

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,

$$E_p = q\mathcal{E}x. \quad (1)$$

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

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

So, the Schrödinger equation is,

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

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

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

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

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(x + i \frac{p}{m\omega}\right), \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(x - i \frac{p}{m\omega}\right), \quad [a, a^\dagger] = \mathbb{I}. \quad (5)$$

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

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

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

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

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

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

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

$$b := a + \kappa, \quad [a, b] = a(a + \kappa) - (a + \kappa)a = aa - aa + \kappa a - \kappa a = 0. \quad (9)$$

With this definition, the new operator b commutes with the old one a . And the adjoint of b is automatically $b^\dagger = a^\dagger + \kappa$.

$$[b, b^\dagger] = [(a + \kappa), (a + \kappa)^\dagger] = \mathbb{I}. \quad (10)$$

Then the hamiltonian with a constant electric field H' is,

$$\begin{aligned} H' &= \hbar\omega \left((a^\dagger + \kappa)(a + \kappa) - \kappa(a + a^\dagger) - \kappa^2 + \frac{1}{2} - \frac{q\mathcal{E}}{2} \sqrt{\frac{2\hbar}{m\omega}} (a + a^\dagger) \right) \\ &= \hbar\omega \left(b^\dagger b - \kappa^2 + \frac{1}{2} - \left(\kappa + \frac{q\mathcal{E}}{2} \sqrt{\frac{2\hbar}{m\omega}} \right) (a + a^\dagger) \right) \end{aligned} \quad (11)$$

. Setting κ as,

$$\kappa = -\frac{q\mathcal{E}}{2} \sqrt{\frac{2\hbar}{m\omega}}, \quad \kappa + \frac{q\mathcal{E}}{2} \sqrt{\frac{2\hbar}{m\omega}} = 0. \quad (12)$$

Then H' is,

$$H' = \hbar\omega \left(b^\dagger b - \kappa^2 + \frac{1}{2} \right). \quad (13)$$

We can write the eigenvalue equation with the new operator.

$$H' \psi'_n = E'_n \psi'_n. \quad (14)$$

Or,

$$\hbar\omega \left(b^\dagger b + \frac{1}{2} \right) \psi'_n = (E'_n + \kappa^2) \psi'_n. \quad (15)$$

(3)

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

$$S(x, t) = e^{x^2 - (t-x)^2} = e^{-t^2 + 2tx} = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} t^n. \quad (16)$$

- (1) Using this generating function, derive the Hermite differential equation.
 (2) Derive the following formula from Eq. (16):

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}, \quad (17)$$

which is called the Rodrigues representation of the Hermite polynomial.

- (3) Using Eq. (16), derive the orthogonal relation of the Hermite polynomials

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) dx = 2^n \sqrt{\pi} n! \delta_{nm}. \quad (18)$$

- (4) Prove that

$$\left(2x - \frac{d}{dx} \right)^n 1 = H_n(x), \quad (19)$$

- (5) Prove

$$\int_{-\infty}^{\infty} x e^{-x^2} H_n(x) H_m(x) dx = \sqrt{\pi} 2^{n-1} n! \delta_{m,n-1} + \sqrt{\pi} 2^n (n+1)! \delta_{m,n+1}. \quad (20)$$

- (6) Prove

$$\int_{-\infty}^{\infty} x^2 e^{-x^2} H_n(x) H_n(x) dx = \sqrt{\pi} 2^n n! \left(n + \frac{1}{2} \right). \quad (21)$$

Answer :

- (1) The Hermite differential equation is,

$$\frac{d^2 y}{dx^2} - 2x \frac{dy}{dx} + \lambda y = 0, \quad (22)$$

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

$$\begin{aligned} \frac{dS}{dx} &= 2tS = \sum_{n=0}^{\infty} \frac{H'_n(x)}{n!} t^n \\ \frac{d^2 S}{dx^2} &= 4t^2 S = \sum_{n=0}^{\infty} \frac{H''_n(x)}{n!} t^n. \end{aligned} \quad (23)$$

And,

$$\frac{dS}{dt} = 2(-t + x)S = \sum_{n=0}^{\infty} \frac{H_n(x)}{n!} n t^{n-1} = -\frac{dS}{dx} + 2xS. \quad (24)$$

From Eq. (23),

$$\begin{aligned} \frac{dS}{dx} &= \frac{1}{2t} \frac{d^2 S}{dx^2} = \frac{1}{2} \sum_{n=0}^{\infty} \frac{H''_n(x)}{n!} t^{n-1} \\ 2xS &= 2x \frac{1}{2t} \frac{dS}{dt} = x \sum_{n=0}^{\infty} \frac{H'_n(x)}{n!} t^{n-1} \end{aligned}$$

Then Eq. (24) 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,

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0. \quad (25)$$

(2) From Eq. (16),

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

And,

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

Since the series representation is unique,

$$H_n(x) = e^{x^2} \frac{d^n}{dt^n} e^{-(t-x)^2} \Big|_{t=0}. \quad (26)$$

If we regard t as just the parameter, Eq. (26) is true for any t . A differential part of a LHS is,

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

Finally we obtain,

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

(3) First, when $t = 1$ and $t = -1$, Eq. (16) 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,

$$\int_{-\infty}^{\infty} e^{-x^2} H_m(x) e^{2x-1} dx = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x) dx \quad (28)$$

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. (28) 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. (25),

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

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,

$$\int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_m(x) dx = 2^n n! \sqrt{\pi} \delta_{nm}. \quad (29)$$

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

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

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. (27),

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

Hence this statement is true for $n = k + 1$.

By mathematical induction, this statement is true for any n . □

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

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

From Eq. (27),

$$\begin{aligned}
H'_n(x) &= \frac{d}{dx} \left((-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \right) = (-1)^n \left(2x e^{x^2} \frac{d^n}{dx^n} e^{-x^2} + e^{x^2} \frac{d^{n+1}}{dx^{n+1}} e^{-x^2} \right) \\
&= 2x H_n(x) - H_{n+1}(x).
\end{aligned} \tag{30}$$

Then I_{nm} is,

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

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. (29), we obtain that,

$$\begin{aligned}
I_{nm} &= \frac{1}{2} (2^{n+1} \sqrt{\pi} (n+1)! \delta_{n+1,m} + 2^n \sqrt{\pi} n! \delta_{n,m+1}) \\
&= 2^n \sqrt{\pi} (n+1)! \delta_{n+1,m} + 2^{n-1} \sqrt{\pi} n! \delta_{n,m+1}.
\end{aligned} \tag{31}$$

Therefore the statement is true. □

(6) *Proof.* Eq. (21) 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. (30), 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. (31) and (29),

$$\begin{aligned}\int_{-\infty}^{\infty} x^2 e^{-x^2} H_n H_n dx &= \sqrt{\pi} 2^{n-1} n! \delta_{n+1, n-1} + \sqrt{\pi} 2^n (n+1)! \delta_{n+1, n+1} - \sqrt{\pi} 2^{n-1} n! \\ &= \sqrt{\pi} 2^n n! \left(n + \frac{1}{2} \right).\end{aligned}\tag{32}$$

Therefore the statement is true. \square

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

$$\Delta x \Delta p = \left(n + \frac{1}{2} \right) \hbar.\tag{33}$$

Answer :

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

$$\psi_n(x) = \psi_n^*(x) = (n! 2^n)^{-\frac{1}{2}} \left(\frac{m\omega}{\hbar\pi} \right)^{\frac{1}{4}} \exp\left(-\frac{m\omega}{2\hbar} x^2\right) H_n \left(\sqrt{\frac{m\omega}{\hbar}} x \right), \quad E_n = \left(n + \frac{1}{2} \right) \hbar\omega.\tag{34}$$

The expectation value of the kinetic energy is,

$$\langle T_n \rangle = \frac{1}{2m} \int \psi_n^* p^2 \psi_n dx = \frac{\langle p^2 \rangle}{2m}.\tag{35}$$

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,

$$\langle p^2 \rangle = -\hbar^2 \int \psi_n^* \frac{\partial^2 \psi_n}{\partial x^2} dx = \hbar^2 \int \frac{\partial \psi_n^*}{\partial x} \frac{\partial \psi_n}{\partial x} dx\tag{36}$$

Changing the variable,

$$\sqrt{\frac{m\omega}{\hbar}} x = \xi, \quad \frac{\partial \psi_n}{\partial x} = \frac{\partial \psi_n}{\partial \xi} \frac{\partial \xi}{\partial x} = \sqrt{\frac{m\omega}{\hbar}} \frac{\partial \psi_n}{\partial \xi}\tag{37}$$

Then,

$$\frac{\partial \psi_n}{\partial \xi} = (n! 2^n)^{-\frac{1}{2}} \left(\frac{m\omega}{\hbar\pi} \right)^{\frac{1}{4}} (-\xi H_n(\xi) + H_n'(\xi)) e^{-\frac{\xi^2}{2}}.\tag{38}$$

The integration of Eq. (36) is,

$$\begin{aligned}\int \frac{\partial \psi_n^*}{\partial x} \frac{\partial \psi_n}{\partial x} dx &= (n! 2^n)^{-1} \sqrt{\frac{m\omega}{\hbar\pi}} \frac{m\omega}{\hbar} \int (-\xi H_n(\xi) + H_n'(\xi))^2 e^{-\xi^2} \sqrt{\frac{\hbar}{m\omega}} d\xi \\ &= (n! 2^n)^{-1} \frac{m\omega}{\hbar\sqrt{\pi}} \int (-\xi H_n(\xi) + H_n'(\xi))^2 e^{-\xi^2} d\xi\end{aligned}\tag{39}$$

From Eq. (30)

$$\begin{aligned}
\int (-\xi H_n(\xi) + H'_n(\xi))^2 e^{-\xi^2} d\xi &= \int (-\xi H_n(\xi) + 2\xi H_n(\xi) - H_{n+1}(\xi))^2 e^{-\xi^2} d\xi \\
&= \int (\xi H_n(\xi) - H_{n+1}(\xi))^2 e^{-\xi^2} d\xi \\
&= \int ((\xi^2 H_n H_n - 2\xi H_n H_{n+1} + H_{n+1} H_{n+1}) e^{-\xi^2} d\xi.
\end{aligned} \tag{40}$$

We can use Eq. (29), (31) and (32) to calculate this integration.

$$\begin{aligned}
\int \xi^2 H_n H_n e^{-\xi^2} dx &= 2^n n! \sqrt{\pi} \left(n + \frac{1}{2} \right) \\
\int \xi H_n H_{n+1} e^{-\xi^2} dx &= 2^n (n+1)! \sqrt{\pi} \\
\int H_{n+1} H_{n+1} e^{-\xi^2} dx &= 2^{n+1} (n+1)! \sqrt{\pi}
\end{aligned} \tag{41}$$

Then,

$$\begin{aligned}
\int (-\xi H_n(\xi) + H'_n(\xi))^2 e^{-\xi^2} d\xi &= \sqrt{\pi} 2^n n! \left(n + \frac{1}{2} - 2(n+1) + 2(n+1) \right) \\
&= \sqrt{\pi} 2^n n! \left(n + \frac{1}{2} \right).
\end{aligned} \tag{42}$$

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

$$\langle p^2 \rangle = \hbar^2 (n! 2^n)^{-1} \frac{m\omega}{\hbar \sqrt{\pi}} \sqrt{\pi} 2^n n! \left(n + \frac{1}{2} \right) = \hbar m \omega \left(n + \frac{1}{2} \right). \tag{43}$$

We obtain the expectation value of the kinetic energy.

$$\langle T_n \rangle = \frac{\langle p^2 \rangle}{2m} = \frac{1}{2} \hbar \omega \left(n + \frac{1}{2} \right). \tag{44}$$

The expectation value of the potential energy is,

$$\langle V_n \rangle = \int \psi_n^* \frac{1}{2} m \omega^2 x^2 \psi_n dx = \frac{1}{2} m \omega^2 \int \psi_n^* x^2 \psi_n dx = \frac{1}{2} m \omega^2 \langle x^2 \rangle. \tag{45}$$

From Eq. (37), the expectation value of the square of x is,

$$\begin{aligned}
\langle x^2 \rangle &= \int \psi_n^* x^2 \psi_n dx = \langle x^2 \rangle = \left(\frac{\hbar}{m\omega} \right)^{\frac{3}{2}} \int \psi_n^*(\xi) \xi^2 \psi_n(\xi) d\xi \\
&= (n! 2^n)^{-1} \sqrt{\frac{m\omega}{\hbar \pi}} \left(\frac{\hbar}{m\omega} \right)^{\frac{3}{2}} \int \xi^2 H_n(\xi) H_n(\xi) e^{-\xi^2} d\xi
\end{aligned} \tag{46}$$

The integration part can be calculated by Eq. (32).

$$\int \xi^2 H_n(\xi) H_n(\xi) e^{-\xi^2} d\xi = \sqrt{\pi} 2^n n! \left(n + \frac{1}{2} \right). \tag{47}$$

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

$$\langle x^2 \rangle = \frac{\hbar}{m\omega} \left(n + \frac{1}{2} \right). \tag{48}$$

Finally we obtain the expectation value of the potential energy.

$$\langle V_n \rangle = \frac{1}{2} m \omega^2 (n! 2^n)^{-1} \sqrt{\frac{m\omega}{\hbar \pi}} \left(\frac{\hbar}{m\omega} \right)^{\frac{3}{2}} \sqrt{\pi} 2^n n! \left(n + \frac{1}{2} \right) = \frac{1}{2} \hbar \omega \left(n + \frac{1}{2} \right). \tag{49}$$

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

$$\left\langle x \frac{\partial V}{\partial x} \right\rangle = 2 \langle T \rangle. \quad (50)$$

Substituting Eq. (44) and (49),

$$\left\langle x \frac{\partial V}{\partial x} \right\rangle = m\omega^2 \int \psi_n^* x^2 \psi_n dx = 2 \langle V_n \rangle = 2 \langle T_n \rangle. \quad (51)$$

The results satisfy the virial theorem.

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

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}, \quad \Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}. \quad (52)$$

$\langle x \rangle$ is,

$$\langle x \rangle = \int x \psi^* \psi dx = (n!2^n)^{-1} \sqrt{\frac{m\omega}{\hbar\pi}} \left(\frac{\hbar}{m\omega} \right) \int \xi H_n H_n e^{-\xi^2} d\xi. \quad (53)$$

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

$$\langle x \rangle = 0. \quad (54)$$

With Eq. (48) Δx is,

$$\Delta x = \sqrt{\langle x^2 \rangle} = \sqrt{\frac{\hbar}{m\omega} \left(n + \frac{1}{2} \right)}. \quad (55)$$

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

$$\langle p \rangle = \int \psi^* p \psi dx = -i\hbar \int \psi_n^* \frac{\partial \psi_n}{\partial x} dx. \quad (56)$$

The integration by part is,

$$\langle p \rangle = -i\hbar \int \psi_n^* \frac{\partial \psi_n}{\partial x} dx = i\hbar \int \frac{\partial \psi_n^*}{\partial x} \psi_n dx. \quad (57)$$

From Eq. (34), $\psi = \psi^*$. So,

$$\langle p \rangle = i\hbar \int \frac{\partial \psi_n^*}{\partial x} \psi_n dx = i\hbar \int \psi_n^* \frac{\partial \psi_n}{\partial x} dx = -\langle p \rangle. \quad (58)$$

Therefore,

$$\langle p \rangle = 0. \quad (59)$$

With Eq. (43) Δp is,

$$\Delta p = \sqrt{\langle p^2 \rangle} = \sqrt{\hbar m\omega \left(n + \frac{1}{2} \right)}. \quad (60)$$

Finally $\Delta x \Delta p$ si,

$$\Delta x \Delta p = \sqrt{\frac{\hbar}{m\omega} \left(n + \frac{1}{2} \right)} \sqrt{\hbar m\omega \left(n + \frac{1}{2} \right)} = \hbar \left(n + \frac{1}{2} \right). \quad (61)$$

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

$$\psi(x, t) = \frac{1}{\sqrt{2}}[\psi_0(x, t) + \psi_1(x, t)], \quad (62)$$

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

(2) Prove the following relations

$$\begin{aligned} \langle E \rangle &= \langle H \rangle = \hbar\omega, \\ \langle x \rangle &= \frac{1}{\sqrt{2\alpha}} \cos \omega t, \\ \langle p \rangle &= -\sqrt{\frac{\alpha}{2}} \hbar \sin \omega t, \end{aligned} \quad (63)$$

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

(3) If

$$\psi(x, t) = \frac{1}{\sqrt{2}}[e^{i\delta_0}\psi_0(x, t) + e^{i\delta}\psi_1(x, t)], \quad (64)$$

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, $\psi_n(x)$.

Answer : We already know that the solution of the Schrödinger equation in the coordinate space is,

$$\psi_n(x) = (n!2^n)^{-\frac{1}{2}} \left(\frac{m\omega}{\hbar\pi} \right)^{\frac{1}{4}} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right). \quad (65)$$

It satisfies the equation,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_n}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \psi_n = E_n \psi_n, \quad E_n = \left(n + \frac{1}{2}\right) \hbar\omega. \quad (66)$$

And the wave function in the momentum space satisfies that,

$$\frac{p^2}{2m} \phi_n - \frac{1}{2} m \omega^2 \hbar^2 \frac{\partial^2 \phi_n}{\partial p^2} = \mathcal{E}_n \phi_n. \quad (67)$$

Multiplying $1/m^2\omega^2$ to Eq. (80),

$$\frac{p^2}{2m^3\omega^2} \phi_n - \frac{\hbar^2}{2m} \frac{\partial^2 \phi_n}{\partial p^2} = \frac{\mathcal{E}_n}{m^2\omega^2} \phi_n. \quad (68)$$

Set $1/m^4\omega^2 = \omega_p^2$. Then,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \phi_n}{\partial p^2} + \frac{1}{2} m \omega_p^2 p^2 \phi_n = m^2 \omega_p^2 \mathcal{E}_n \phi_n. \quad (69)$$

Since the form of the equation corresponds to Eq. (66), the form of the solution will be the same. Comparing the two equations,

$$\omega^2 x^2 \longrightarrow \omega_p^2 p^2, \quad E_n \longrightarrow m^2 \omega_p^2 \mathcal{E}_n. \quad (70)$$

Then $\phi_n(p)$ and \mathcal{E} are,

$$\phi_n(p) = (n!2^n)^{-\frac{1}{2}} \left(\frac{m\omega_p}{\hbar\pi} \right)^{\frac{1}{4}} \exp\left(-\frac{m\omega_p}{2\hbar}p^2\right) H_n\left(\sqrt{\frac{m\omega_p^2}{\hbar\omega}}p\right), \quad \mathcal{E}_n = \left(n + \frac{1}{2}\right) m^2 \hbar \omega^3. \quad (71)$$

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

$$\psi(x, 0) = \sum_n A_n u_n(x) = \left(\frac{\alpha^2}{\pi}\right)^{1/4} e^{-\alpha^2(x-a)^2/2}. \quad (72)$$

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

$$|\psi(x, t)|^2 = \left(\frac{\alpha^2}{\pi}\right)^{1/4} e^{-\alpha^2(x-a \cos \omega t)^2} \quad (73)$$

and discuss the result.

Answer : The wave function in the momentum space $\phi(p, 0)$ at $t = 0$ is,

$$\phi(p, 0) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{-\frac{i}{\hbar}px} \psi(x, 0) dx = \frac{1}{\sqrt{2\pi\hbar}} \left(\frac{\alpha^2}{\pi}\right)^{1/4} \int \exp\left(-\frac{i}{\hbar}px - \frac{\alpha^2}{2}(x-a)^2\right) dx. \quad (74)$$

The exponential of the integrated term can be represented into the complete square form about x .

$$\begin{aligned} -\frac{i}{\hbar}px - \frac{\alpha^2}{2}(x-a)^2 &= -\frac{\alpha^2}{2}x^2 + \left(\alpha^2a - \frac{i}{\hbar}p\right)x - \frac{\alpha^2a^2}{2} \\ &= -\frac{\alpha^2}{2}\left(x - \left(a - \frac{i}{\alpha^2\hbar}p\right)\right)^2 + \frac{\alpha^2}{2}\left(a - \frac{i}{\alpha^2\hbar}p\right)^2 - \frac{\alpha^2a^2}{2}. \end{aligned} \quad (75)$$

Since the last two terms in the RHS are independent on x , we just integrate the first term in the RHS and it is the gaussian integration.

$$\begin{aligned} \phi(p, 0) &= \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{\alpha^2}{2}\left(a - \frac{i}{\alpha^2\hbar}p\right)^2 - \frac{\alpha^2a^2}{2}\right) \int \exp\left(-\frac{\alpha^2}{2}\left[x - \left(a - \frac{i}{\alpha^2\hbar}p\right)\right]^2\right) dx \\ &= \frac{1}{\sqrt{2\pi\hbar}} \sqrt{\frac{2\pi}{\alpha^2}} \exp\left(\frac{\alpha^2}{2}\left(a - \frac{i}{\alpha^2\hbar}p\right)^2 - \frac{\alpha^2a^2}{2}\right) \\ &= \frac{1}{\alpha\sqrt{\hbar}} \exp\left(-\frac{p^2}{2\alpha^2\hbar^2} - i\frac{a}{\hbar}p\right). \end{aligned} \quad (76)$$

The wave function in the momentum space $\phi(p, t)$ at any time t that is not a zero is,

$$\begin{aligned} \phi(p, t) &= \exp(-i\omega t) \phi(p, 0) = \frac{1}{\alpha\sqrt{\hbar}} \exp\left(-i\omega t - \frac{p^2}{2\alpha^2\hbar^2} - i\frac{a}{\hbar}p\right) \\ &= \frac{1}{\alpha\sqrt{\hbar}} \exp(). \end{aligned} \quad (77)$$

To obtain the wave function in the coordinate space at time t that is not a zero, we operate Fourier transform into the $\phi(p, t)$.

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

$$P_n = \frac{1}{Z} e^{-E_n/kT} \quad (78)$$

with

$$Z = \sum_n e^{-E_n/kT}, \quad (79)$$

where

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega. \quad (80)$$

(1) Derive the mean energy per an SHO

$$\langle E \rangle = \frac{\hbar\omega}{e^{\hbar\omega/kT} - 1} + \frac{1}{2}\hbar\omega. \quad (81)$$

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

$$C_V = \frac{\partial U}{\partial T}. \quad (82)$$

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,

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

Define β as,

$$\beta = \frac{1}{kT}. \quad (83)$$

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 regreded as the deriavtive for β .

$$\langle E \rangle = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = -\frac{\partial(\ln Z)}{\partial \beta}. \quad (84)$$

From Eq. (80), 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 $e^{-\frac{1}{2}\beta \hbar\omega}$.

$$Z = \frac{e^{-\frac{1}{2}\beta \hbar\omega}}{1 - e^{-\beta \hbar\omega}}. \quad (85)$$

Then $\ln Z$ is,

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

And Eq. (84) 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,

$$\begin{aligned} \langle E \rangle &= \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{e^{\beta \hbar\omega} - 1} \\ &= \frac{\hbar\omega}{e^{\hbar\omega/kT} - 1} + \frac{1}{2}\hbar\omega. \end{aligned} \quad (86)$$

(2) The first law of the thermodynamics is,

$$dU = dQ - dW. \quad (87)$$

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 the constant and the work is a zero.

$$dW = PdV = 0, \quad dU = dQ. \quad (88)$$

By the definition of the specific heat with constant volume,

$$C_V = \left(\frac{\partial Q}{\partial T} \right)_V = \frac{\partial U}{\partial T}. \quad (89)$$

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

$$U = N \langle E \rangle = \frac{N\hbar\omega}{e^{\hbar\omega/kT} - 1} + \frac{1}{2}N\hbar\omega. \quad (90)$$

Hence the specific heat C_V is,

$$C_V = \frac{\partial U}{\partial T} = \frac{\partial}{\partial T} \left(\frac{N\hbar\omega}{e^{\hbar\omega/kT} - 1} \right) = \frac{N\hbar^2\omega^2 e^{\hbar\omega/kT}}{kT^2 (e^{\hbar\omega/kT} - 1)^2}. \quad (91)$$

Consdiering that the degree of freedom is 3,

$$C_V = \frac{3N\hbar^2\omega^2 e^{\hbar\omega/kT}}{kT^2 (e^{\hbar\omega/kT} - 1)^2}. \quad (92)$$

From Eq. (83), Eq. (91) can be rewritten as,

$$C_V = \frac{3Nk\beta^2\hbar^2\omega^2 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}. \quad (93)$$

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

$$\lim_{\beta \rightarrow 0} \frac{\beta}{e^{\beta\hbar\omega} - 1} = \frac{1}{\hbar\omega}. \quad (94)$$

Finally C_V is,

$$C_V = \frac{3Nk\hbar^2\omega^2}{\hbar^2\omega^2} = 3Nk = 3nR. \quad (95)$$

(3) From Eq. (86), when the temperature is large, the mean energy per an SHO behaves approximately as the linear function.

$$\begin{aligned} \langle E \rangle &= \frac{1}{2}\hbar\omega + \hbar\omega [e^{\beta\hbar\omega} - 1]^{-1} = \frac{1}{2}\hbar\omega + \hbar\omega [(1 + \hbar\omega\beta + \dots) - 1]^{-1} \\ &= \end{aligned} \quad (96)$$