Ex7684: Dot - Ring System

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The problem:

A particle of mass M is confined to a site. The undisturbed bond energy is ϵ_0.
The site is coupled to a large ring of length L at one point, so that $\langle \epsilon_0 | H | \Psi \rangle = \alpha \Psi(x_0)$.
In the first question assume that the energy ϵ_0 is underneath the potential floor of the ring.

(1) Calculate the correction Δ to the bond energy, by using second order perturbation theory.
(2) Repeat the first question under the assumption that ϵ_0 is above the potential floor.
(3) In the last case, calculate the decay constant Γ of the bound state, by using Fermi's golden rule.
(4) Find a domain of values for ϵ_0, in which the previous results are unreliable.
(5) The bond energy from the first question can be found accurately, by solving a third degree equation. Write the equation.

Guidance:

- It would be convenient to work in the momentum basis $|k\rangle$ of the ring.
- Assume that the ring is very big, so that the discrete sum can be approximated by an integral.
- Write the final answer using the constants α, M, ϵ_0.
- If it helps it is allowed, and advisable to use the notation: $v_0 = \left(\frac{2\epsilon_0}{M}\right)^{\frac{1}{2}}$.

The solution:

For clarity reasons let us denote by Ψ a general linear combination of the momentum states on the ring, and by ψ the general wave function.

(1) The system is a combination of two separate systems; the undisturbed site and the states of the ring. Therefore the general wave function for the system is:

$$|\psi\rangle = |\epsilon_0\rangle + \sum_x \Psi(x) |x\rangle$$

The previous statement can be refined by using the eigenstates of a ring of length L:

$$|\psi\rangle = a |\epsilon_0\rangle + \frac{1}{\sqrt{L}} \sum_x e^{ik_n x} |x\rangle$$

with:

$$k_n = \frac{2\pi}{L} \times n, \quad E_n = \frac{2\pi^2}{m\text{Ł}^2} \times n^2, \quad n = 0, \pm 1, \pm 2, ...$$

Now that the undisturbed Hamiltonian is clear, lets evaluate the disturbance.
All of the momentum states of the ring are coupled to the site. The coupling occurs in a specific site in the position basis, and because we have the freedom to choose the x-axis origin, let us call the site of the coupling $x = 0$. Thus:

$$\langle \epsilon_0 | H | \Psi_k \rangle = \langle \epsilon_0 | H \Psi^k(0) | 0 \rangle = \langle \epsilon_0 | H \frac{e^{ik_n \cdot 0}}{\sqrt{L}} | 0 \rangle = \frac{\alpha}{\sqrt{L}}$$

Therefore the coupling of each of the momentum states to the standalone state is identical:

$$V_{n,\epsilon_0} = \frac{\alpha}{\sqrt{L}}$$

Remembering $\epsilon_0 < 0$ and assuming the disturbance is small:

$$V_{n,\epsilon_0} << |\epsilon_0|$$

We can now use second order perturbation theory approximation.

$$\Delta = \sum_{n=-\infty}^{\infty} \frac{|V_{n,\epsilon_0}|^2}{-|\epsilon_0| - E_n} = -\frac{\alpha^2}{L} \sum_{n=-\infty}^{\infty} \frac{1}{|\epsilon_0| + \frac{2\pi^2}{M\text{Ł}^2}\, n^2} = -\frac{M\text{Ł}\alpha^2}{2\pi^2} \int_{-\infty}^{\infty} \frac{\mathrm{d}n}{\frac{M\text{Ł}^2}{2\pi^2}\,|\epsilon_0| + n^2} = -\frac{\alpha^2}{\left(\frac{2\epsilon_0}{M}\right)^{\frac{1}{2}}} = -\frac{\alpha^2}{v_0}$$

The discrete sum turned into the integral since the ring is large enough.

(2) Let us repeat the process, only now $\epsilon_0 > 0$:

$$\Delta = \frac{\alpha^2}{L} \sum_{n=-\infty}^{\infty} \frac{1}{\epsilon_0 - \frac{2\pi^2}{M\text{Ł}^2}\, n^2} = \frac{\alpha^2}{2\, L\sqrt{\epsilon_0}} \int_{n=-\infty}^{\infty} \frac{1}{\sqrt{\epsilon_0} - \sqrt{\frac{2\pi^2}{M\text{Ł}^2}}\, n} + \frac{1}{\sqrt{\epsilon_0} + \sqrt{\frac{2\pi^2}{M\text{Ł}^2}}\, n} =$$

$$\frac{d}{b} \times \ln\left(\frac{|a+bn|}{|a-bn|}\right)\Big|_{-\infty}^{\infty} = 0$$

We know that : $d \int \frac{1}{a+bn}\, \mathrm{d}n = \frac{d}{b} \times \ln|a+bn| + c$

$$ln(1) = 0$$

(3) Let us use δ for mean level spacing and not the usual Δ, which we defined as the perturbation. Using the dispersion relation to find the mean level spacing, and assuming that the decay into the continuum occurs at the energy of the standalone state ($v_E = v_0$):

$$\mathrm{d}E = v_E \mathrm{d}p \quad \Rightarrow \quad \delta = v_0 \frac{\pi}{L}$$

Now according to Fermi's Golden Rule:

$$\Gamma = \frac{2\pi}{\delta} |V_{n,\epsilon_0}|^2 = \frac{2\alpha^2}{v_0}$$

(4) We shall find the values of ϵ_0 for which our approximations are valid, and deduce that the results are unreliable for the exact opposite conditions.

In order for the perturbation theory to be valid, one must require:

$$|V_{n,\epsilon_0}| << \epsilon_0 \;\rightarrow\; \Delta << \epsilon_0$$

The requirement for the validity of Fermi's Golden Rule is obvious out of basic unit analysis:

$$\Gamma << \epsilon_0$$

This can be interpreted as the bandwidth of decay being small in relation to the original energy level.

(5) The Schrödinger equation can be written as follows:

$$\epsilon_0|\epsilon_0\rangle + \frac{\alpha}{\sqrt{L}}\sum_k \Psi_k = E|\epsilon_0\rangle$$

$$\epsilon_k\Psi_k + \frac{\alpha}{\sqrt{L}}|\epsilon_0\rangle = E\Psi_k, \qquad k = 1,2,3,...$$

the k-th equation may be written as:

$$\Psi_k \;=\; \frac{\frac{\alpha}{\sqrt{L}}}{E_k - \epsilon_k}|\epsilon_0\rangle$$

Now by substituting this expression into the 0-th equation:

$$\frac{\alpha^2}{L}\sum_k \frac{1}{E-\epsilon_k} \;=\; E - \epsilon_0$$

This sum has been calculated in the first clause, and for an arbitrary energy E:

$$-\frac{\alpha^2}{v_E} = E - \epsilon_0$$

By writing v_E explicitly ($v_E = \sqrt{\frac{2E}{M}}$), we find the third degree equation for the exact energy:

$$M\alpha^2 = 2E\cdot(E-\epsilon_0)^2$$

Additional information: When using a computer program to find the roots, we see the complex part of the solution in accordance to whats expected when using "P+Q" formalism and finding the rezolvent and its pole:

$$E_n = \epsilon_0 + \Delta - i\frac{\Gamma}{2}$$

Here the requirement of clause (4) is made clear for those familiar with this process.