Discretizing Schrödinger's equation

Consider the Schrödinger's equation

$$i\frac{\partial}{\partial t}\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x) \tag{1}$$

The second derivative at a coordinate x may then be written as

$$\begin{aligned}\frac{\partial^2}{\partial x^2}\psi(x) &= \overset{\lim}{\delta x \to 0}\ \frac{\partial}{\partial x}\frac{\psi(x+\delta x/2)-\psi(x-\delta x/2)}{\delta x} \\ &= \overset{\lim}{\delta x \to 0}\ \frac{\psi(x+\delta x)-2\psi(x)-\psi(x-\delta x)}{(\delta x)^2} \end{aligned} \tag{2}$$

"Discretize" the coordinate x, i.e. consider it to be a series of points x_i with $x_{i+1} = x_i + \delta x$. Also, make the substitution $\psi(x) \to \psi_i/\sqrt{\delta x}$ to preserve the normalization of ψ.

Schrödonger's equation then becomes

$$i\frac{\partial}{\partial t}\psi_i = -\frac{\hbar^2}{2m(\delta x)^2}(\psi_{i+1} - 2\psi_i + \psi_{i-1}) + V(x_i)\psi_i \tag{3}$$

This may be written in the matrix form as

$$H = -\frac{\hbar^2}{2m(\delta x)^2}\begin{pmatrix} ... & ... & ... & ... & ... \\ ... & -2 & 1 & 0 & ... \\ ... & 1 & -2 & 1 & ... \\ ... & 0 & 1 & -2 & ... \\ ... & ... & ... & ... & ... \end{pmatrix} + \begin{pmatrix} ... & ... & ... & ... & ... \\ ... & V(x_{i-1}) & 0 & 0 & ... \\ ... & 0 & V(x) & 0 & ... \\ ... & 0 & 0 & V(x_{i+1}) & ... \\ ... & ... & ... & ... & ... \end{pmatrix} \tag{4}$$

where ψ_i form the basis. Schrödinger's equation can then be solved in this discretized form (useful for solving the evolution equation numerically).

Eq. (4) explicitly shows how the momentum operator (which involves the derivatives) mixes different ψ_i states. Not surprising, since $\psi_i = \psi(x_i)/\sqrt{\delta x}$, and position and momentum do not commute. From the equation, it is clear that

$$\langle x_{i+1}|H|x_i\rangle = -\frac{\hbar^2}{2m(\delta x)^2} \tag{5}$$

where $|x_i\rangle \equiv \psi_i$.

Aharonov-Bohm effect in discretized notation

In the presence of an electromagnetic field (or the vector potential A), the Hamiltonian becomes

$$\begin{aligned} H &= \frac{1}{2m}\left(p - \frac{eA}{c}\right)^2 \\ &= \frac{1}{2m}\left(p^2 - \frac{e}{c}(pA + Ap) + \frac{e^2A^2}{c^2}\right) \end{aligned} \tag{6}$$

We have already calculated the contribution of the p^2 term to the discretized Hamiltonian, it is given by the first matrix in eq. 4). The A^2 term will give a diagonal matrix similar to the second matrix in eq. 4), since it has no momentum dependence. It will then not contribute to $\langle x_{i+1}|H|x_i\rangle$

The $(pA + Ap)$ term may be written as

$$\begin{aligned} -\frac{e}{2mc}(pA + Ap)\psi &= \frac{i\hbar e}{2mc}(\nabla \cdot A\psi + A \cdot \nabla\psi) \\ &= \frac{i\hbar e}{2mc}\left((\nabla \cdot A)\psi + 2A \cdot (\nabla\psi)\right) \end{aligned} \tag{7}$$

Clearly, the contribution of this term to $\langle x_{i+1}|H|x_i\rangle$ is equal to $(i\hbar e)/(2mc\delta x)A(x_i)$.

In the presence of the vector potential, we thus have

$$\begin{aligned} \langle x_{i+1}|H|x_i\rangle &= -\frac{\hbar^2}{2m(\delta x)^2} + \frac{i\hbar e}{2mc\delta x}A(x_i) \\ &= -\frac{\hbar^2}{2m(\delta x)^2}\left(1 - \frac{ie\delta x}{\hbar c}A(x_i)\right) \\ &\equiv H_0(1 - \Delta_i) \end{aligned} \tag{8}$$

For the propagation along any particular path $x_1(t_1) \to x_n(t_n)$ such that $x_{i+1} - x_i = \delta x$, the transition matrix element is

$$\begin{aligned} \langle x_n|e^{-iHt}|x_1\rangle &= \langle x_n|1 - iH\delta t|x_{n-1}\rangle ... \langle x_3|1 - iH\delta t|x_2\rangle\langle x_2|1 - iH\delta t|x_1\rangle \\ &= \langle x_n| - iH_0\delta t(1 - \Delta_{n-1})|x_{n-1}\rangle ... \\ &\quad \langle x_3| - iH_0\delta t(1 - \Delta_2)|x_2\rangle\langle x_2| - iH_0\delta t(1 - \Delta_1)|x_1\rangle \\ &= \langle x_n| - iH_0\delta t|x_{n-1}\rangle ... \langle x_3| - iH_0\delta t|x_2\rangle\langle x_2| - iH_0\delta t|x_1\rangle \end{aligned}$$

$$
\begin{aligned}
&\times \prod_i (1-\Delta_i) \\
= \quad & \langle x_n | e^{-iH_0 t} | x_1 \rangle \prod_i (1-\Delta_i) \qquad (9)
\end{aligned}
$$

(I have jumped a few steps here, but I guess the basic idea is clear).

Now,

$$
\prod_i (1-\Delta_i) = \prod \left(1 - \frac{ie\delta x}{\hbar c} A(x_i)\right) = \exp\left[-\frac{ie}{\hbar c}\int_{\text{path}} dx \cdot A(x)\right] \qquad (10)
$$

(where we have jumped to 3-dim).

Thus, the presence of the potential A contributes an additional phase to the transition amplitude.