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. Derivatives for x of generating function S are,

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

And,

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

From Eq. (24),

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

Then Eq. (25) 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,

$$H_n''(x)-2xH_n'(x)+2nH_n(x)=0. \tag{26}$$

(2) From Eq. (17),

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

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,

$$H_n(x)=e^{x^2}\frac{d^n}{dt^n}e^{-(t-x)^2}\bigg|_{t=0}. \tag{27}$$

If we regard t as just the parameter, Eq. (27) 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,

$$H_n(x)=(-1)^ne^{x^2}\frac{d^n}{dx^n}e^{-x^2}. \tag{28}$$

(3) First, when $t=1$ and $t=-1$, Eq. (17) 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,

$$\int_{-\infty}^{\infty}e^{-x^2}H_m(x)e^{2x-1}\,dx=\sum_{n=0}^{\infty}\frac{1}{n!}\int_{-\infty}^{\infty}e^{-x^2}H_m(x)H_n(x)\,dx \tag{29}$$

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,

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

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. (29) 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. (26),

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

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,

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

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,

$$\int_{-\infty}^{\infty} e^{-x^2}H_n(x)H_m(x)dx = 2^n n!\sqrt{\pi}\delta_{nm}. \tag{30}$$

(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. (28),

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

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. (28),

$$\begin{aligned}H_n'(x) &= \frac{d}{dx}\left((-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}\right) = (-1)^n\left(2xe^{x^2}\frac{d^n}{dx^n}e^{-x^2}+e^{x^2}\frac{d^{n+1}}{dx^{n+1}}e^{-x^2}\right)\\ &= 2xH_n(x)-H_{n+1}(x).\end{aligned} \tag{31}$$

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. (30), we obtain that,

$$\begin{aligned}I_{nm} &= \frac{1}{2}\left(2^{n+1}\sqrt{\pi}(n+1)!\delta_{n+1,m}+2^n\sqrt{\pi}n!\delta_{n,m+1}\right)\\ &= 2^n\sqrt{\pi}(n+1)!\delta_{n+1,m}+2^{n-1}\sqrt{\pi}n!\delta_{n,m+1}.\end{aligned} \tag{32}$$

Therefore the statement is true. □

(6) *Proof.* Eq. (22) is,

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

From Eq. (31), the second term of the RHS is,

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

Hence,

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

From Eq. (32) and (30),

$$\begin{aligned}\int_{-\infty}^{\infty} x^2 e^{-x^2} H_n H_n \, dx &= \sqrt{\pi}2^{n-1} n! \delta_{n+1,n-1} + \sqrt{\pi}2^n (n+1)! \delta_{n+1,n+1} - \sqrt{\pi}2^{n-1} n! \\ &= \sqrt{\pi}2^n n! \left(n + \frac{1}{2}\right).\end{aligned} \tag{33}$$

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

$$\Delta x \Delta p = \left(n + \frac{1}{2}\right)\hbar. \tag{34}$$

Answer :

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

$$\psi_n(x) = \psi_n^*(x) = (n! 2^n)^{-\frac{1}{2}} \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right), \quad E_n = \left(n + \frac{1}{2}\right)\hbar\omega. \tag{35}$$

The expectation value of the kinetic energy is,

$$\langle T_n \rangle = \frac{1}{2m}\int \psi_n^* p^2 \psi_n \, dx = \frac{\langle p^2 \rangle}{2m}. \tag{36}$$

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,

$$\langle p^2 \rangle = -\hbar^2 \int \psi_n^* \frac{\partial^2 \psi_n}{\partial x^2} \, dx = \hbar^2 \int \frac{\partial \psi_n^*}{\partial x}\frac{\partial \psi_n}{\partial x} \, dx \tag{37}$$

Changing the variable,

$$\sqrt{\frac{m\omega}{\hbar}}x = \xi, \quad \frac{\partial \psi_n}{\partial x} = \frac{\partial \psi_n}{\partial \xi}\frac{\partial \xi}{\partial x} = \sqrt{\frac{m\omega}{\hbar}}\frac{\partial \psi_n}{\partial \xi} \tag{38}$$

Then,

$$\frac{\partial \psi_n}{\partial \xi} = (n! 2^n)^{-\frac{1}{2}} \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} (-\xi H_n(\xi) + H_n'(\xi)) e^{-\frac{\xi^2}{2}}. \tag{39}$$

The integration of Eq. (37) is,

$$\begin{aligned}\int \frac{\partial \psi_n^*}{\partial x}\frac{\partial \psi_n}{\partial x} \, dx &= (n! 2^n)^{-1} \sqrt{\frac{m\omega}{\hbar\pi}} \frac{m\omega}{\hbar} \int (-\xi H_n(\xi) + H_n'(\xi))^2 e^{-\xi^2} \sqrt{\frac{\hbar}{m\omega}} d\xi \\ &= (n! 2^n)^{-1} \frac{m\omega}{\hbar\sqrt{\pi}} \int (-\xi H_n(\xi) + H_n'(\xi))^2 e^{-\xi^2} \, d\xi\end{aligned} \tag{40}$$

From Eq. (31)

$$\begin{aligned}\int (-\xi H_n\,(\xi) + H_n'\,(\xi))^2 e^{-\xi^2}\,d\xi &= \int (-\xi H_n\,(\xi) + 2\xi H_n(\xi) - H_{n+1}(\xi))^2 e^{-\xi^2}\,d\xi \\ &= \int (\xi H_n\,(\xi) - H_{n+1}(\xi))^2 e^{-\xi^2}\,d\xi \\ &= \int ((\xi^2 H_n H_n - 2\xi H_n H_{n+1} + H_{n+1}H_{n+1}) e^{-\xi^2}\,d\xi.\end{aligned} \tag{41}$$

We can use Eq. (30), (32) and (33) to calculate this integration.

$$\begin{aligned}\int \xi^2 H_n H_n e^{-\xi^2}\,dx &= 2^n n!\sqrt{\pi}\left(n+\frac{1}{2}\right) \\ \int \xi H_n H_{n+1} e^{-\xi^2}\,dx &= 2^n (n+1)!\sqrt{\pi} \\ \int H_{n+1} H_{n+1} e^{-\xi^2}\,dx &= 2^{n+1}(n+1)!\sqrt{\pi}\end{aligned} \tag{42}$$

Then,

$$\begin{aligned}\int (-\xi H_n\,(\xi) + H_n'\,(\xi))^2 e^{-\xi^2}\,d\xi &= \sqrt{\pi}2^n n!\left(n+\frac{1}{2} - 2(n+1) + 2(n+1)\right) \\ &= \sqrt{\pi}2^n n!\left(n+\frac{1}{2}\right).\end{aligned} \tag{43}$$

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

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

We obtain the expectation value of the kinetic energy.

$$\langle T_n\rangle = \frac{\langle p^2\rangle}{2m} = \frac{1}{2}\hbar\omega\left(n+\frac{1}{2}\right). \tag{45}$$

The expectation value of the potential energy is,

$$\langle V_n\rangle = \int \psi_n^* \frac{1}{2} m\omega^2 x^2 \psi_n\,dx = \frac{1}{2}m\omega^2 \int \psi_n^* x^2 \psi_n\,dx = \frac{1}{2}m\omega^2\langle x^2\rangle. \tag{46}$$

From Eq. (38), the expectation value of the square of x is,

$$\begin{aligned}\langle x^2\rangle &= \int \psi_n^* x^2 \psi_n\,dx = \langle x^2\rangle = \left(\frac{\hbar}{m\omega}\right)^{\frac{3}{2}} \int \psi_n^*(\xi)\xi^2\psi_n(\xi)\,d\xi \\ &= (n!2^n)^{-1}\sqrt{\frac{m\omega}{\hbar\pi}}\left(\frac{\hbar}{m\omega}\right)^{\frac{3}{2}}\int \xi^2 H_n(\xi)H_n(\xi)e^{-\xi^2}\,d\xi\end{aligned} \tag{47}$$

The integration part can be calculated by Eq. (33).

$$\int \xi^2 H_n(\xi)H_n(\xi)e^{-\xi^2}\,d\xi = \sqrt{\pi}2^n n!\left(n+\frac{1}{2}\right). \tag{48}$$

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,

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

Substituting Eq. (45) and (49),

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

The results satisfy the virial theorem.

(2)

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

$$\psi(x,t) = \frac{1}{\sqrt{2}}[\psi_0(x,t)+\psi_1(x,t)], \tag{52}$$

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

(2) Prove the following relations

$$\begin{aligned}\langle E\rangle &= \langle H\rangle = \hbar\omega,\\ \langle x\rangle &= \frac{1}{\sqrt{2\alpha}}\cos\omega t,\\ \langle p\rangle &= -\sqrt{\frac{\alpha}{2}}\hbar\sin\omega t,\end{aligned} \tag{53}$$

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

(3) If

$$\psi(x,t) = \frac{1}{\sqrt{2}}[e^{i\delta_0}\psi_0(x,t)+e^{i\delta}\psi_1(x,t)], \tag{54}$$

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

$$\psi(x,0) = \sum_n A_n u_n(x) = \left(\frac{\alpha^2}{\pi}\right)^{1/4} e^{-\alpha^2(x-a)^2/2}. \tag{55}$$

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

$$|\pi(x,t)|^2 = \left(\frac{\alpha^2}{\pi}\right)^{1/4} e^{-\alpha^2(x-a\cos\omega t)^2} \tag{56}$$

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

$$P_n = \frac{1}{Z} e^{-E_n/kT} \tag{57}$$

with

$$Z = \sum_n e^{-E_n/kT}, \tag{58}$$

where

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega. \tag{59}$$

(1) Derive the mean energy per an SHO

$$\langle E \rangle = \frac{\hbar\omega}{e^{\hbar\omega/kT} - 1} + \frac{1}{2}\hbar\omega. \tag{60}$$

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

$$C_V = \frac{\partial U}{\partial T}. \tag{61}$$

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

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