Homework 7 - The Harmonic Oscillator

Question 1:

Hermite polynomials H_n are defined using the generating function

$$F(z,\lambda) = e^{-\lambda^2+2z\lambda} = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} H_n(z).$$

Prove the following identities regarding Hermite polynomials:

1. $\frac{dH_n(z)}{dz} = 2nH_{n-1}(z)$.
2. $H_n(z) = 2zH_{n-1}(z) - 2nH_{n-2}(z)$.
3. $H_n(z) = (-1)^n e^{z^2} \frac{d^n}{dz^n} e^{-z^2}$.
4. $\frac{d^2H_n}{dz^2} - 2z\frac{dH_n}{dz} + 2nH_n = 0$.

Solution:

1. Taking the derivative of $F(z,\lambda)$ with respect to (wrt) z we find

$$2\lambda e^{-\lambda^2+2z\lambda} = 2\lambda \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} H_n = 2\sum_{n=0}^{\infty} \frac{\lambda^{n+1}}{(n+1)!}(n+1) H_n = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!}\frac{dH_n}{dz},$$

   comparing powers of λ we immediately get

$$\boxed{\frac{dH_n}{dz} = 2nH_{n-1}}.$$

2. Taking the derivative of $F(z,\lambda)$ with respect to λ we find

$$(-2\lambda+2z)\, e^{-\lambda^2+2z\lambda} = (-2\lambda+2z)\sum_{n=0}^{\infty} \frac{\lambda^n}{n!} H_n = \sum_{n=0}^{\infty}\left(-2(n+1)\frac{\lambda^{n+1}}{(n+1)!} + 2z\frac{\lambda^n}{n!}\right) H_n = \sum_{n=0}^{\infty} \frac{\lambda^{n-1}}{(n-1)!} H_n,$$

   comparing powers of λ we immediately get

$$\boxed{H_n = 2zH_{n-1} - 2(n-1)H_{n-2}}.$$

3. The generating function generates H_n by taking the derivatives wrt λ and taking the $\lambda = 0$ limit:

$$\begin{aligned}
\frac{d^n}{d\lambda^n} F(z,\lambda)\big|_{\lambda=0} &= \frac{d^n}{d\lambda^n}\left[e^{-\lambda^2+2z\lambda}\right]\big|_{\lambda=0} \\
&= \frac{d^n}{d\lambda^n}\left[e^{-(\lambda-z)^2} e^{z^2}\right]\big|_{\lambda=0} \\
&= e^{z^2}\frac{d^n}{d\lambda^n}\left[e^{-(\lambda-z)^2}\right]\big|_{\lambda=0} \\
&= e^{z^2}\frac{d^n}{dx^n}\left[e^{-x^2}\right]\big|_{x=-z} \\
&= (-1)^n e^{z^2}\frac{d^n}{dz^n}\left[e^{-z^2}\right],
\end{aligned}$$

while

$$\frac{d^n}{d\lambda^n}\sum_{m=0}^{\infty}\frac{\lambda^m}{m!}H_m\big|_{\lambda=0}=\sum_{m=n}^{\infty}\frac{\lambda^{m-n}}{(m-n)!}H_m\big|_{\lambda=0}=H_n\left(z\right),$$

thus

$$\boxed{H_n\left(z\right)=\left(-1\right)^n e^{z^2}\frac{d^n}{dz^n}\left[e^{-z^2}\right]}.$$

4. Differentiating wrt z the relation we have found in (1) gives us

$$\frac{d^2H_n}{dz^2}=2n\frac{d}{dz}H_{n-1},$$

taking a look at the relation from (2), combining it with (1), we may write it as

$$H_n=2zH_{n-1}-2\left(n-1\right)H_{n-2}=2zH_{n-1}-\frac{d}{dz}H_{n-1}.$$

Plugging this relation into the equation above yields

$$\begin{aligned}\frac{d^2H_n}{dz^2}&=2n\left(2zH_{n-1}-H_n\right)\\&=2z\frac{d}{dz}H_n-2nH_n,\end{aligned}$$

where we used (1) again in the last equality. Therefore, the equation for H_n reads

$$\boxed{\frac{d^2H_n}{dz^2}-2z\frac{dH_n}{dz}+2nH_n=0}.$$

Question 2:

Consider a simple harmonic oscillator of mass m and frequency ω. It is given that at time $t=0$ the following is true:

- The probability of measuring any energy greater than $2\hbar\omega$ is zero.
- $\langle E\rangle_{t=0}=\hbar\omega$.
- $\langle x\rangle_{t=0}=\frac{1}{2}\sqrt{\frac{\hbar}{m\omega}}$.

Find:

1. $\Psi\left(x,t\right)$.
2. $\langle\hat{x}\rangle\left(t\right)$, $\langle\hat{p}\rangle\left(t\right)$ and $\left\langle\hat{H}\right\rangle\left(t\right)$.
3. $\sigma_p\left(t\right)$ and $\sigma_x\left(t\right)$, and show that Heisenberg's uncertainty principle holds.

Solution:

1. If $P\left(E>2\hbar\omega\right)=0$, recalling that $E_n=\hbar\omega\left(n+\frac{1}{2}\right)$, then the wave function is

$$\psi=c_0\psi_0+c_1\psi_1,$$

where

$$\left|c_0\right|^2+\left|c_1\right|^2=1.$$

Using the expectation value $\langle E\rangle_{t=0}$ we have

$$\langle E\rangle_{t=0}=\left\langle\psi|\hat{H}\psi\right\rangle=E_0\left|c_0\right|^2+E_1\left|c_1\right|^2=\frac{1}{2}\hbar\omega\left|c_0\right|^2+\frac{3}{2}\hbar\omega\left(1-\left|c_0\right|^2\right)=\hbar\omega,$$

we find

$$|c_0|^2 = |c_1|^2 = \frac{1}{2},$$

or

$$|c_0| = \frac{1}{\sqrt{2}} \quad \text{and} \quad |c_1| = \frac{1}{\sqrt{2}}e^{i\theta}.$$

Now, using the expectation value $\langle x \rangle_{t=0}$ we get

$$\begin{aligned}
\langle x \rangle_{t=0} &= \langle \psi | \hat{x}\psi \rangle \\
&= \frac{1}{2}\left(\cancel{\langle \psi_0 | x\psi_0 \rangle} + e^{i\theta}\langle \psi_0 | x\psi_1 \rangle + e^{-i\theta}\langle \psi_1 | x\psi_0 \rangle + \cancel{\langle \psi_1 | x\psi_1 \rangle}\right) \\
&= \frac{1}{2}\left(e^{i\theta} + e^{-i\theta}\right)\sqrt{\frac{\hbar}{2m\omega}} \\
&= \sqrt{\frac{\hbar}{2m\omega}}\cos\theta,
\end{aligned}$$

where we used the result $\langle \psi_n | \hat{x}\psi_l \rangle = \langle \psi_l | \hat{x}\psi_n \rangle = \delta_{n,l+1}\sqrt{\hbar/2m\omega}$, thus

$$\sqrt{\frac{\hbar}{2m\omega}}\cos\theta = \frac{1}{2}\sqrt{\frac{\hbar}{m\omega}} \quad \rightarrow \quad \cos\theta = \frac{1}{\sqrt{2}} \quad \rightarrow \quad \theta = \frac{\pi}{4}.$$

Finally we can write

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2}}\left(\psi_0 e^{-i\frac{\omega}{2}t} + \psi_1 e^{i\left(\frac{\pi}{4} - \frac{3\omega}{2}t\right)}\right)}.$$

2. The time dependent expectation values are

$$\langle x \rangle(t) = \langle \Psi | \hat{x}\Psi \rangle = \frac{1}{2}\left(\cancel{\langle \psi_0 | \hat{x}\psi_0 \rangle} + e^{i\left(\frac{\pi}{4} - \omega t\right)}\langle \psi_0 | \hat{x}\psi_1 \rangle + e^{-i\left(\frac{\pi}{4} - \omega t\right)}\langle \psi_1 | \hat{x}\psi_0 \rangle + \cancel{\langle \psi_0 | \hat{x}\psi_0 \rangle}\right),$$

$$\boxed{\langle x \rangle(t) = \sqrt{\frac{\hbar}{2m\omega}}\cos\left(\omega t - \frac{\pi}{4}\right)}.$$

$$\langle p \rangle(t) = \langle \Psi | \hat{p}\Psi \rangle = \frac{1}{2}\left(\cancel{\langle \psi_0 | \hat{p}\psi_0 \rangle} + e^{i\left(\frac{\pi}{4} - \omega t\right)}\langle \psi_0 | \hat{p}\psi_1 \rangle + e^{-i\left(\frac{\pi}{4} - \omega t\right)}\langle \psi_1 | \hat{p}\psi_0 \rangle + \cancel{\langle \psi_0 | \hat{p}\psi_0 \rangle}\right),$$

$$\boxed{\langle p \rangle(t) = \sqrt{\frac{\hbar m\omega}{2}}\sin\left(\omega t - \frac{\pi}{4}\right)},$$

where we used the result $\langle \psi_l | \hat{p}\psi_n \rangle = -\langle \psi_n | \hat{p}\psi_l \rangle = i\delta_{n,l+1}\sqrt{\hbar m\omega/2}$.

$$\langle H \rangle(t) = \left\langle \Psi | \hat{H}\Psi \right\rangle = \frac{1}{2}\left(\left\langle \psi_0 | \hat{H}\psi_0 \right\rangle + e^{i\left(\frac{\pi}{4} - \omega t\right)}\cancel{\left\langle \psi_0 | \hat{H}\psi_1 \right\rangle} + e^{-i\left(\frac{\pi}{4} - \omega t\right)}\cancel{\left\langle \psi_1 | \hat{H}\psi_0 \right\rangle} + \left\langle \psi_0 | \hat{H}\psi_0 \right\rangle\right),$$

$$\boxed{\langle H \rangle(t) = h\omega},$$

as we expect, the energy is conserved.

3. We need to find $\left\langle x^2 \right\rangle(t)$ and $\left\langle p^2 \right\rangle(t)$, using the result $\left\langle \psi_n | \hat{x}^2\psi_l \right\rangle = \frac{\hbar}{m\omega}\delta_{nl}$, we find

$$\left\langle x^2 \right\rangle(t) = \left\langle \Psi | \hat{x}^2\Psi \right\rangle = \frac{1}{2}\left(\left\langle \psi_0 | \hat{x}^2\psi_0 \right\rangle + e^{i\left(\frac{\pi}{4} - \omega t\right)}\cancel{\left\langle \psi_0 | \hat{x}^2\psi_1 \right\rangle} + e^{-i\left(\frac{\pi}{4} - \omega t\right)}\cancel{\left\langle \psi_1 | \hat{x}^2\psi_0 \right\rangle} + \left\langle \psi_0 | \hat{x}^2\psi_0 \right\rangle\right),$$

$$\underline{\left\langle x^2 \right\rangle(t) = \frac{\hbar}{m\omega}}.$$

We could do the same for $\hat{p}^2$, but it is easier to take advantage of the fact that

$$\langle E \rangle = \frac{\left\langle p^2 \right\rangle}{2m} + \frac{1}{2}m\omega^2\left\langle x^2 \right\rangle = \hbar\omega \quad \rightarrow \quad \underline{\left\langle p^2 \right\rangle(t) = \hbar m\omega}.$$

Therefore, using $\sigma_Q(t) = \sqrt{\langle Q^2\rangle(t) - \langle Q\rangle^2(t)}$, we find

$$\boxed{\sigma_x(t) = \sqrt{\frac{\hbar}{m\omega}}\sqrt{1 - \frac{1}{2}\cos^2\left(\omega t - \frac{\pi}{4}\right)} \quad \text{and} \quad \sigma_p(t) = \sqrt{\hbar m\omega}\sqrt{1 - \frac{1}{2}\sin^2\left(\omega t - \frac{\pi}{4}\right)}},$$

thus

$$\begin{aligned}\sigma_x(t)\sigma_p(t) &= \hbar\sqrt{1 + \frac{1}{4}\cos^2\left(\omega t - \frac{\pi}{4}\right)\sin^2\left(\omega t - \frac{\pi}{4}\right) - \frac{1}{2}\left[\cos^2\left(\omega t - \frac{\pi}{4}\right) + \sin^2\left(\omega t - \frac{\pi}{4}\right)\right]} \\ &= \frac{\hbar}{\sqrt{2}}\sqrt{1 + \frac{1}{2}\cos^2\left(\omega t - \frac{\pi}{4}\right)\sin^2\left(\omega t - \frac{\pi}{4}\right)},\end{aligned}$$

hence

$$\boxed{\sigma_x(t)\sigma_p(t) \geq \frac{\hbar}{\sqrt{2}} > \frac{\hbar}{2}}.$$

Question 3:

Consider a particle moving under the potential

$$V(x) = \begin{cases} \frac{m\omega^2 x^2}{2}, & x > 0, \\ \infty, & \text{else.} \end{cases}$$

Find the particle's eigenfunctions and the corresponding allowed energies.

Hint: Solve Schrödinger equation for $x < 0$ and $x > 0$ separately, and then demand continuity of the wave function.

Solution:

In the regime of $x > 0$, the solution is that of harmonic oscillator,

$$\psi = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sum_n \frac{c_n}{\sqrt{2^n n!}}H_n(\xi)e^{-\xi^2/2}, \quad \text{with} \quad E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad \text{and} \quad \xi \equiv \sqrt{\frac{m\omega}{\hbar}}x,$$

whereas at $\psi(x \leq 0) = 0$, hence, recalling that the $H_n = 0$ only for odd n,

$$c_n = 0 \quad \text{for} \quad n = 2, 4, 6, \ldots$$

So we can write

$$\boxed{\psi = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sum_{2n+1} \frac{c_n}{\sqrt{2^n n!}}H_n(\xi)e^{-\xi^2/2}}.$$

Question 4:

Consider an isotropic three-dimensional harmonic oscillator.

1. Perform separation of variables and find the eigenstates of the system.
2. Find the allowed energies and determine the degeneracy of each level.

Solution:

The Schrödinger equation is

$$\hat{H}\psi = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi + \frac{1}{2}m\omega^2\left(x^2 + y^2 + z^2\right)\psi = \left(\hat{H}_x + \hat{H}_y + \hat{H}_z\right)\psi = (E_n + E_m + E_l)\psi.$$

1. These are 3 copies of the same Hamiltonian, thus

$$\psi(x,y,z) = \psi_n(x)\,\psi_m(y)\,\psi_l(z) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} \sum_{n,m,l} \frac{c_{nml}}{\sqrt{2^{n+m+l} n!m!l!}} H_n(\xi_x)\,H_m(\xi_y)\,H_l(\xi_z)\,e^{-\left(\xi_x^2+\xi_y^2+\xi_z^2\right)/2}.$$

2. The corresponding energies are

$$E_{nml} = \hbar\omega\sqrt{n+m+l+\frac{3}{2}},$$

where there is a degeneracy g_n of the nth energy level. In order to find the form of g_n let us look at the degeneracy of the nth level for each n_x:

	$n=0$	$n=1$	$n=2$	$\cdots$	degeneracy
$n_x = 0:$	$(0,0,0)$	$(0,1,0)$ $(0,0,1)$	$(0,2,0)$ $(0,1,1)$ $(0,0,2)$	$\cdots$	$n+1$
$n_x = 1:$		$(1,0,0)$	$(1,1,0)$ $(1,0,1)$	$\cdots$	n
$n_x = 2:$			$(2,0,0)$	$\cdots$	$n-1$

thus, summing on n_x we get

$$g_n = \sum_{n_x=0}^{n} (n+1-n_x) = (n+1)(n+1) - \frac{n(n+1)}{2} \quad \rightarrow \quad \boxed{g_n = \frac{(n+2)(n+1)}{2}}.$$

Question 5:

The Morse potential, is a convenient model for the potential energy of a diatomic molecule. It is given by

$$V(r) = D_e\left(1-e^{-a(r-r_e)}\right)^2,$$

Where r is the distance between molecules, r_e is equilibrium bond distance, D_e is potential well depth and a controls the width of the well. Estimate the ground state energy of a molecule which consists of two atoms of masses m_1 and m_2 in their center-of-mass system.

Solution:

Noting that $V(r) \geq 0$, and the only zero is at $V(r_e) = 0$, we may Taylor expand the potential around its minimum

$$V(r) = a^2 D_e (r-r_e)^2 + \mathcal{O}\left[(r-r_e)^3\right] \approx a^2 D_e (r-r_e)^2.$$

In the center-of-mass system the Schrödinger equation is that of a harmonic oscillator,

$$\hat{H}\psi = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2}\psi + \frac{1}{2}\mu\omega^2(r-r_e)^2 = E_n\psi, \quad \text{with} \quad \mu \equiv \frac{m_1 m_2}{m_1+m_2} \quad \text{and} \quad \omega \equiv \sqrt{\frac{2a^2 D_e}{\mu}},$$

thus the ground state is approximated by $\boxed{E_0 = \frac{1}{2}\hbar\omega}$.