§1 Quantum Dynamics Basics

In this chapter, we will simulate the dynamics of a particle, such as an electron, which follows the law of quantum mechanics [1]. Basics of the quantum-dynamics (QD) method [2-5] are described, along with corresponding data structures in program, qd.c.

§1.1 Schrödinger Wave Equation

WAVE FUNCTION

The state of an electron at time t is specified by a complex-valued wave function, $\psi(\vec{r},t) = \mathrm{Re}\psi(\vec{r},t) + i\,\mathrm{Im}\psi(\vec{r},t) \in \mathbf{C}$ (where $i = \sqrt{-1}$), which is spread in the 3-dimensional space, $\vec{r} = (x,y,z) \in \mathbf{R}^3$. Given the wave function, we can calculate various physical properties such as:

- $P(\vec{r},t) = \psi^*(\vec{r},t)\psi(\vec{r},t) = |\psi(\vec{r},t)|^2 = |\mathrm{Re}\psi(\vec{r},t)|^2 + |\mathrm{Im}\psi(\vec{r},t)|^2$: The probability to find the electron at position $\vec{r}$ at time t.
- $\langle \vec{r}(t) \rangle = \int dx \int dy \int dz |\psi(\vec{r},t)|^2 \vec{r}$: The expected position of the electron at time t.

Here, $\psi^*(\vec{r},t) = \mathrm{Re}\psi(\vec{r},t) - i\,\mathrm{Im}\psi(\vec{r},t)$ is the complex conjugate of the wave function.

Normalization: The electron wave function must be normalized such that the electron must be found somewhere in the entire space with probability 1, i.e.,

$$\int dx \int dy \int dz |\psi(\vec{r},t)|^2 = 1. \tag{1}$$

WAVE EQUATION

The time evolution of the electron state, subjected to a time-independent, real-valued potential, $V(\vec{r})$, is described by the following partial differential equation:

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) \right] \psi(\vec{r},t), \tag{2}$$

where $\hbar = 1.05457\times10^{-27}$ g•cm^2/s is the Planck constant, $m = 9.10938\times10^{-28}$ g is the electron mass, and $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is the Laplacian operator.

Dimensionless equation: In the following, we measure length (x, y, z) in unit of $\hbar^2/me^2 = 0.529177\times10^{-8}$ cm, time (t) in unit of $\hbar^3/me^4 = 2.41889\times10^{-17}$ s, and energy (V) in unit of $me^4/\hbar^2 = 4.35974\times10^{-11}$ g•cm^2/s^2, where $e = 4.80321\times10^{-10}$ esu is the electron charge in the CGS unit. Substituting

$$\begin{cases} x = \dfrac{\hbar^2}{me^2}x', y = \dfrac{\hbar^2}{me^2}y', z = \dfrac{\hbar^2}{me^2}z' \\ t = \dfrac{\hbar^3}{me^4}t' \\ V = \dfrac{me^4}{\hbar^2}V' \end{cases} \tag{3}$$

in Eq. (2), we obtain

$$i\hbar \bullet \frac{me^4}{\hbar^3}\frac{\partial}{\partial t'}\psi(\vec{r}',t') = \left[-\frac{\hbar^2}{2m}\bullet\left(\frac{me^2}{\hbar^2}\right)^2\nabla'^2 + \frac{me^4}{\hbar^2}V(\vec{r}')\right]\psi(\vec{r}',t'),$$

or the dimensionless equation,

$$i\frac{\partial}{\partial t'}\psi(\vec{r}',t') = \left[-\frac{\nabla'^2}{2} + V(\vec{r}')\right]\psi(\vec{r}',t'). \tag{4}$$

In the following, we will use the dimensionless variables discussed above but omit the ´ symbol for brevity.

TWO-DIMENSIONAL ELECTRON

As a specific example, the program qd.c simulates the time evolution of an electron confined in the 2-dimensional plane ($z = 0$). Such electrons are common at the interface between two heterogeneous materials in semiconductor devices. The electron state is now specified by the 2-dimensional wave function, $\psi(x,y,t)$, where $0 \le x \le L_x$ and $0 \le y \le L_y$ (L_x and L_y are the system sizes in the x and y directions, respectively), and its time evolution is governed by the 2-dimensional Schrödinger equation,

$$i\frac{\partial}{\partial t}\psi(x,y,t) = H\psi(x,y,t). \tag{5}$$

In Eq. (5), the Hamiltonian operator, H, is defined as

$$\begin{aligned} H &= -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} + V(x,y) \\ &= T_x + T_y + V \end{aligned}. \tag{6}$$

Boundary condition: We impose the periodic boundary condition on the wave function such that

$$\begin{cases} \psi(x + L_x, y) = \psi(x,y) \\ \psi(x, y + L_y) = \psi(x,y) \end{cases}. \tag{7}$$

DISCRETIZATION

The wave function is discretized on a regular mesh of size Δx and Δy in the x and y directions, respectively. Here $\Delta x = L_x/N_x$ and $\Delta y = L_y/N_y$, where N_x and N_y are the numbers of mesh points in the x and y directions, respectively. We denote the discretized wave function as $\psi_{j,k} = \psi(j\Delta x, k\Delta y)$, see the figure below.

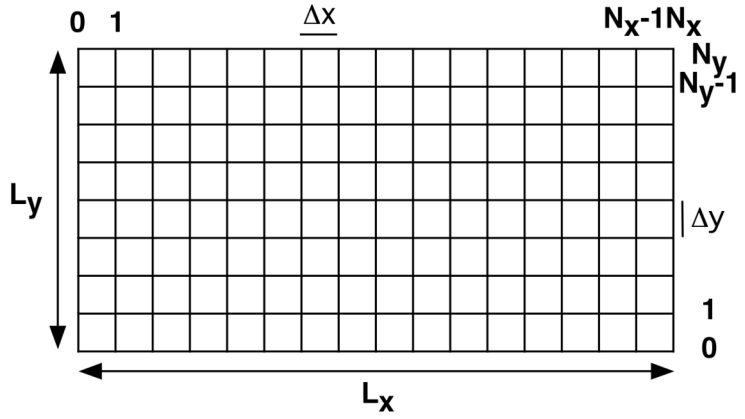

Figure: 2-dimensional mesh, on which the wave function is discretized.

In the discretized form, the Hamiltonian operator in Eq. (6) acts as

$$\left(H\psi\right)_{j,k} = \left(T_x\psi\right)_{j,k} + \left(T_y\psi\right)_{j,k} + \left(V\psi\right)_{j,k}, \tag{8}$$

where

$$\begin{cases} \left(T_x\psi\right)_{j,k} = -\dfrac{1}{2}\dfrac{\psi_{j-1,k} - 2\psi_{j,k} + \psi_{j+1,k}}{(\Delta x)^2} \\ \left(T_y\psi\right)_{j,k} = -\dfrac{1}{2}\dfrac{\psi_{j,k-1} - 2\psi_{j,k} + \psi_{j,k+1}}{(\Delta y)^2} \\ \left(V\psi\right)_{j,k} = V_{j,k}\psi_{j,k} \end{cases} \tag{9}$$

and the potential-energy function is discretized as $V_{j,k} = V(j\Delta x, k\Delta y)$.

Note that the discretized H is a mapping from an $N_x \times N_y$ array ψ ($\psi_{j,k}$ is its element at the j-th column and k-th row) to another $N_x \times N_y$ array $H\psi$. The (j, k)-th element, $(H\psi)_{j,k}$, of the output array, $H\psi$, is a linear combination of the input array with different indices, as specified in Eqs. (8) and (9).

§1.2 Numerical Integration of Schrödinger Equation

The time evolution of the wave function is formally written down as

$$\psi(t + \Delta t) = \exp\left(-iH\Delta t\right)\psi(t), \tag{10}$$

where we omit the indices for simplicity. Here the exponential function of an operator is defined as a series expansion,

$$\exp\left(-iH\Delta t\right) = \sum_{n=0}^{\infty} \frac{1}{n!}\left(-iH\Delta t\right)^n. \tag{11}$$

In the split-operator method [2-5], the wave function is propagated for a small time interval, Δt, as

$$\begin{aligned} \psi(t + \Delta t) = {} & \exp\left(-iV\Delta t/2\right)\exp\left(-iT_x\Delta t\right)\exp\left(-iT_y\Delta t\right)\exp\left(-iV\Delta t/2\right)\psi(t) \\ & + O\left(\left[\Delta t\right]^3\right) \end{aligned}. \tag{12}$$

In Eq. (12), the application of the potential propagator, $\exp(-iV\Delta t/2)$, is straightforward.

$$\begin{aligned} \left(\exp\left(-iV\Delta t/2\right)\psi\right)_{j,k} &= \psi_{j,k} - \frac{i\Delta t}{2}\left(V\psi\right)_{j,k} + \frac{\left(-i\dfrac{\Delta t}{2}\right)^2}{2!}\left(V^2\psi\right)_{j,k} + \cdots \\ &= \psi_{j,k} - \frac{i\Delta t}{2}V_{j,k}\psi_{j,k} + \frac{\left(-i\dfrac{\Delta t}{2}\right)^2}{2!}\left(V_{j,k}\right)^2\psi_{j,k} + \cdots. \\ &= \exp\left(-iV_{j,k}\Delta t/2\right)\psi_{j,k} \end{aligned} \tag{13}$$

Note that, for real number a,

$$\begin{aligned}\exp(ia) &= 1 + ia + \frac{1}{2!}(-a^2) + \frac{1}{3!}(-ia^3) + \frac{1}{4!}(a^4) + \frac{1}{4!}(ia^5) + \cdots \\ &= \left(1 - \frac{1}{2!}a^2 + \frac{1}{4!}a^4 + \cdots\right) + i\left(a - \frac{1}{3!}a^3 + \frac{1}{5!}a^5 + \cdots\right) \\ &= \cos(a) + i\sin(a)\end{aligned} \quad . \tag{14}$$

Using Eq. (14) in Eq. (13),

$$\begin{aligned}\left(\exp(-iV\Delta t/2)\psi\right)_{j,k} &= \left[\cos\left(V_{j,k}\Delta t/2\right) - i\sin\left(V_{j,k}\Delta t/2\right)\right]\left[\mathrm{Re}\psi_{j,k} + i\,\mathrm{Im}\psi_{j,k}\right] \\ &= \left[\cos\left(V_{j,k}\Delta t/2\right)\mathrm{Re}\psi_{j,k} + \sin\left(V_{j,k}\Delta t/2\right)\mathrm{Im}\psi_{j,k}\right] \\ &\quad + i\left[\cos\left(V_{j,k}\Delta t/2\right)\mathrm{Im}\psi_{j,k} - \sin\left(V_{j,k}\Delta t/2\right)\mathrm{Re}\psi_{j,k}\right]\end{aligned} \quad . \tag{15}$$

Many algorithms have been proposed to apply the kinetic propagators such as $\exp(-iT_x\Delta t)$. Among these algorithms, the space-splitting method (SSM) [4,5] is highly scalable on massively parallel computers. To understand the SSM, we first note that the operation of T_x on $\psi_{j,k}$ is expressed as

$$T_x\psi_{j,k} = b\psi_{j-1,k} + 2a\psi_{j,k} + b\psi_{j+1,k} \tag{16}$$

where

$$\begin{cases} a = 1/2(\Delta x)^2 \\ b = -1/2(\Delta x)^2 \end{cases} \tag{17}$$

For each index k, the operation of T_x on $\psi_{j,k}$ thus amounts to the multiplication of a tridiagonal matrix,

$$T_x = \begin{bmatrix} 2a & b & & & & & & \\ b & 2a & b & & & & & \\ & b & 2a & b & & & & \\ & & \ddots & \ddots & \ddots & & & \\ & & & b & 2a & b & & \\ & & & & b & 2a & b & \\ & & & & & b & 2a & \end{bmatrix}. \tag{18}$$

In the SSM, this tridiagonal matrix is expressed as a direct sum of 2×2 submatrices,

$$T_x = \begin{bmatrix} 2a & b & & & & & \\ b & 2a & b & & & & \\ & b & 2a & b & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & b & 2a & b & \\ & & & & b & 2a & b \\ & & & & & b & 2a \end{bmatrix}$$

$$= \frac{1}{2}\begin{bmatrix} a & b & & & & & \\ b & a & & & & & \\ & & a & b & & & \\ & & b & a & & & \\ & & & & \ddots & & \\ & & & & & b & a \\ & & & & & b & a \end{bmatrix} + \begin{bmatrix} a & & & & & & \\ & a & b & & & & \\ & b & a & & & & \\ & & & \ddots & & & \\ & & & & a & b & \\ & & & & b & a & \\ & & & & & & a \end{bmatrix} + \frac{1}{2}\begin{bmatrix} a & b & & & & & \\ b & a & & & & & \\ & & a & b & & & \\ & & b & a & & & \\ & & & & \ddots & & \\ & & & & & b & a \\ & & & & & b & a \end{bmatrix} \tag{19}$$

where we have omitted the index k. The exponential of a 2×2 matrix on the right-hand side of Eq. (19) is calculated analytically as follows:

$$\exp\left(-i\Delta t T_x\right) = U_x^{(\text{half})} U_x^{(\text{full})} U_x^{(\text{half})} + O\left((\Delta t)^3\right) =$$

$$\begin{bmatrix} \varepsilon_2^+ & \varepsilon_2^- & & & & & \\ \varepsilon_2^- & \varepsilon_2^+ & & & & & \\ & & \varepsilon_2^+ & \varepsilon_2^- & & & \\ & & \varepsilon_2^- & \varepsilon_2^+ & & & \\ & & & & \ddots & & \\ & & & & & \varepsilon_2^+ & \varepsilon_2^- \\ & & & & & \varepsilon_2^- & \varepsilon_2^+ \end{bmatrix} \begin{bmatrix} \varepsilon_1^+ & & & & & & \\ & \varepsilon_1^+ & \varepsilon_1^- & & & & \\ & \varepsilon_1^- & \varepsilon_1^+ & & & & \\ & & & \ddots & & & \\ & & & & \varepsilon_1^+ & \varepsilon_1^- & \\ & & & & \varepsilon_1^- & \varepsilon_1^+ & \\ & & & & & & \varepsilon_1^+ \end{bmatrix} \begin{bmatrix} \varepsilon_2^+ & \varepsilon_2^- & & & & & \\ \varepsilon_2^- & \varepsilon_2^+ & & & & & \\ & & \varepsilon_2^+ & \varepsilon_2^- & & & \\ & & \varepsilon_2^- & \varepsilon_2^+ & & & \\ & & & & \ddots & & \\ & & & & & \varepsilon_2^+ & \varepsilon_2^- \\ & & & & & \varepsilon_2^- & \varepsilon_2^+ \end{bmatrix} \tag{20}$$

where

$$\begin{cases} \varepsilon_n^+ = \dfrac{1}{2}\left[\exp\left(-\dfrac{i\Delta t}{n}(a+b)\right) + \exp\left(-\dfrac{i\Delta t}{n}(a-b)\right)\right] \\ \varepsilon_n^- = \dfrac{1}{2}\left[\exp\left(-\dfrac{i\Delta t}{n}(a+b)\right) - \exp\left(-\dfrac{i\Delta t}{n}(a-b)\right)\right] \end{cases} \tag{21}$$

The operation of $\exp(-iT_y\Delta t)$ is executed in a similar manner.

§1.3 Data Structures of qd.c

NX, NY: Number of mesh points in the x and y directions.
psi[NX+2][NY+2][2]: psi[i][j][0|1] is the real|imaginary part of the wave function on mesh point (i, j) in the xy plane.

The wave function to be simulated is in the range, 1 ≤ i ≤ NX and 1 ≤ j ≤ NY. To simplify the operation of the finite-difference operators considering the periodic boundary condition, the wave function values at the edge are duplicated as follows:

```
for (sy=1; sy<=NY; sy++)
   for (s=0; s<=1; s++) {
      psi[0][sy][s] = psi[NX][sy][s];
      psi[NX+1][sy][s] = psi[1][sy][s];
   }
for (sx=1; sx<=NX; sx++)
   for (s=0; s<=1; s++) {
      psi[sx][0][s] = psi[sx][NY][s];
      psi[sx][NY+1][s] = psi[sx][1][s];
   }
```

v[NX+2][NY+2]: v[i][j] is the potential energy at mesh point (i, j).
u[NX+2][NY+2][2]: u[i][j][0|1] is the reallimaginary part of the potential propagator at mesh point (i, j).

The potential propagator, $\exp(-iV\Delta t/2)$, is operated in qd.c as follows, see Eq. (15).

```
for (sx=1; sx<=NX; sx++)
   for (sy=1; sy<=NY; sy++) {
      wr=u[sx][sy][0]*psi[sx][sy][0]-u[sx][sy][1]*psi[sx][sy][1];
      wi=u[sx][sy][0]*psi[sx][sy][1]+u[sx][sy][1]*psi[sx][sy][0];
      psi[sx][sy][0]=wr;
      psi[sx][sy][1]=wi;
   }
```

The program qd.c simulates an electron incident on a potential barrier of height B_H and width B_W, see the figure below. In addition, an edge potential of height E_H is applied at i = 1 or NX or j = 1 or NY in v[i][j]. The potential v[i][j] = 0 at all the other mesh points.

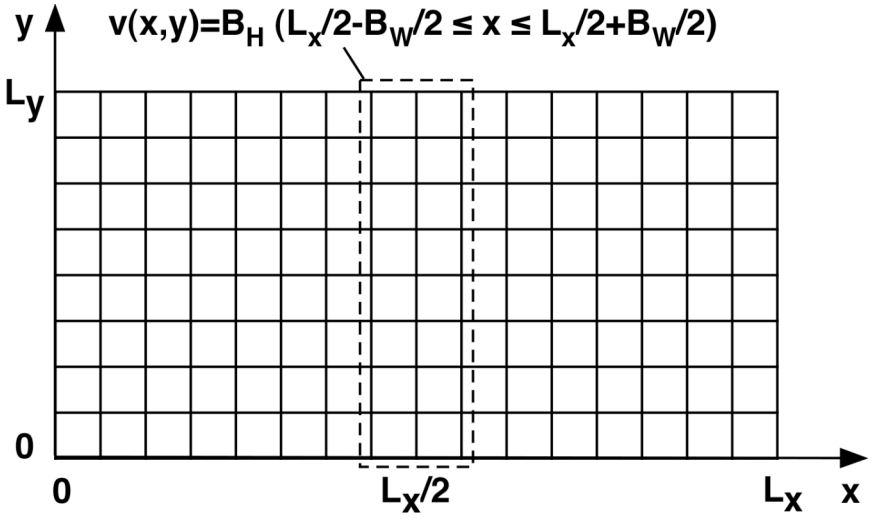

Figure: The potential energy function.

In classical mechanics, a particle coming from one side of the potential barrier with a higher kinetic energy than B_H will pass through the barrier to the other side; otherwise, the particle will bounce back at the barrier. In quantum mechanics, a part of the electron wave function is transmitted through the barrier and the other part is reflected at the barrier.

ND: The number of spatial dimensions = 2.
al[ND][2][2]: al[0|1][0|1][0|1] is the x|y-direction, half ($\Delta t/2$)|full (Δt)-step, reallimaginary-part of the diagonal element of the kinetic propagator, see Eqs. (20) and (21).
bux|y[2][NX+2|Y+2][2]: bux|y[0|1][i][0|1] is the x|y-direction, half ($\Delta t/2$)|full (Δt)-step, reallimaginary-part of the upper off-diagonal kinetic propagator on mesh i, see Eqs. (20) and (21).
blx|y[2][NX+2|Y+2][2]: blx|y[0|1][i][0|1] is the x|y-direction, half ($\Delta t/2$)|full (Δt)-step, reallimaginary-part of the lower off-diagonal kinetic propagator on mesh i, see Eqs. (20) and (21).

The 2×2 block-diagonal form of the kinetic propagator, Eq. (20), can be handled

$$\left(U_x^{(\text{half})}\psi\right)_{i,j} = \varepsilon_2^- \delta_{\text{mod}(i,2),0}\psi_{i-1,j} + \varepsilon_2^+ \psi_{i,j} + \varepsilon_2^- \delta_{\text{mod}(i,2),1}\psi_{i+1,j} \tag{22}$$

$$\left(U_x^{(\text{full})}\psi\right)_{i,j} = \varepsilon_1^- \delta_{\text{mod}(i,2),1}\psi_{i-1,j} + \varepsilon_1^+ \psi_{i,j} + \varepsilon_1^- \delta_{\text{mod}(i,2),0}\psi_{i+1,j} \tag{23}$$

where $\delta_{\text{mod}(i,2),0} = 1$ (if mod(i, 2) = 0) and 0 (else), *etc*. The above kinetic propagator is used in qd.c to update the wave function as follows, where d (= 0 for x; 1 for y) is the direction and t (= 0 for $\Delta t/2$—half; 1 for Δt—full) is the time step:

```
/* WRK|PSI holds the new|old wave function */
for (sx=1; sx<=NX; sx++) {
   for (sy=1; sy<=NY; sy++) {
      wr=al[d][t][0]*psi[sx][sy][0]-al[d][t][1]*psi[sx][sy][1];
      wi=al[d][t][0]*psi[sx][sy][1]+al[d][t][1]*psi[sx][sy][0];
      if (d==0) {
         wr+=(blx[t][sx][0]*psi[sx-1][sy][0]-blx[t][sx][1]*psi[sx-1][sy][1]);
         wi+=(blx[t][sx][0]*psi[sx-1][sy][1]+blx[t][sx][1]*psi[sx-1][sy][0]);
         wr+=(bux[t][sx][0]*psi[sx+1][sy][0]-bux[t][sx][1]*psi[sx+1][sy][1]);
         wi+=(bux[t][sx][0]*psi[sx+1][sy][1]+bux[t][sx][1]*psi[sx+1][sy][0]);
      }
      else if (d==1) {
         wr+=(bly[t][sy][0]*psi[sx][sy-1][0]-bly[t][sy][1]*psi[sx][sy-1][1]);
         wi+=(bly[t][sy][0]*psi[sx][sy-1][1]+bly[t][sy][1]*psi[sx][sy-1][0]);
         wr+=(buy[t][sy][0]*psi[sx][sy+1][0]-buy[t][sy][1]*psi[sx][sy+1][1]);
         wi+=(buy[t][sy][0]*psi[sx][sy+1][1]+buy[t][sy][1]*psi[sx][sy+1][0]);
      }
      wrk[sx][sy][0]=wr;
      wrk[sx][sy][1]=wi;
   }
}
/* Copy the new wave function back to PSI */
for (sx=1; sx<=NX; sx++)
   for (sy=1; sy<=NY; sy++)
      for (s=0; s<=1; s++)
         psi[sx][sy][s]=wrk[sx][sy][s];
```

INITIAL WAVE FUNCTION

$$\psi(x,y,t=0) = C\exp\left(-\frac{(x-x_0)^2}{4\sigma^2}\right)\exp\left(ik_0x\right)\sin\left(\frac{\pi y}{L_y}\right) \tag{24}$$

To understand the meaning of this wave function, consider

$$\psi(x,y) = C\exp\left(ik_0x\right), \tag{25}$$

where $C = \sqrt{L_xL_y}$ is the normalization constant such that

$$\int_0^{L_x} dx \int_0^{L_y} dy\, |\psi(x,y)|^2 = \int_0^{L_x} dx \int_0^{L_y} dy C^2\left(\cos^2(k_0x) + \sin^2(k_0x)\right) = 1. \tag{26}$$

Then

$$
\begin{aligned}
H\psi(x,y) &= -\frac{1}{2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)C\exp\left(ik_0x\right) \\
&= -\frac{C}{2}\frac{d^2}{dx^2}\exp\left(ik_0x\right) \\
&= -\frac{ik_0C}{2}\frac{d}{dx}\exp\left(ik_0x\right) \\
&= \frac{k_0^2C}{2}\exp\left(ik_0x\right) = \frac{k_0^2}{2}\psi(x,y)
\end{aligned}
\quad , \tag{27}
$$

and thus the expectation value of its energy is

$$
\begin{aligned}
E_0 &= \int_0^{L_x}dx\int_0^{L_y}dy\psi^*(x,y)H\psi(x,y) \\
&= \int_0^{L_x}dx\int_0^{L_y}dy\psi^*(x,y)\frac{k_0^2}{2}\psi(x,y). \\
&= \frac{k_0^2}{2}
\end{aligned}
\tag{28}
$$

or $k_0 = \sqrt{2E_0}$.

We can show that the following 'traveling' wave function is a solution to the time-dependent Schrödinger equation, if the potential energy function is 0:

$$\psi(x,y,t) = C\exp\left(ik_0\left(x - v_0t\right)\right), \tag{29}$$

where $v_0 = E_0/k_0$ is the wave speed.

The last factor in Eq. (24) also satisfies the Schrödinger equation and follows the boundary condition, $\psi(x,0) = \psi(x,L_y) = 0$, which is required if there is a very high potential barrier at $y = 0$ and L_y (the electron then cannot exist). Finally, the first Gaussian factor in Eq. (24) acts to localize the wave function around $x = x_0$ and spread σ.

References

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§2 Quantum Dynamics Basics II—One Dimensional System

This lecture note explains the quantum dynamics (QD) simulation program, `qd1.c`, which simulates the time evolution of a wave function in one spatial dimension. Here, we only highlight differences from the two-dimensional QD simulation program, `qd.c`, explained in the lecture note on Quantum Dynamics Basics.

Schrödinger Wave Equation

WAVE EQUATION

The program qd1.c simulates the time evolution of a wave function in one-dimensional space, $0 \le x \le L_x$ (L_x is the system size). The one-dimensional wave function, $\psi(x,t) = \mathrm{Re}\psi(x,t) + i\,\mathrm{Im}\psi(x,t) \in \mathbf{C}$ (where $i = \sqrt{-1}$), satisfies the normalization condition:

$$\int dx|\psi(x,t)|^2 = 1. \tag{1}$$

The time evolution of the wave function, subjected to a time-independent, real-valued potential, $V(x)$, is described (in the dimensionless form as explained in the lecture note) by the time-dependent Schrödinger equation:

$$i\frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t). \tag{2}$$

In Eq. (2), the Hamiltonian operator, H, is defined as

$$\begin{aligned} H &= -\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x) \\ &= T_x + V \end{aligned}. \tag{3}$$

Boundary condition: We impose the periodic boundary condition on the wave function such that

$$\psi(x + L_x) = \psi(x). \tag{4}$$

DISCRETIZATION

The wave function is discretized on a regular mesh of size Δx. Here $\Delta x = L_x/N_x$, and N_x is the number of mesh points. We denote the discretized wave function as $\psi_j = \psi(j\Delta x)$, see the figure below.

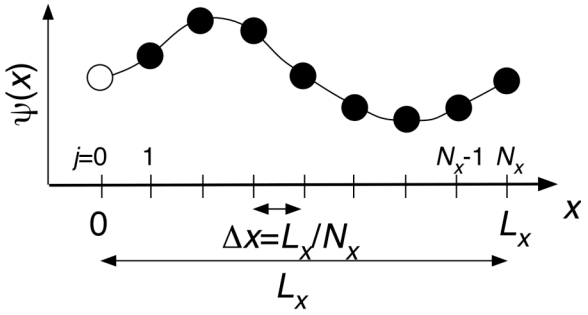


Figure: One-dimensional mesh, on which the wave function is discretized.

In the discretized form, the Hamiltonian operator in Eq. (3) acts as

$$(H\psi)_j = (T_x\psi)_j + (V\psi)_j, \tag{5}$$

where

$$\begin{cases} (T_x\psi)_j = -\dfrac{1}{2}\dfrac{\psi_{j-1} - 2\psi_j + \psi_{j+1}}{(\Delta x)^2} \\ (V\psi)_j = V_j\psi_j \end{cases} \tag{6}$$

and the potential-energy function is discretized as $V_j = V(j\Delta x)$.

Numerical Integration of Schrödinger Equation

The time evolution of the wave function is formally written down as

$$\psi(t + \Delta t) = \exp(-iH\Delta t)\psi(t), \tag{7}$$

where we omit the indices for simplicity. Here the exponential function of an operator is defined as a series expansion,

$$\exp(-iH\Delta t) = \sum_{n=0}^{\infty} \frac{1}{n!}(-iH\Delta t)^n. \tag{8}$$

In the split-operator method, the wave function is propagated for a small time interval, Δt, as

$$\psi(t + \Delta t) = \exp(-iV\Delta t/2)\exp(-iT_x\Delta t)\exp(-iV\Delta t/2)\psi(t) + O\left([\Delta t]^3\right). \tag{9}$$

In Eq. (9), the application of the potential propagator, exp(-$iV\Delta t$/2), is straightforward.

$$\begin{aligned} \left(\exp(-iV\Delta t/2)\psi\right)_j &= \psi_j - \frac{i\Delta t}{2}(V\psi)_j + \frac{(-i\Delta t/2)^2}{2!}\left(V^2\psi\right)_j + \cdots \\ &= \psi_j - \frac{i\Delta t}{2}V_j\psi_j + \frac{(-i\Delta t/2)^2}{2!}\left(V_j\right)^2\psi_j + \cdots. \\ &= \exp\left(-iV_j\Delta t/2\right)\psi_j \end{aligned} \tag{10}$$

Note that, for real number a,

$$\begin{aligned} \exp(ia) &= 1 + ia + \frac{1}{2!}(-a^2) + \frac{1}{3!}(-ia^3) + \frac{1}{4!}(a^4) + \frac{1}{4!}(ia^5) + \cdots \\ &= \left(1 - \frac{1}{2!}a^2 + \frac{1}{4!}a^4 + \cdots\right) + i\left(a - \frac{1}{3!}a^3 + \frac{1}{5!}a^5 + \cdots\right) \\ &= \cos(a) + i\sin(a) \end{aligned} \tag{11}$$

Using Eq. (11) in Eq. (10),

$$\begin{aligned} \left(\exp(-iV\Delta t/2)\psi\right)_j &= \left[\cos\left(V_j\Delta t/2\right) - i\sin\left(V_j\Delta t/2\right)\right]\left[\mathrm{Re}\psi_j + i\,\mathrm{Im}\psi_j\right] \\ &= \left[\cos\left(V_j\Delta t/2\right)\mathrm{Re}\psi_j + \sin\left(V_j\Delta t/2\right)\mathrm{Im}\psi_j\right] \\ &\quad + i\left[\cos\left(V_j\Delta t/2\right)\mathrm{Im}\psi_j - \sin\left(V_j\Delta t/2\right)\mathrm{Re}\psi_j\right] \end{aligned} \tag{12}$$

To apply the kinetic propagator, exp(-$iT_x\Delta t$), we use the space-splitting method (SSM). To understand the SSM, we first note that the operation of T_x on ψ_j is expressed as

$$T_x\psi_j = b\psi_{j-1} + 2a\psi_j + b\psi_{j+1} \tag{13}$$

where

$$\begin{cases} a = 1/2(\Delta x)^2 \\ b = -1/2(\Delta x)^2 \end{cases} \tag{14}$$

The operation of T_x on ψ_j thus amounts to the multiplication of a tridiagonal matrix,

$$T_x = \begin{bmatrix} 2a & b & & & & & & \\ b & 2a & b & & & & & \\ & b & 2a & b & & & & \\ & & \ddots & \ddots & \ddots & & & \\ & & & b & 2a & b & & \\ & & & & b & 2a & b & \\ & & & & & b & 2a \end{bmatrix}. \tag{15}$$

In the SSM, this tridiagonal matrix is expressed as a direct sum of 2 × 2 submatrices,

$$\begin{aligned} T_x &= \begin{bmatrix} 2a & b & & & & & & \\ b & 2a & b & & & & & \\ & b & 2a & b & & & & \\ & & \ddots & \ddots & \ddots & & & \\ & & & b & 2a & b & & \\ & & & & b & 2a & b & \\ & & & & & b & 2a \end{bmatrix} \\ &= \frac{1}{2}\begin{bmatrix} a & b & & & & & & \\ b & a & & & & & & \\ & & a & b & & & & \\ & & b & a & & & & \\ & & & & \ddots & & & \\ & & & & & b & a & \\ & & & & & b & a \end{bmatrix} + \begin{bmatrix} a & & & & & & & \\ & a & b & & & & & \\ & b & a & & & & & \\ & & & \ddots & & & & \\ & & & & a & b & & \\ & & & & b & a & & \\ & & & & & & a & \end{bmatrix} + \frac{1}{2}\begin{bmatrix} a & b & & & & & & \\ b & a & & & & & & \\ & & a & b & & & & \\ & & b & a & & & & \\ & & & & \ddots & & & \\ & & & & & b & a & \\ & & & & & b & a \end{bmatrix}. \end{aligned} \tag{16}$$

The exponential of a 2×2 matrix on the right-hand side of Eq. (16) is calculated analytically as follows:

$$\exp(-i\Delta t T_x) = U_x^{(\text{half})} U_x^{(\text{full})} U_x^{(\text{half})} + O\left((\Delta t)^3\right) =$$

$$\begin{bmatrix} \varepsilon_2^+ & \varepsilon_2^- & & & & & & \\ \varepsilon_2^- & \varepsilon_2^+ & & & & & & \\ & & \varepsilon_2^+ & \varepsilon_2^- & & & & \\ & & \varepsilon_2^- & \varepsilon_2^+ & & & & \\ & & & & \ddots & & & \\ & & & & & \varepsilon_2^+ & \varepsilon_2^- & \\ & & & & & \varepsilon_2^- & \varepsilon_2^+ \end{bmatrix} \begin{bmatrix} \varepsilon_1^+ & & & & & & & \\ & \varepsilon_1^+ & \varepsilon_1^- & & & & & \\ & \varepsilon_1^- & \varepsilon_1^+ & & & & & \\ & & & \ddots & & & & \\ & & & & \varepsilon_1^+ & \varepsilon_1^- & & \\ & & & & \varepsilon_1^- & \varepsilon_1^+ & & \\ & & & & & & \varepsilon_1^+ & \end{bmatrix} \begin{bmatrix} \varepsilon_2^+ & \varepsilon_2^- & & & & & & \\ \varepsilon_2^- & \varepsilon_2^+ & & & & & & \\ & & \varepsilon_2^+ & \varepsilon_2^- & & & & \\ & & \varepsilon_2^- & \varepsilon_2^+ & & & & \\ & & & & \ddots & & & \\ & & & & & \varepsilon_2^+ & \varepsilon_2^- & \\ & & & & & \varepsilon_2^- & \varepsilon_2^+ \end{bmatrix} \tag{17}$$

where

$$\begin{cases} \varepsilon_n^+ = \frac{1}{2}\left[\exp\left(-\frac{i\Delta t}{n}(a+b)\right) + \exp\left(-\frac{i\Delta t}{n}(a-b)\right)\right] \\ \varepsilon_n^- = \frac{1}{2}\left[\exp\left(-\frac{i\Delta t}{n}(a+b)\right) - \exp\left(-\frac{i\Delta t}{n}(a-b)\right)\right] \end{cases} \tag{18}$$

Data Structures of `qd1.c`

`NX`: Number of mesh points.
`psi[NX+2][2]`: `psi[i][0|1]` is the reallimaginary part of the wave function on mesh point i.

The wave function to be simulated is in the range, $1 \le i \le$ `NX`. To simplify the operation of the finite-difference operators considering the periodic boundary condition, the wave function values at the edges are duplicated as follows:

```
for (s=0; s<=1; s++) {
   psi[0   ][s] = psi[NX][s];
   psi[NX+1][s] = psi[1 ][s];
}
```

`v[NX+2]`: `v[i]` is the potential energy at mesh point i.
`u[NX+2][2]`: `u[i][0|1]` is the reallimaginary part of the potential propagator at mesh point *i*.

The potential propagator, $\exp(-iV\Delta t/2)$, is operated in qd1.c as follows, see Eq. (12).

```
for (sx=1; sx<=NX; sx++) {
   wr = u[sx][0]*psi[sx][0]-u[sx][1]*psi[sx][1];
   wi = u[sx][0]*psi[sx][1]+u[sx][1]*psi[sx][0];
   psi[sx][0] = wr;
   psi[sx][1] = wi;
}
```

The program `qd1.c` simulates an electron incident on a potential barrier of height B_H and width B_W, see the figure below. In addition, an edge potential of height E_H is applied at i = 1 or `NX` in `v[i]`. The potential `v[i]` = 0 at all the other mesh points.

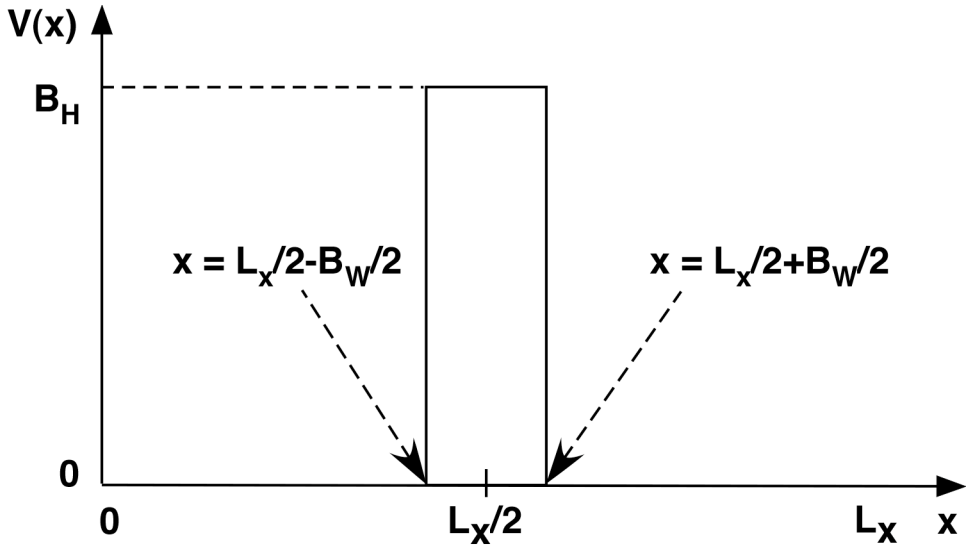


Figure: The potential energy function.

al[2][2]: al[0|1][0|1] is the half (Δt/2)|full (Δt)-step, reallimaginary-part of the diagonal element of the kinetic propagator, see Eqs. (17) and (18).

`bu[2][NX+2][2]: bu[0|1][i][0|1]` is the half ($\Delta t/2$)|full (Δt)-step, real|imaginary-part of the upper off-diagonal kinetic propagator on mesh point i, see Eqs. (17) and (18).
`bl[2][NX+2][2]: bl[0|1][i][0|1]` is the half ($\Delta t/2$)|full (Δt)-step, real|imaginary-part of the lower off-diagonal kinetic propagator on mesh point i, see Eqs. (17) and (18).

The 2×2 block-diagonal form of the kinetic propagator, Eq. (17), can be handled

$$\left(U_x^{(\text{half})}\psi\right)_i = \varepsilon_2^- \delta_{\text{mod}(i,2),0}\psi_{i-1} + \varepsilon_2^+ \psi_i + \varepsilon_2^- \delta_{\text{mod}(i,2),1}\psi_{i+1} \tag{19}$$

$$\left(U_x^{(\text{full})}\psi\right)_i = \varepsilon_1^- \delta_{\text{mod}(i,2),1}\psi_{i-1} + \varepsilon_1^+ \psi_i + \varepsilon_1^- \delta_{\text{mod}(i,2),0}\psi_{i+1} \tag{20}$$

where $\delta_{\text{mod}(i,2),0} = 1$ (if mod(i, 2) = 0) and 0 (else), etc. The above kinetic propagator is used in `qd1.c` to update the wave function as follows, where t (= 0 for $\Delta t/2$—half; 1 for Δt—full) is the time step:

```
/* WRK|PSI holds the new|old wave function */
for (sx=1; sx<=NX; sx++) {
   wr = al[t][0]*psi[sx][0]-al[t][1]*psi[sx][1];
   wi = al[t][0]*psi[sx][1]+al[t][1]*psi[sx][0];
   wr += (bl[t][sx][0]*psi[sx-1][0]-bl[t][sx][1]*psi[sx-1][1]);
   wi += (bl[t][sx][0]*psi[sx-1][1]+bl[t][sx][1]*psi[sx-1][0]);
   wr += (bu[t][sx][0]*psi[sx+1][0]-bu[t][sx][1]*psi[sx+1][1]);
   wi += (bu[t][sx][0]*psi[sx+1][1]+bu[t][sx][1]*psi[sx+1][0]);
   wrk[sx][0] = wr;
   wrk[sx][1] = wi;
}
/* Copy the new wave function back to PSI */
for (sx=1; sx<=NX; sx++)
   for (s=0; s<=1; s++)
      psi[sx][s] = wrk[sx][s];
```

INITIAL WAVE FUNCTION

We choose the initial wave function at time $t = 0$ to be

$$\psi(x, t=0) = C\exp\left(-\frac{(x-x_0)^2}{4\sigma^2}\right)\exp\left(ik_0 x\right). \tag{21}$$

where $k_0 = \sqrt{2E_0}$ (E_0 is the energy of the wave packet) and C is the normalization constant such that

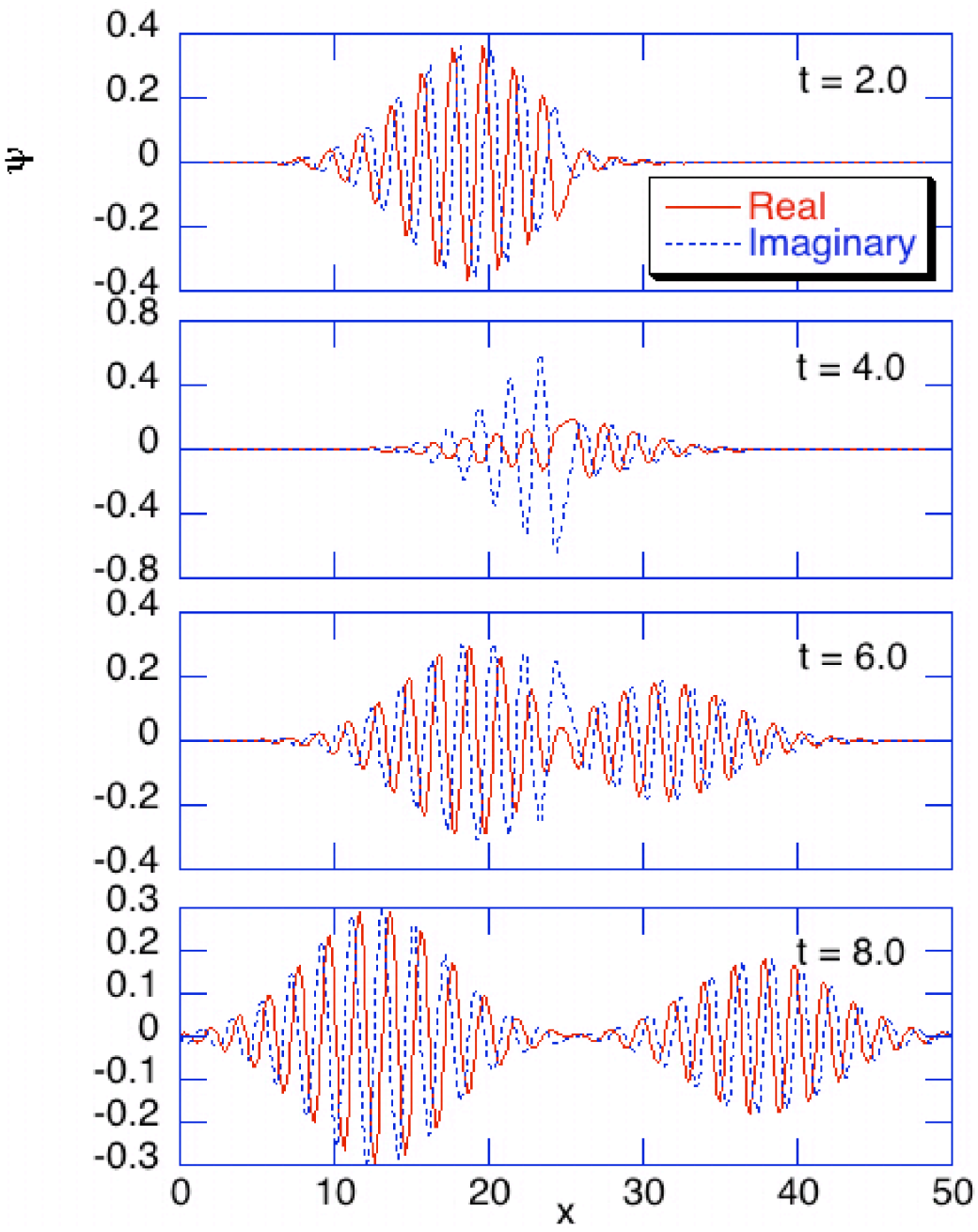
$$\int_0^{L_x} dx\, |\psi(x)|^2 = 1. \tag{22}$$

The first Gaussian factor in Eq. (21) acts to localize the wave function around $x = x_0$ and spread σ.

NUMERICAL EXAMPLE

The following figure shows the real and imaginary parts of the wave function at four different times, t = 2.0, 4.0, 6.0, and 8.0, for the following parameter set:

$L_X = 50.0$
$N_x = 512$
$\Delta t = 10^{-3}$
$x_0 = 12.5$
$\sigma = 3.0$
$E_0 = 5.0$
$B_H = 5.0$
$B_W = 1.0$
$E_H = 50.0$


ψ
t = 2.0
Real
Imaginary
t = 4.0
t = 6.0
t = 8.0
0.4
0.2
0
-0.2
-0.4
0.8
0.4
0
-0.4
-0.8
0.4
0.2
0
-0.2
-0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
10
20
30
40
50
x