0.1 Discrete Schrodinger Equation

0.1.1 Schrodinger Equation on an infinite discrete lattice

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t)$$

Let the lattice points be labelled x_i with lattice spacing a. The wavefunction at i^{th} site is

$$\psi(x_i,t) = \langle x_i|\,\psi(t)\rangle$$

where $|x_i\rangle$ is state of definite position with a Dirac delta normalisation $\langle x_i|\,x_j\rangle = \delta\left(x_i - x_j\right)$. The wavefunction normalisation is

$$\int_{-\infty}^{\infty} dx\,|\psi(x,t)|^2 = 1$$

For the discrete system, this reduces to

$$\sum_i a\,|\langle x_i|\,\psi(t)\rangle|^2 = 1$$

This motivates us to define normalisable states of definite position $|\tilde{x_i}\rangle = \sqrt{a}\,|x_i\rangle$. These satisfy $\langle \tilde{x}_i|\,\tilde{x}_j\rangle = \delta_{ij}$ where δ_{ij} is the Kronecker delta (**verify this statement**). Then

$$\begin{aligned}\psi(x_i,t) &= \langle x_i|\,\psi(t)\rangle \\ &= (1/\sqrt{a})\,\langle\tilde{x}_i|\,\psi(t)\rangle \\ &= (1/\sqrt{a})\;\phi_i(t)\end{aligned}$$

where $\phi_i = \langle\tilde{x}_i|\,\psi\rangle$. The discretised second derivative of the wavefunction is

$$\left.\frac{\partial^2\psi(x,t)}{\partial x^2}\right|_{x_i} = \frac{\psi\left(x_i+a,t\right) - 2\psi\left(x_i,t\right) + \psi\left(x_i-a,t\right)}{a^2}$$

Then the Schrodinger equation reduces to

$$i\hbar\,\frac{d\phi_i(t)}{dt} = -\frac{\hbar^2}{2ma^2}\left[\phi_{i+1}(t) - 2\phi_i(t) + \phi_{i-1}(t)\right] + V_i\phi_i(t)$$

This can be written as a matrix equation

$$i\hbar\,\frac{d\phi(t)}{dt} = H\phi$$

where ϕ is a column vector with entries ϕ_i and H is the Hamiltonian matrix with matrix elements

$$H_{ij} = -\frac{\hbar^2}{2ma^2}\left[\delta_{i+1,j} - 2\;\delta_{i,j} + \delta_{i-1,j}\right] + V_i\;\delta_{i,j}$$

It is easy to verify that H is Hermitian (**verify**).
The generic problem is as follows: the state $\phi(0)$ is given at $t = 0$ and the state $\phi(t)$ at instant t is to be determined. First the eigenvalues and (normalised) eigenvectors of H are determined using matrix techniques

$$H\phi_{E_i} = E_i\phi_{E_i}$$

The completeness of the set $\{\phi_{E_i}\}$ allows us to express the state at $t = 0$ as a linear superposition of these states

$$\phi(0) = \sum_i c_i\phi_{E_i}$$

where $c_i = \phi_{E_i}^\dagger \phi(0)$. The state at instant t is then given by

$$\begin{aligned}\phi(t) &= e^{-iHt/\hbar}\phi(0) \\ &= \sum_i c_i\ e^{-iE_it/\hbar}\phi_{E_i}\end{aligned}$$

Example: Harmonic Oscillator interaction with $V(x) = (1/2)m\omega^2 x^2$. The Hamiltonian matrix elements are

$$\begin{aligned}H_{ij} &= -\frac{\hbar^2}{2ma^2}\left[\delta_{i+1,j} - 2\ \delta_{i,j} + \delta_{i-1,j}\right] + (1/2)m\omega^2 x_i^2\ \delta_{i,j} \\ &= -\frac{\hbar^2}{2ma^2}\left[\delta_{i+1,j} - 2\ \delta_{i,j} + \delta_{i-1,j}\right] + (1/2)m\omega^2 a^2\ i^2\ \delta_{i,j}\end{aligned}$$

where $x_i = a \times i,\ i \in \mathbb{Z}$.
Natural scales: Natural length scale is $l_0 = \sqrt{\hbar/m\omega}$, natural energy scale is $E_0 = (1/2)\hbar\omega$ and natural time scale is $t_0 = 2/\omega$. We express the lattice spacing a in terms of l_0 as $a = l_0\Delta$ where Δ is dimensionless. Then the Hamiltonian simplifies to

$$H_{ij} = \frac{\hbar\omega}{2}\left[-\frac{\delta_{i+1,j} - 2\ \delta_{i,j} + \delta_{i-1,j}}{\Delta^2} + i^2\delta_{i,j}\right]$$

The eigenvalue equation is

$$H\phi_{E_i} = E_i\phi_{E_i}$$

We measure E_i in natural unit of energy E_0, so that $E_i = \epsilon_i E_0$ where ϵ_i is the dimensionless energy eigenvalue. Then the eigenvalue equation becomes

$$\tilde{H}\phi_{E_i} = \epsilon_i\phi_{E_i}$$

where $\tilde{H} = H/E_0$. To compute the time-evolution, we use time $\tau = t/t_0$. Then the time evolution gives

$$\phi(\tau) = \sum_i c_i\ e^{-i\epsilon_i\tau}\phi_{E_i}$$

which solves the problem.

0.1.2 Creation-Annihilation Operators

The quantum evolution on a discretised lattice is enormously simplified if we introduce the creation-annihilation formalism. This formalism allows us to scale the system to any number of (identical) particles. Here, we are assuming that the particles are bosons. For now, we assume there is only one particle. Define a 'vacuum' state $|0\rangle$ as one in which there is no particle. Next, define operator $\hat{a}_i$ (annihilation operator) and its Hermitian adjoint $\hat{a}_i^\dagger$ (creation operator) associated with the i^{th} lattice site. These operators are assumed to satisfy the algebra

$$\begin{aligned}\left[\hat{a}_i, \hat{a}_j^\dagger\right] &= \hat{I}\delta_{ij} \\ \left[\hat{a}_i, \hat{a}_j\right] &= 0 \\ \left[\hat{a}_i^\dagger, \hat{a}_j^\dagger\right] &= 0\end{aligned}$$

The state $|0\rangle$ is then defined as $\hat{a}_i\,|0\rangle = 0\ \forall i$. Further, the (normalised) state of definite position $|\tilde{x_i}\rangle$ is defined by $|\tilde{x_i}\rangle = \hat{a}_i^\dagger\,|0\rangle$. Then, it is easy to check that it follows from the algebra of these operators that $\langle\tilde{x}_i|\ \tilde{x}_j\rangle = \delta_{ij}$.

Exercise: Write the Hamiltonian $\hat{H}$ for a particle on a lattice in terms of creation-annihilation operators such that the matrix elements of H in the $|\tilde{x_i}\rangle$ basis are

$$\langle\tilde{x}_i|\,\hat{H}\,|\tilde{x}_j\rangle = -\frac{\hbar^2}{2ma^2}\left[\delta_{i+1,j} - 2\ \delta_{i,j} + \delta_{i-1,j}\right] + V_i\ \delta_{i,j}$$

Hint: Play around with terms such as $\sum_i \hat{a}_i^\dagger\ \hat{a}_{i+1}$, $\sum_i \hat{a}_i^\dagger\ \hat{a}_i$, etc. where the sum is over all lattice sites (assume an infinitely long lattice) and use algebra of creation-annihilation operators to get the right factors so as to reproduce the form of H_{ij}.