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Homework #4#

Course 314, Introduction In Quantum Mechanics, Professor K. Griffioen

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1 Problem 6.2

For the harmonic oscillator [$V(x) = (1/2)kx^2$], the allowed energies are :

$$E_n = (n + 1/2)\hbar\omega, (n = 0, 1, 2, \dots), \quad (1)$$

where $\omega = \sqrt{k}/m$ is the classical frequency. now suppose the spring constant increases slightly : $k \rightarrow (1 + \epsilon)k$. (Perhaps we cool the spring, so it becomes less flexible.)

(a) Find the *exact* new energies (trivial, in this case). Expand your formula as a power series in ϵ , up to second order.

(b) Now calculate the first- order perturbation in the energy, using Equation 6.9. What is H' ? Compare your result with part (a). *Hint*: It is not necessary - in fact, it is not *permitted* - to calculate a single integral in doing this problem.

2 Solution

(a)

$$\begin{aligned} V &= \frac{1}{2}kx^2 \\ E &= (n + \frac{1}{2})\hbar\omega \\ \omega &= \sqrt{\frac{k}{m}} \\ V' &= \frac{1}{2}(1 + \epsilon)kx^2 \end{aligned} \quad (2)$$

then the perturbation of energy will be :

$$\begin{aligned}
 E' &= (n + \frac{1}{2})\hbar\omega', & (3) \\
 \omega' &= \sqrt{\frac{(1 + \epsilon)k}{m}} = \sqrt{1 + \epsilon}\omega \\
 E' &= (n + \frac{1}{2})(\hbar\omega)(1 + \frac{\epsilon}{2} - \frac{\epsilon^2}{8} + \dots)
 \end{aligned}$$

and $\sqrt{1 + \epsilon} = 1 + \frac{\epsilon}{2} - \frac{\epsilon^2}{8} + \dots$, represent the Taylor expansion of $(1 + \epsilon)^{1/2}$.

(b) The first-order correction of energy is given by :

$$E_1 = \langle \psi_n | H' | \psi_n \rangle = \langle \psi_n | \frac{1}{2} k \epsilon x^2 | \psi_n \rangle = \epsilon \langle \psi_n | \frac{1}{2} k x^2 | \psi_n \rangle = \epsilon \langle V \rangle \quad (4)$$

The virial theorem states that :

$$\begin{aligned}
 2 \langle T \rangle &= \langle \bar{r} \cdot \bar{\nabla} V \rangle = \langle x \cdot \frac{d}{dx} V \rangle = \langle x \cdot \frac{2}{2} k x \rangle = 2 \langle V \rangle, \text{ but} & (5) \\
 E &= \langle V \rangle + \langle T \rangle, \text{ then} \\
 \langle V \rangle &= \frac{1}{2} (n + \frac{1}{2}) \hbar \omega \\
 E_1 &= \frac{\epsilon}{2} (n + \frac{1}{2}) \hbar \omega
 \end{aligned}$$

This result is just what we get for the ϵ power of the exact expansion.

3 Problem 6.3

Two identical bosons are placed in an infinite square well(Equation 2.15.) They interact weakly with one another, via the potential

$$V(x_1, x_2) = -aV_0\delta(x_1 - x_2) \quad (6)$$

(where V_0 is a constant with dimensions of energy and a is the width of the well).

(a) First, ignoring the interaction between particles, find the ground state and first excited state - both

the wave functions and the associated energies.

(b) Use first - order perturbation theory to calculate the affect of the particle - particle interaction on the ground and first excited state energies.

4 Solution

(a)

$$\begin{aligned} V(x_1, x_2) &= -aV_0\delta(x_1 - x_2), \\ \psi_n(x) &= \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a} \\ E_n &= \frac{n^2\pi^2\hbar^2}{2ma^2} \end{aligned} \tag{7}$$

where ψ_n represent the general wave function which characterize the bosons in an infinite square well potential.

The ground state will have the following wave function :

$$\psi_{gs} = \psi_1(x_1)\psi_2(x_2) = \frac{2}{a}\sin\frac{\pi x_1}{a}\sin\frac{\pi x_2}{a} \tag{8}$$

The associated ground state energy will be :

$$E_{gs} = \frac{\pi^2\hbar^2}{ma^2} \tag{9}$$

For the first excited state the wave function will be :

$$\psi_{1st} = \frac{1}{\sqrt{2}}\left(\psi_1(x_1)\psi_2(x_2) + \psi_1(x_2)\psi_2(x_1)\right) = \frac{\sqrt{2}}{a}\left(\sin\frac{\pi x_1}{a}\sin\frac{2\pi x_2}{a} + \sin\frac{2\pi x_1}{a}\sin\frac{\pi x_2}{a}\right) \tag{10}$$

The corresponding energy for the first excited state will be :

$$E_{1st} = \frac{5\pi^2\hbar^2}{2ma^2} \tag{11}$$

(b) Under the interaction between particles the first-order correction of the energy in the ground state will be :

$$\begin{aligned}
E'_{gs} &= \int_0^a dx_1 \int_0^a \psi_1(x_1)^2 \psi_1(x_2)^2 (-aV_0) \delta(x_1 - x_2) dx_2 \\
&= -aV_0 \int_0^a \psi_1(x_1)^4 dx_1 \\
&= -aV_0 \left(\frac{2}{a}\right)^2 \int_0^a \sin \frac{\pi x}{a} dx \\
&= -\frac{3}{2}V_0
\end{aligned} \tag{12}$$

and for the first excited state :

$$\begin{aligned}
E_{1st} &= \left(\frac{2}{a}\right)^2 \int_0^a dx_1 \int_0^a (-aV_0) \delta(x_1 - x_2) \left(\frac{1}{\sqrt{2}}\psi_1(x_1)\psi_2(x_2) + \frac{1}{\sqrt{2}}\psi_1(x_2)\psi_2(x_1)\right)^2 dx_2 \\
&= \left(\frac{2}{a}\right)^2 \int_0^a dx_1 \int_0^a (-aV_0) \left(\frac{2}{\sqrt{2}}\psi_1(x_1)\psi_2(x_1)\right)^2 dx_1 \\
&= -\frac{8}{a}V_0 \int_0^a \sin \frac{\pi x}{a} \sin \frac{2\pi x}{a} dx \\
E_{1st} &= -2V_0
\end{aligned} \tag{13}$$

5 Problem 6.7

Consider a particle of mass m that is free to move in a one - dimensional region of length L that closes on itself (for instance, a bead which slides frictionlessly on a circular wire of circumference L ; Problem 2.43).

(a) Show that the stationary states can be written in the form

$$\psi_n(x) = \frac{1}{\sqrt{L}} e^{2\pi i n x / L}, (-L/2 < x < L/2), \tag{14}$$

where $n = 0, \pm 1, \pm 2, \dots$, and the allowed energies are

$$E_n = \frac{2}{m} \left(\frac{n\pi\hbar}{L}\right)^2. \tag{15}$$

Notice that - with the exception of the ground state ($n = 0$) - these are all doubly degenerate.

Xcy(b) Now suppose we introduce the perturbation

$$H' = -V_0 e^{-x^2/a^2}, \quad (16)$$

where $a \ll L$. (This puts a little " dimple " in the potential at $x = 0$, as though we bent the wire slightly to make a " trap. ") Find the first-order correction to E_n , using Equation 6.26. *Hint:* To evaluate the integrals, exploit the fact that $a \ll L$ to extend the limits from $\pm L/2$ to $\pm\infty$; after all, H' is essentially zero outside $-a \ll x \ll a$.

(c) What are the " good " linear combinations of ψ_n and ψ_{-n} for this problem ? Show that with these states you get the first-order correction using Equation 6.9.

(d) Find a Hermitin operator A that fits the requirement of the theorem, and show that the simultaneous eigenstates of H^0 and A are precisely the ones you found in (c).

6 Solution

(a) From Shrodinger equation we have :

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} &= E\psi, \\ k^2 &= \frac{2mE}{\hbar^2}, \\ \frac{d^2\psi}{dx^2} + k^2\psi &= 0, \\ \psi &= e^{\pm ikx} \end{aligned} \quad (17)$$

Applying the boundary condition $\psi(x+L) = \psi(x)$, we'll find :

$$\begin{aligned} e^{\pm ik(x+L)} &= e^{\pm ikx}, \\ e^{\pm ikx} e^{\pm ikL} &= e^{\pm ikx}, \\ e^{\pm ikL} &= 1, \\ kL &= 2\pi n, n = 0, \pm 1, \pm 2, \dots \end{aligned} \quad (18)$$

Applying the normalization condition of wave function we'll have :

$$\begin{aligned}\int_{-L/2}^{L/2} \psi^* \psi dx &= 1, \\ \int_{-L/2}^{L/2} A^2 dx &= 1, \\ A &= \frac{1}{\sqrt{L}}\end{aligned}\tag{19}$$

Then we'll plug into $\psi = e^{\pm ikx}$ and we'll obtain :

$$\begin{aligned}\psi_n &= \frac{1}{\sqrt{L}} e^{2\pi i n x / L}, n = 0, \pm 1, \pm 2, \dots \\ E_n &= \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 (2\pi)^2 n^2}{2m L^2} = \frac{2}{m} \left(\frac{n \hbar \pi}{L} \right)^2\end{aligned}\tag{20}$$

(b) Under the small perturbation $H' = -V_0 e^{-x^2/a^2}$, where $a \ll L$, the first-order correction of E_n is given by :

$$E'_\pm = \frac{1}{2} \left[W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2} \right],\tag{21}$$

where the matrix elements $W_{aa}, W_{bb}, W_{ab} = W_{ba}$ can be computed as follows :

$$\begin{aligned}W_{aa} = W_{bb} &= \langle \psi_a | H' | \psi_a \rangle = \int_{-L/2}^{L/2} \psi_a^* H' \psi_a dx = -\frac{V_0}{L} \int_{-L/2}^{L/2} e^{-x^2/a^2} dx, \\ W_{ab} = W_{ba} &= \langle \psi_a | H' | \psi_b \rangle = \langle \psi_b | H' | \psi_a \rangle = -\frac{V_0}{L} \int_{-L/2}^{L/2} \psi_a^* H' \psi_b dx = -\frac{V_0}{L} \int_{-L/2}^{L/2} e^{-4\pi i n x / L} e^{-x^2/a^2} dx \\ \psi_a &= \frac{1}{\sqrt{L}} e^{+2\pi i n x / L} \\ \psi_b &= \frac{1}{\sqrt{L}} e^{-2\pi i n x / L}\end{aligned}\tag{22}$$

We can make the approximation $L/2 \rightarrow \infty$, since $L \gg a$, so vthen we'll have :

$$W_{aa} = W_{bb} = -\frac{a V_0 \sqrt{\pi}}{L},\tag{23}$$

$$W_{ab} = W_{ba} = -\frac{aV_0\sqrt{\pi}}{L}e^{-4\pi^2n^2a^2/L^2}$$

We'll make the subscript $e^{-4\pi^2n^2a^2/L^2} = \epsilon$, and then the first - order correction of E_n will be :

$$E'_\pm = -\frac{aV_0}{L}(1 \mp \epsilon) \quad (24)$$

(c) We resolve the eigenvalue problem knowing that the transformation matrix has the following form :

$$W = \begin{pmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{pmatrix} = -\frac{aV_0\pi}{l} \begin{pmatrix} 1 & \epsilon \\ \epsilon & 1 \end{pmatrix} \quad (25)$$

Then we'll determine the eigenstates of the matrix operator W :

$$\begin{aligned} \begin{pmatrix} 1-\epsilon & \epsilon \\ \epsilon & 1-\epsilon \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} &= 0 \rightarrow \frac{1}{\sqrt{L}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \\ \begin{pmatrix} -\epsilon & \epsilon \\ \epsilon & -\epsilon \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} &= 0 \rightarrow \frac{1}{\sqrt{L}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \end{aligned} \quad (26)$$

The "good" combinations of ψ_n and ψ_{-n} will be :

$$\begin{aligned} \psi_n &= \frac{1}{\sqrt{2L}} \left(e^{2\pi inx/L} + e^{-2\pi inx/L} \right) \\ \psi_{-n} &= \frac{1}{\sqrt{2L}} \left(e^{2\pi inx/L} - e^{-2\pi inx/L} \right) \end{aligned} \quad (27)$$

(d) We have to find an operator A that fits the requirement to be Hermitian, and the H^0 and A to have the same eigenstates :

$$\begin{aligned} A^\dagger &= A, \\ [A, H^0] &= 0 \end{aligned} \quad (28)$$

Under theorem conditions :

$$A\psi_n = 1\psi_n, \quad (29)$$

$$A\psi_{-n} = -1\psi_{-n}$$

So the operator A takes x to the $-x$ (parity operator), and since $e^{-(-x)^2/a^2} = e^{-x^2/a^2}$, the eigenfunctions $\psi_{\pm n}$ are simultaneous eigenstates for A and H^0 .

References

- [1] D. J. Griffiths, Introduction To Quantum Mechanics, 1995