

Quantum Dynamics

Aiichiro Nakano

Collaboratory for Advanced Computing & Simulations

Department of Computer Science

Department of Physics & Astronomy

Department of Chemical Engineering & Materials Science

Department of Quantitative & Computational Biology

University of Southern California

Email: anakano@usc.edu

Goals:

1. Partial differential equation
2. Spectral method
(Fourier transform)

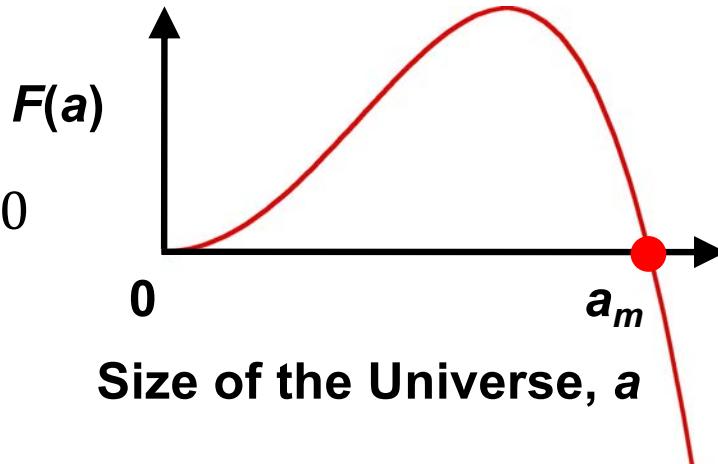


Quantum Universe

- Wheeler-deWitt equation

$$\left[-\hbar^2 \frac{d^2}{da^2} + \left(\frac{3\pi c^3}{2G} \right)^2 \left(a^2 - \frac{a^4}{a_m^2} \right) \right] \psi(a) = 0$$

$F(a)$



CREATION OF UNIVERSES FROM NOTHING

Alexander VILENIN

Physics Department, Tufts University, Medford, MA 02155, USA

Received 11 June 1982

A cosmological model is proposed in which the universe is created by quantum tunneling from literally nothing into a de Sitter space. After the tunneling, the model evolves along the lines of the inflationary scenario. This model does not have a big-bang singularity and does not require any initial or boundary conditions.

IS IT POSSIBLE TO CREATE A UNIVERSE IN THE LABORATORY BY QUANTUM TUNNELING?

Edward FARHI*

*Center for Theoretical Physics, Laboratory for Nuclear Science and Department of Physics,
Massachusetts Institute of Technology, Cambridge, MA 02139, USA*

Alan H. GUTH**

*Center for Theoretical Physics, Laboratory for Nuclear Science and Department of Physics,
Massachusetts Institute of Technology, Cambridge, MA 02139, USA
and
Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138, USA*

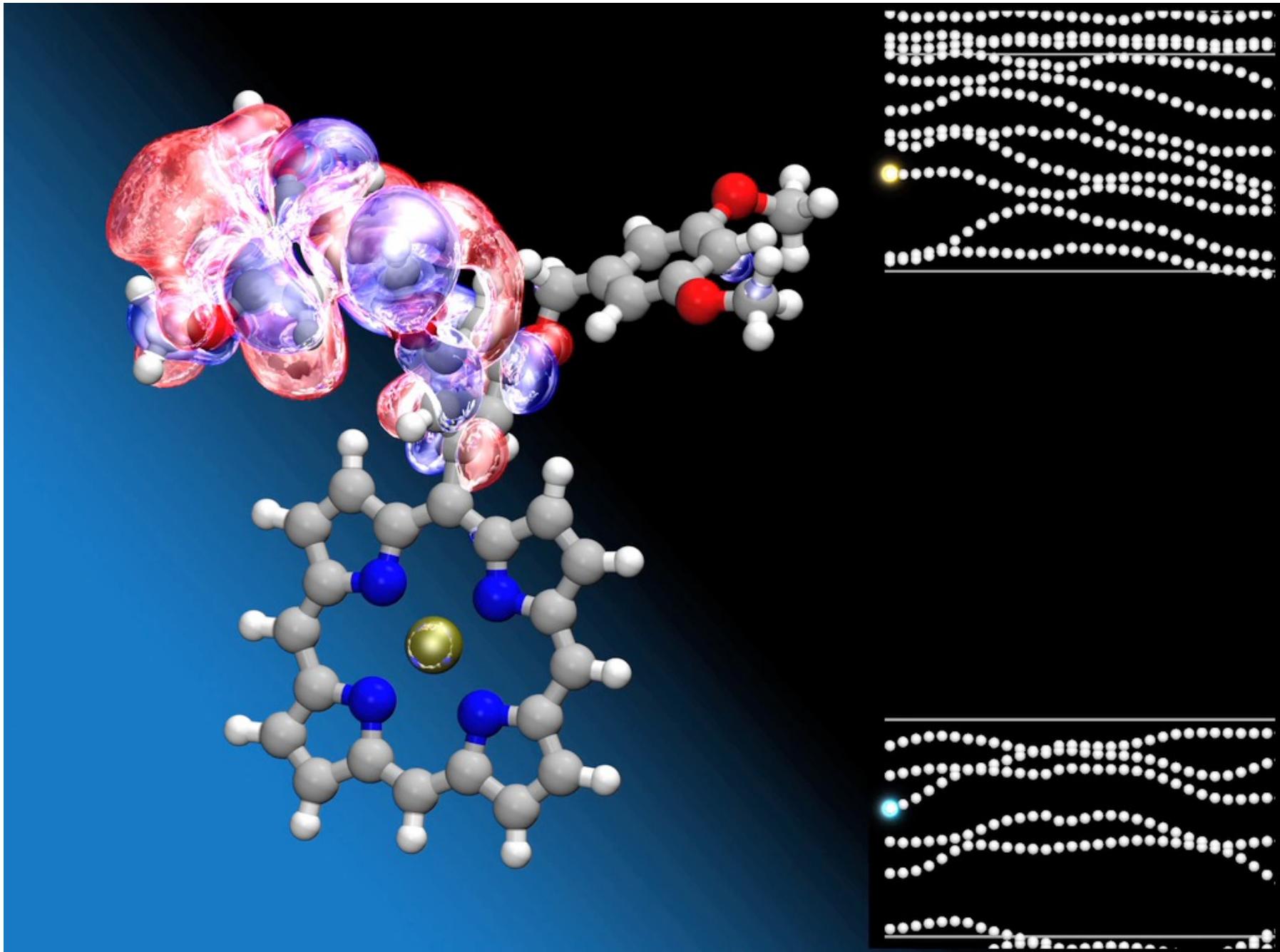
Jemal GUVEN

*Instituto de Ciencias Nucleares, Universidad Nacional Autonoma de Mexico, Circuito Exterior
C.U.A. Postal 70-543, 04510 Mexico D.F. Mexico*

Phys. Lett. 117B, 25 ('82)

Nucl. Phys. B339, 417 ('90)

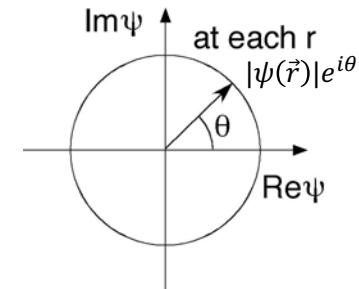
Photoexcited Electron Dynamics



Wave Equation

- **Complex wave function**

$$\psi(\vec{r}, t) = \text{Re}\psi(\vec{r}, t) + i\text{Im}\psi(\vec{r}, t) \in \mathbb{C} \quad (i = \sqrt{-1})$$



- **Probability**

$$P(\vec{r}, t) = \psi^*(\vec{r}, t)\psi(\vec{r}, t) = |\psi(\vec{r}, t)|^2 = |\text{Re}\psi(\vec{r}, t)|^2 + |\text{Im}\psi(\vec{r}, t)|^2$$

$$\psi^*\psi = (\psi_0 - i\psi_1)(\psi_0 + i\psi_1) = \psi_0^2 + \psi_1^2 \geq 0$$

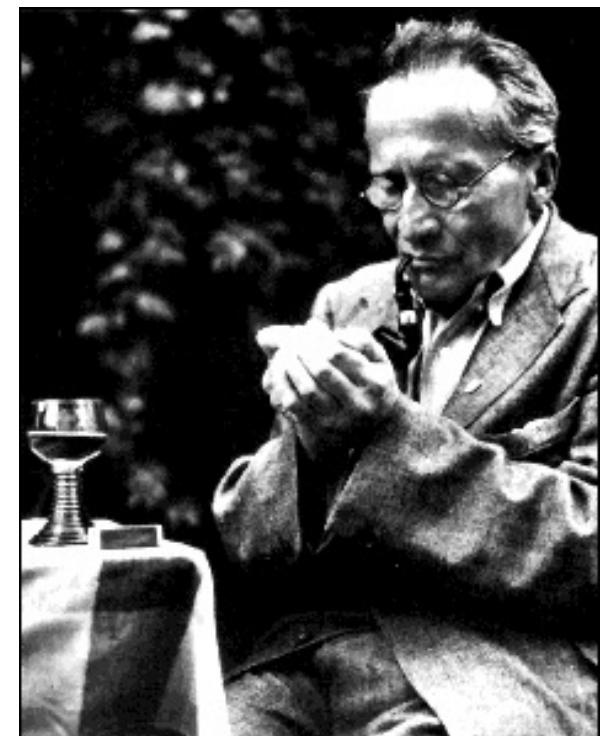
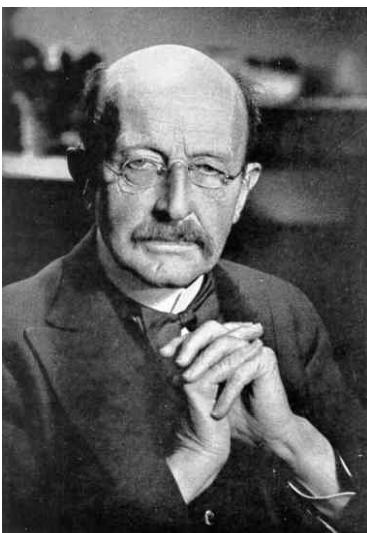
- **Normalization**

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

- **Schrödinger (partial differential) equation**

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

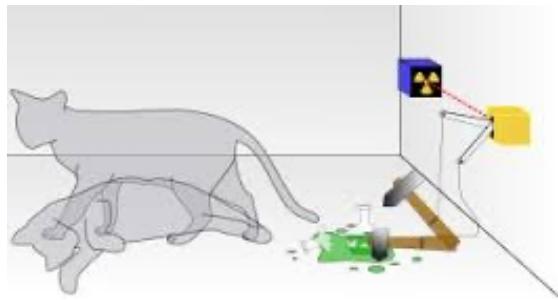
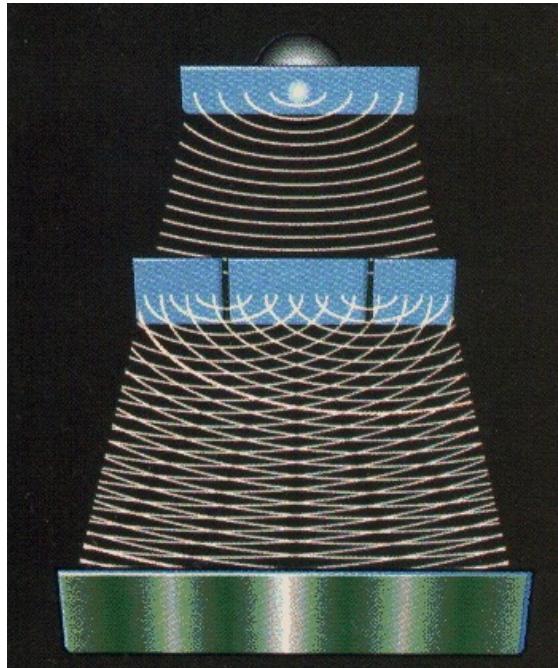
Laplacian: $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$



Planck constant: $\hbar = 1.05457 \times 10^{-27} \text{ g} \cdot \text{cm}^2/\text{s}$

Single-Electron Double-Slit Experiment

What wave?



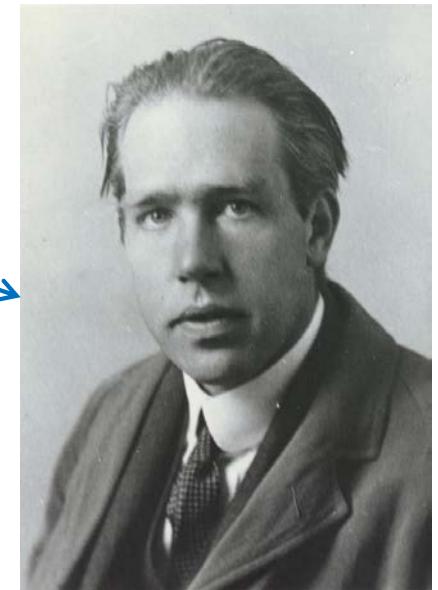
<http://rdg.ext.hitachi.co.jp/rd/moviee/doubleslite-n.mpeg>

Akira Tonomura (Hitachi, Ltd.)

Atomic Unit

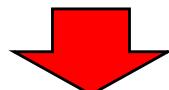
Length, energy & time in atomic unit

$$\begin{aligned} \frac{e^2}{r} &= \frac{\hbar^2}{mr^2} & \vec{r} &= \frac{\hbar^2}{me^2} \vec{r}' & \frac{\hbar^2}{me^2} &= 0.529177 \text{ \AA} & \text{Bohr} \\ E &= \frac{e^2}{r} & V &= \frac{me^4}{\hbar^2} V' & \frac{me^4}{\hbar^2} &= 27.2116 \text{ eV} & \text{Hartree} \\ E &= \frac{\hbar}{t} & t &= \frac{\hbar^3}{me^4} t' & \frac{\hbar^3}{me^4} &= 0.0241889 \text{ fs} \end{aligned}$$



Time-dependent Schrödinger equation
in atomic unit

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



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



Two-Dimensional Electron

- Schrödinger equation (in atomic unit)

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

- Hamiltonian operator

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



The Nobel Prize in Physics 1985

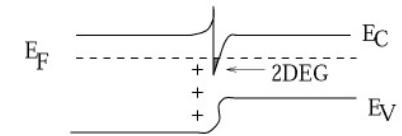
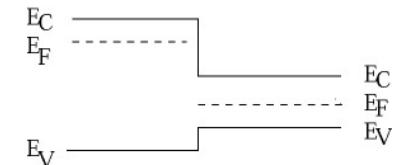
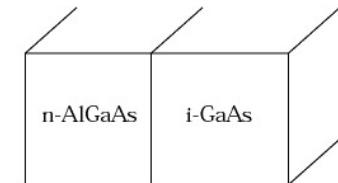
"for the discovery of the quantized Hall effect"



Klaus von Klitzing

Federal Republic of Germany

Max-Planck-Institut für Festkörperforschung
Stuttgart, Federal Republic of Germany
b. 1943



The Nobel Prize in Physics 1998

"for their discovery of a new form of quantum fluid with fractionally charged excitations"

- Periodic boundary condition

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



Robert B.
Laughlin

1/3 of the prize
USA



Horst L. Störmer

1/3 of the prize
Federal Republic of
Germany



Daniel C. Tsui

1/3 of the prize
USA

Stanford University
Stanford, CA, USA
b. 1950

Columbia University
New York, NY, USA
b. 1949

Princeton University
Princeton, NJ, USA
b. 1939
(In Henan, China)

Layered Materials Genome

- Atomically-thin layered materials will dominate materials science in this century

Geim & Grigorieva, *Nature* **499**, 419 ('13)

The Nobel Prize in Physics
2010



© The Nobel Foundation.
Photo: U. Montan
Andre Geim
Prize share: 1/2



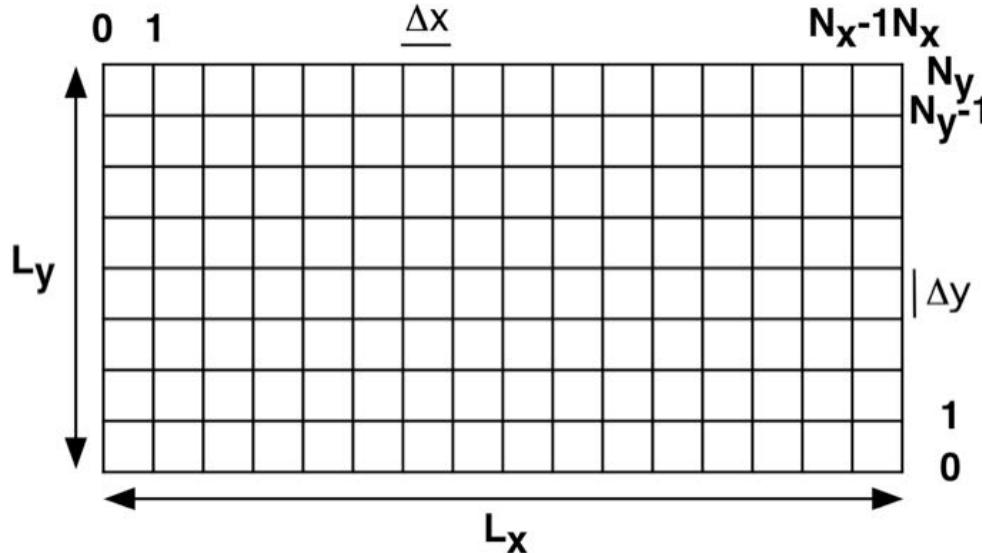
© The Nobel Foundation.
Photo: U. Montan
Konstantin
Novoselov
Prize share: 1/2

- Tuning material properties in desired ways by building heterostructures composed of unlimited combinations of atomically thin layers in a way similar to genetics



Spatial Discretization

- Regular 2D mesh: $\psi_{jk} = \psi(j\Delta x, k\Delta y)$ ($\Delta x = L_x/N_x$ & $\Delta y = L_y/N_y$)



- Finite differencing

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

$$\begin{aligned} \frac{\partial^2}{\partial x^2} \psi(x, y, t) &= \frac{\partial \psi(x + \Delta/2, y, t)/\partial x - \partial \psi(x - \Delta/2, y, t)/\partial x}{\Delta} \\ &= \frac{\psi(x + \Delta, y, t) - \psi(x, y, t) - \psi(x, y, t) - \psi(x - \Delta, y, t)}{\Delta} \\ &= \frac{\psi(x + \Delta, y, t) - 2\psi(x, y, t) + \psi(x - \Delta, y, t)}{\Delta^2} \end{aligned}$$

Temporal Propagation

- **Formal solution to the Schrödinger equation:** $i \frac{\partial}{\partial t} \psi(t) = H\psi(t)$

$$\psi(t + \Delta t) = \exp(-iH\Delta t)\psi(t)$$

- **Split-operator method (Trotter-expansion): unitary!**

$$\begin{aligned} \psi(t + \Delta t) &= \exp(-i(T_x + T_y + V)\Delta t)\psi(t) \stackrel{\substack{T_x T_y = T_y T_x \\ \exp(-i(T_x + T_y)\Delta t)}}{\iff} \exp(-iT_x\Delta t)\exp(-iT_y\Delta t) \\ &= \exp(-iV\Delta t/2)\exp(-iT_x\Delta t)\exp(-iT_y\Delta t)\exp(-iV\Delta t/2)\psi(t) + O([\Delta t]^3) \end{aligned}$$

- **Potential propagator (mesh point-by-point complex-number multiplications)**

$$(u_0 + iu_1)(\psi_0 + i\psi_1) = (u_0\psi_0 - u_1\psi_1) + i(u_0\psi_1 + u_1\psi_0)$$

$$\begin{aligned} (\exp(-iV\Delta t/2)\psi)_{jk} &= \exp(-iV_{jk}\Delta t/2)\psi_{jk} \\ &= [\cos(V_{jk}\Delta t/2) - i \sin(V_{jk}\Delta t/2)][\text{Re}\psi_{jk} + i \text{Im}\psi_{jk}] \\ &= [\cos(V_{jk}\Delta t/2)\text{Re}\psi_{jk} + \sin(V_{jk}\Delta t/2)\text{Im}\psi_{jk}] \\ &\quad + i[\cos(V_{jk}\Delta t/2)\text{Im}\psi_{jk} - \sin(V_{jk}\Delta t/2)\text{Re}\psi_{jk}] \end{aligned}$$

$$\exp(ia) = \sum_{n=0}^{\infty} \frac{(ia)^n}{n!} = \left(1 - \frac{a^2}{2!} + \frac{a^4}{4!} - \dots\right) + i \left(a - \frac{a^3}{3!} + \frac{a^5}{5!} - \dots\right) = \cos(a) + i\sin(a)$$

Kinetic Propagator

- Mesh-point coupling

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

- Tridiagonal matrix representation

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



Note the periodic boundary condition

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

Space Splitting Method (SSM)

- 2x2 block-diagonal decomposition & split-operator exponentiation

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

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

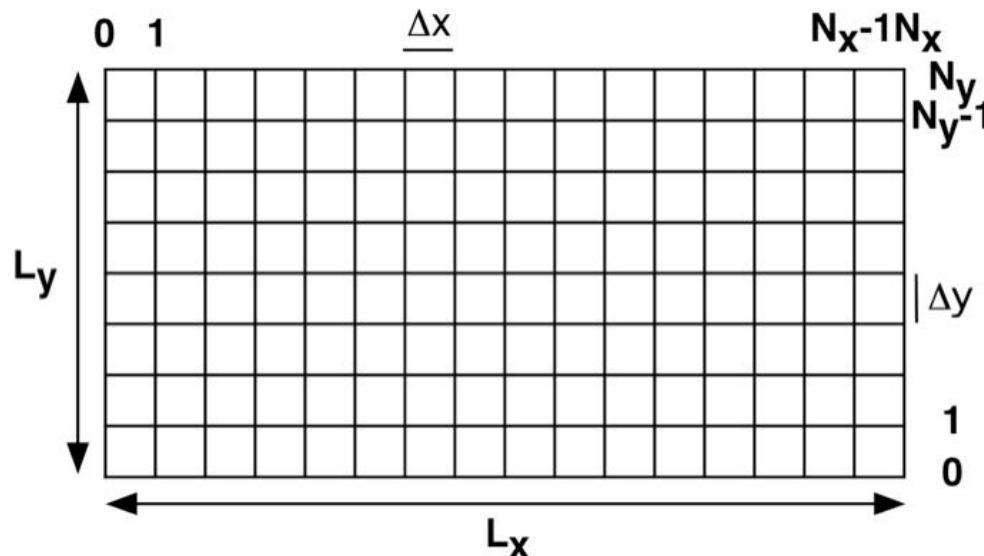
$$\exp(-i\Delta t T_x) = U_x^{(\text{half})} U_x^{(\text{full})} U_x^{(\text{half})} + O([\Delta t]^3) =$$

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

Data Structures in Program qd.c

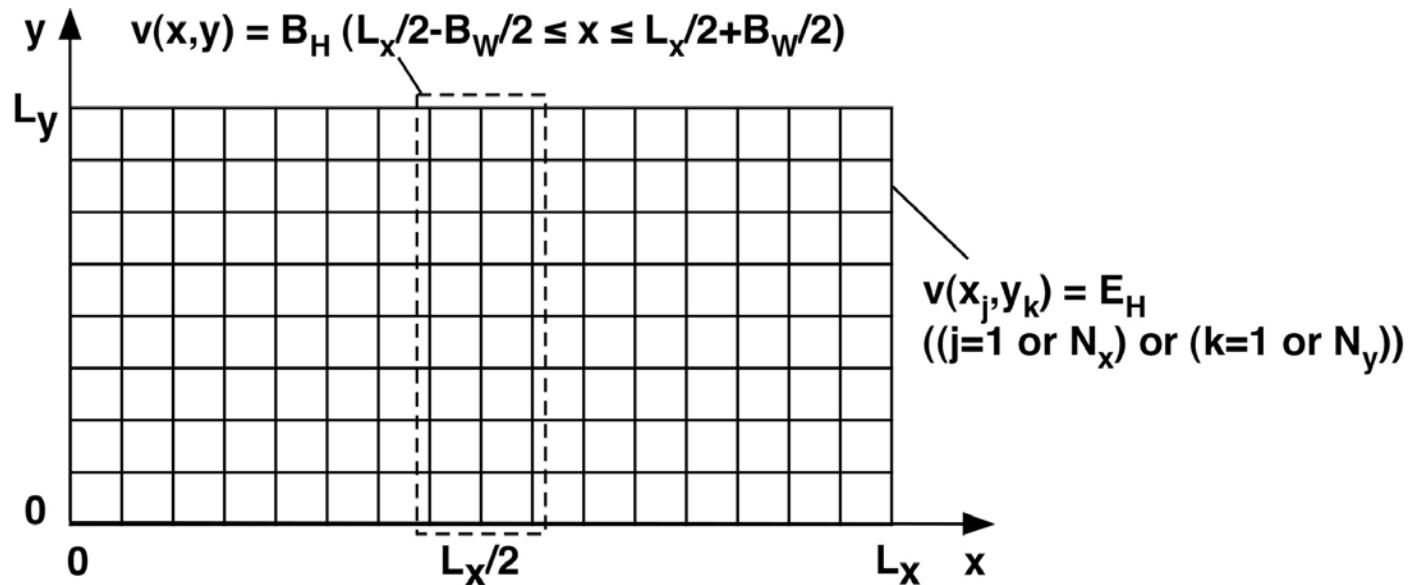
- Wave function: $\psi[NX+2][NY+2][2]$
- Periodic boundary condition by auxiliary elements

```
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];}
```



Potential Propagator in qd.c

- Potential barrier: $v[NX+2][NY+2]$



- Potential propagator: $\exp(-iV\Delta t/2)$, $u[NX+2][NY+2][2]$
- Potential propagation: $\psi \leftarrow \exp(-iV\Delta t/2) \psi$

```
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; }
```

Kinetic Propagator in qd.c

$$\begin{aligned} \left(U_x^{(\text{half})} \psi \right)_{i,j} &= \varepsilon_2^- \delta_{\text{mod}(i,2),0} \psi_{i-1,j} + \varepsilon_2^+ \psi_{i,j} + \varepsilon_2^- \delta_{\text{mod}(i,2),1} \psi_{i+1,j} \\ \left(U_x^{(\text{full})} \psi \right)_{i,j} &= \varepsilon_1^- \delta_{\text{mod}(i,2),1} \psi_{i-1,j} + \varepsilon_1^+ \psi_{i,j} + \varepsilon_1^- \delta_{\text{mod}(i,2),0} \psi_{i+1,j} \end{aligned}$$

```
/* 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

- Gaussian wave packet

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

<u>Symbol</u>	<u>Variable in qd.c</u>
x_0 (packet center)	X0
σ (packet spread)	S0
$k_0^2/2$ (energy)	E0

Quantum Dynamics—II

One Dimensional System

Aiichiro Nakano

Collaboratory for Advanced Computing & Simulations

Department of Computer Science

Department of Physics & Astronomy

Department of Chemical Engineering & Materials Science

Department of Quantitative & Computational Biology

University of Southern California

Email: anakano@usc.edu



Goal: Understand `qd1.c`



Wave Equation

- Complex wave function

$$\psi(x, t) = \text{Re}\psi(x, t) + i\text{Im}\psi(x, t) \in \mathbb{C} \quad (i = \sqrt{-1})$$

- Normalization

$$\int dx |\psi(x, t)|^2 = 1$$

- Schrödinger equation (in atomic unit)

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

- Hamiltonian operator

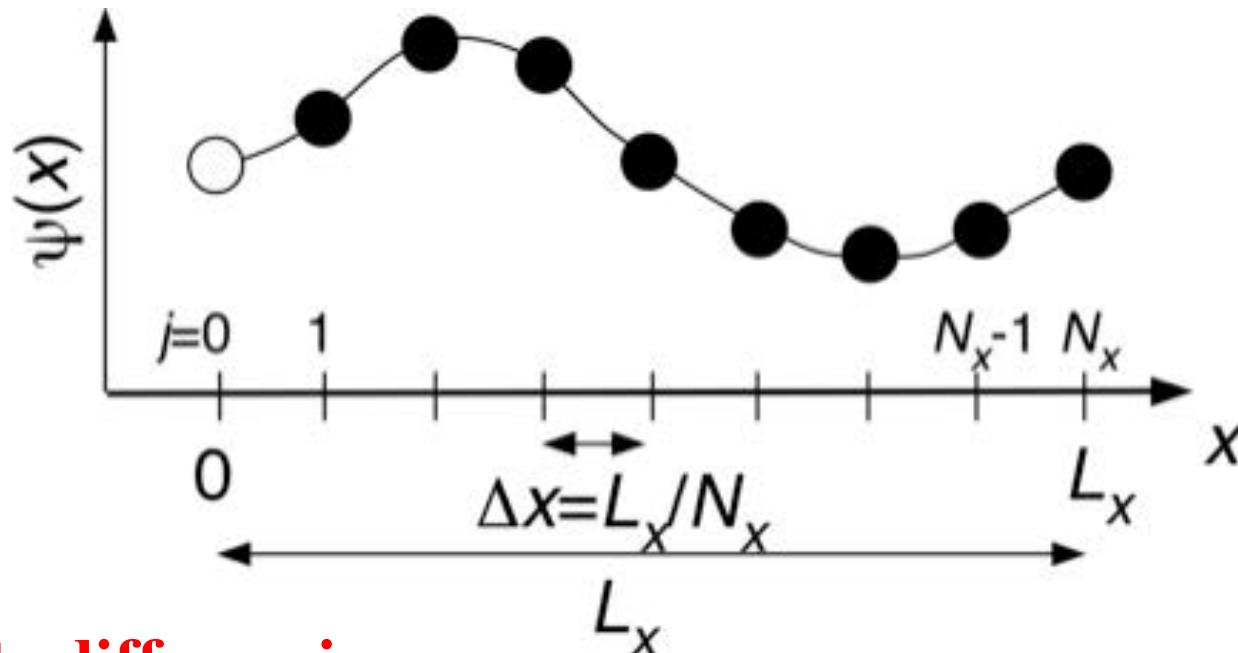
$$H = -\frac{1}{2} \frac{\partial^2}{\partial x^2} + V(x) = T_x + V$$

- Periodic boundary condition

$$\psi(x + L_x) = \psi(x)$$

Spatial Discretization

- Regular 1D mesh: $\psi_j = \psi(j\Delta x)$ ($\Delta x = L_x/N_x$)



- Finite differencing

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

$$\begin{aligned} \frac{\partial^2}{\partial x^2} \psi(x, t) &= \frac{\partial \psi(x + \Delta/2, t) / \partial x - \partial \psi(x - \Delta/2, t) / \partial x}{\Delta} \\ &= \frac{\psi(x + \Delta, t) - \psi(x, t)}{\Delta} - \frac{\psi(x, t) - \psi(x - \Delta, t)}{\Delta} \\ &= \frac{\psi(x + \Delta, t) - 2\psi(x, t) + \psi(x - \Delta, t)}{\Delta^2} \end{aligned}$$

Temporal Propagation

- **Formal solution to the Schrödinger equation:** $\frac{\partial}{\partial t}\psi(t) = -iH\psi(t)$
$$\psi(t + \Delta t) = \exp(-iH\Delta t)\psi(t)$$
- **Split-operator method: unitary!**

$$\begin{aligned}\psi(t + \Delta t) &= \exp(-i(T_x + V)\Delta t)\psi(t) \\ &= \exp(-iV\Delta t/2)\exp(-iT_x\Delta t)\exp(-iV\Delta t/2)\psi(t) + O([\Delta t]^3)\end{aligned}$$

- **Potential propagator (mesh point-by-point complex-number multiplications)** $(u_0 + iu_1)(\psi_0 + i\psi_1) = (u_0\psi_0 - u_1\psi_1) + i(u_0\psi_1 + u_1\psi_0)$

$$\begin{aligned}(\exp(-iV\Delta t/2)\psi)_j &= \exp(-iV_j\Delta t/2)\psi_j \\ &= [\cos(V_j\Delta t/2) - i \sin(V_j\Delta t/2)][\operatorname{Re}\psi_j + i \operatorname{Im}\psi_j] \\ &= [\cos(V_j\Delta t/2)\operatorname{Re}\psi_j + \sin(V_j\Delta t/2)\operatorname{Im}\psi_j] \\ &\quad + i[\cos(V_j\Delta t/2)\operatorname{Im}\psi_j - \sin(V_j\Delta t/2)\operatorname{Re}\psi_j]\end{aligned}$$

$$\exp(ia) = \sum_{n=0}^{\infty} \frac{(ia)^n}{n!} = \left(1 - \frac{a^2}{2!} + \frac{a^4}{4!} - \dots\right) + i\left(a - \frac{a^3}{3!} + \frac{a^5}{5!} - \dots\right) = \cos(a) + i\sin(a)$$

Kinetic Propagator: It's a Matrix!

- Mesh-point coupling

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

- Tridiagonal matrix representation

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



Note the periodic boundary condition

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

Space Splitting Method (SSM)

- **2x2 block-diagonal decomposition & split-operator exponentiation**

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

Block-by-block exponentiation

$$\exp \left[\begin{bmatrix} \blacksquare & & \\ & \blacksquare & \\ & & \blacksquare \end{bmatrix} \right] = \sum_{n=0}^{\infty} \frac{1}{n!} \left[\begin{bmatrix} \blacksquare^n & & \\ & \blacksquare^n & \\ & & \blacksquare^n \end{bmatrix} \right]^n = \begin{bmatrix} e^{\blacksquare} & & \\ & e^{\blacksquare} & \\ & & e^{\blacksquare} \end{bmatrix}$$

Split-operator (Trotter expansion) again

$$= \frac{1}{2} \left[\begin{bmatrix} a & b & & & & \\ b & a & & & & \\ & a & b & & & \\ & b & a & & & \\ & & \ddots & & & \\ & & & a & b & \\ & & & b & a & \end{bmatrix} + \begin{bmatrix} a & & & & & b \\ & a & b & & & \\ & b & a & & & \\ & & \ddots & & & \\ & & & a & b & \\ & & & b & a & \\ & & & & & a \end{bmatrix} + \frac{1}{2} \begin{bmatrix} a & b & & & & \\ b & a & & & & \\ & a & b & & & \\ & b & a & & & \\ & & \ddots & & & \\ & & & a & b & \\ & & & b & a & \end{bmatrix} \right]$$

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

$$= \exp \left(-\frac{i\Delta t}{2} \left[\begin{bmatrix} a & b & & & & \\ b & a & & & & \\ & a & b & & & \\ & b & a & & & \\ & & \ddots & & & \\ & & & a & b & \\ & & & b & a & \end{bmatrix} \right] \right) \exp \left(-i\Delta t \left[\begin{bmatrix} a & & & & & b \\ & a & b & & & \\ & b & a & & & \\ & & \ddots & & & \\ & & & a & b & \\ & & & b & a & \\ & & & & & a \end{bmatrix} \right] \right) \exp \left(-\frac{i\Delta t}{2} \left[\begin{bmatrix} a & b & & & & \\ b & a & & & & \\ & a & b & & & \\ & b & a & & & \\ & & \ddots & & & \\ & & & a & b & \\ & & & b & a & \end{bmatrix} \right] \right)$$

How? Block diagonal → block-by-block exponentiation

Space Splitting Method (SSM)

$$\begin{aligned}
 & \exp(-i\Delta t T_x) = U_x^{(\text{half})} U_x^{(\text{full})} U_x^{(\text{half})} + O([\Delta t]^3) \\
 &= \exp\left(-\frac{i\Delta t}{2}\begin{bmatrix} a & b \\ b & a \\ & \ddots \\ & & a & b \\ & & b & a \\ & & & \ddots \\ & & & & a & b \\ & & & & b & a \end{bmatrix}\right) \exp\left(-i\Delta t \begin{bmatrix} a & & & b \\ & a & b & \\ & b & a & \\ & & \ddots & \\ & & & a & b \\ & & & b & a \\ & & & & \ddots \\ & & & & & a & b \\ & & & & & b & a \end{bmatrix}\right) \exp\left(-\frac{i\Delta t}{2}\begin{bmatrix} a & b \\ b & a \\ & \ddots \\ & & a & b \\ & & b & a \\ & & & \ddots \\ & & & & a & b \\ & & & & b & a \end{bmatrix}\right) \\
 &= \begin{bmatrix} \varepsilon_2^+ & \varepsilon_2^- \\ \varepsilon_2^- & \varepsilon_2^+ \\ & \ddots \\ & & \varepsilon_2^+ & \varepsilon_2^- \\ & & \varepsilon_2^- & \varepsilon_2^+ \\ & & & \ddots \\ & & & & \varepsilon_2^+ & \varepsilon_2^- \\ & & & & \varepsilon_2^- & \varepsilon_2^+ \end{bmatrix} \begin{bmatrix} \varepsilon_1^+ & & & \varepsilon_1^- \\ & \varepsilon_1^+ & \varepsilon_1^- & \\ & \varepsilon_1^- & \varepsilon_1^+ & \\ & & \ddots & \\ & & & \varepsilon_1^+ & \varepsilon_1^- \\ & & & \varepsilon_1^- & \varepsilon_1^+ \\ & & & & \varepsilon_1^+ \end{bmatrix} \begin{bmatrix} \varepsilon_2^+ & \varepsilon_2^- \\ \varepsilon_2^- & \varepsilon_2^+ \\ & \ddots \\ & & \varepsilon_2^+ & \varepsilon_2^- \\ & & \varepsilon_2^- & \varepsilon_2^+ \\ & & & \ddots \\ & & & & \varepsilon_2^+ & \varepsilon_2^- \\ & & & & \varepsilon_2^- & \varepsilon_2^+ \end{bmatrix}
 \end{aligned}$$

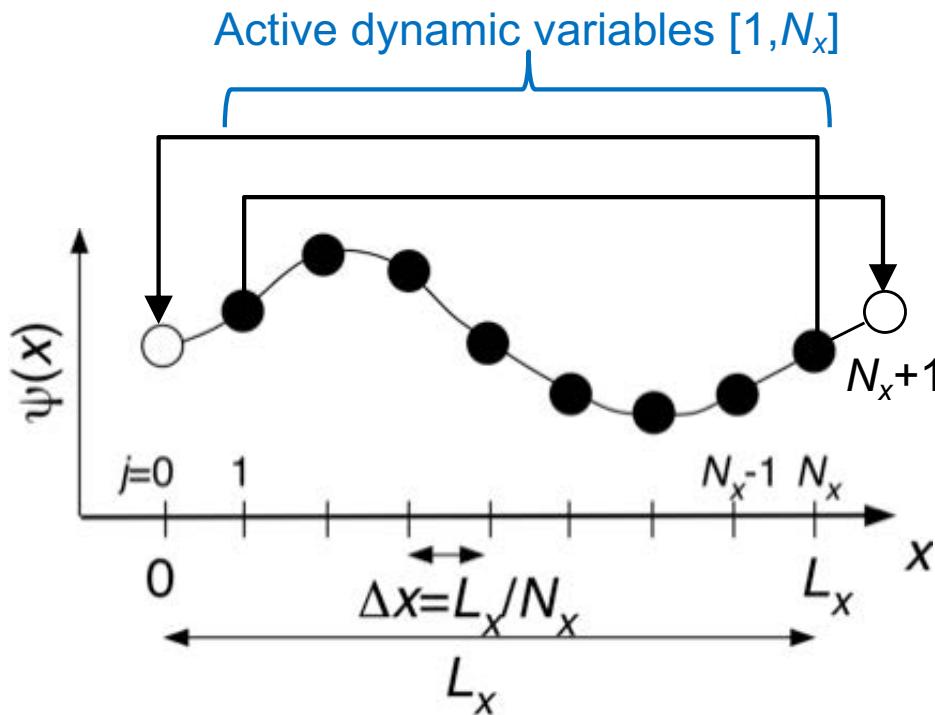
$$\begin{cases} \varepsilon_n^+ = \frac{1}{2} \left[\exp\left(-\frac{i\Delta t}{n}(a+b)\right) + \exp\left(-\frac{i\Delta t}{n}(a-b)\right) \right] \\ \varepsilon_n^- = \frac{1}{2} \left[\exp\left(-\frac{i\Delta t}{n}(a+b)\right) - \exp\left(-\frac{i\Delta t}{n}(a-b)\right) \right] \end{cases} \quad \text{Just need } 2 \times 2 \text{ exponentiation} \\
 \exp\left(-\frac{i\Delta t}{(2)} \begin{bmatrix} a & b \\ b & a \end{bmatrix}\right)$$

Use eigen-decomposition & telescoping

Data Structures in Program qd1.c

- Wave function: $\text{psi}[NX+2][2]$ $\text{psi}[j][0|1] = (\text{Re}|\text{Im})\psi_{j\Delta x}$
- Periodic boundary condition by auxiliary elements

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



Potential Propagator in qd1.c

- Potential barrier: $v[NX+2]$
- Potential propagator: $\exp(-iV\Delta t/2)$, $u[NX+2][2]$
- Potential propagation: $\psi \leftarrow \exp(-iV\Delta t/2) \psi$

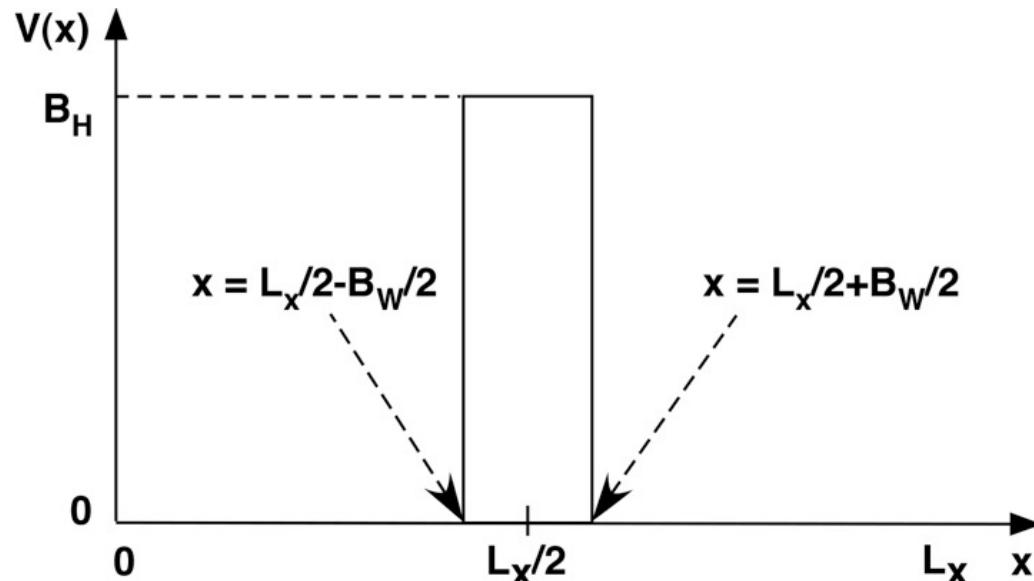
```

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;
}

```

$$\begin{cases} u[j][0] = \cos\left(-\frac{\Delta}{2}V_j\right) \\ u[j][1] = \sin\left(-\frac{\Delta}{2}V_j\right) \end{cases}$$

$$\exp\left(-\frac{iV_j\Delta}{2}\right)\psi_j \equiv u\psi = (u_0 + iu_1)(\psi_0 + i\psi_1) = \overbrace{(u_0\psi_0 - u_1\psi_1)}^{\text{new } \psi_0} + i\overbrace{(u_0\psi_1 + u_1\psi_0)}^{\text{new } \psi_1}$$



Kinetic Propagator in qd1.c

$$\begin{aligned} \left(U_x^{(\text{half})} \psi \right)_i &= \varepsilon_2^- \delta_{\text{mod}(i,2),0} \psi_{i-1} + \varepsilon_2^+ \psi_i + \varepsilon_2^- \delta_{\text{mod}(i,2),1} \psi_{i+1} \\ \left(U_x^{(\text{full})} \psi \right)_i &= \varepsilon_1^- \delta_{\text{mod}(i,2),1} \psi_{i-1} + \varepsilon_1^+ \psi_i + \varepsilon_1^- \delta_{\text{mod}(i,2),0} \psi_{i+1} \end{aligned}$$

```

for (sx=1; sx<=NX; sx++) { // WRK[][][]|PSI[][] holds the new|old wave function
    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;}  $\psi_j \leftarrow \beta_l \psi_{j-1} + \alpha \psi_j + \beta_u \psi_{j+1}$ 

```

```

for (sx=1; sx<=NX; sx++) // Copy the new wave function back to PSI
    for (s=0; s<=1; s++)
        psi[sx][s]=wrk[sx][s];

```

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

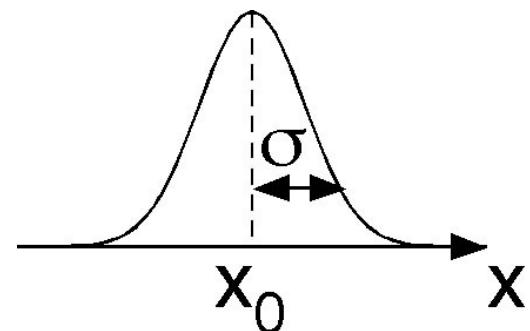
$$= \begin{bmatrix} \varepsilon_2^+ & \varepsilon_2^- \\ \varepsilon_2^- & \varepsilon_2^+ \\ & \ddots \\ & & \varepsilon_2^+ & \varepsilon_2^- \\ & & \varepsilon_2^- & \varepsilon_2^+ \end{bmatrix} \begin{bmatrix} \varepsilon_1^+ & & & \varepsilon_1^- \\ & \varepsilon_1^+ & \varepsilon_1^- & \\ & \varepsilon_1^-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

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

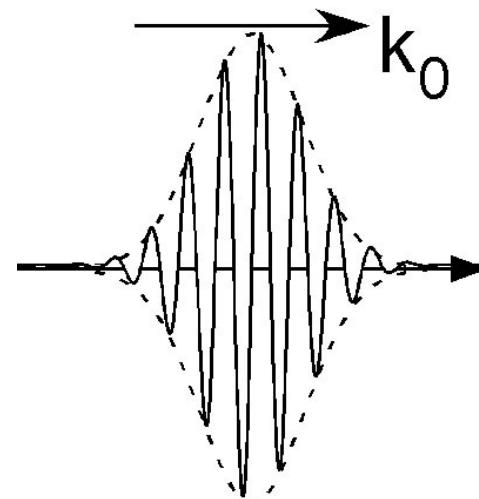
Initial Wave Function

- Gaussian wave packet

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



Symbol	Variable in qd1.c
x_0 (packet center)	X0
σ (packet spread)	S0
$k_0^2/2$ (energy)	E0



Quantum Dynamics—III

Spectral Method

Aiichiro Nakano

Collaboratory for Advanced Computing & Simulations

Department of Computer Science

Department of Physics & Astronomy

Department of Chemical Engineering & Materials Science

Department of Quantitative & Computational Biology

University of Southern California

Email: anakano@usc.edu

Goal: Understand Fourier transform in the context of the orthonormal plane-wave basis set in a vector space

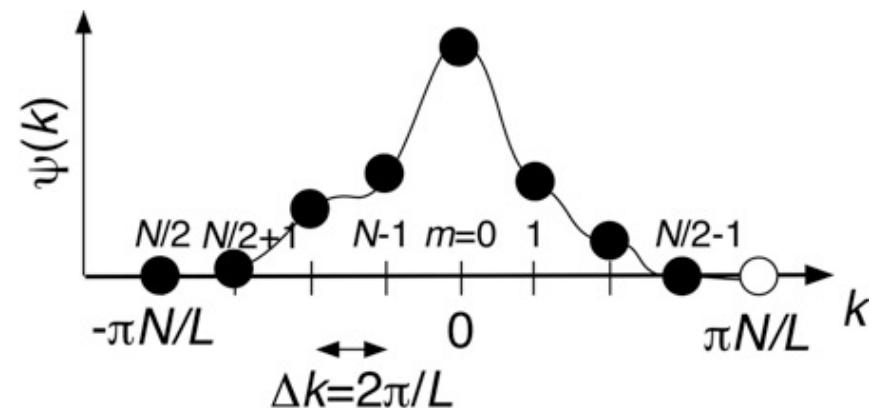
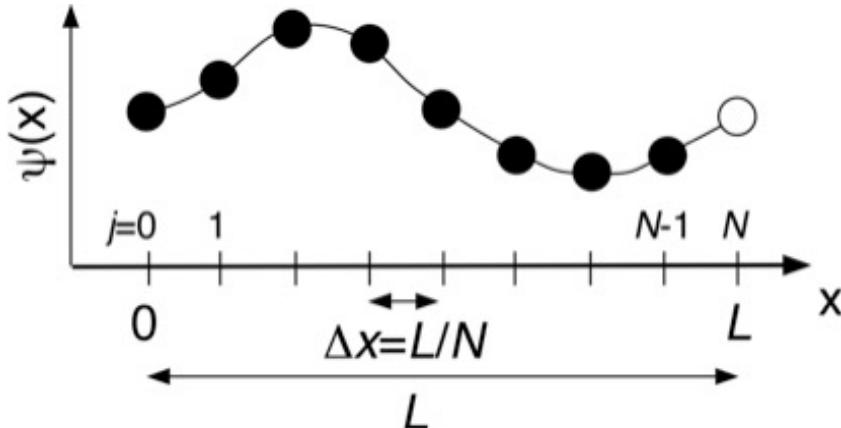
Resolution of identity:

$$1 = \sum_n |n\rangle\langle n|$$



Discrete Fourier Transform

- Discretize $\psi(x) \in C (x \in [0, L])$ on N mesh points, $x_j = j\Delta x (j = 0, \dots, N-1)$, with equal mesh spacing, $\Delta x = L/N$
- Periodic boundary condition: $\psi(x + L) = \psi(x)$

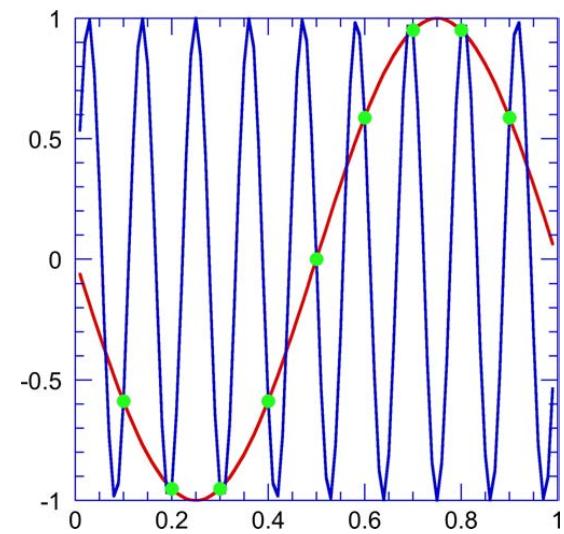


- Discrete Fourier transform: Represents $\psi(x)$ as a linear combination of $\exp(ikx) = \cos(kx) + i \sin(kx)$, with different wave numbers, k

$$\psi_j = \sum_{m=0}^{N-1} \tilde{\psi}_m \exp(i k_m x_j)$$

$$k_m = \begin{cases} 2\pi m / L & (m = 0, 1, \dots, N/2 - 1) \\ 2\pi(m - N)/L & (m = N/2, N/2 + 1, \dots, N - 1) \end{cases}$$

$$\tilde{\psi}_m = \frac{1}{N} \sum_{j=0}^{N-1} \psi_j \exp(-i k_m x_j)$$



Wave Numbers

- Periodic boundary condition, $\psi(x + L) = \psi(x)$, is guaranteed by choosing $k_m = 2\pi m/L$

$$e^{i\left(\frac{2\pi m}{L}(x+L)\right)} = e^{i\left(\frac{2\pi m}{L}x + 2\pi m\right)} = e^{i\frac{2\pi m}{L}x} \underbrace{e^{i2\pi m}}_{(e^{i2\pi})^{m=1} = 1} = e^{i\frac{2\pi m}{L}x}$$

- Folding back the latter half of wave numbers by $\frac{2\pi N}{L} = 2\pi/\Delta x$ (cf. first Brillouin zone):

$$\text{From } \left[0, \frac{2\pi N}{L}\right] = \left[0, \frac{2\pi}{\Delta x}\right] \text{ to } \left[-\frac{2\pi}{L} \cdot \frac{N}{2}, \frac{2\pi}{L} \cdot \frac{N}{2}\right] = \left[-\frac{\pi}{\Delta x}, \frac{\pi}{\Delta x}\right]$$

$$\Delta x = \frac{L}{N}$$

The shift won't change wave-function value on any grid point

$$e^{i\left(k_m - \frac{2\pi N}{L}\right)x_j} = e^{ik_m x_j} e^{-i\frac{2\pi N}{L} \cdot \frac{L}{N} j} = e^{ik_m x_j} e^{\overbrace{-i2\pi j}^1} = e^{i k_m x_j}$$

Orthonormal Basis Set

- **N -dimensional vector space:** $|\psi\rangle = (\psi_0, \psi_1, \dots, \psi_{N-1})$
- **Plane-wave basis set:** $\left\{ |m\rangle = b_m(x_j) = \frac{1}{\sqrt{N}} \exp(i k_m x_j) \mid m = 0, 1, \dots, N-1 \right\}$
- **Orthonormality:** $\langle m|n\rangle \equiv \sum_{j=0}^{N-1} b_m^*(x_j) b_n(x_j) = \delta_{m,n} = \begin{cases} 1 & m = n \\ 0 & m \neq n \end{cases}$

$$\therefore \langle m|n\rangle = \frac{1}{N} \sum_{j=0}^{N-1} \exp(i(k_n - k_m)x_j) = \frac{1}{N} \sum_{j=0}^{N-1} \exp\left(i \frac{2\pi}{N}(n-m)j\right)$$

$$(k_n - k_m)x_j = \frac{2\pi(n-m)}{L} \cdot \frac{L}{N}j$$

$$= \begin{cases} \frac{1}{N} \frac{\exp(i2\pi(n-m)) - 1}{\exp(i \frac{2\pi}{N}(n-m)) - 1} = 0 & m \neq n \\ \frac{1}{N} \bullet N = 1 & m = n \end{cases}$$

Geometric series

$$S = \sum_{j=0}^{N-1} \left(e^{i \frac{2\pi}{N}(n-m)} \right)^j = 1 + \dots + r^{N-1}$$

$$rS = r + \dots + r^N$$

$$\therefore (r-1)S = (r^N - 1)$$

- **Completeness:** $|\psi\rangle = \sum_{m=0}^{N-1} |m\rangle \langle m|\psi\rangle$ or $1 = \sum_{m=0}^{N-1} |m\rangle \langle m|$

- **Fourier transform:** $\psi_j = \sum_{m=0}^{N-1} \exp(ik_m x_j) \boxed{\frac{1}{N} \sum_{l=0}^{N-1} \exp(-ik_m x_l) \psi_l}$ $\tilde{\psi}_m(k_m)$

Spectral Method

- Kinetic-energy operator is diagonal in the momentum space: $\tilde{\psi}_m \xrightarrow[T]{\frac{k_m^2}{2}} \tilde{\psi}_m$

$$-\frac{1}{2} \frac{\partial^2}{\partial x^2} \sum_{m=0}^{N-1} \tilde{\psi}_m \exp(ik_m x) = \sum_{m=0}^{N-1} \frac{k_m^2}{2} \tilde{\psi}_m \exp(ik_m x)$$

- Potential-energy operator is diagonal in the real space: $\psi_j \xrightarrow[V]{\quad} V_j \psi_j$
- Split-operator technique & spectral method

$$\psi(t + \Delta t) = \exp(-iV\Delta t / 2)^F \exp(-iT\Delta t)^{F^{-1}} \exp(-iV\Delta t / 2)\psi(t) + O((\Delta t)^3)$$

1. $\psi_j \xrightarrow[\exp(-iV\Delta t / 2)]{} \exp(-iV_j \Delta t / 2)\psi_j$
2. $\psi_j \xrightarrow[F^{-1}]{\quad} F^{-1}\psi_j = \tilde{\psi}_m = \frac{1}{N} \sum_{j=1}^N \psi_j \exp(-ik_m x_j)$
3. $\tilde{\psi}_m \xrightarrow[\exp(-iT\Delta t)]{} \exp(-ik_m^2 \Delta t / 2)\tilde{\psi}_m \quad \exp\left(\frac{i\Delta t}{2} \frac{\partial^2}{\partial x^2}\right) \sum_m \tilde{\psi}_m e^{-ik_m x} = \sum_m \exp\left(-\frac{i\Delta t k_m^2}{2}\right) \tilde{\psi}_m e^{-ik_m x}$
4. $\tilde{\psi}_m \xrightarrow[F]{\quad} F\tilde{\psi}_m = \psi_j = \sum_{m=1}^N \tilde{\psi}_m \exp(ik_m x_j)$
5. $\psi_j \xrightarrow[\exp(-iV\Delta t / 2)]{} \exp(-iV_j \Delta t / 2)\psi_j$

Numerical Recipes FFT: four1()

- Spectral method requires

$$\psi_j \xrightarrow[F^{-1}]{F^{-1}} F^{-1}\psi_j = \tilde{\psi}_m = \frac{1}{N} \sum_{j=1}^N \psi_j \exp(-ik_m x_j)$$

$$\tilde{\psi}_m \xrightarrow[F]{F} F\tilde{\psi}_m = \psi_j = \sum_{m=1}^N \tilde{\psi}_m \exp(ik_m x_j)$$

- `four1(double data[], unsigned long nn, int isign)`

On input, the `data[]` array contains $2*nn$ elements that represent nn complex function values, such that `data[2*j-1]` & `data[2*j]` ($j = 1, \dots, nn$) are the real & imaginary parts of the function value on the j -th grid point

- On output `data[]` is replaced by:

—`isign = 1`
$$data_j \leftarrow \sum_{m=1}^N data_m \exp(i2\pi m j / N)$$

$$k_m x_j = \frac{2\pi m}{L} \times \frac{L}{N} j = \frac{2\pi m j}{N}$$

—`isign = -1`
$$data_m \leftarrow \sum_{j=1}^N data_j \exp(-i2\pi m j / N)$$

- Note that `four1()` does not perform the division by N in F^{-1}

See `four1.c` in the class home page

Using four1()

- Define double psi[2*N], where psi[2*j] & psi[2*j+1] ($j = 0, \dots, N-1$) are the real & imaginary parts of ψ_j

```
/* Fourier transform */
four1(psi-1, (unsigned long) N, 1);

/* Inverse Fourier transform */
four1(psi-1, (unsigned long) N, -1);
for (j=0; j<2*N; j++)
    psi[j] /= N;
```

- Note that four1() assumes 1 offset for the first argument but psi[] is 0 offset

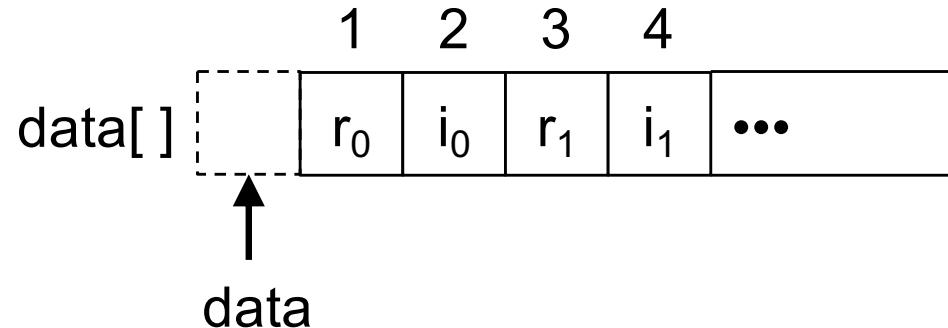
$$\begin{aligned}\psi_j &\xrightarrow[F^{-1}]{\quad} F^{-1}\psi_j = \tilde{\psi}_m = \frac{1}{N} \sum_{j=1}^N \psi_j \exp(-ik_m x_j) \\ \tilde{\psi}_m &\xrightarrow[F]{\quad} F\tilde{\psi}_m = \psi_j = \sum_{m=1}^N \tilde{\psi}_m \exp(ik_m x_j)\end{aligned}$$

0	1	2	3		$2N-2$	$2N-1$
psi[]	Re ψ_0	Im ψ_0	Re ψ_1	Im ψ_1	...	Re ψ_{N-1} Im ψ_{N-1}

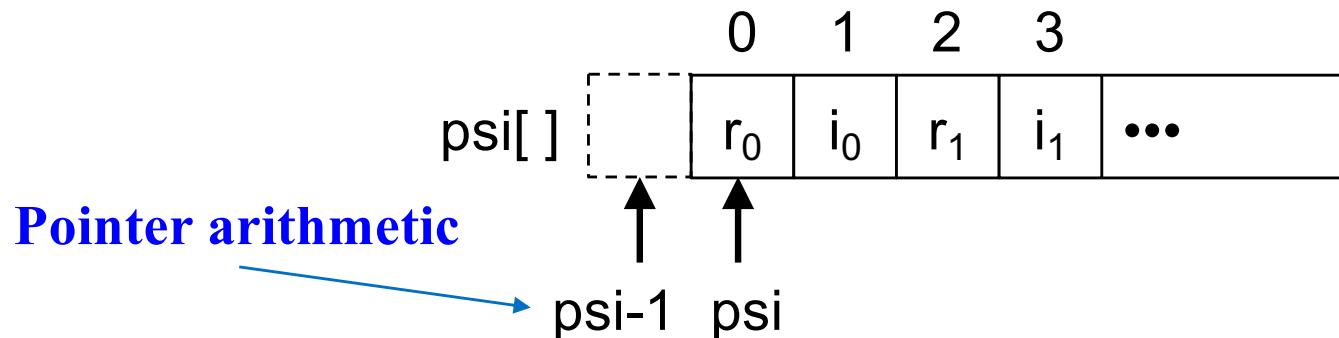
Array Offset

```
four1(psi-1, (unsigned long) N, 1);
```

- four1() assumes 1-offset (because of its Fortran origin)



- But psi[] uses 0-offset (C convention)



Energy

$$\langle H \rangle = \langle T \rangle + \langle V \rangle$$

$$= \int dx \psi^*(x) \left(-\frac{1}{2} \frac{\partial^2}{\partial x^2} \right) \psi(x) + \int dx \psi^*(x) V(x) \psi(x)$$

discretize

$$\cong dx \sum_{j=0}^{N-1} \psi_j^* \left(-\frac{1}{2} \frac{\partial^2}{\partial x^2} \right) \psi_j + dx \sum_{j=0}^{N-1} V_j |\psi_j|^2$$
$$= dx N \sum_{m=0}^{N-1} \frac{k_m^2}{2} |\tilde{\psi}_m|^2 + dx \sum_{j=0}^{N-1} V_j |\psi_j|^2 \quad \text{weighted sums}$$

In calc_energy():

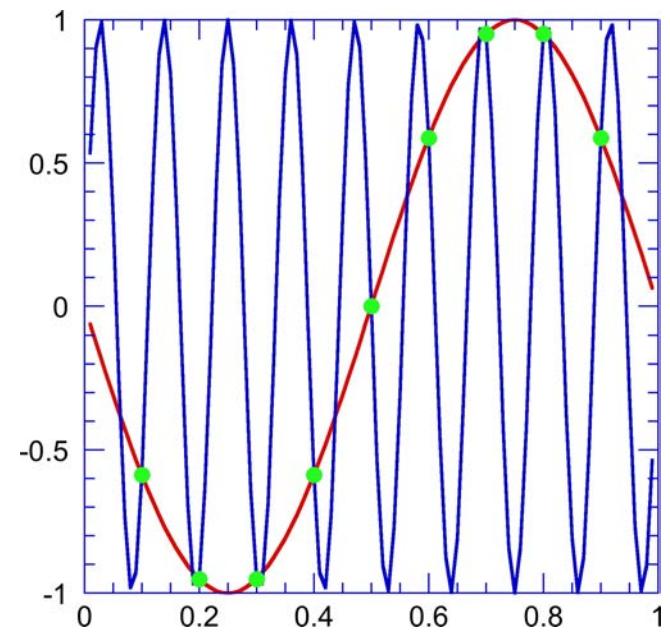
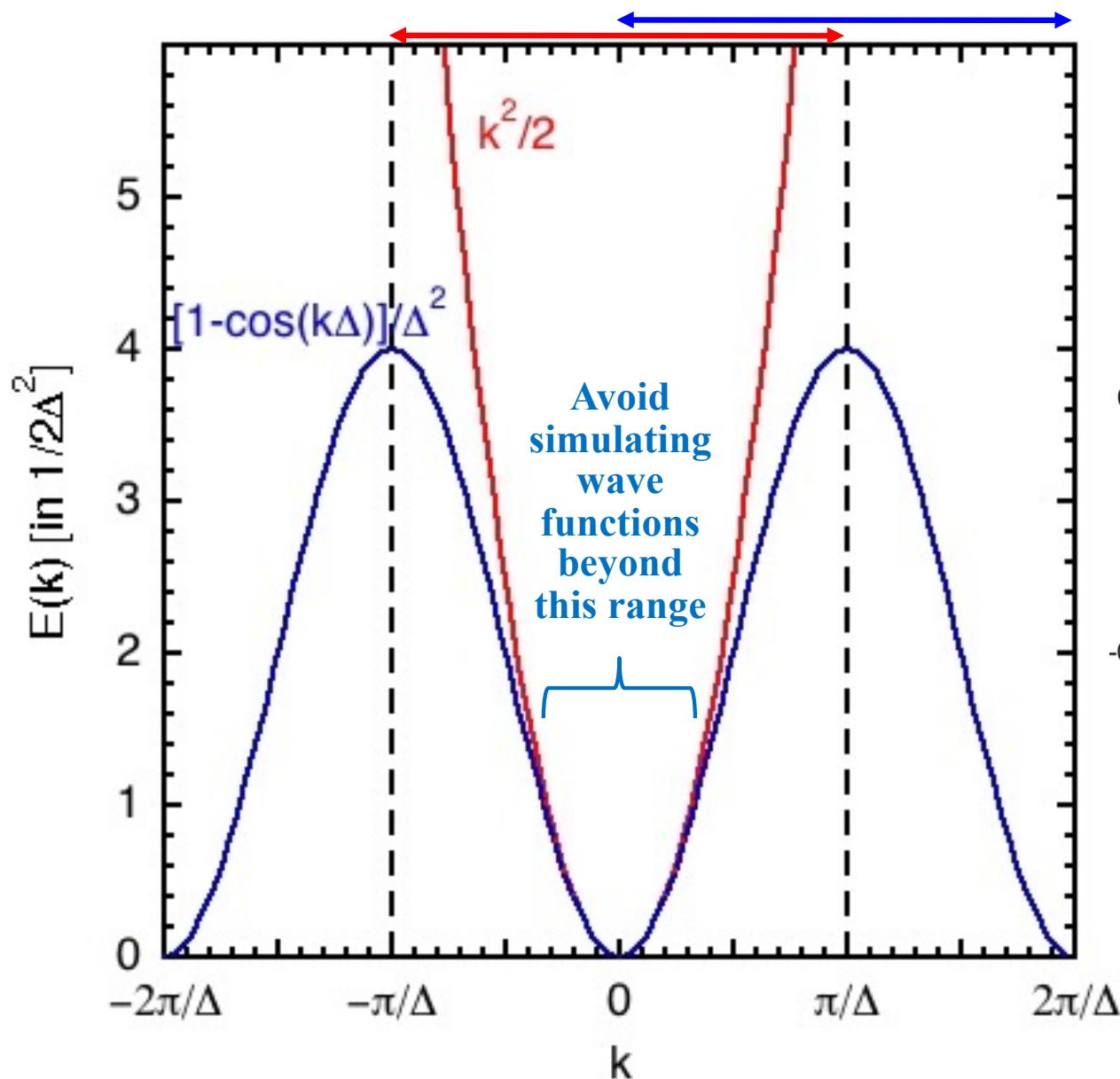
1. $\tilde{\psi}_m \leftarrow F^{-1}[\psi_j]$
2. $E_{\text{kin}} \leftarrow dx N \sum_{m=0}^{N-1} \frac{k_m^2}{2} |\tilde{\psi}_m|^2$
3. $\psi_j \leftarrow F[\tilde{\psi}_m] \text{ // don't forget}$
4. $E_{\text{pot}} \leftarrow dx \sum_{j=0}^{N-1} V_j |\psi_j|^2$



Kinetic Energy

$$\begin{aligned}
 \langle T \rangle &= dx \sum_{j=0}^{N-1} \overbrace{\sum_{m=0}^{N-1} \tilde{\psi}_m^* \exp(-ik_m x_j)}^{\psi^*(x_j)} \left(-\frac{1}{2} \frac{\partial^2}{\partial x^2} \right) \overbrace{\sum_{n=0}^{N-1} \tilde{\psi}_n \exp(ik_n x_j)}^{\psi(x_j)} \\
 &= dx \sum_{j=0}^{N-1} \sum_{m=0}^{N-1} \tilde{\psi}_m^* \exp(-ik_m x_j) \sum_{n=0}^{N-1} \frac{k_n^2}{2} \tilde{\psi}_n \exp(ik_n x_j) \\
 &= dx \sum_{m=0}^{N-1} \tilde{\psi}_m^* \sum_{n=0}^{N-1} \frac{k_n^2}{2} \tilde{\psi}_n \underbrace{\sum_{j=0}^{N-1} \exp(i(k_n - k_m)x_j)}_{N\langle m|n \rangle} \\
 &\quad \text{addition theorem} \quad \frac{1 - \cos(k_n \Delta x)}{\Delta x^2} \\
 &= dx \sum_{m=0}^{N-1} \tilde{\psi}_m^* \sum_{n=0}^{N-1} \frac{k_n^2}{2} \tilde{\psi}_n N \delta_{m,n} \\
 &= dx N \sum_{m=0}^{N-1} \frac{k_m^2}{2} |\tilde{\psi}_m|^2 \\
 &\quad \xrightarrow[\Delta x \rightarrow 0]{k_n^2} \frac{k_n^2}{2} \\
 &\quad \frac{d^2}{dx^2} e^{ik_n x_j} \cong \frac{e^{-ik_n \Delta x} - 2 + e^{ik_n \Delta x}}{\Delta x^2} e^{ik_n x_j} \\
 &\quad = \frac{2[\cos(k_n \Delta x) - 1]}{\Delta x^2} e^{ik_n x_j}
 \end{aligned}$$

Continuum vs. Discrete Kinetic Energy



Total Energy Conservation

- Energy eigenvalues & eigenvectors: $H|n\rangle = \varepsilon_n|n\rangle$ ($n = 0, \dots, N - 1$)
- Time evolution of a wave function

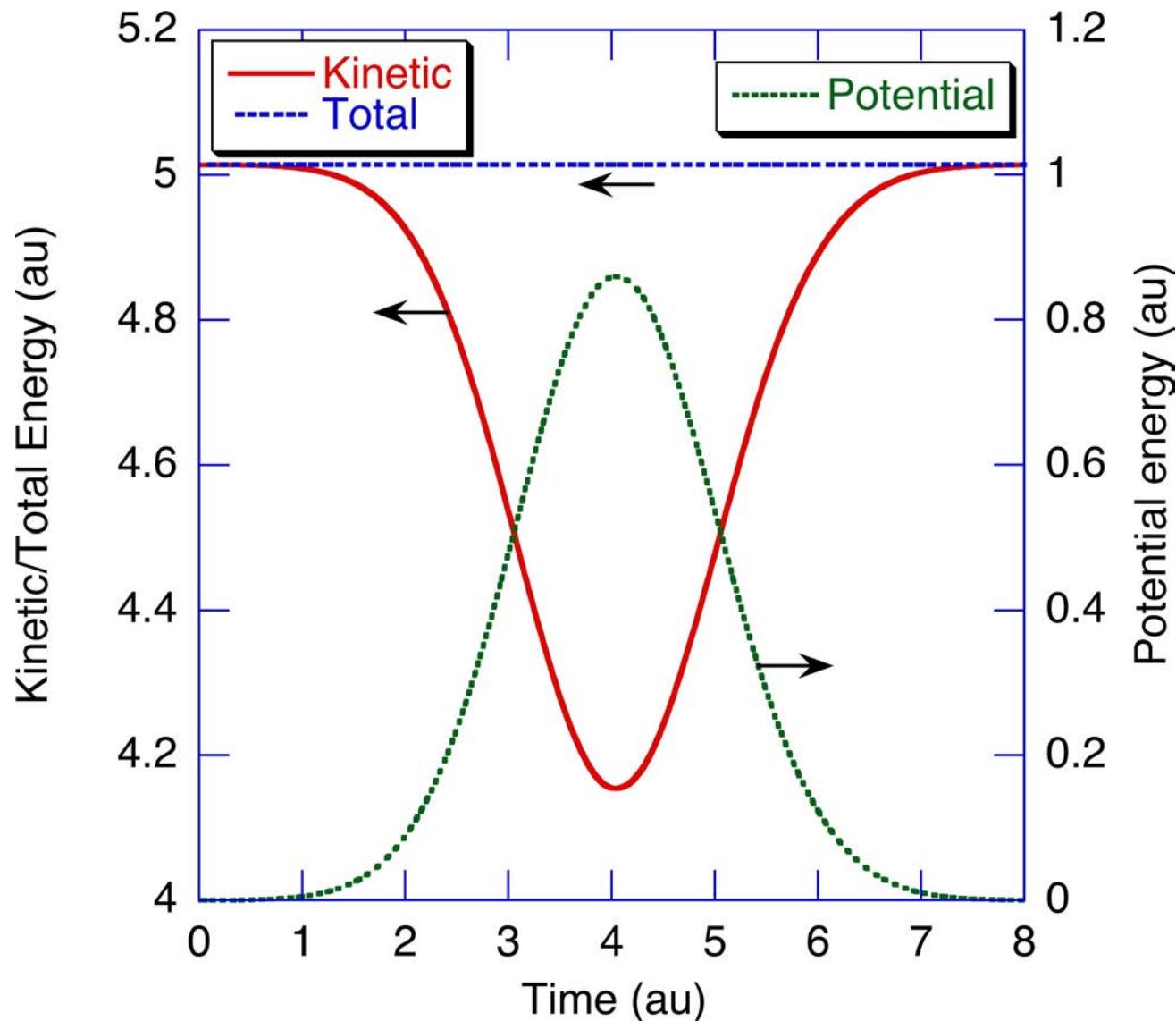
$$|\psi(t)\rangle = \exp(-iHt) \sum_{n=0}^{N-1} |n\rangle\langle n| \psi(0)\rangle = \sum_{n=0}^{N-1} \exp(-i\varepsilon_n t) |n\rangle\langle n| \psi(0)\rangle$$

- Total energy

$$\begin{aligned} \langle \psi(t) | H | \psi(t) \rangle &= \left(\sum_{m=0}^{N-1} \langle \psi(0) | m \rangle \exp(i\varepsilon_m t) \langle m | \right) H \left(\sum_{n=0}^{N-1} \exp(-i\varepsilon_n t) |n\rangle\langle n| \psi(0)\rangle \right) \\ &= \left(\sum_{m=0}^{N-1} \langle \psi(0) | m \rangle \exp(i\varepsilon_m t) \langle m | \right) \left(\sum_{n=0}^{N-1} \exp(-i\varepsilon_n t) \varepsilon_n |n\rangle\langle n| \psi(0)\rangle \right) \\ &= \sum_{m=0}^{N-1} \sum_{n=0}^{N-1} \exp(i(\varepsilon_m - \varepsilon_n)t) \varepsilon_n \langle \psi(0) | m \rangle \langle n | \psi(0) \rangle \langle m | n \rangle \\ &= \sum_{n=0}^{N-1} \varepsilon_n |\langle n | \psi(0) \rangle|^2 = \text{constant} \end{aligned}$$

$\delta_{m,n}$

Energy Conservation for 1D Square Barrier

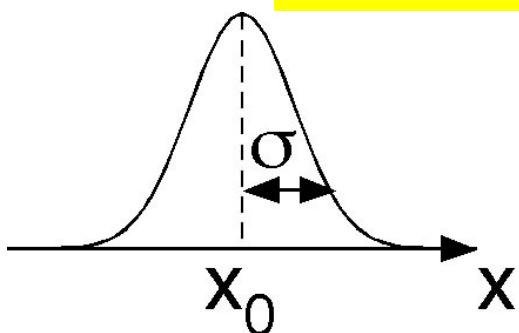


Energy conservation: good program verification

Initial Wave Function

- Gaussian wave packet

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



$$i \frac{\partial}{\partial t} \exp \left(ik_0 x - i \frac{k_0^2}{2} t \right) = \frac{k_0^2}{2} \exp \left(ik_0 x - i \frac{k_0^2}{2} t \right)$$

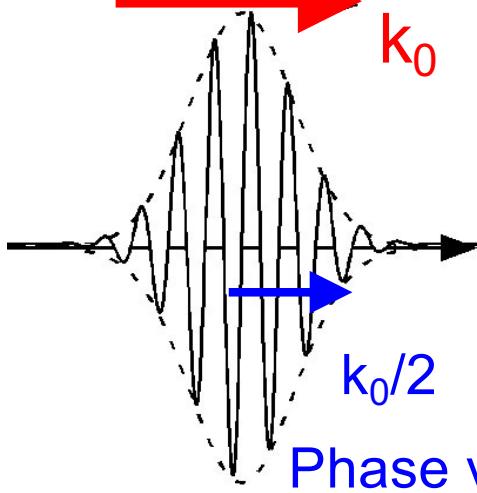
Free-space solution

Free-space solution

1

Group velocity

k₀



$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + 0 \right] \exp\left(ik_0x - i \frac{k_0^2}{2}t\right) = \frac{k_0^2}{2} \exp\left(ik_0x - i \frac{k_0^2}{2}t\right)$$

$$\psi(x, t) = \int dk \tilde{\psi}(k) \exp(ikx - i\omega(k)t) \quad \text{Here, } \omega(k) = k^2/2$$

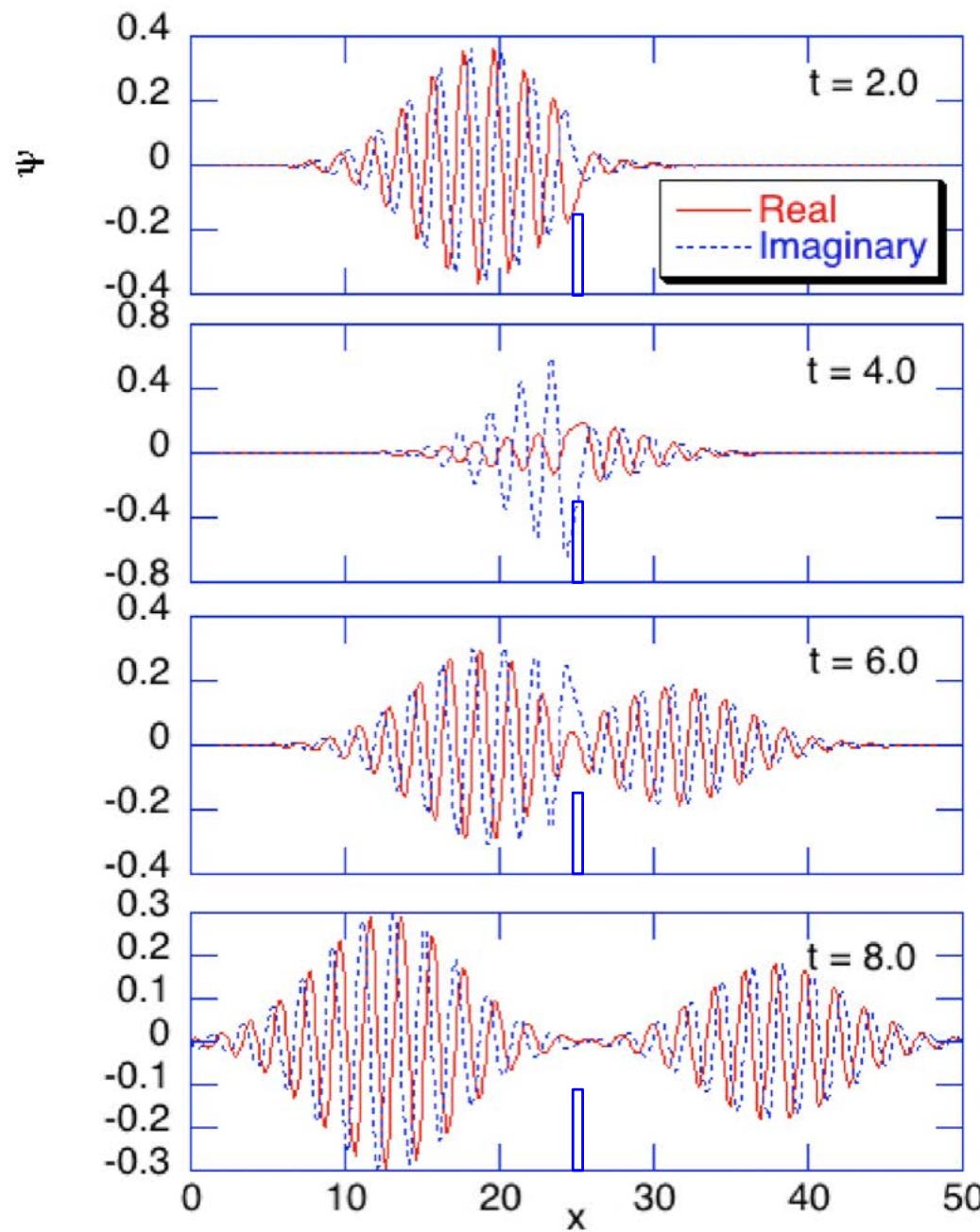
$$= \int dk \tilde{\psi}(k) \exp \left(i \frac{k_0 + k - k_0}{\tilde{k}} x - i \overline{\omega(k)} t \right)$$

Phase velocity

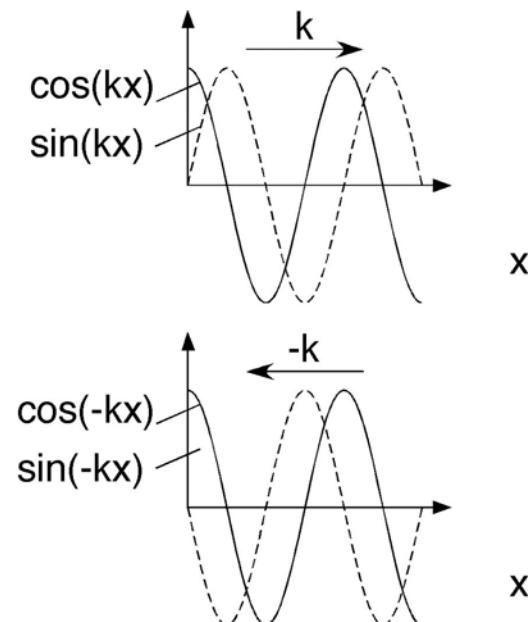
Group velocity

See Gaussian wave-packet movie at <https://www.cond-mat.de/teaching/QM/JSim/wpack.html>

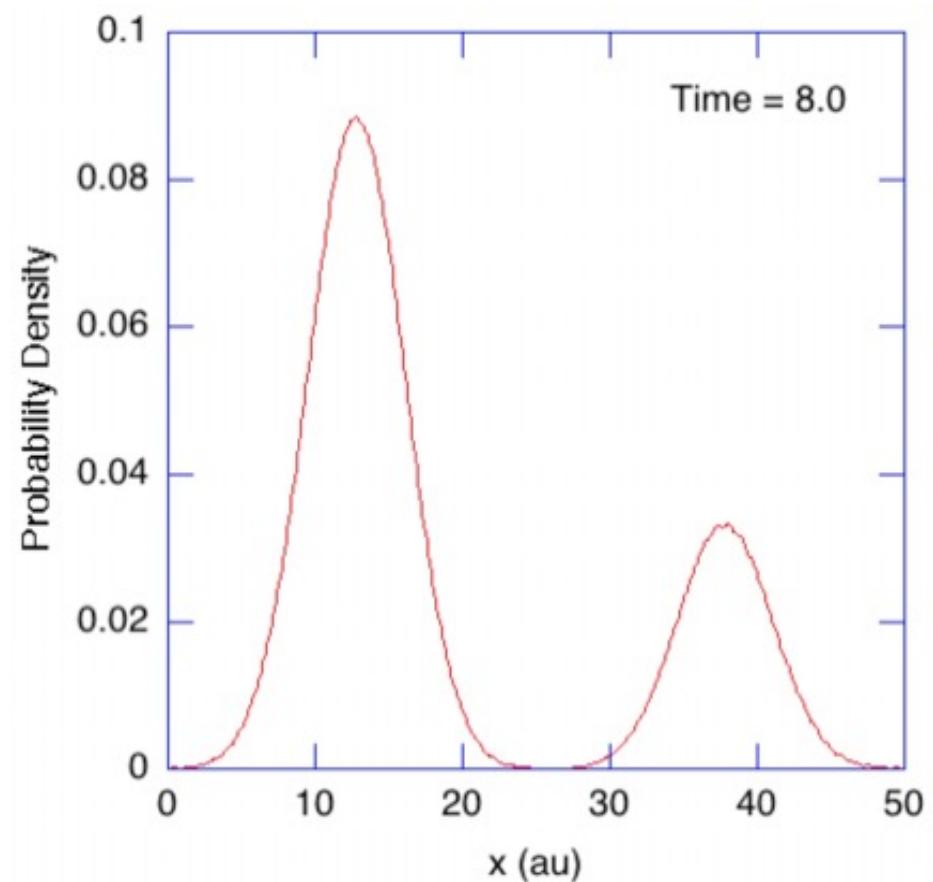
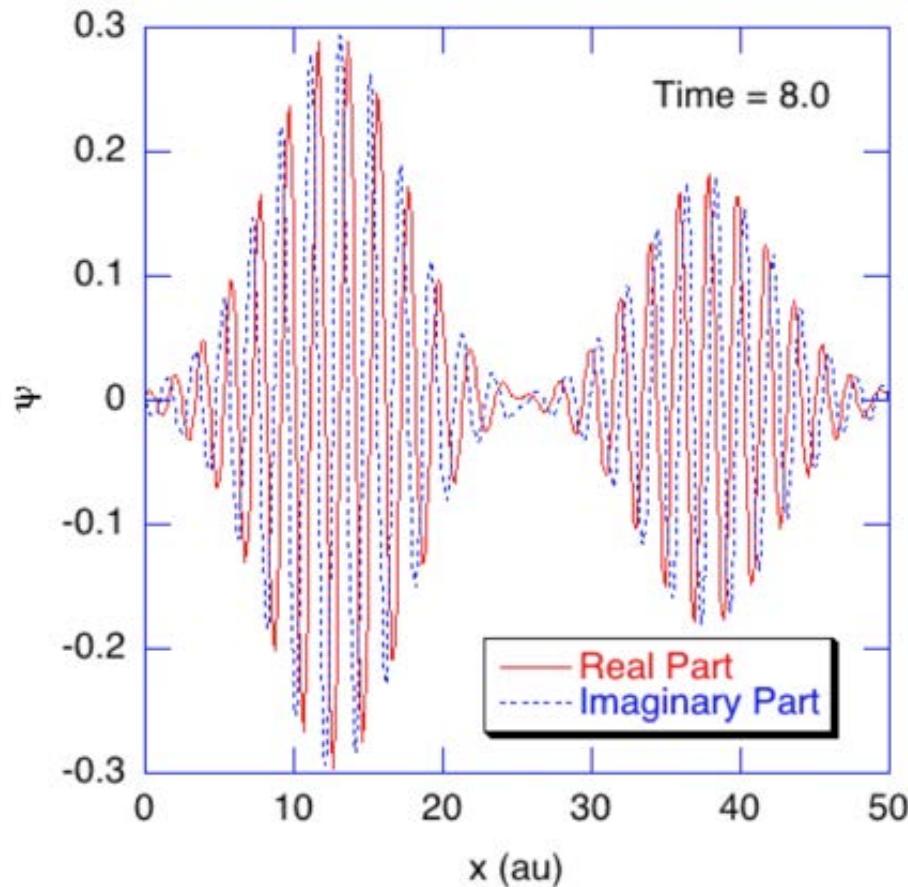
Numerical Example



$\Delta t = 2 \times 10^{-3}$ au



Wave Function & Probability

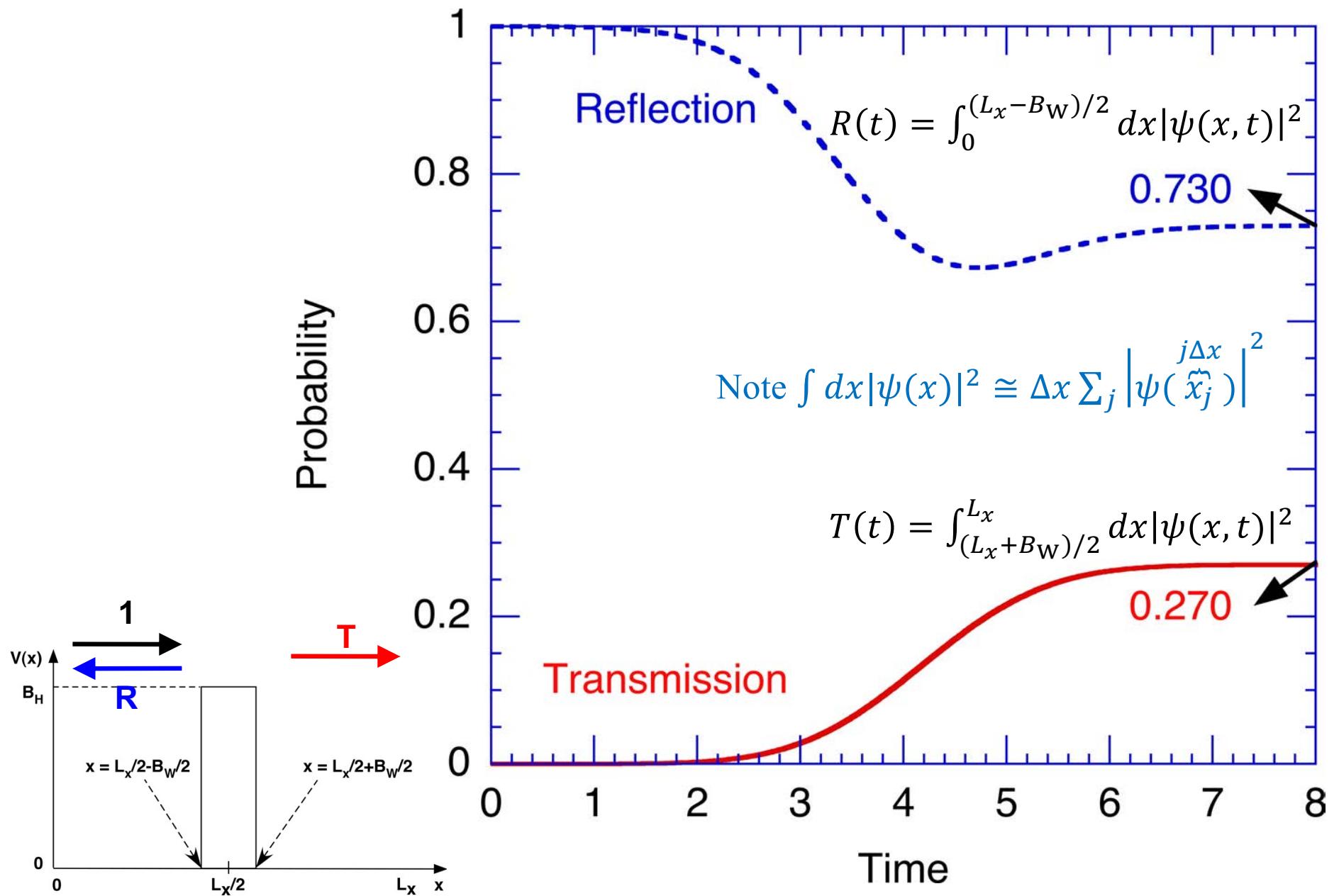


qd1.in

50.0	LX
2.0e-3	DT
4000	NSTEP
10	NECAL
12.5 3.0 5.0	X0 S0 E0
5.0 1.0	BH BW
50.0	EH

qd1.h #define NX 512

Transmission & Reflection Coefficients



Top 10 Algorithms in History

In putting together this issue of *Computing in Science & Engineering*, we knew three things: it would be difficult to list just 10 algorithms; it would be fun to assemble the authors and read their papers; and, whatever we came up with in the end, it would be controversial. We tried to assemble the 10 algorithms with the greatest influence on the development and practice of science and engineering in the 20th century.

Following is our list (here, the list is in chronological order; however, the articles appear in no particular order):

- Metropolis Algorithm for Monte Carlo
- Simplex Method for Linear Programming
- Krylov Subspace Iteration Methods
- The Decompositional Approach to Matrix Computations
- The Fortran Optimizing Compiler
- QR Algorithm for Computing Eigenvalues
- Quicksort Algorithm for Sorting
- Fast Fourier Transform
- Integer Relation Detection
- Fast Multipole Method

PHYS 516
CSCI 596
CSCI 653

IEEE CiSE, Jan/Feb (2000)

Fast Fourier Transform

- Danielson-Lanczos algorithm:

$$\begin{aligned}\psi_j &= \sum_{m=0}^{N-1} \tilde{\psi}_m \exp(ik_m x_j) = \sum_{m=0}^{N-1} \tilde{\psi}_m \exp(i2\pi m j / N) \quad O(N^2)! \\ &= \sum_{m=0}^{N/2-1} \tilde{\psi}_{2m} \exp(i2\pi(2m)j / N) + \sum_{m=0}^{N/2-1} \tilde{\psi}_{2m+1} \exp(i2\pi(2m+1)j / N) \\ &\quad \text{even terms} \qquad \qquad \qquad \text{odd terms} \\ &= \sum_{m=0}^{N/2-1} \tilde{\psi}_{2m} \exp(i2\pi m j / (N/2)) + \exp(i2\pi j / N) \sum_{m=0}^{N/2-1} \tilde{\psi}_{2m+1} \exp(i2\pi m j / (N/2))\end{aligned}$$

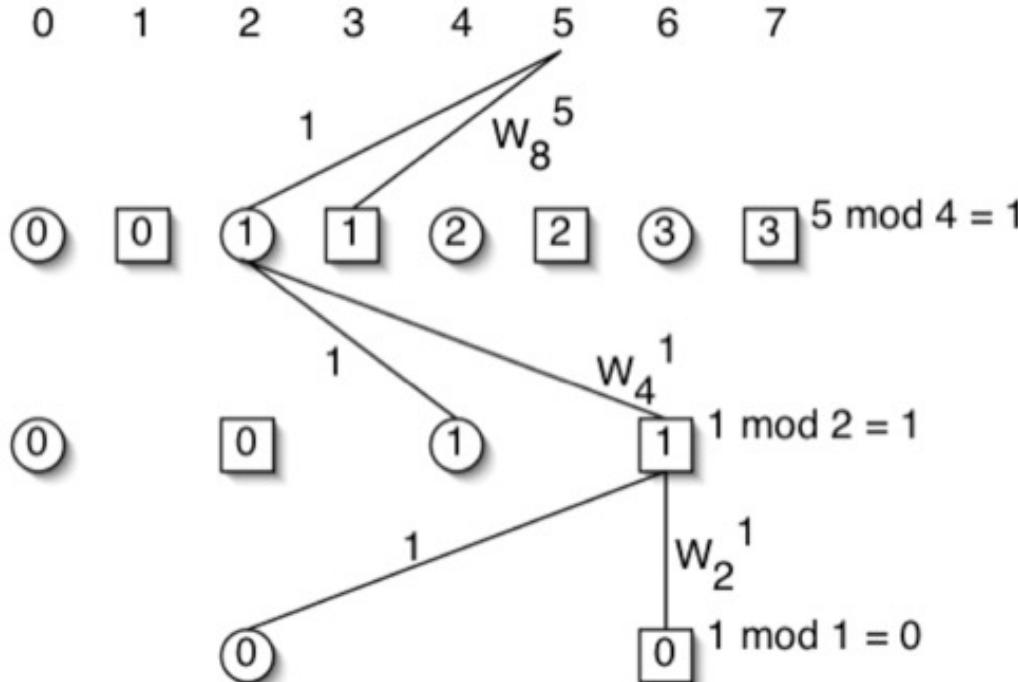
$$\left. \begin{array}{l} \psi_j^0 = \sum_{m=0}^{N/2-1} \tilde{\psi}_{2m} \exp(i2\pi m j / (N/2)) \\ \psi_j^1 = \sum_{m=0}^{N/2-1} \tilde{\psi}_{2m+1} \exp(i2\pi m j / (N/2)) \\ W_N = \exp(i2\pi j / N) \end{array} \right\} \begin{array}{l} \text{subarray Fourier decompositions} \\ j \text{ read as } j \bmod N/2 \end{array}$$

Divide-and-conquer

Fast Fourier Transform

- Recursive sub-Fourier transforms: $\psi_j = \psi_j^0 + W_N^j \psi_j^1$

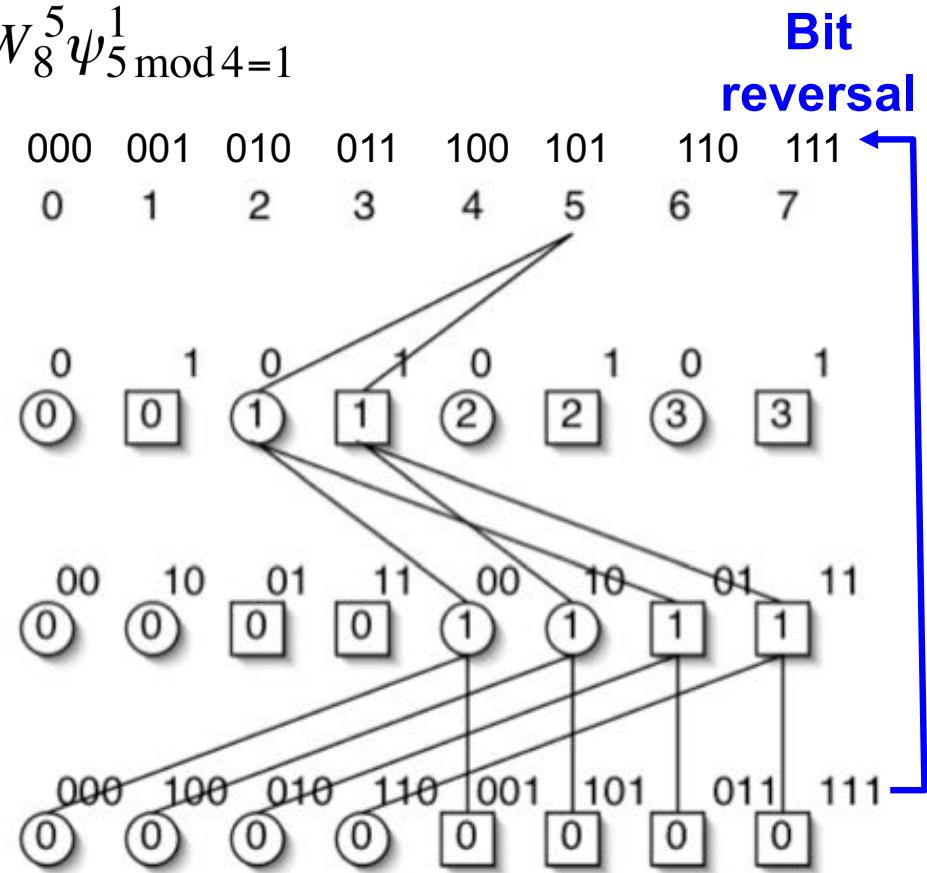
$$\psi_5 = \psi_{5 \bmod 4=1}^0 + W_8^5 \psi_{5 \bmod 4=1}^1$$



$010 \rightarrow 010 \rightarrow 2$

$011 \rightarrow 110 \rightarrow 6$

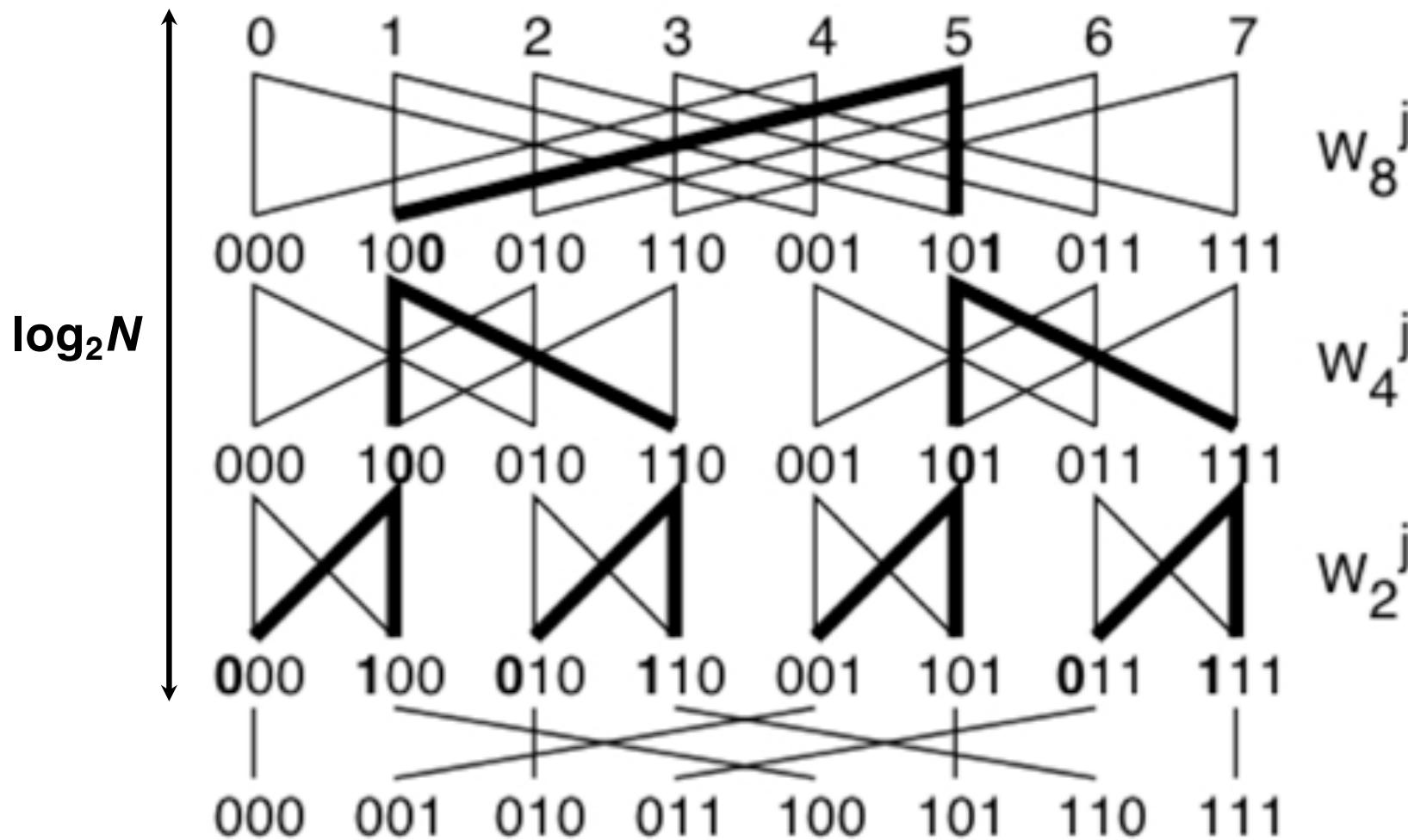
Path bit reversal = element



Recursion tree
 $O(N)$ operations per element

Fast Fourier Transform Algorithm

- Butterfly (hypercube) data exchange after bit-reversal:



- Many computations are shared among the recursion trees
- $2N \log_2 N$ arithmetic operations

Parallelizing Quantum Dynamics

Aiichiro Nakano

Collaboratory for Advanced Computing & Simulations

Department of Computer Science

Department of Physics & Astronomy

Department of Chemical Engineering & Materials Science

Department of Quantitative & Computational Biology

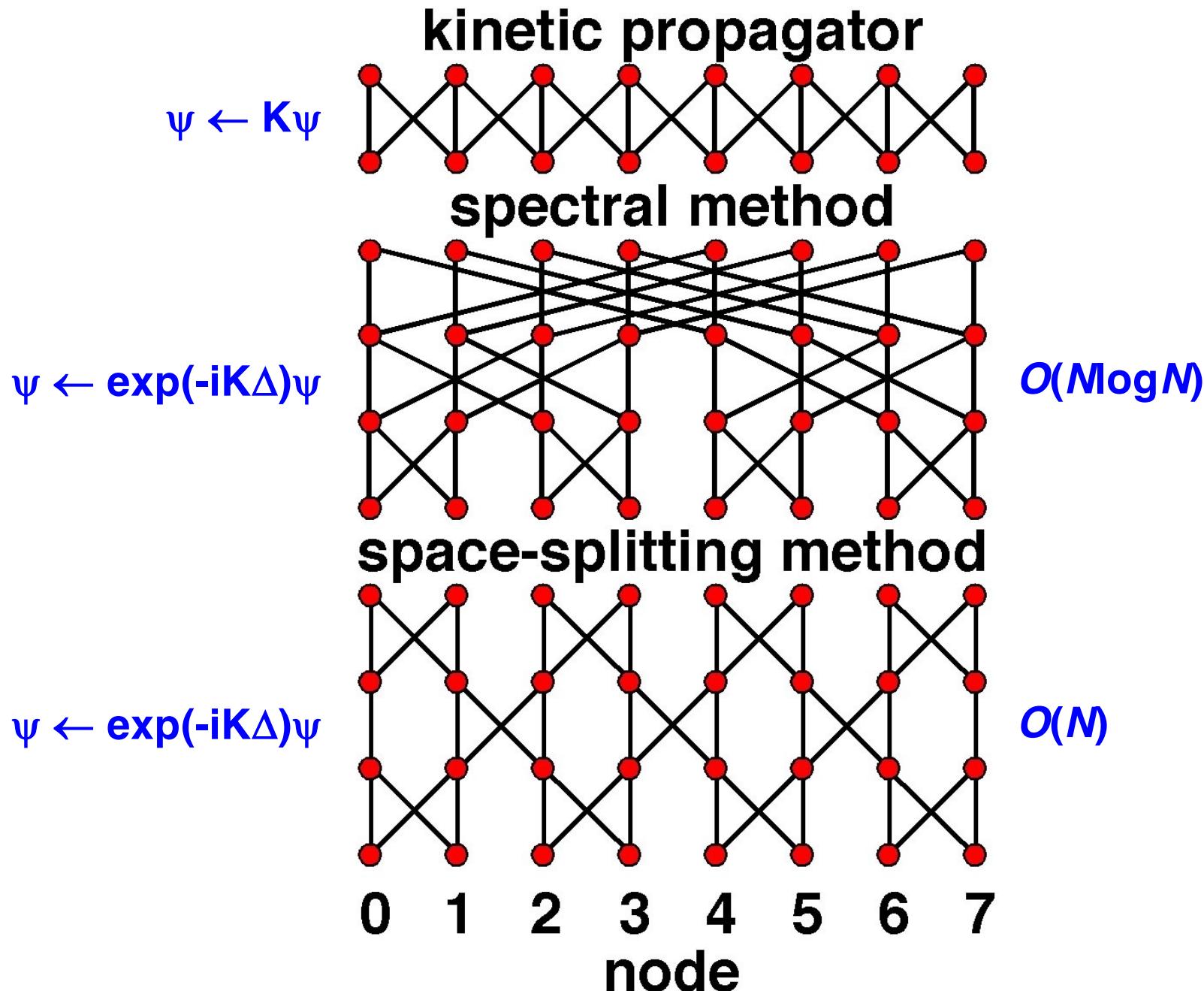
University of Southern California

Email: anakano@usc.edu

See <https://aiichironakano.github.io/cs596.html>

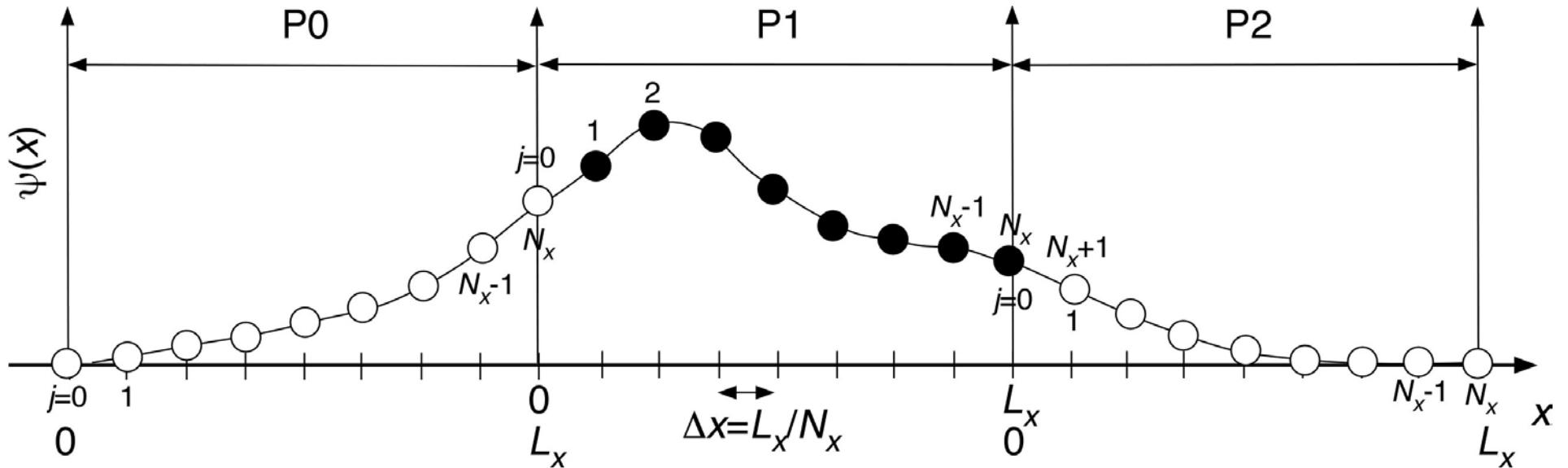


Parallel QD Communications



Parallelization of Space Splitting Method

- Self-centric spatial decomposition



- Local & global coordinates

$$\begin{cases} x_j = j\Delta x \\ x_j^{(\text{global})} = j\Delta x + pL_x \end{cases}$$

- Global coordinates only in `init_prop()` & `init_wavefn()`

Boundary Wave Function Caching

- Parallelized `periodic_bc()`

```
plw = (myid-1+nproc)%nproc; /* Lower partner process */
pup = (myid+1           )%nproc; /* Upper partner process */

/* Cache boundary wave function value at the lower end */
dbuf[0:1] ← psi[NX][0:1];
Send dbuf to pup;
Receive dbufr from plw;
psi[0][0:1] ← dbufr[0:1];

/* Cache boundary wave function value at the upper end */
dbuf[0:1] ← psi[1][0:1];
Send dbuf to plw;
Receive dbufr from pup;
psi[NX+1][0:1] ← dbufr[0:1];
```

