

3.3 One-dimensional quantum-mechanical harmonic oscillator

The 1D harmonic oscillator is a system used to solve the Schrödinger equation analytically.

The Schrödinger equation is a linear partial differential equation that governs the wave function of a quantum-mechanical system. A large number of systems behave similar to the harmonic oscillator as they approach the limit of small oscillations. These small oscillations are particularly relevant to the vibrations of atoms about their equilibrium position in a diatomic molecule, the oscillations of atoms, and the oscillators of ions in a crystal lattice.

3.3.1 Schrödinger equation

The time-independent Schrodinger equation is used to solve several practical problems. The equation for one particle with mass m and energy E in one-dimensional space is defined as:

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{d\hat{x}^2} + V(x)\psi = E\psi \quad (3.3.1.1)$$

where \hbar is the reduced Planck constant (1.05457×10^{-34} Js), $\psi(x)$ is the wavefunction giving the probability of finding a particle at the position x , and $V(x)$ is the potential energy that is operated to the particle at the position x . The wavefunction contains all the information about the motion of the particle.

3.3.2 1D harmonic oscillation

In classical mechanics, a harmonic oscillator is a system that, when displaced from its equilibrium position, experiences a restoring force F proportional to the displacement x . It is defined as:

$$F = -kx \quad (3.3.2.1)$$

where k is the force constant. The force can be related to the potential energy as:

$$F = -dV/dx \quad (3.3.2.2)$$

The potential energy stored during the harmonic oscillation is defined as a parabolic function:

$$V = (1/2)kx^2 \quad (3.3.2.3)$$

Thus, the time-independent Schrödinger equation in 1D can be written as:

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{d\hat{x}^2} + \frac{1}{2}kx^2\psi = E\psi \quad (3.3.2.4)$$

3.3.3 Solution of the 1D harmonic oscillation

In classical mechanism, the force applied to a spring is defined as $F = -kx$, and the motion is defined as $F = m \frac{d^2x}{dt^2}$, where t is time. Thus, we can write:

$$m \frac{d^2x}{dt^2} = \frac{1}{2}kx^2 \quad (3.3.3.1)$$

The solution to this equation has the form $x = A\cos(\omega t + \theta)$, with $\omega = \sqrt{k/m}$. Equation (3.3.2.4) can be written in terms of the angular frequency.

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{d\hat{x}^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi \quad (3.3.3.2)$$

Considering that this equation is difficult to solve, we may write:

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{d\hat{x}^2} = (E - \frac{1}{2}m\omega^2x^2)\psi(x) \quad (3.3.3.3)$$

The valuables x and E can be replaced by:

$$x = \sqrt{\frac{\hbar}{m\omega}} \xi \quad (3.3.3.4)$$

$$E = \frac{\hbar\omega}{2} \xi \quad (3.3.3.5)$$

Then, the equation become in a simple form:

$$\frac{d^2\phi(\xi)}{d\xi^2} + (\varepsilon - \xi^2)\phi(\xi) = 0 \quad (3.3.3.6)$$

where $\phi(\xi) = \psi(x)$. Still, this equation is difficult to solve. Let's consider the first term of the previous equation. This can be written as:

$$\begin{aligned} \frac{d^2}{d\xi^2} [H(\xi)e^{-\frac{\xi^2}{2}}] &= \frac{d^2}{d\xi^2} \left[\frac{dH(\xi)}{d\xi} e^{-\frac{\xi^2}{2}} - H(\xi) \frac{d}{d\xi} e^{-\frac{\xi^2}{2}} \right] \\ &= \frac{d}{d\xi} \left[\frac{dH(\xi)}{d\xi} e^{-\frac{\xi^2}{2}} - \xi H(\xi) e^{-\frac{\xi^2}{2}} \right] = e^{-\frac{\xi^2}{2}} \left[\frac{d^2H(\xi)}{d\xi^2} - 2\xi \frac{dH(\xi)}{d\xi} + (\xi^2 - 1)H(\xi) \right] \end{aligned} \quad (3.3.3.7)$$

Simplifying the second term of equation (3.3.3.6) and incorporation (3.3.3.7), we can write:

$$e^{-\frac{\xi^2}{2}} \left[\frac{d^2H(\xi)}{d\xi^2} - 2\xi \frac{dH(\xi)}{d\xi} + (\xi^2 - 1)H(\xi) \right] + (\varepsilon - \xi^2)H(\xi)e^{-\frac{\xi^2}{2}} = 0 \quad (3.3.3.8)$$

Simplifying one more time gives:

$$\frac{d^2H(\xi)}{d\xi^2} - 2\xi \frac{dH(\xi)}{d\xi} + (\varepsilon - 1)H(\xi) = 0 \quad (3.3.3.9)$$

Now, assuming $H(\xi) = \sum_{k=0}^{\infty} a_k \xi^k$ and substituting this into the previous equation gives:

$$\begin{aligned} \sum_{k=2}^{\infty} k(k-1)a_k \xi^{k-2} - 2\xi \sum_{k=1}^{\infty} k a_k \xi^{k-1} + (\varepsilon - 1) \sum_{k=0}^{\infty} a_k \xi^k &= 0 \\ \sum_{k=2}^{\infty} k(k-1)a_k \xi^{k-2} - 2(0 \cdot a_0 \cdot \xi^0 + \sum_{k=1}^{\infty} k a_k \xi^k) + (\varepsilon - 1) \sum_{k=0}^{\infty} a_k \xi^k &= 0 \\ \sum_{k=0}^{\infty} (k+2)(k+1)a_{k+2} \xi^k - 2 \sum_{k=0}^{\infty} k a_k \xi^k + (\varepsilon - 1) \sum_{k=0}^{\infty} a_k \xi^k &= 0 \\ \sum_{k=0}^{\infty} [(k+2)(k+1)a_{k+2} - (2k - \varepsilon + 1)a_k] \xi^k &= 0 \end{aligned} \quad (3.3.3.10)$$

To satisfy this condition, the interior of the sum must be equal to 0. Thus, we can write:

$$a_{k+2} = \frac{(2k - \varepsilon + 1)}{(k+2)(k+1)} a_k \quad (3.3.3.11)$$

Using this to rewrite $H(\xi)$ we have:

$$\begin{aligned} H(\xi) &= a_0 \left(1 - \frac{\varepsilon-1}{1 \cdot 2} \xi^2 + \frac{\varepsilon-1}{1 \cdot 2} \frac{\varepsilon-4-1}{3 \cdot 4} \xi^4 - \dots \right) + a_1 \left(\xi - \frac{\varepsilon-1}{2 \cdot 3} \xi^3 \right. \\ &\quad \left. + \frac{\varepsilon-2-1}{2 \cdot 3} \frac{\varepsilon-6-1}{4 \cdot 5} \xi^5 - \dots \right) \end{aligned} \quad (3.3.3.12)$$

Without special conditions, the series diverges at large ξ . The conditions for the convergence at any ξ can be described by $\varepsilon = 2n - 1$. Then, a_n is non-zero while the higher terms are zero. Therefore, the series becomes finite. We can write:

$$a_{n+2} = \frac{\varepsilon - 2n + 1}{(n + 2)(n + 1)} a_n = 0 \quad (3.3.3.13)$$

Thus, $H(\xi)$ is characterized by $\varepsilon = 2n - 1$ and Hermite polynomials $H_n(\xi)$. The first few Hermite polynomials are described as:

$$\begin{aligned} H_0(\xi) &= a_0 \\ H_1(\xi) &= a_1 \xi \\ H_2(\xi) &= a_0 \left(1 - \frac{4}{1 \cdot 2} \xi^2\right) \\ H_3(\xi) &= a_1 \left(1 - \frac{4}{2 \cdot 3} \xi^3\right) \\ H_4(\xi) &= a_0 \left(1 - \frac{8}{1 \cdot 2} \xi^2 + \frac{8}{1 \cdot 2 \cdot 3 \cdot 4} \xi^4\right) \\ H_5(\xi) &= a_1 \left(1 - \frac{8}{2 \cdot 3} \xi^3 + \frac{8}{2 \cdot 3 \cdot 4 \cdot 5} \xi^5\right) \end{aligned} \quad (3.3.3.14)$$

The wavefunction under the potential of the harmonic oscillator can now be written as $\phi(\xi) = cH(\xi)e^{-\frac{\xi^2}{2}}$ and $\psi(x) = cH\left(\sqrt{\frac{m\omega}{\hbar}}x\right)e^{-\frac{m\omega}{2\hbar}x^2}$. The allowed energies are $E = \frac{\hbar\omega}{2}(2n + 1) = \hbar\omega(n + \frac{1}{2})$.

3.3.4 Energy level

The permitted energy levels can be written as:

$$E = \frac{\hbar\omega}{2} \varepsilon_v = \frac{\hbar\omega}{2} \left(v + \frac{1}{2}\right) \quad (3.3.3.15)$$

where $v=0,2, \dots$, or any quantum number. The angular frequency increases with increasing k and decreasing m , such that at $v=0$, $E_0 = \frac{\hbar\omega}{2}$. This is also referred to as the non-zero, zero-point energy. The separation between the adjacent levels can be written as $E_{v+1} - E_v = \hbar\omega$, which is identical for all v . The energy levels $\hbar\omega$ form a uniform ladder of spacing, see Fig. 1.

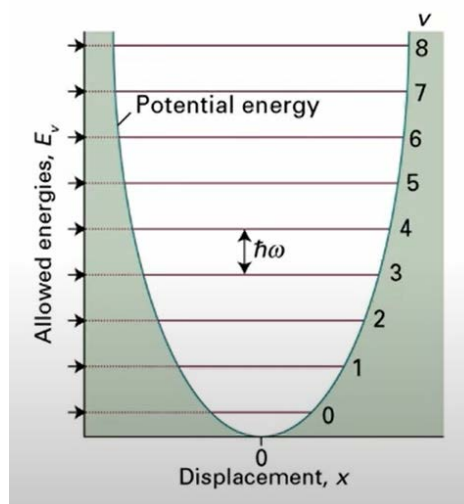


Fig.1. Diagram of a potential well illustrating the allowed energy levels as a function of displacement.

3.3.5 Time dependent Schrödinger equation of the harmonic oscillator

The time dependent Schrödinger equation of the harmonic oscillator requires further analysis of the particle's oscillation. The particle's oscillation can be investigated via the ladder operator \hat{a} and its adjoint \hat{a}^+ .

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i}{m\omega} \hat{p} \right) \quad (3.3.5.1)$$

$$\hat{a}^+ = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - \frac{i}{m\omega} \hat{p} \right) \quad (3.3.5.2)$$

where \hat{x} is the particle's displacement and \hat{p} is the momentum. This notation becomes particularly useful when investigating the time (t) dependent solution. The solution is a simple superposition of the lowest two eigenstates (n=0 and 1), such that:

$$|\psi\rangle = \cos\theta|0\rangle + e^{i\varphi}\sin\theta|1\rangle \quad (3.3.5.3)$$

where φ is the phase lag of the oscillation and θ is the angle of the oscillation. The time evolution is thus given by:

$$|\psi, t\rangle = e^{-\frac{iH}{\hbar}t} |\psi\rangle = e^{-\frac{iH}{\hbar}t} \cos\theta|0\rangle + e^{-\frac{iH}{\hbar}t} e^{i\varphi} \sin\theta|1\rangle \quad (3.3.5.4)$$

In terms of energy, E_0 and E_1 , we can write:

$$\begin{aligned} |\psi, t\rangle &= e^{-\frac{iE_0}{\hbar}t} \cos\theta |0\rangle + e^{-\frac{iE_1}{\hbar}t} e^{i\varphi} \sin\theta |1\rangle \\ &= e^{-\frac{i\omega}{2}t} (\cos\theta|0\rangle + e^{i\varphi} \sin\theta|1\rangle) \end{aligned} \quad (3.3.5.5)$$

We can now write this solution in terms of ladder operators using $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^+)$:

$$\begin{aligned} &\langle \psi, t | \hat{x} | \psi, t \rangle \\ &= e^{-\frac{i\omega}{2}t} (\cos\theta|0\rangle + e^{i\varphi} \sin\theta|1\rangle) \hat{x} e^{\frac{i\omega}{2}t} (\cos\theta|0\rangle + e^{i\varphi} \sin\theta|1\rangle) \\ &= e^{-\frac{i\omega}{2}t} (\cos\theta|0\rangle + e^{i\varphi} \sin\theta|1\rangle) \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^+) e^{\frac{i\omega}{2}t} (\cos\theta|0\rangle \\ &\quad + e^{i\varphi} \sin\theta|1\rangle) \end{aligned} \quad (3.3.5.6)$$

This can be simplified to using $\langle \hat{a}|0\rangle = |0\rangle$, $\langle \hat{a}|1\rangle = |0\rangle$, $\langle \hat{a}^+|0\rangle = |1\rangle$ and $\langle \hat{a}^+|1\rangle = \sqrt{2}|2\rangle$:

$$\begin{aligned} &\langle \psi, t | \hat{x} | \psi, t \rangle \\ &= (\cos\theta|0\rangle + e^{i\varphi} \sin\theta|1\rangle) \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^+) (\cos\theta|0\rangle + e^{i\varphi} \sin\theta|1\rangle) \\ &= \sqrt{\frac{\hbar}{2m\omega}} (\cos\theta|0\rangle + e^{i\varphi} \sin\theta|1\rangle) (\cos\theta|1\rangle + e^{i\varphi} \sin\theta(|0\rangle \\ &\quad + \sqrt{2}|2\rangle)) \end{aligned} \quad (3.3.5.7)$$

Finally, when processing the multiplication among the similar energy states, this results in:

$$\begin{aligned} \langle \psi, t | \hat{x} | \psi, t \rangle &= \sqrt{\frac{\hbar}{2m\omega}} (e^{i\varphi} \sin\theta \cos\theta + e^{i\varphi} \sin\theta \cos\theta) \\ &= \sqrt{\frac{\hbar}{2m\omega}} (\cos(\omega t - \varphi) \sin 2\theta) \end{aligned} \quad (3.3.5.8)$$

In other words, the position oscillates between $\pm \sqrt{\frac{\hbar}{2m\omega}} \sin 2\theta$ at a frequency ω .

3.3.6 Phonons

The harmonic oscillator is used to describe vibrations in a crystal lattice, such as phonons, using quantum-mechanics. The quantum-mechanical description is used to derive the lattice properties, such as the specific heat, of the system. Let's consider a system defined as a monoatomic crystal formed by ions in a lattice. The equilibrium position of the ions can be described as $R_n = nd$, where d is the lattice constant. Considering a significant displacement x_n from the equilibrium position, the actual position of the ions would be $r_n = x_n + R_n$. The interaction potential among the ions can be written as:

$$V = \frac{1}{2} \sum_{n,m} V(r_n - r_m) = \frac{1}{2} \sum_{n,m} V(R_n - R_m + x_n - x_m) \quad (3.3.6.1)$$

In the case of a negligible displacement, the potential can be expanded as:

$$\begin{aligned} V &= \frac{1}{2} \sum_{n,m} V(R_n - R_m) + \frac{1}{2} \sum_{n,m} (x_n - x_m) \partial V(R_n - R_m) \\ &+ \frac{1}{2} \sum_{n,m} (x_n - x_m)^2 \partial^2 V(R_n - R_m) \end{aligned} \quad (3.3.6.2)$$

The first term represents the interaction potential at equilibrium, which is not significant in this case. Extending the second term gives:

$$\begin{aligned} \frac{1}{2} \sum_{n,m} (x_n - x_m) \partial V(R_n - R_m) &= \frac{1}{2} \sum_n x_n \sum_m \partial V(R_n - R_m) - \partial V(R_m - R_n) \\ &= \sum_n x_n \sum_m \partial V(R_n - R_m) \end{aligned} \quad (3.3.6.3)$$

The last sum is the total force F_n exerted on the atom n by all the other atoms. At equilibrium, this force is null and thus the second term of (3.3.6.1) can also be ignored. Assuming only neighboring atoms interact with each other, extending the third term of (3.3.6.1) gives:

$$\frac{1}{2} \sum_{n,m} (x_n - x_m)^2 \partial^2 V(R_n - R_m) = \frac{1}{2} K \sum_{n,m} (x_n - x_{n+1})^2 \quad (3.3.6.4)$$

The potential energy of the lattice can now be written as:

$$\begin{aligned} V &= \frac{1}{2} K \sum_{n,m} (x_n - x_{n+1})^2 \\ &= - \frac{K}{2NM} \sum_k \frac{4 \sin^2(kd/2)}{2\omega_k} [-a_k^+ a_{-k}^+ - a_k^+ a_k - a_k a_{-k} - a_k a_k^+] \end{aligned} \quad (3.3.6.5)$$

The Hamiltonian can be written as:

$$H = \sum_n \frac{p_n^2}{2M} + \frac{1}{2} K \sum_{n,m} (x_n - x_{n+1})^2 \quad (3.3.6.6)$$

where M is the mass of the ions. After some algebra, this can be simplified to:

$$H = \sum_k \omega_k [a_k^+ a_k + \frac{1}{2}] \quad (3.3.6.7)$$

We can now define $n_k = a_k^\dagger a_k$, which describes the excitation number of a normal mode of the ion vibration. Quasi-particles, such as phonons, can also be described by n_k .

The heat capacity describes how much heat is required to raise the temperature of a given system. The specific heat capacity is a measure particular to a material and only depends on the type and phase of that material. This is described in terms of heat capacity per unit mass and is defined by $C_v = \frac{\partial u}{\partial T}$, where T is temperature. The thermal energy density (u) requires the investigation of the lattice vibration, which is governed by the partition function. The resulting thermal energy density in terms of volume (V) is:

$$u = \frac{1}{V} \sum_k \omega_k \left[n(k) + \frac{1}{2} \right] \quad (3.3.6.8)$$

Taking the derivative gives:

$$C_v = \sum_k \frac{\omega_k^2}{4Vk_b T^2 \sinh^2\left(\frac{\omega_k}{2k_b T}\right)} \quad (3.3.6.9)$$

3.3.7 References

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