Quantum Mechanics

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PROBLEM SET 2

Problem 1. A constant electric field $\mathcal{E}$ is exerted on a charged linear harmonic oscillator.

(1) Write down the corresponding Schrödinger equation.

(2) Derive the eigenvalues and eigenvectors of the charged linear oscillators under a uniform electric field.

(3) Discuss the change in energy levels and physics. eigenstates.

Hint: Use the operator method.
Answer :

(1) A charged particle away from the equilibrium position has the potential energy when it is in the electric field. Let a distance from equilibrium position to a particle is x. In the constant electric field, the electric potential energy E_p is,

$$E_p = q\mathcal{E}x. \tag{1}$$

Then, the Hamiltonain of the charged linear harmonic oscillator is,

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - q\mathcal{E}x. \tag{2}$$

So, the Schrödinger equation is,

$$-\frac{\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\psi - q\mathcal{E}x\psi = E\psi. \tag{3}$$

(2) First, Suppose that there is no electric field, that is, $\mathcal{E}$ is zero. Then the Schrödinger equation and the energy is,

$$-\frac{\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi, \;\; E_n = \left(\frac{1}{2} + n\right)\hbar\omega. \tag{4}$$

It is the Schrödinger equation of the simple harmonic oscillator. In the algebric method to solve the equation, we defined new operators,

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + i\frac{p}{m\omega}\right), \;\; a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - i\frac{p}{m\omega}\right). \tag{5}$$

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And,

$$x=\sqrt{\frac{2\hbar}{m\omega}}\left(\frac{a+a^\dagger}{2}\right),\ \ p=\sqrt{2\hbar m\omega}\left(\frac{a-a^\dagger}{2i}\right) \tag{6}$$

It is said to ladder operators. Operators is from the hamiltonian of simple harmonic oscillator,

$$H=\frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2=\hbar\omega\left(a^\dagger a+\frac{1}{2}\right)=\hbar\omega\left(aa^\dagger-\frac{1}{2}\right). \tag{7}$$

Now, recall a constant electric field $\mathcal{E}$. From Eq. (2) and (7), hamiltonian is,

$$H=\hbar\omega\left(a^\dagger a+\frac{1}{2}-q\mathcal{E}x\right)=\hbar\omega\left(a^\dagger a+\frac{1}{2}-q\mathcal{E}\sqrt{\frac{2\hbar}{m\omega}}\left(\frac{a+a^\dagger}{2}\right)\right), \tag{8}$$

or,

$$H=\hbar\omega\left(aa^\dagger-\frac{1}{2}\right)-q\mathcal{E}\sqrt{\frac{2\hbar}{m\omega}}\left(\frac{a+a^\dagger}{2}\right). \tag{9}$$

If ψ_n is the eigenvector and E_n is the eigenvalue of ψ_n, the Schrödinger equation is,

$$-\frac{\hbar}{2m}\frac{\partial^2\psi_n}{\partial x^2}+\frac{1}{2}m\omega^2x^2\psi_n-q\mathcal{E}x\psi_n=E_n\psi_n,\ \ E_n=\left(\frac{1}{2}+n\right)\hbar\omega+E_m. \tag{10}$$

E_m is a energy due to a constant electric field. Then we write the reduced equation,

$$-q\mathcal{E}x\psi_n=-q\mathcal{E}\sqrt{\frac{2\hbar}{m\omega}}\left(\frac{a+a^\dagger}{2}\right)\psi_n=E_m\psi_n. \tag{11}$$

Define κ as,

$$\kappa=-\frac{q\mathcal{E}}{2\hbar\omega}\sqrt{\frac{2\hbar}{m\omega}}=-\frac{1}{\omega}\frac{q\mathcal{E}}{\sqrt{2\hbar m\omega}}. \tag{12}$$

Then Eq. (9) is,

$$H=\hbar\omega\left[a^\dagger a-\kappa\left(a+a^\dagger\right)+\frac{1}{2}\right]=\hbar\omega\left[(a^\dagger-\kappa)(a-\kappa)-\kappa^2.+\frac{1}{2}\right] \tag{13}$$

Now we define new operators from ladder operators,

$$b=a-\kappa,\ \ b^\dagger=a^\dagger-\kappa. \tag{14}$$

The hamiltonian can be repersented by new operators.

$$H=\hbar\omega\left(b^\dagger b-\left(\kappa^2-\frac{1}{2}\right)\right). \tag{15}$$

The Schrödinger equation and reduced equation from Eq. (3) and (11) are,

$$\begin{aligned}&\hbar\omega\left(b^\dagger b-\left(\kappa^2-\frac{1}{2}\right)\right)\psi_n=E_n\psi_n\\ &\hbar\omega\kappa\left(b+b^\dagger+2\kappa\right)\psi_n=E_m\psi_n,\ \ E_n=\left(\frac{1}{2}+n\right)\hbar\omega+E_m.\end{aligned} \tag{16}$$

(3)

Problem 2. The generating function $S(x,t)$ for the Hermite polynomial $H_n(x)$ is defined as

$$S(x,t)=e^{x^2-(t-x)^2}=e^{-t^2+2tx}=\sum_{n=0}^{\infty}\frac{H_n(x)}{n!}t^n. \tag{17}$$

(1) Using this generating function, derive the Hermite differential equation.

(2) Derive the following formula from Eq. (17):

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}, \tag{18}$$

which is called the Rodrigues representation of the Hermite polynomial.

(3) Using Eq. (17), derive the orthogonal relation of the Hermite polynomials

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) dx = 2^n \sqrt{\pi} n! \delta_{nm}. \tag{19}$$

(4) Prove that

$$\left(2x - \frac{d}{dx}\right)^n 1 = H_n(x), \tag{20}$$

(5) Prove

$$\int_{-\infty}^{\infty} x e^{-x^2} H_n(x) H_m(x) dx = \sqrt{\pi} 2^{n-1} n! \delta_{m,n-1} + \sqrt{\pi} 2^n (n+1)! \delta_{m,n+1}. \tag{21}$$

(6) Prove

$$\int_{-\infty}^{\infty} x^2 e^{-x^2} H_n(x) H_n(x) dx = \sqrt{\pi} 2^n n! \left(n + \frac{1}{2}\right). \tag{22}$$

Answer :

(1) The Hermite differential eqaution is,

$$\frac{d^2 y}{dx^2} - 2x \frac{dy}{dx} + \lambda y = 0, \tag{23}$$

λ is a any constant. Then,

$$\begin{aligned} \frac{dS}{dx} &= 2tS = \sum_{n=0}^{\infty} \frac{H'_n(x)}{n!} t^n \\ \frac{d^2 S}{dx^2} &= 4t^2 S = \sum_{n=0}^{\infty} \frac{H''_n(x)}{n!} t^n. \end{aligned} \tag{24}$$

And,

$$\frac{dS}{dt} = 2(-t + x) S = \sum_{n=0}^{\infty} \frac{H_n(x)}{(n-1)!} t^{n-1}. \tag{25}$$

Substituting Eq. (24) and (25) into Eq. (17),

$$asd \tag{26}$$

(2)

(3)

(4)

(5)

(6)

Problem 3. Given the eigenfunctions and eigenenergies of the SHO,

(1) Compute the kinetic and potential energies at the n^{th} level. Show that the results satisfy the virial theorem.

(2) Show that the n^{th} state of the SHO satisfies

$$\Delta x \Delta p = \left(n + \frac{1}{2}\right)\hbar. \tag{27}$$

Problem 4. If a wavefunction desribes a mixed state of the eigenstates of the SHO given as

$$\psi(x,t) = \frac{1}{\sqrt{2}}[\psi_0(x,t) + \psi_1(x,t)], \tag{28}$$

(1) Investigate how the probability density changes in time.

(2) Prove the following relations

$$\begin{aligned}
\langle E \rangle &= \langle H \rangle = \hbar\omega, \\
\langle x \rangle &= \frac{1}{\sqrt{2\alpha}} \cos \omega t, \\
\langle p \rangle &= -\sqrt{\frac{\alpha}{2}}\hbar \sin \omega t,
\end{aligned} \tag{29}$$

where $\alpha = \sqrt{m\omega/\hbar}$.

(3) If

$$\psi(x,t) = \frac{1}{\sqrt{2}}[e^{i\delta_0}\psi_0(x,t) + e^{i\delta}\psi_1(x,t)], \tag{30}$$

discuss the effects of the phase factors δ_0 and δ on $\langle x \rangle$ and $\langle p \rangle$.

Problem 5. Derive the wavefunction in momentum space, which corresponds to the eigenfunctions for the SHO in coordinates, $\psi_n(x)$.

Problem 6. At $t = 0$, the wavefunction for a state is described by

$$\psi(x,0) = \sum_n A_n u_n(x) = \left(\frac{\alpha^2}{\pi}\right)^{1/4} e^{-\alpha^2(x-a)^2/2}. \tag{31}$$

show that after some time t, the probability density changes in time as

$$|\pi(x,t)|^2 = \left(\frac{\alpha^2}{\pi}\right)^{1/4} e^{-\alpha^2(x-a\cos\omega t)^2} \tag{32}$$

and discuss the result.

Problem 7. THe Einstein model for a solid assumes that it consists of many SHOs. If the N atoms are similar each other and oscillate similarly in average, the solid can be explained in terms of N SHOs. At a given temperature T, N atoms are in thermal equilibrium. Then, the Boltzmann distribution is given by

$$P_n = \frac{1}{Z}e^{-E_n/kT} \tag{33}$$

with

$$Z = \sum_n e^{-E_n/kT}, \tag{34}$$

where

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega. \tag{35}$$

(1) Derive the mean energy per an SHO

$$\langle E \rangle = \frac{\hbar\omega}{e^{\hbar\omega/kT} - 1} + \frac{1}{2}\hbar\omega. \tag{36}$$

(2) If U is the internal energy of the solid, derive the specific heat with constant volume

$$C_V = \frac{\partial U}{\partial T}. \tag{37}$$

Show that when T is large, $C_V = 3R$.

(3) Discuss the physics related to this problem as far as you can.