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 Hamiltonian 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. Then the Schrödinger equation and the energy are,

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

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

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

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$\mathbb{I}$ is the identity operator. And,

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

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

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) = \hbar\omega \left(a a^\dagger - \frac{1}{2} \right). \tag{4}$$

Now, recall that there is a constant electric field $\mathcal{E}$. From Eq. (2) and (4), hamiltonian with a constant electric field is,

$$H = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) - q\mathcal{E}x = \hbar\omega \left(a^\dagger a + \frac{1}{2} - \frac{q\mathcal{E}}{2\hbar\omega} \sqrt{\frac{2\hbar}{m\omega}} \left(a + a^\dagger \right) \right) = \hbar\omega \left(a^\dagger a + \frac{1}{2} + \kappa \left(a + a^\dagger \right) \right), \tag{5}$$

where

$$\kappa = -\frac{q\mathcal{E}}{2\hbar\omega} \sqrt{\frac{2\hbar}{m\omega}} = -\frac{q\mathcal{E}}{\omega\sqrt{2\hbar m\omega}}. \tag{6}$$

To eliminate the terms of a and $a^\dagger$, we define the new operator b.

$$b \coloneqq a + \kappa. \tag{7}$$

With this definition, the new operator b commutes with the a.

$$\begin{aligned} &[a, b] = a(a + \kappa) - (a + \kappa)a = aa - aa + \kappa a - \kappa a = 0, \\ &\left[b, b^\dagger\right] = \left[(a + \kappa), (a + \kappa)^\dagger\right] = \mathbb{I}. \end{aligned} \tag{8}$$

Then the hamiltonian with a constant electric field H is

$$\begin{aligned} H &= \hbar\omega \left((a^\dagger + \kappa)(a + \kappa) - \kappa(a + a^\dagger) - \kappa^2 + \frac{1}{2} + \kappa \left(a + a^\dagger \right) \right) \\ &= \hbar\omega \left(b^\dagger b - \kappa^2 + \frac{1}{2} \right). \end{aligned} \tag{9}$$

Then H is

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

We can write the eigenvalue equation with the new operator.

$$H\psi'_n = E'_n \psi'_n, \tag{10}$$

$$\hbar\omega \left(b^\dagger b + \frac{1}{2} \right) \psi'_n = \left(E'_n + \hbar\omega\kappa^2 \right) \psi'_n. \tag{11}$$

The operator b and $b^\dagger$ behave to $H + \hbar\omega\kappa^2$ and ψ'_n as a and $a^\dagger$ did to H and ψ_n. From Eq. (8) and Eq. (11),

$$\begin{aligned} \hbar\omega \left(b^\dagger b + \frac{1}{2} \right) (b\psi'_n) &= \hbar\omega \left(b^\dagger b b + \frac{1}{2} b \right) \psi'_n = \hbar\omega \left(b b^\dagger b - \frac{1}{2} b \right) \psi'_n = \hbar\omega b \left(b^\dagger b - \frac{1}{2} \right) \psi'_n \\ &= \hbar\omega b \left(b^\dagger b + \frac{1}{2} - 1 \right) \psi'_n = \left(E'_n + \hbar\omega\kappa^2 - \hbar\omega \right) (b\psi'_n). \end{aligned} \tag{12}$$

Evidently, there is the ground state of ψ'_n, that is,

$$b\psi'_0 = \left(\sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{\hbar}{m\omega} \frac{d}{dx} \right) + \kappa \right) \psi'_0(x) = 0. \tag{13}$$

It is ODE of the first order about x.

$$\frac{d\psi_0'}{dx} = -\frac{m\omega}{\hbar}\left(\sqrt{\frac{2\hbar}{m\omega}}\kappa^2 + x\right)\psi_0' = -\left(\sqrt{\frac{2m\omega}{\hbar}}\kappa + \frac{m\omega}{\hbar}x\right)\psi_0'.$$

The solution of this ODE is,

$$\psi_0' = A\exp\left(-\left(\frac{m\omega}{2\hbar}x^2 + \sqrt{\frac{2m\omega}{\hbar}}\kappa x\right)\right) = A\exp\left(-\frac{m\omega}{2\hbar}\left(x + \sqrt{\frac{2\hbar}{m\omega}}\kappa\right)^2 + \kappa^2\right)$$

Normalization constant A is,

$$|A|^2\int\exp\left(-\frac{m\omega}{\hbar}\left(x + \sqrt{\frac{2\hbar}{m\omega}}\kappa\right)^2 + 2\kappa^2\right)dx = |A|^2 e^{2\kappa^2}\sqrt{\frac{\pi\hbar}{m\omega}} = 1, \tag{14}$$

$$A = \pm\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\kappa^2}. \tag{15}$$

Therefore the ground state of ψ_n' is,

$$\psi_0' = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\exp\left(-\frac{m\omega}{2\hbar}\left(x + \sqrt{\frac{2\hbar}{m\omega}}\kappa\right)^2\right).$$

Use Eq. (11) and Eq. (13) to obtain E_0'.

$$\frac{1}{2}\hbar\omega\psi_0' = (E_0' + \hbar\omega\kappa)\,\psi_0',\ \ E_0' = \left(\frac{1}{2} - \kappa\right)\hbar\omega. \tag{16}$$

From the application of Eq. (12), as n increases by 1, so does energy by a $\hbar\omega$. And ψ_n' is,

$$\psi_n' = A_n'(b^\dagger)^n\psi_0' = A_n'\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\left(\sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{\hbar}{m\omega}\frac{d}{dx}\right) + \kappa\right)^n\exp\left(-\frac{m\omega}{2\hbar}\left(x + \sqrt{\frac{2\hbar}{m\omega}}\kappa\right)^2\right). \tag{17}$$

A_n' is the normalization constant. Substituting ξ as,

$$\xi \coloneqq \sqrt{\frac{m\omega}{2\hbar}}x + \kappa,\ \ dx = \sqrt{\frac{2\hbar}{m\omega}}d\xi. \tag{18}$$

Then,

$$\psi_n' = A_n'\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\left(\xi - \frac{1}{2}\frac{d}{d\xi}\right)^n e^{-\frac{1}{2}\xi^2} = A_n'\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} 2^{-n}H_n(\xi)e^{-\xi^2}. \tag{19}$$

From Eq.(6) and (18),

$$\xi = \sqrt{\frac{m\omega}{2\hbar}}x - \frac{q\mathcal{E}}{2\hbar\omega}\sqrt{\frac{2\hbar}{m\omega}} = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{q\mathcal{E}}{m\omega^2}\right). \tag{20}$$

Finally we obtain the exact form of the nth eigenvector ψ'.

$$\psi_n' = A_n'\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} 2^{-n}H_n\left(\sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{q\mathcal{E}}{m\omega^2}\right)\right)\exp\left(-\frac{m\omega}{2\hbar}\left(x - \frac{q\mathcal{E}}{m\omega^2}\right)^2\right). \tag{21}$$

Eigenvalue E_0' can be obtained Substituting Eq. (21) into Eq. (11).

$$\frac{1}{2}\hbar\omega\psi_0' = (E_0' + \hbar\omega\kappa^2)\psi_0',\ \ E_0' = \left(\frac{1}{2} - \kappa^2\right)\hbar\omega. \tag{22}$$

From Eq. (8) and (12) E_n' is,

$$E_n' = \left(\frac{1}{2} + n - \kappa^2\right)\hbar\omega = \left(\frac{1}{2} + n - \frac{q^2\mathcal{E}^2}{2\hbar^2 m^2\omega^3}\right)\hbar\omega. \tag{23}$$

(3) Let us compare the energy levels and eigenstate of SHO with not charged.

$$\psi_n = B_n H_n\left(\sqrt{\frac{m\omega}{2\hbar}}x\right)\exp\left(-\frac{m\omega}{2\hbar}x^2\right),\ \ E_n = \left(n+\frac{1}{2}\right)\hbar\omega \tag{24}$$

$$\psi'_n = B'_n H_n\left(\sqrt{\frac{m\omega}{2\hbar}}\left(x-\frac{q\mathcal{E}}{m\omega^2}\right)\right)\exp\left(-\frac{m\omega}{2\hbar}\left(x-\frac{q\mathcal{E}}{m\omega^2}\right)^2\right),\ \ E'_n = \left(\frac{1}{2}+n-\frac{q^2\mathcal{E}^2}{2\hbar^2 m^2\omega^3}\right)\hbar\omega. \tag{25}$$

The energy levels with a constant electric field are as small as $\frac{q^2\mathcal{E}^2}{2\hbar m^2\omega^2}$and the eigenvectors with a constant electric field get the effect of shift by $-\frac{q\mathcal{E}}{m\omega^2}$ without the change of the shape for any n.

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

$$S(x,t) = e^{x^2-(t-x)^2} = e^{-t^2+2tx} = \sum_{n=0}^{\infty}\frac{H_n(x)}{n!}t^n. \tag{26}$$

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

(2) Derive the following formula from Eq. (26):

$$H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}, \tag{27}$$

which is called the Rodrigues representation of the Hermite polynomial.

(3) Using Eq. (26), derive the orthogonal relation of the Hermite polynomials

$$\int_{-\infty}^{\infty} e^{-x^2}H_n(x)H_m(x)dx = 2^n\sqrt{\pi}n!\delta_{nm}. \tag{28}$$

(4) Prove that

$$\left(2x-\frac{d}{dx}\right)^n 1 = H_n(x), \tag{29}$$

(5) Prove

$$\int_{-\infty}^{\infty} xe^{-x^2}H_n(x)H_m(x)dx = \sqrt{\pi}2^{n-1}n!\delta_{m,n-1} + \sqrt{\pi}2^n(n+1)!\delta_{m,n+1}. \tag{30}$$

(6) Prove

$$\int_{-\infty}^{\infty} x^2e^{-x^2}H_n(x)H_n(x)dx = \sqrt{\pi}2^n n!\left(n+\frac{1}{2}\right). \tag{31}$$

Answer :

(1) The Hermite differential eqaution is,

$$\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + \lambda y = 0, \tag{32}$$

λ is a any constant. Derivatives for x of generating function S are,

$$\begin{aligned}\frac{dS}{dx} &= 2tS = \sum_{n=0}^{\infty}\frac{H'_n(x)}{n!}t^n \\ \frac{d^2S}{dx^2} &= 4t^2S = \sum_{n=0}^{\infty}\frac{H''_n(x)}{n!}t^n.\end{aligned} \tag{33}$$

And,

$$\frac{dS}{dt} = 2(-t+x)S = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} n t^{n-1} = -\frac{dS}{dx} + 2xS. \tag{34}$$

From Eq. (33),

$$\frac{dS}{dx} = \frac{1}{2t}\frac{d^2S}{dx^2} = \frac{1}{2}\sum_{n=0}^{\infty} \frac{H_n''(x)}{n!} t^{n-1}$$

$$2xS = 2x\frac{1}{2t}\frac{dS}{dt} = x\sum_{n=0}^{\infty} \frac{H_n'(x)}{n!} t^{n-1}$$

Then Eq. (34) is,

$$\sum_{n=0}^{\infty} \frac{H_n(x)}{n!} n t^{n-1} = -\frac{1}{2}\sum_{n=0}^{\infty} \frac{H_n''(x)}{n!} t^{n-1} + x\sum_{n=0}^{\infty} \frac{H_n'(x)}{n!} t^{n-1}.$$

Finally we obtain,

$$\sum_{n=0}^{\infty} \left(\frac{H_n''(x) - 2xH_n'(x) + 2nH_n(x)}{n!} t^{n-1} \right) = 0.$$

It is true for any t when all coefficient is zero. So,

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0. \tag{35}$$

(2) From Eq. (26),

$$e^{-(t-x)^2+x^2} = e^{x^2} e^{-(t-x)^2}.$$

And,

$$e^{x^2} e^{-(t-x)^2} = e^{x^2} \sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{d^n}{dt^n} e^{-(t-x)^2} \bigg|_{t=0} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^n.$$

Since the series representation is unique,

$$H_n(x) = e^{x^2} \frac{d^n}{dt^n} e^{-(t-x)^2} \bigg|_{t=0}. \tag{36}$$

If we regard t as just the parameter, Eq. (36) is true for any t. A differential part of a LHS is,

$$\frac{d^n}{dt^n} e^{-(t-x)^2} \bigg|_{t=0} = (-1)^n \frac{d^n}{dx^n} e^{-(t-x)^2} \bigg|_{t=0} = (-1)^n \frac{d^n}{dx^n} e^{-x^2}$$

Finally we obtain,

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}. \tag{37}$$

(3) First, when $t = 1$ and $t = -1$, Eq. (26) is,

$$e^{2x-1} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!}$$

$$e^{-2x-1} = \sum_{n=0}^{\infty} (-1)^n \frac{H_n(x)}{n!}.$$

For checking the value $2^n\sqrt{\pi}n!$, consider a integration as,

$$\int_{-\infty}^{\infty} e^{-x^2} H_m(x) e^{2x-1}\,dx = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x)\,dx \tag{38}$$

The RHS is,

$$\int_{-\infty}^{\infty} e^{-x^2} H_m(x) e^{2x-1}\,dx = (-1)^m \int_{-\infty}^{\infty} e^{2x-1} \frac{d^m}{dx^m} e^{-x^2}\,dx$$

Using the integration by part to RHS,

$$\begin{aligned}\int_{-\infty}^{\infty} e^{2x-1} \frac{d^m}{dx^m} e^{-x^2}\,dx &= e^{2x-1} \frac{d^{m-1}}{dx^{m-1}} e^{-x^2}\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} 2e^{2x-1} \frac{d^{m-1}}{dx^{m-1}} e^{-x^2}\,dx \\ &= -2 \int_{-\infty}^{\infty} e^{2x-1} \frac{d^{m-1}}{dx^{m-1}} e^{-x^2}\,dx.\end{aligned}$$

Repetition of the integration by part for m times conserves the form in the integration multiplying $(-2)^m$.

$$\int_{-\infty}^{\infty} e^{2x-1} \frac{d^m}{dx^m} e^{-x^2}\,dx = (-2)^m \int_{-\infty}^{\infty} e^{2x-1} e^{-x^2}\,dx = (-2)^m \sqrt{\pi}.$$

Therefore, Eq. (38) is,

$$\sum_{n=0}^{\infty} \frac{1}{n!} \int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x)\,dx = (-1)^m (-2)^m \sqrt{\pi} = 2^m \sqrt{\pi}.$$

Now, check the orthogonality. From Eq. (35),

$$e^{x^2} \frac{d}{dx} \left(e^{-x^2} H_n'(x) \right) + 2n H_n(x) = 0.$$

Multiplying e^{-x^2},

$$\int_{-\infty}^{\infty} \frac{d}{dx} \left(e^{-x^2} H_n'(x) \right) H_m(x)\,dx + 2n \int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x)\,dx = 0.$$

Change m and n each other, subtract the previous one,

$$\int_{-\infty}^{\infty} \frac{d}{dx} \left(e^{-x^2} H_n' \right) H_m - \frac{d}{dx} \left(e^{-x^2} H_m' \right) H_n\,dx + 2(n-m) \int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x)\,dx = 0.$$

Integrations by part of first two terms are,

$$\begin{aligned}&\int_{-\infty}^{\infty} \frac{d}{dx} \left(e^{-x^2} H_n' \right) H_m - \frac{d}{dx} \left(e^{-x^2} H_m' \right) H_n\,dx \\ &= e^{-x^2} H_n' H_m\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} e^{-x^2} H_n' H_m'\,dx - e^{-x^2} H_n H_m'\Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} e^{-x^2} H_n' H_m'\,dx \\ &= 0.\end{aligned}$$

It means that,

$$2(n-m) \int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x)\,dx = 0.$$

If $n \neq m$, the integration is a zero. For this reason,

$$\sum_{n=0}^{\infty} \frac{1}{n!} \int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x)\,dx = \frac{1}{m!} \int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_m(x)\,dx = 2^m \sqrt{\pi}.$$

Finally we obtain,

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) dx = 2^n n! \sqrt{\pi} \delta_{nm}. \tag{39}$$

(4) *Proof.* We use the mathematical induction. If $n = 0$ and $n = 1$, then,

$$H_0(x) = 1, \;\; H_1(x) = 2x.$$

The statement is true. Suppose it is true:

$$H_k(x) = \left(2x - \frac{d}{dx}\right)^k 1.$$

Then,

$$H_{k+1}(x) = \left(2x - \frac{d}{dx}\right)\left(2x - \frac{d}{dx}\right)^k 1 = \left(2x - \frac{d}{dx}\right) H_k(x)$$

From Eq. (37),

$$\begin{aligned}
\left(2x - \frac{d}{dx}\right) H_k(x) &= \left(2x - \frac{d}{dx}\right)(-1)^k e^{x^2} \frac{d^k}{dx^k} e^{-x^2} \\
&= (-1)^k 2xe^{x^2} \frac{d^k}{dx^k} e^{-x^2} - (-1)^k 2xe^{x^2} \frac{d^k}{dx^k} e^{-x^2} - (-1)^k e^{x^2} \frac{d^{k+1}}{dx^{k+1}} e^{-x^2} \\
&= (-1)^{k+1} = e^{x^2} \frac{d^{k+1}}{dx^{k+1}} e^{-x^2} = H_{k+1}(x).
\end{aligned}$$

Hence this statement is true for $n = k + 1$.
By mathematical induction, this statement is true for any n. □

(5) *Proof.* Set I_{nm},

$$\begin{aligned}
I_{nm} &= \int_{-\infty}^{\infty} xe^{-x^2} H_n(x) H_m(x)\, dx \\
&= -\frac{1}{2} e^{-x^2} H_n(x) H_m(x) \Big|_{-\infty}^{\infty} + \frac{1}{2} \int_{-\infty}^{\infty} e^{-x^2} \left(H_n'(x) H_m(x) + H_n(x) H_m'(x)\right) dx \\
&= \frac{1}{2} \int_{-\infty}^{\infty} e^{-x^2} H_n'(x) H_m(x)\, dx + \frac{1}{2} \int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m'(x)\, dx.
\end{aligned}$$

From Eq. (37),

$$\begin{aligned}
H_n'(x) &= \frac{d}{dx}\left((-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}\right) = (-1)^n \left(2xe^{x^2} \frac{d^n}{dx^n} e^{-x^2} + e^{x^2} \frac{d^{n+1}}{dx^{n+1}} e^{-x^2}\right) \\
&= 2xH_n(x) - H_{n+1}(x).
\end{aligned} \tag{40}$$

Then I_{nm} is,

$$\begin{aligned}
I_{nm} &= \frac{1}{2} \int_{-\infty}^{\infty} e^{-x^2} (2xH_n(x) - H_{n+1}(x)) H_m(x)\, dx + \frac{1}{2} \int_{-\infty}^{\infty} e^{-x^2} H_n(x)(2xH_m(x) - H_{m+1}(x))\, dx \\
&= 2I_{nm} - \frac{1}{2} \int_{-\infty}^{\infty} e^{-x^2} H_{n+1}(x) H_m(x)\, dx - \frac{1}{2} \int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_{m+1}(x)\, dx.
\end{aligned}$$

Hence,

$$I_{nm} = \frac{1}{2}\left(\int_{-\infty}^{\infty} e^{-x^2} H_{n+1}(x) H_m(x)\, dx + \int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_{m+1}(x)\, dx\right).$$

From Eq. (39), we obtain that,

$$\begin{aligned}
I_{nm} &= \frac{1}{2}\left(2^{n+1}\sqrt{\pi}(n+1)!\delta_{n+1,m} + 2^n \sqrt{\pi} n! \delta_{n,m+1}\right) \\
&= 2^n \sqrt{\pi}(n+1)!\delta_{n+1,m} + 2^{n-1}\sqrt{\pi} n! \delta_{n,m+1}.
\end{aligned} \tag{41}$$

Therefore the statement is true. □

(6) *Proof.* Eq. (31) is,

$$\int_{-\infty}^{\infty} x^2 e^{-x^2} H_n H_n \, dx = -\frac{1}{2} x e^{-x^2} H_n H_n \Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} x e^{-x^2} H_n' H_n \, dx - \frac{1}{2} \int_{-\infty}^{\infty} e^{-x^2} H_n H_n \, dx.$$

From Eq. (40), the second term of the RHS is,

$$\int_{-\infty}^{\infty} x e^{-x^2} H_n' H_n \, dx = \int_{-\infty}^{\infty} 2x^2 e^{-x^2} H_n H_n \, dx - \int_{-\infty}^{\infty} x e^{-x^2} H_{n+1} H_n \, dx.$$

Hence,

$$\begin{aligned}\int_{-\infty}^{\infty} x^2 e^{-x^2} H_n H_n \, dx &= \int_{-\infty}^{\infty} 2x^2 e^{-x^2} H_n H_n \, dx - \int_{-\infty}^{\infty} x e^{-x^2} H_{n+1} H_n \, dx - \frac{1}{2} \int_{-\infty}^{\infty} e^{-x^2} H_n H_n \, dx \\ &= \int_{-\infty}^{\infty} x e^{-x^2} H_{n+1} H_n \, dx + \frac{1}{2} \int_{-\infty}^{\infty} e^{-x^2} H_n H_n \, dx.\end{aligned}$$

From Eq. (41) and (39),

$$\begin{aligned}\int_{-\infty}^{\infty} x^2 e^{-x^2} H_n H_n \, dx &= \sqrt{\pi} 2^{n-1} n! \delta_{n+1,n-1} + \sqrt{\pi} 2^n (n+1)! \delta_{n+1,n+1} - \sqrt{\pi} 2^{n-1} n! \\ &= \sqrt{\pi} 2^n n! \left(n + \frac{1}{2}\right).\end{aligned} \tag{42}$$

Therefore the statement is true. □

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

$$\Delta x \Delta p = \left(n + \frac{1}{2}\right) \hbar. \tag{43}$$

Answer :

(1) The eigenvector and eigenfunction of the SHO are,

$$\psi_n(x) = \psi_n^*(x) = (n! 2^n)^{-\frac{1}{2}} \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega}{2\hbar} x^2\right) H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right), \quad E_n = \left(n + \frac{1}{2}\right) \hbar\omega. \tag{44}$$

The expectation value of the kinetic energy is,

$$\langle T_n \rangle = \frac{1}{2m} \int \psi_n^* p^2 \psi_n \, dx = \frac{\langle p^2 \rangle}{2m}. \tag{45}$$

Since the expectation value of the kinetic energy is an integer multiple of the square of momentum, we just calculate the expectation value of the square of momentum. Using the integration by part,

$$\langle p^2 \rangle = -\hbar^2 \int \psi_n^* \frac{\partial^2 \psi_n}{\partial x^2} \, dx = \hbar^2 \int \frac{\partial \psi_n^*}{\partial x} \frac{\partial \psi_n}{\partial x} \, dx \tag{46}$$

Changing the variable,

$$\sqrt{\frac{m\omega}{\hbar}} x = \xi, \quad \frac{\partial \psi_n}{\partial x} = \frac{\partial \psi_n}{\partial \xi} \frac{\partial \xi}{\partial x} = \sqrt{\frac{m\omega}{\hbar}} \frac{\partial \psi_n}{\partial \xi} \tag{47}$$

Then,

$$\frac{\partial \psi_n}{\partial \xi} = (n!2^n)^{-\frac{1}{2}} \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} (-\xi H_n(\xi) + H_n'(\xi)) e^{-\frac{\xi^2}{2}}.$$

The integration of Eq. (46) is,

$$\begin{aligned}
\int \frac{\partial \psi_n^*}{\partial x}\frac{\partial \psi_n}{\partial x}\, dx &= (n!2^n)^{-1} \sqrt{\frac{m\omega}{\hbar\pi}}\frac{m\omega}{\hbar} \int (-\xi H_n(\xi) + H_n'(\xi))^2 e^{-\xi^2} \sqrt{\frac{\hbar}{m\omega}} d\xi \\
&= (n!2^n)^{-1} \frac{m\omega}{\hbar\sqrt{\pi}} \int (-\xi H_n(\xi) + H_n'(\xi))^2 e^{-\xi^2}\, d\xi
\end{aligned}$$

From Eq. (40)

$$\begin{aligned}
\int (-\xi H_n(\xi) + H_n'(\xi))^2 e^{-\xi^2}\, d\xi &= \int (-\xi H_n(\xi) + 2\xi H_n(\xi) - H_{n+1}(\xi))^2 e^{-\xi^2}\, d\xi \\
&= \int (\xi H_n(\xi) - H_{n+1}(\xi))^2 e^{-\xi^2}\, d\xi \\
&= \int ((\xi^2 H_n H_n - 2\xi H_n H_{n+1} + H_{n+1} H_{n+1}) e^{-\xi^2}\, d\xi.
\end{aligned}$$

We can use Eq. (39), (41) and (42) to calculate this integration.

$$\begin{aligned}
\int \xi^2 H_n H_n e^{-\xi^2}\, dx &= 2^n n! \sqrt{\pi}\left(n + \frac{1}{2}\right) \\
\int \xi H_n H_{n+1} e^{-\xi^2}\, dx &= 2^n (n+1)! \sqrt{\pi} \\
\int H_{n+1} H_{n+1} e^{-\xi^2}\, dx &= 2^{n+1} (n+1)! \sqrt{\pi}.
\end{aligned}$$

Then,

$$\begin{aligned}
\int (-\xi H_n(\xi) + H_n'(\xi))^2 e^{-\xi^2}\, d\xi &= \sqrt{\pi} 2^n n! \left(n + \frac{1}{2} - 2(n+1) + 2(n+1)\right) \\
&= \sqrt{\pi} 2^n n! \left(n + \frac{1}{2}\right).
\end{aligned}$$

Therefore the expectation value of the square of the momentum is,

$$\langle p^2 \rangle = \hbar^2 (n!2^n)^{-1} \frac{m\omega}{\hbar\sqrt{\pi}} \sqrt{\pi} 2^n n! \left(n + \frac{1}{2}\right) = \hbar m\omega \left(n + \frac{1}{2}\right). \tag{48}$$

We obtain the expectation value of the kinetic energy.

$$\langle T_n \rangle = \frac{\langle p^2 \rangle}{2m} = \frac{1}{2}\hbar\omega\left(n + \frac{1}{2}\right). \tag{49}$$

The expectation value of the potential energy is,

$$\langle V_n \rangle = \int \psi_n^* \frac{1}{2} m\omega^2 x^2 \psi_n\, dx = \frac{1}{2} m\omega^2 \int \psi_n^* x^2 \psi_n\, dx = \frac{1}{2} m\omega^2 \langle x^2 \rangle.$$

From Eq. (47), the expectation value of the square of x is,

$$\begin{aligned}
\langle x^2 \rangle = \int \psi_n^* x^2 \psi_n\, dx = \langle x^2 \rangle &= \left(\frac{\hbar}{m\omega}\right)^{\frac{3}{2}} \int \psi_n^*(\xi) \xi^2 \psi_n(\xi)\, d\xi \\
&= (n!2^n)^{-1} \sqrt{\frac{m\omega}{\hbar\pi}} \left(\frac{\hbar}{m\omega}\right)^{\frac{3}{2}} \int \xi^2 H_n(\xi) H_n(\xi) e^{-\xi^2}\, d\xi
\end{aligned}$$

The integration part can be calculated by Eq. (42).

$$\int \xi^2 H_n(\xi) H_n(\xi) e^{-\xi^2}\, d\xi = \sqrt{\pi} 2^n n! \left(n + \frac{1}{2}\right).$$

So, $\langle x^2 \rangle$ is,

$$\langle x^2 \rangle = \frac{\hbar}{m\omega}\left(n + \frac{1}{2}\right). \tag{50}$$

Finally we obtain the expectation value of the potential energy.

$$\langle V_n \rangle = \frac{1}{2} m\omega^2 (n! 2^n)^{-1} \sqrt{\frac{m\omega}{\hbar\pi}} \left(\frac{\hbar}{m\omega}\right)^{\frac{3}{2}} \sqrt{\pi} 2^n n! \left(n + \frac{1}{2}\right) = \frac{1}{2}\hbar\omega \left(n + \frac{1}{2}\right). \tag{51}$$

Let us confirm that the results satisfy the virial theorem. In this condition the virial theorem is,

$$\left\langle x \frac{\partial V}{\partial x} \right\rangle = 2 \langle T \rangle .$$

Substituting Eq. (49) and (51),

$$\left\langle x \frac{\partial V}{\partial x} \right\rangle = m\omega^2 \int \psi_n^* x^2 \psi_n \, dx = 2 \langle V_n \rangle = 2 \langle T_n \rangle .$$

The results satisfy the virial theorem.

(2) Let us calculate Δx and Δp. From the definition, Δx and Δp are,

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}, \ \ \Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}.$$

$\langle x \rangle$ is,

$$\langle x \rangle = \int x \psi^* \psi \, dx = (n! 2^n)^{-1} \sqrt{\frac{m\omega}{\hbar\pi}} \left(\frac{\hbar}{m\omega}\right) \int \xi H_n H_n e^{-\xi^2} \, d\xi.$$

Since the integrated term is an even function and the integration interval is symmetric, the integration is a zero. Therefore,

$$\langle x \rangle = 0.$$

With Eq. (50) Δx is,

$$\Delta x = \sqrt{\langle x^2 \rangle} = \sqrt{\frac{\hbar}{m\omega}\left(n + \frac{1}{2}\right)}.$$

To calculate Δp, $\langle p \rangle$ is,

$$\langle p \rangle = \int \psi^* p \psi \, dx = -i\hbar \int \psi_n^* \frac{\partial \psi_n}{\partial x} \, dx.$$

The integration by part is,

$$\langle p \rangle = -i\hbar \int \psi_n^* \frac{\partial \psi_n}{\partial x} \, dx = i\hbar \int \frac{\partial \psi_n^*}{\partial x} \psi_n \, dx.$$

From Eq. (44), $\psi = \psi^*$. So,

$$\langle p \rangle = i\hbar \int \frac{\partial \psi_n^*}{\partial x} \psi_n \, dx = i\hbar \int \psi_n^* \frac{\partial \psi_n}{\partial x} \, dx = -\langle p \rangle.$$

Therefore,

$$\langle p \rangle = 0.$$

With Eq. (48) Δp is,

$$\Delta p = \sqrt{\langle p^2 \rangle} = \sqrt{\hbar m\omega \left(n + \frac{1}{2}\right)}.$$

Finally $\Delta x \Delta p$ is,

$$\Delta x \Delta p = \sqrt{\frac{\hbar}{m\omega}\left(n + \frac{1}{2}\right)}\sqrt{\hbar m\omega \left(n + \frac{1}{2}\right)} = \hbar \left(n + \frac{1}{2}\right). \tag{52}$$

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

$$\psi(x,t) = \frac{1}{\sqrt{2}}[\psi_0(x,t) + \psi_1(x,t)], \tag{53}$$

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

(2) Prove the following relations

$$\begin{aligned} \langle E \rangle &= \langle H \rangle = \hbar\omega, \\ \langle x \rangle &= \frac{1}{\sqrt{2}\alpha}\cos\omega t, \\ \langle p \rangle &= -\frac{\alpha}{\sqrt{2}}\hbar \sin\omega t, \end{aligned} \tag{54}$$

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

(3) If

$$\psi(x,t) = \frac{1}{\sqrt{2}}[e^{i\delta_0}\psi_0(x,t) + e^{i\delta}\psi_1(x,t)], \tag{55}$$

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

Answer :

(1) The probability density of this wavefunction is,

$$\rho = |\psi(x,t)|^2 = \frac{1}{2}\left[|\psi_0(x,t)|^2 + |\psi_1(x,t)|^2 + \psi_0^*(x,t)\psi_1(x,t) + \psi_0(x,t)\psi_1^*(x,t)\right]. \tag{56}$$

To consider the time factor $\exp\left(-\frac{iE_n}{\hbar}t\right)$, we have to know the energy of the SHO. The Schrödinger equation of the SHO is,

$$H\psi_n(x,0) = E_n\psi_n(x,0) = \left(\frac{1}{2} + n\right)\hbar\omega\psi_n(x,0). \tag{57}$$

And,

$$\psi_0(x,t) = \psi_0(x,0)\exp\left(-\frac{iE_0}{\hbar}t\right), \quad \psi_1(x,t) = \psi_1(x,0)\exp\left(-\frac{iE_1}{\hbar}t\right)$$

Therefore energys of ψ_0 and ψ_1 are,

$$\begin{aligned} E_0 &= \frac{1}{2}\hbar\omega, \quad \psi_0(x,t) = \psi_0(x,0)e^{-\frac{1}{2}i\omega t}, \\ E_1 &= \frac{3}{2}\hbar\omega, \quad \psi_1(x,t) = \psi_1(x,0)e^{-\frac{3}{2}i\omega t}. \end{aligned} \tag{58}$$

Then Eq. (56) is,

$$\rho = \frac{1}{2}\left[|\psi_0(x,0)|^2 + |\psi_1(x,0)|^2 + \psi_0^*(x,0)\psi_1(x,0)e^{-i\omega t} + \psi_0(x,0)\psi_1^*(x,0)e^{i\omega t}\right]$$

Since $\psi_0(x,0)$ and $\psi_0(x,0)$ are the eigenstate of the SHO,

$$\psi_0(x,0) = \psi_0^*(x,0), \ \ \psi_1(x,0) = \psi_1^*(x,0) \tag{59}$$

Then the last two terms are,

$$\psi_0^*(x,0)\psi_1(x,0)e^{-i\omega t} + \psi_0(x,0)\psi_1^*(x,0)e^{i\omega t} = 2\psi_0(x,0)\psi_1(x,0)\cos\omega t.$$

The probability density is,

$$\rho = \frac{1}{2}\left[|\psi_0(x,0)|^2 + |\psi_1(x,0)|^2 + 2\psi_0(x,0)\psi_1(x,0)\cos\omega t\right] \tag{60}$$

Because $-1 \leq \cos\omega t \leq 1$, the probability density oscillates having the amplitude between ρ_{min} and ρ_{max}.

$$\rho_{min} = \frac{1}{2}\left(\psi_0(x,0) - \psi_1(x,0)\right)^2, \ \ \rho_{max} = \frac{1}{2}\left(\psi_0(x,0) + \psi_1(x,0)\right)^2. \tag{61}$$

(2) From Eq. (57), Eq. (58) and Eq. (59), the expectation value of the hamiltonian is,

$$\begin{aligned}
\langle H\rangle &= \int \psi^*(x,t)H\psi(x,t)\,dx = \int \psi^*(x,t)E\psi(x,t)\,dx = \langle E\rangle \\
&= \frac{1}{2}\int [\psi_0^*(x,t) + \psi_1^*(x,t)][H\psi_0(x,t) + H\psi_1(x,t)]\,dx \\
&= \frac{1}{2}\int \left[e^{\frac{1}{2}i\omega t}\psi_0(x,0) + e^{\frac{3}{2}i\omega t}\psi_1(x,0)\right]\left[\frac{1}{2}\hbar\omega e^{-\frac{1}{2}i\omega t}\psi_0(x,0) + \frac{3}{2}\hbar\omega e^{-\frac{3}{2}i\omega t}\psi_1(x,0)\right]\,dx.
\end{aligned} \tag{62}$$

Since $\psi_0(x,0)$ and $\psi_1(x,0)$ are orthogonal to each other, the term of $\psi_0(x,0)\psi_1(x,0)$ can be canceled out.

$$\langle H\rangle = \frac{1}{2}\int\left[\frac{1}{2}\hbar\omega|\psi_0(x,0)|^2 + \frac{3}{2}\hbar\omega|\psi_1(x,0)|^2\right]\,dx = \frac{1}{2}\left[\frac{1}{2}\hbar\omega + \frac{3}{2}\hbar\omega\right] = \hbar\omega. \tag{63}$$

The expectation value of the x is,

$$\langle x\rangle = \int \psi^*(x,t)x\psi(x,t)\,dx = \int x|\psi(x,t)|^2\,dx = \int x\rho\,dx \tag{64}$$

From the Eq. (60),

$$\langle x\rangle = \frac{1}{2}\int x\left[|\psi_0(x,0)|^2 + |\psi_1(x,0)|^2 + 2\psi_0(x,0)\psi_1(x,0)\cos\omega t\right]\,dx. \tag{65}$$

Since the first two terms in the braket are the even functions, these terms can be canceled out.

$$\langle x\rangle = \int x\psi_0(x,0)\psi_1(x,0)\cos\omega t\,dx. \tag{66}$$

$\psi_0(x,0)$ and $\psi_1(x,0)$ are the eigenstate of the SHO. Therefore,

$$\begin{aligned}
\psi_0(x,0) &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\exp\left(-\frac{m\omega}{2\hbar}x^2\right) \\
\psi_1(x,0) &= \sqrt{2}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\sqrt{\frac{m\omega}{\hbar}}x\exp\left(-\frac{m\omega}{2\hbar}x^2\right).
\end{aligned}$$

Then the expectation value of x is,

$$\langle x\rangle = \sqrt{\frac{2}{\pi}}\frac{m\omega}{\hbar}\cos\omega t\int x^2\exp\left(-\frac{m\omega}{\hbar}x^2\right)\,dx.$$

Substituting $\alpha = \sqrt{m\omega/\hbar}$,

$$\langle x \rangle = \sqrt{\frac{2}{\pi}}\alpha^2 \cos\omega t \left(-\frac{1}{2\alpha}\right)\left(\frac{d}{d\alpha}\right)\int e^{-\alpha^2 x^2}\,dx = -\sqrt{\frac{1}{2\pi}}\alpha\cos\omega t\left(\frac{d}{d\alpha}\right)\frac{\sqrt{\pi}}{\alpha}$$
$$= \sqrt{\frac{1}{2\pi}}\alpha\cos\omega t\left(\frac{\sqrt{\pi}}{\alpha^2}\right) = \frac{1}{\sqrt{2}\alpha}\cos\omega t.$$

Before finding expectation value of p, let us show that,

$$\langle p \rangle = m\frac{d}{dt}\langle x \rangle. \tag{67}$$

From the Generalized Ehrenfest's Theorem,

$$i\hbar\frac{d}{dt}\langle x \rangle = \langle [x, H] \rangle + i\hbar\left\langle \frac{\partial x}{\partial t}\right\rangle = \left\langle \left[x, \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2\right]\right\rangle = \frac{1}{2m}\left\langle \left[x, p^2\right]\right\rangle.$$

Since $\left[x, p^2\right] = 2i\hbar p$,

$$i\hbar\frac{d}{dt}\langle x \rangle = \frac{i\hbar}{m}\langle p \rangle.$$

Hence,

$$\langle p \rangle = m\frac{d}{dt}\langle x \rangle = -\frac{m\omega}{\sqrt{2}\alpha}\sin\omega t = -\frac{\alpha}{\sqrt{2}}\hbar\sin\omega t. \tag{68}$$

(3) If there are the phase factors δ_0 and δ, Eq. (66) changes into,

$$\langle x \rangle = \frac{1}{2}\left(e^{i(\delta_0-\delta)} + e^{-i(\delta_0-\delta)}\right)\int x\left[\psi_0(x,0)\psi_1(x,0)\cos\omega t\right]\,dx$$
$$= \cos(\delta_0 - \delta)\int x\left[\psi_0(x,0)\psi_1(x,0)\cos\omega t\right]\,dx.$$

Let define $\Delta\delta$ as $\Delta\delta = \delta_0 - \delta$. Then $\langle x \rangle$ is,

$$\langle x \rangle = \cos\Delta\delta\int x\left[\psi_0(x,0)\psi_1(x,0)\cos\omega t\right]\,dx.$$

The integration part equals the expectation value of x without the phase factors. Therefore,

$$\langle x \rangle = \frac{1}{\sqrt{2}\alpha}\cos\Delta\delta\cos\omega t.$$

From Eq. (68), the expectation value of p is,

$$\langle p \rangle = -\frac{\alpha}{\sqrt{2}}\hbar\cos\Delta\delta\sin\omega t.$$

If $\Delta\delta = \left(n + \frac{1}{2}\right)\pi$, the expectation value of x and p are zeros. And when $\Delta\delta = n\pi$, the expectation value of x and p has the maximum value.

Problem 5. Derive the wavefunction in momentum space, which corresponds to the eigenfunctions for the SHO in coordinates, $\psi_n(x)$.
Answer : The solution of the Schrödinger equation in the coordinate space is,

$$\psi_n(x) = (n!2^n)^{-\frac{1}{2}}\left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}}\exp\left(-\frac{m\omega}{2\hbar}x^2\right)H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right). \tag{69}$$

It satisfies the equation,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_n}{\partial x^2}+\frac{1}{2}m\omega^2x^2\psi_n=E_n\psi_n,\ \ E_n=\left(n+\frac{1}{2}\right)\hbar\omega. \tag{70}$$

The wavefunction in the momentum space $\phi_n(p)$ is the Inverse Fourier Transformation of the wavefunction in the coordinate space $\psi_n(x)$.

$$\begin{aligned}\phi_n(p)&=\frac{1}{\sqrt{2\pi\hbar}}\int\psi_n(x)e^{-\frac{i}{\hbar}px}\,dx\\&=\frac{1}{\sqrt{2\pi\hbar}}(n!2^n)^{-\frac{1}{2}}\left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}}\int H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)\exp\left(-\frac{m\omega}{2\hbar}x^2-\frac{i}{\hbar}px\right)dx.\end{aligned} \tag{71}$$

Changing x and p into the dimensionless variables ξ and p_ξ.

$$\xi=\sqrt{\frac{m\omega}{\hbar}}x,\ \ p_\xi=\frac{1}{\sqrt{\hbar m\omega}}p. \tag{72}$$

Then $\phi_n(p)$ is,

$$\phi_n(p)=\frac{1}{\sqrt{2\pi\hbar}}(n!2^n)^{-\frac{1}{2}}\left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}}\sqrt{\frac{\hbar}{m\omega}}\int H_n\left(\xi\right)e^{-\frac{1}{2}\xi^2-ip_\xi\xi}\,d\xi. \tag{73}$$

To find the Inverse Fourier Transformation of the Hermite polynomial, let us consider the generating function of the Hermite polynomial.

$$\int e^{-t^2+2\xi t-\frac{1}{2}\xi^2-ip_\xi\xi}\,d\xi=\sum_n\frac{t^n}{n!}\int H_n(\xi)e^{-\frac{1}{2}\xi^2-ip_\xi\xi}\,d\xi. \tag{74}$$

The LHS is the gaussian integration of ξ.

$$\begin{aligned}\int e^{-t^2+2\xi t-\frac{1}{2}\xi^2-ip_\xi\xi}\,d\xi&=e^{-t^2}\int e^{-\frac{1}{2}\xi^2+\xi(2t-ip_\xi)}\,d\xi=e^{-t^2}\int e^{-\frac{1}{2}(\xi-(2t-ip_\xi))^2+\frac{1}{2}(2t-ip_\xi)^2}\,d\xi\\&=e^{-t^2+\frac{1}{2}(2t-ip_\xi)^2}\sqrt{2\pi}=\sqrt{2\pi}e^{t^2-2ip_\xi-\frac{1}{2}p_\xi^2}.\end{aligned} \tag{75}$$

We can obtain the generating function about $-it$ and p_ξ.

$$\int e^{-t^2+2\xi t-\frac{1}{2}\xi^2-ip_\xi\xi}\,d\xi=\sqrt{2\pi}e^{t^2-2ip_\xi-\frac{1}{2}p_\xi^2}=\sqrt{2\pi}e^{-\frac{1}{2}p_\xi^2}\sum_m\frac{(-it)^m}{m!}H_m(p_\xi). \tag{76}$$

From Eq. (74), the coefficients of nth order have to be the same.

$$\begin{aligned}&\sum_n\frac{t^n}{n!}\int H_n(\xi)e^{-\frac{1}{2}\xi^2-ip_\xi\xi}\,d\xi=\sum_m\frac{(-it)^m}{m!}H_m(p_\xi)\sqrt{2\pi}e^{-\frac{1}{2}p_\xi^2},\\&\int H_n(\xi)e^{-\frac{1}{2}\xi^2-ip_\xi\xi}\,d\xi=(-i)^mH_m(p_\xi)\sqrt{2\pi}e^{-\frac{1}{2}p_\xi^2}.\end{aligned} \tag{77}$$

Therefore the wavefunction in the momentum space $\phi_n(p)$ is,

$$\phi_n(p)=(n!2^n)^{-\frac{1}{2}}\left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}}\sqrt{\frac{1}{m\omega}}(-i)^nH_n(p_\xi)e^{-\frac{1}{2}p_\xi^2}. \tag{78}$$

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

$$\psi(x,0)=\sum_nA_nu_n(x)=\left(\frac{\alpha^2}{\pi}\right)^{1/4}e^{-\alpha^2(x-a)^2/2}. \tag{79}$$

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

$$|\psi(x,t)|^2 = \left(\frac{\alpha^2}{\pi}\right)^{1/4} e^{-\alpha^2(x-a\cos\omega t)^2} \tag{80}$$

and discuss the result.
Answer : First we change the form of the exponential more similarly with Eq. (26), the generating function for the Hermite polynomial.

$$\begin{aligned}\exp\left(-\frac{\alpha^2}{2}(x-a)^2\right) &= \exp\left(-\frac{1}{2}\alpha^2x^2+\alpha^2ax-\frac{1}{2}\alpha^2a^2\right) = \exp\left(-\frac{1}{2}\alpha^2x^2\right)\exp\left(\alpha^2ax-\frac{1}{2}\alpha^2a^2\right)\\ &= \exp\left(-\frac{1}{2}\alpha^2x^2\right)\exp\left(2\left(\frac{\alpha a}{2}\right)(\alpha x)-\left(\frac{\alpha a}{2}\right)^2\right)\exp\left(-\left(\frac{\alpha a}{2}\right)^2\right).\end{aligned} \tag{81}$$

The second exponential of the RHS is the generating function of $S\left(\alpha x, \frac{\alpha a}{2}\right)$.

$$\exp\left(-\frac{\alpha^2}{2}(x-a)^2\right) = \exp\left(-\frac{1}{2}\alpha^2\left(x^2+\frac{1}{2}a^2\right)\right)\sum_{m=0}^{\infty}\frac{H_m(\alpha x)}{m!}\left(\frac{\alpha a}{2}\right)^n.$$

Hence $\psi(x,0)$ is,

$$\psi(x,0) = \sum_n A_n u_n(x) = \left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{4}}\exp\left(-\frac{1}{2}\alpha^2\left(x^2+\frac{1}{2}a^2\right)\right)\sum_n\frac{H_n(\alpha x)}{n!}\left(\frac{\alpha a}{2}\right)^n \tag{82}$$

$$= \sum_n\left(\left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{4}}\exp\left(-\frac{1}{4}\alpha^2a^2\right)\frac{1}{n!}\left(\frac{\alpha a}{2}\right)^n\right)\left(\exp\left(-\frac{1}{2}\alpha^2x^2\right)H_n(\alpha x)\right). \tag{83}$$

From Eq. (79) the wavefunction at the time t is,

$$\begin{aligned}\psi(x,t) &= \sum_n A_n u_n(x)e^{-i\frac{E_n}{\hbar}t} = \sum_n A_n u_n(x)e^{-i\left(n+\frac{1}{2}\right)\omega t}\\ &= e^{-\frac{1}{2}i\omega t}\sum_n A_n u_n(x)e^{-in\omega t}.\end{aligned}$$

Substituting Eq. (82),

$$\begin{aligned}\psi(x,t) &= \left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\alpha^2\left(x^2+\frac{1}{2}a^2\right)}e^{-\frac{1}{2}i\omega t}\sum_n\left(\frac{H_n(\alpha x)}{n!}\left(\frac{\alpha a}{2}\right)^n e^{-in\omega t}\right)\\ &= \left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\alpha^2\left(x^2+\frac{1}{2}a^2\right)}e^{-\frac{1}{2}i\omega t}\sum_n\left(\frac{H_n(\alpha x)}{n!}\left(\frac{\alpha a}{2}e^{-i\omega t}\right)^n\right).\end{aligned}$$

The summation can be expressed as the generating function for the Hermite polynomial.

$$\sum_n\left(\frac{H_n(\alpha x)}{n!}\left(\frac{\alpha a}{2}e^{-i\omega t}\right)^n\right) = S\left(\alpha x, \frac{\alpha a}{2}e^{-i\omega t}\right) = \exp\left(-\frac{1}{4}\alpha^2a^2e^{-2i\omega t}+\alpha^2axe^{-i\omega t}\right), \tag{84}$$

$$\psi(x,t) = \left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\alpha^2\left(x^2+\frac{1}{2}a^2\right)}e^{-\frac{1}{2}i\omega t}\exp\left(-\frac{1}{4}\alpha^2a^2e^{-2i\omega t}+\alpha^2axe^{-i\omega t}\right) \tag{85}$$

From Eq. (85) we obtain the probability density at the time t.

$$\begin{aligned}|\psi(x,t)|^2 &= \left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{2}} e^{-\alpha^2\left(x^2+\frac{1}{2}a^2\right)}\exp\left(-\frac{1}{4}\alpha^2a^2(e^{2i\omega t}+e^{-2i\omega t})+\alpha^2ax(e^{i\omega t}+e^{-i\omega t})\right)\\ &= \left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{2}}\exp\left(-\alpha^2x^2-\frac{1}{2}\alpha^2a^2(1+\cos 2\omega t)+2\alpha^2ax\cos\omega t\right).\end{aligned}$$

From the Half angle identity, $1 + \cos 2\omega t = 2\cos^2 \omega t$.

$$\begin{aligned}
|\psi(x,t)|^2 &= \left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{2}} \exp\left(-\alpha^2 x^2 - \alpha^2 a^2 \cos^2 \omega t + 2\alpha^2 a x \cos \omega t\right) \\
&= \left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{2}} \exp\left(-\alpha^2 (x^2 + a^2 \cos^2 \omega t - 2ax \cos \omega t)\right) \\
&= \left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{2}} \exp\left(-\alpha^2 (x - a\cos \omega t)\right)^2.
\end{aligned}$$

Finally the probability density is,

$$|\psi(x,t)|^2 = \left(\frac{\alpha^2}{\pi}\right)^{\frac{1}{2}} e^{-\alpha^2 (x - a\cos\omega t)^2}. \tag{86}$$

With this probability density, the wavefunction moves between intervals of $2a$ periodically without change in the shape and energy. Since, the expectation value of the position and the momentum oscillate with the probability density.

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

$$P_n = \frac{1}{Z} e^{-E_n/kT} \tag{87}$$

with

$$Z = \sum_n e^{-E_n/kT}, \tag{88}$$

where

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega. \tag{89}$$

(1) Derive the mean energy per an SHO

$$\langle E \rangle = \frac{\hbar\omega}{e^{\hbar\omega/kT} - 1} + \frac{1}{2}\hbar\omega. \tag{90}$$

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

$$C_V = \frac{\partial U}{\partial T}. \tag{91}$$

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

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

Answer :

(1) By the definition, the expectation value of the energy is,

$$\langle E \rangle = \sum_n E_n P_n = \frac{1}{Z}\sum_n E_n e^{-E_n/kT}, \;\; Z = \sum_n P_n.$$

Define β as,

$$\beta = \frac{1}{kT}. \tag{92}$$

Then,

$$\langle E \rangle = \frac{1}{Z} \sum_n E_n e^{-\beta E_n}, \quad Z = \sum_n e^{-\beta E_n}.$$

The summation term is regraded as the deriavtive for β.

$$\langle E \rangle = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = -\frac{\partial (\ln Z)}{\partial \beta}. \tag{93}$$

From Eq. (89), Z is,

$$Z = \sum_n e^{-\beta \hbar \omega (\frac{1}{2} + n)} = e^{-\frac{1}{2}\beta \hbar \omega} \sum_n e^{-n\beta \hbar \omega}.$$

It is power series with a common ratio $e^{-\beta \hbar \omega}$ and first term $e^{-\frac{1}{2}\beta \hbar \omega}$.

$$Z = \frac{e^{-\frac{1}{2}\beta \hbar \omega}}{1 - e^{-\beta \hbar \omega}}. \tag{94}$$

Then $\ln Z$ is,

$$\ln Z = \ln \left(e^{-\frac{1}{2}\beta \hbar \omega} \right) - \ln \left(1 - e^{-\beta \hbar \omega} \right) = -\frac{1}{2}\beta \hbar \omega - \ln \left(1 - e^{-\beta \hbar \omega} \right).$$

And Eq. (93) is,

$$\langle E \rangle = -\frac{\partial (\ln Z)}{\partial \beta} = \frac{1}{2}\hbar \omega + \frac{\hbar \omega e^{-\beta \hbar \omega}}{1 - e^{-\beta \hbar \omega}}$$

Multiplying $e^{\beta \hbar \omega}$ to the second term of the RHS,

$$\begin{aligned} \langle E \rangle &= \frac{1}{2}\hbar \omega + \frac{\hbar \omega}{e^{\beta \hbar \omega} - 1} \\ &= \frac{\hbar \omega}{e^{\hbar \omega / kT} - 1} + \frac{1}{2}\hbar \omega. \end{aligned} \tag{95}$$

(2) The first law of the thermodynamics is,

$$dU = dQ - dW. \tag{96}$$

Q and W are the heat supplied to the system and the work done on the system respectively. In the case of the solid, the volume is constant and the work is a zero.

$$dW = PdV = 0, \quad dU = dQ. \tag{97}$$

By the definition of the specific heat with constant volume,

$$C_V = \left(\frac{\partial Q}{\partial T} \right)_V = \frac{\partial U}{\partial T}. \tag{98}$$

Since U is the total energy of the solid and there are the N atoms,

$$U = N \langle E \rangle = \frac{N \hbar \omega}{e^{\hbar \omega / kT} - 1} + \frac{1}{2} N \hbar \omega. \tag{99}$$

Hence the specific heat C_V is,

$$C_V = \frac{\partial U}{\partial T} = \frac{\partial}{\partial T} \left(\frac{N \hbar \omega}{e^{\hbar \omega / kT} - 1} \right) = \frac{N \hbar^2 \omega^2 e^{\hbar \omega / kT}}{kT^2 \left(e^{\hbar \omega / kT} - 1 \right)^2}. \tag{100}$$

Considering that the degree of freedom is 3,

$$C_V = \frac{3N\hbar^2\omega^2 e^{\hbar\omega/kT}}{kT^2\left(e^{\hbar\omega/kT}-1\right)^2}. \tag{101}$$

From Eq. (92), Eq. (100) can be rewritten as,

$$C_V = \frac{3Nk\beta^2\hbar^2\omega^2 e^{\beta\hbar\omega}}{\left(e^{\beta\hbar\omega}-1\right)^2}. \tag{102}$$

When T is large, β is converged to a zero and $e^{-\beta\hbar\omega}$ is converged to 1. Then,

$$\lim_{\beta\to 0}\frac{\beta}{e^{\beta\hbar\omega}-1} = \frac{1}{\hbar\omega}. \tag{103}$$

Finally C_V is,

$$C_V = \frac{3Nk\hbar^2\omega^2}{\hbar^2\omega^2} = 3Nk = 3nR. \tag{104}$$

(3) Let us consider when the temperature is very small. From Eq. (101),

$$\lim_{T\to 0}\frac{3N\hbar^2\omega^2 e^{\hbar\omega/kT}}{kT^2\left(e^{\hbar\omega/kT}-1\right)^2} = 0. \tag{105}$$

C_v is converged to a zero. From Eq. (95), when the temperature is large, the mean energy per an SHO behaves approximately as the linear function.

$$\begin{aligned}\langle E\rangle &= \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{e^{\beta\hbar\omega}-1} \approx \frac{1}{2}\hbar\omega + \frac{1}{\beta} - \frac{1}{2}\hbar\omega + \frac{1}{12}\hbar\omega^2\beta + \cdots \\ &\approx \frac{1}{\beta} = kT.\end{aligned} \tag{106}$$

In high temperatures, the mean energy per an SHO by The Einstein model is directly proportional to temperature.