$\varphi_A \equiv \varphi_{1,2} = \frac{2}{a}\cos\frac{\pi x}{a}\sin\frac{2\pi y}{a} \qquad (20.11)$$

$$\varphi_B \equiv \varphi_{2,1} = \frac{2}{a}\cos\frac{2\pi x}{a}\sin\frac{\pi y}{a} \qquad (20.12)$$

Degenerate Perturbation Theory

- **We now consider what happens if we add a PERTURBATION to the potential in the well**

$$V(x,y) = -Kxy\,, \quad K > 0 \qquad (20.14)$$

*** The idea in degenerate perturbation theory is to solve the Schrödinger equation EXACTLY but only for the degenerate states**

*** For the doubly-degenerate level of interest here we therefore need to recast the Hamiltonian as a 2 x 2 matrix**

$$\mathrm{H} = \begin{bmatrix} <A|H|A> & <B|H|A> \\ <A|H|B> & <B|H|B> \end{bmatrix} \qquad (20.15)$$

*** The first matrix element is easily evaluated**

$$<A|H|A> = <A|H_o|A> + <A|V|A> = \varepsilon + 0 = \varepsilon \qquad (20.16)$$

REMEMBER THAT φ_A IS AN EIGENSTATE OF H_o WITH ENERGY ε

THIS INTEGRAL VANISHES BECAUSE OF THE SYMMETRY OF V (Eq. 20.14)

Degenerate Perturbation Theory

- **The next matrix element is similarly evaluated**

$$< A | H | B > = \varepsilon \cancel{< A | B >} - < A | Kxy | B > = - < A | Kxy | B > \qquad (20.17)$$

*** The last term on the RHS of Eq. 20.17 is just the integral**

$$-\frac{4K}{a^2}\int_{-a/2}^{+a/2} \cos\frac{\pi x}{a} \sin\frac{2\pi y}{a}\, xy \cos\frac{2\pi x}{a} \sin\frac{\pi y}{a}\, dxdy = -\frac{16}{9\pi^2} Ka^2 \equiv -\Delta \qquad (20.18)$$

*** The matrix Schrödinger equation therefore reduces to**

$$\begin{bmatrix} \varepsilon & -\Delta \\ -\Delta & \varepsilon \end{bmatrix} \mathbf{a} = E\mathbf{a} \qquad (20.19)$$

Degenerate Perturbation Theory

- **The condition for solution to Eq, 20.19 is**

$$\begin{vmatrix} E-\varepsilon & \Delta \\ \Delta & E-\varepsilon \end{vmatrix} = (E-\varepsilon)^2 - \Delta^2 = 0 \qquad (20.20)$$

*** Solution of Eq. 20.20 now yields TWO distinct energy solutions**

$$E = \varepsilon \pm \Delta \qquad (20.21)$$

⇒ **Thus we see that the effect of the perturbation is to LIFT the degeneracy yielding TWO non-degenerate solutions**

⇒ **The degeneracy is lifted since the perturbation to the Hamiltonian BREAKS the symmetry of the potential well**

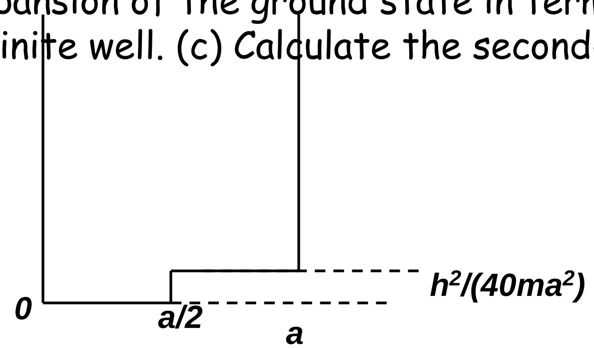
⇒ **We will discuss some examples of degenerate perturbation theory in the following classes**

Homework

P20.1 Assuming hydrogen nucleus (proton) is a uniformly charged sphere with a radius of 10^{-15} m, instead of a point as we have assumed in lecture 17. Using perturbation theory, calculate the corresponding correction in the ground state energy. Hint: The potential energy inside the sphere is changed to

$$-\frac{1}{4\pi\varepsilon_0}\frac{e}{a}$$

P20.2 A particle of mass m is in an infinite potential well perturbed as shown in the figure below. (a) Calculate the first-order energy shift of the n^{th} eigenvalue due to the perturbation. (b) Write out the first three nonvanishing terms for the perturbation expansion of the ground state in terms of the unperturbed eigenfunctions of the infinite well. (c) Calculate the second-order energy shift for the ground state.



P20.3 Consider the perturbed 2-D oscillator Hamiltonian

$$H = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{1}{2}k(x^2 + y^2) + \lambda xy$$

Use perturbation theory to calculate the energy shift of the degenerate first excited state to first order due to the perturbation λxy. What are the first order wave functions?