Tutorial 6 - The Harmonic Oscillator

The Harmonic Oscillator

Perhaps the most important potential function is that of the harmonic oscillator, a motion the is governed by *Hooke's law*,

$$m\frac{d^2x}{dt^2} = -kx \quad \rightarrow \quad x(t) = A\sin(\omega t) + B\cos(\omega t), \quad \text{where} \quad \omega \equiv \sqrt{\frac{k}{m}}.$$

The reason for this is that any potential $V(x)$ is *approximately* parabolic, in the neighborhood of a local minimum x_0, as can we can see by expanding it in a *Taylor series*,

$$V(x) = \underbrace{V(x_0)}_{\text{constant}} + \underbrace{V'(x_0)}_{=0}(x - x_0) + \frac{1}{2}V''(x_0)(x - x_0)^2 + \cdots \approx \frac{1}{2}V''(x_0)(x - x_0)^2.$$

The time-independent Schrödinger equation for the potential $V(x) = \frac{1}{2}m\omega^2 x^2$ is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi,$$

which can be written more simply in terms of $\xi \equiv \sqrt{\frac{m\omega}{\hbar}}x$, as

$$\left(\frac{d^2}{d\xi^2} - 2\xi\frac{d}{d\xi} + K - 1\right)h(\xi) = 0,$$

where

$$\psi(\xi) = h(\xi)\, e^{-\xi^2/2}, \quad \text{and} \quad K \equiv \frac{2E}{\hbar\omega}.$$

The solutions to this equations are

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-\frac{m\omega}{2\hbar}x^2}, \quad \text{with} \quad E_n = \hbar\omega\left(n + \frac{1}{2}\right) \quad n = 0, 1, 2, \ldots$$

where H_n are the Hermite polynomials. Many times it is useful to use the parametrized form

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n(\xi)\, e^{-\xi^2/2}.$$

Additional reading: David Griffiths, Introduction to Quantum Mechanics (3$^{\text{nd}}$ edition), Ch. 2.3.2, p.48-54.

Hermite Polynomials

The Hermite polynomials are defined through the derivatives of the Gaussian function

$$g(z) = e^{-z^2}.$$

The successive derivatives of a Gaussian are given by

$$g'(z) = -2ze^{-z^2}.$$
$$g''(z) = \left(4z^2 - 2\right) e^{-z^2},$$

then we would like to state that the nth-order derivative can be written as

$$g^{(n)}(z) = (-1)^n H_n(z)\, g(z),$$

where $H(z)$ is an nth-degree polynomial in z.
The Hermite polynomials can be generated using the *generating function* $F(z, \lambda)$ as follows:

$$F(z, \lambda) \equiv e^{-\lambda^2 + 2\lambda z} \quad \rightarrow \quad H_n(z) = \left\{ \frac{\partial^n}{\partial \lambda^n} F(z, \lambda) \right\}_{\lambda=0}.$$

Differentiating the generating function with respect to z or λ leads to recurrence relations of H_n:

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

The differential equation for the Hermite polynomials is:

$$\left(\frac{d^2}{dz^2} - 2z\frac{d}{dz} + 2n \right) H_n(z) = 0,$$

which is precisely the differential equation for the quantum harmonic oscillator.Properties:

- The parity of H_n is $(-1)^n$.
- H_n has n real zeros, between which one finds those of H_{n-1}.

The first Hermite polynomials are:

$$\begin{aligned} H_0 &= 1, & H_1 &= 2\xi, \\ H_2 &= 4\xi^2 - 2, & H_3 &= 8\xi^3 - 12\xi, \\ H_4 &= 16\xi^4 - 48\xi^2 + 12, & H_5 &= 32\xi^5 - 160\xi^3 + 120\xi. \end{aligned}$$

Additional reading: Cohen Tannoudji, Quantum Mechanics (2^{nd} edition), Ch. V Complement B_v, p.547-550.

Question 1:

Consider a particle with energy $E_n = \hbar\omega\left(n+\frac{1}{2}\right)$, moving under an harmonic potential of frequency ω.

1. For the ground state, calculate the probability of finding a particle outside the classically allowed region.
2. Repeat (1) for $n=1$ and $n=2$. Interpret the result.

Solution:

1. Classically we have
$$x_c = A\cos\omega t, \qquad \text{and} \qquad p_c = -m\omega A\sin\omega t,$$
thus, the boundary position of the particle (i.e. the amplitude), in terms of energy, is
$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = \frac{m\omega^2 A^2}{2} \quad \rightarrow \quad A_n = \sqrt{\frac{2E_n}{m\omega^2}} = \sqrt{\frac{\hbar\left(2n+1\right)}{m\omega}}.$$
Therefore, the probability for finding the particle outside the classical region is
$$\begin{aligned} P_n\left(|x| > A_n\right) &= 1 - P\left(|x| < A_n\right) \\ &= 1 - \int_{-A_n}^{A_n} \psi_n^*\left(x\right)\psi_n\left(x\right)dx \\ &= 1 - \sqrt{\frac{m\omega}{\pi\hbar}}\int_{-A_n}^{A_n}\frac{1}{2^n n!}H_n^2\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-\frac{m\omega}{\hbar}x^2}dx \\ &= 1 - \frac{1}{2^n n!\sqrt{\pi}}\int_{-\sqrt{2n+1}}^{\sqrt{2n+1}} H_n^2\left(\xi\right)e^{-\xi^2}d\xi \end{aligned}$$
At the ground state ($n=0$), $A_0 = \sqrt{\hbar/m\omega}$
$$\boxed{P_0 = 1 - \frac{1}{\sqrt{\pi}}\int_{-1}^{1} e^{-\xi^2}d\xi = 1 - \text{erf}\left(1\right) \approx 0.1578}.$$

2. Plugging in $n=1$ and $n=2$ we get
$$\begin{aligned} P_1 &= 1 - \frac{1}{2\sqrt{\pi}}\int_{-\sqrt{3}}^{\sqrt{3}} 4\xi^2 e^{-\xi^2}d\xi \\ &= 1 - \frac{1}{\sqrt{\pi}}\int_{-\sqrt{3}}^{\sqrt{3}}\left[e^{-\xi^2} - \frac{d}{d\xi}\left(\xi e^{-\xi^2}\right)\right]d\xi \\ &= 1 - \frac{1}{\sqrt{\pi}}\left[\sqrt{\pi}\text{erf}\left(\sqrt{3}\right) - 2\sqrt{3}e^{-3}\right], \end{aligned}$$
and in the same manner
$$\begin{aligned} P_2 &= 1 - \frac{1}{8\sqrt{\pi}}\int_{-\sqrt{5}}^{\sqrt{5}}\left(4\xi^2 - 2\right)^2 e^{-\xi^2}d\xi \\ &= 1 - \frac{1}{2\sqrt{\pi}}\int_{-\sqrt{5}}^{\sqrt{5}}\left(4\xi^4 - 4\xi^2 + 1\right)e^{-\xi^2}d\xi \\ &= 1 - \frac{1}{2\sqrt{\pi}}\left[2\sqrt{\pi}\text{erf}\left(\sqrt{5}\right) - 22\sqrt{5}e^{-5}\right], \end{aligned}$$
thus
$$\boxed{P_1 \approx 0.1116 \qquad \text{and} \qquad P_2 \approx 0.0951}.$$
We see that the probability to find the particle in a classically forbidden region drops as its energy increases, i.e. more energetic particles behave more classically, as one would expect.

Question 2:

Use Heisenberg's uncertainty principle to estimate the ground state energy of a 1D harmonic oscillator. Is this estimate precise? If so, why?

Solution:

Starting from the expectation value of the Hamiltonian

$$\langle H\rangle_n = \frac{\langle p^2\rangle_n}{2m} + \frac{1}{2}m\omega^2\langle x^2\rangle_n .$$

Recalling that $\sigma_Q^2 = \langle Q^2\rangle - \langle Q\rangle^2$, we see that if $\sigma_p^2 = \langle p^2\rangle$ and $\sigma_x^2 = \langle x^2\rangle$, then we can use $\sigma_x\sigma_p \sim \hbar/2$ to estimate $\langle H\rangle$. But in order to do that we first need to show that $\langle x\rangle = \langle p\rangle = 0$. Lets start with

$$\langle x\rangle_n = \int \psi_n^* x\psi_n dx = 0,$$

since $|\psi_n|$ is an even function. Next is

$$\frac{d}{dx} = \sqrt{\frac{m\omega}{\hbar}}\frac{d}{d\xi}$$

$$\begin{aligned}
\langle p\rangle_n &= \int \psi_n^*\left(-i\hbar\frac{d}{dx}\right)\psi_n dx \\
&= -\frac{im\omega}{2^n n!\sqrt{\pi}}\int H_n(\xi)\,e^{-\xi^2/2}\frac{d}{d\xi}\left(H_n(\xi)\,e^{-\xi^2/2}\right)dx \\
&= -\frac{im\omega}{2^n n!\sqrt{\pi}}\int H_n(\xi)\left(H_n'(\xi) - \xi H_n(\xi)\right)e^{-\xi^2}dx \\
&= -\frac{im\omega}{2^n n!\sqrt{\pi}}\int H_n(\xi)\left(2nH_{n-1} - \xi H_n(\xi)\right)e^{-\xi^2}dx,
\end{aligned}$$

but both terms are odd, since H_n^2 is even and H_nH_{n-1} is odd, hence $\langle p\rangle_n = 0$. Therefore, we may write

$$\langle H\rangle_n = E_n = \frac{\sigma_p^2}{2m} + \frac{1}{2}m\omega^2\sigma_x^2 \sim \frac{\hbar^2}{8m\sigma_x^2} + \frac{1}{2}m\omega^2\sigma_x^2,$$

and find the minimum value with respect to σ_x

$$\begin{aligned}
\frac{dE_n}{d\sigma_x} &= -\frac{\hbar^2}{4m\sigma_x^3} + m\omega^2\sigma_x = 0 \quad \rightarrow \quad \sigma_x^2 = \frac{\hbar}{2m\omega}, \\
\left.\frac{d^2E_n}{d\sigma_x^2}\right|_{\sigma_x^2=\frac{\hbar}{2m\omega}} &= -\frac{3\hbar^2}{4m\sigma_x^4} + m\omega^2 = -\frac{1}{2}m\omega^2 < 0 \quad \rightarrow \quad \text{minimum},
\end{aligned}$$

which corresponds to

$$\boxed{(E_n)_{\min} \sim \frac{\hbar\omega}{2}}.$$

In this case the results are accurate since the ground state is a Gaussian, but in case of non-Gaussian ground state we would get $E_n \gtrsim \hbar/2$.

Question 3:

Consider an isotropic two-dimensional harmonic oscillator.

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

Solution:

1. The time-independent Schrödinger equation reads

$$\hat{H}\psi\left(x,y\right)=\left[\frac{1}{2m}\left(\hat{p}_x^2+\hat{p}_y^2\right)+\frac{1}{2}m\omega^2\left(x^2+y^2\right)\right]\psi\left(x,y\right)=E\psi\left(x,y\right),$$

which can be separated into $\hat{H}=\hat{H}_x+\hat{H}_y$ that acts on the wave function

$$\psi\left(x,y\right)=\chi\left(x\right)\eta\left(y\right),$$

so that

$$\left(\hat{H}_x+\hat{H}_y\right)\chi\left(x\right)\eta\left(y\right)=\eta\left(y\right)\hat{H}_x\chi\left(x\right)+\chi\left(x\right)\hat{H}_y\eta\left(y\right)=\eta\left(y\right)E_n^x\chi\left(x\right)+\chi\left(x\right)E_m^y\eta\left(y\right)=\left(E_n^x+E_m^y\right)\chi_n\left(x\right)\eta_m\left(y\right)=E_{n,m}\psi_{n,m}$$

So that the eigenstates are just a multiplication of two copies of one-dimensional harmonic oscillator,

$$\boxed{\psi_{n,m}\left(x,y\right)=\left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\frac{1}{\sqrt{2^{n+m}n!m!}}H_n\left(\xi_x\right)H_m\left(\xi_y\right)e^{-\left(\xi_x^2+\xi_y^2\right)/2}}.$$

2. The energy levels are

$$\boxed{E_{n,m}=\hbar\omega\left(n+m+1\right)},$$

with degeneracies at

$$\left(n,m\right)=\left\{\left(0,0\right),\ \begin{matrix}(0,1)\\(1,0)\end{matrix},\ \begin{matrix}(0,2)\\(1,1)\\(2,0)\end{matrix},\ \begin{matrix}(0,3)\\(1,2)\\(2,1)\\(3,0)\end{matrix},\ \ldots\right\},$$

or in general

$$\boxed{g_n=n+1}.$$