Homework #6 with Solutions

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Problem 6.1

Complete the study (started in class) of bound states of the system of two δ-function quantum wells,

$$U(x) = -W[\delta(x+a) + \delta(x-a)], \qquad W > 0,$$

by exploring the odd eigenstate energy behavior at $a \to 0$. Give a brief physical interpretation of your findings and find limitations (if any) on the validity of your results.

Solution:

In class, we have derived the following general formula for the energy: $\coth \kappa a = 2\frac{mW}{\hbar^2 \kappa} - 1,$

where κ is defined by relation $\frac{\hbar^2 \kappa^2}{2m} = |E| = -E.$ In the limit $\kappa a \to 0,$ we can take $\coth \kappa a \approx 1/\kappa a,$ and the relation yields $\kappa = 2\frac{mW}{\hbar^2} - \frac{1}{a}.$ As a is decreased, so is κ, and it becomes zero at the critical distance $a = a_c = \frac{\hbar^2}{2mW}.$ At $a < a_c$ our formulas are not more valid, because at $a = a_c$ the eigenenergy reaches zero, so that at smaller a the system does not have a bound odd eigenstate (only an even one).

Problem 6.2

The initial state of the system of two similar, weakly coupled quantum wells is prepared as

$$\psi(x,0) = A[u_e(x) + iu_o(x)],$$

where u_e and u_o are, respectively, the even and odd eigenfunctions. Find the time evolution of probability p_R to find the system in the right well.

Solution:

Since u_e and u_o are eigenstates, the wavefunction evolves as

$$\psi(x,t) = A\left[u_e(x)\exp(-i\frac{E_e}{\hbar}t) + iu_o(x)\exp(-i\frac{E_o}{\hbar}t)\right].$$

At weak coupling, $E_e = E_0 - T, E_o = E_0 + T,$ where $E_0 < 0$ is the eigenvalue for a single well, and $T > 0$ is the (small) coupling energy, so that

$$\psi(x,t) = A\exp(-i\frac{E_0}{\hbar}t)\left[u_e(x)\exp(+i\frac{T}{\hbar}t) + u_o(x)\exp(i\frac{\pi}{2})\exp(-i\frac{T}{\hbar}t)\right]$$

$$= A\exp(-i\frac{E_0}{\hbar}t)\left[u_e(x)(\cos\frac{T}{\hbar}t + i\sin\frac{T}{\hbar}t) + u_o(x)(-\sin\frac{T}{\hbar}t - i\cos\frac{T}{\hbar}t)\right].$$

As has been discussed in class, since the wells are weakly coupled, i.e. well separated, we can present the eigenfunctions as linear combinations of the spatially separated "partial" states in each well: $u_e(x) = u_R(x) + u_L(x), \quad u_o(x) = u_R(x) - u_L(x).$ Combining these formulas, we get

$$\psi(x,t) = A\exp(-\frac{E_0}{\hbar}t)\left[u_R(x)(1-i)(\cos\frac{T}{\hbar}t - \sin\frac{T}{\hbar}t) + u_L(x)(1+i)(\cos\frac{T}{\hbar}t + \sin\frac{T}{\hbar}t)\right].$$

The probability of finding the system in the right well is given by the modulus square of the coefficient at $u_R(x)$, i.e.:

$$p_R = 2|A|^2(\cos\frac{T}{\hbar}t - \sin\frac{T}{\hbar}t)^2 = 2|A|^2(1-\sin 2\frac{T}{\hbar}t).$$

We see the same quantum oscillations with frequency $\Omega = 2T/\hbar$ as have been discussed in class. Of course, p_R oscillates in antiphase with

$$p_L = 2|A|^2(1+\sin 2\frac{T}{\hbar}t),$$

because the sum $p_L + p_R$ must be constant.

Problem 6.3

Use the finite difference method with step $h = 2a/3$ to find eigenenergies of the infinitely deep quantum well of width $2a$. Compare the results with the exact formula.

Solution:

Let us denote $u(-2a/3) \equiv u_-$, $u(2a/3) \equiv u_+$, and measure energy in the units of $\hbar^2/ma^2$. Then the two finite-difference Schrödinger equations

$$-\frac{\hbar^2}{2m}\frac{u_{j-1} - 2u_j + u_{j+1}}{h^2} + U_j u_j = Eu_j,$$

which may be written for the internal points of the interval [-a, +a] for h =2a/3, look as follows:

$$-\frac{1}{2}\frac{-2u_- + u_+}{(2/3)^2} = eu_-,$$

$$-\frac{1}{2}\frac{u_- - 2u_+}{(2/3)^2} = eu_+.$$

(We took into account boundary conditions $u(-a) = u(+a) = 0$, as well as the fact that in the internal points $U_j = 0$.) This system of two linear, homogeneous equations is consistent if its determinant equals zero:

$$\begin{vmatrix} \frac{9}{4} - e & -\frac{9}{8} \\ -\frac{9}{8} & \frac{9}{4} - e \end{vmatrix} = 0.$$

This equation gives two solutions:

$$e = \frac{9}{4} \pm \frac{9}{8} = \begin{cases} 27/8 = 3.375, \\ 9/8 = 1.25. \end{cases}$$

These values should be compared with the analytical results $e_1 = \pi^2/8 \approx 1.234$ and $e_2 = \pi^2/2 \approx 4.93$. We see that for the lower (ground) state with its smoother eigenfunction, the finite difference method accuracy with this step h is pretty good, while for the higher (first excited) state the error is still very considerable. Want to reduce it? Take a smaller step (e.g., $h = a/2$) and solve a system of more (e.g., three) linear equations.