Gross-Pitaevksii 方程及其数值模拟

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Outline

1. Gross-Pitaevksii Equation
   - Energy functional of the Hamiltonian
   - Second quantized Hamiltonian
2. Numerical simulation of G-P equation
   - Split-Step Fourier Method
   - Fast Fourier transformation
   - Imaginary Time Method
   - Dimensionless

Hamiltonian

Hamiltonian with contact interaction:

$$H = \sum_{i}^{N} \left[\frac{p_i^2}{2m} + V(\boldsymbol{r}_i) \right] + U_0 \sum_{i<j} \delta(\boldsymbol{r}_i - \boldsymbol{r}_j).$$

- $U_0 = 4\pi\hbar^2 a_s/m$ is given by the pseudopotential.
- N-body wavefunction,

$$\Psi(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_N) = \prod_{i=1}^{N} \phi(\boldsymbol{r}_i),$$

and $\int |\phi_i|^2 d\boldsymbol{r}_i = 1$.

Gross–Pitaevskii equation

- Kinetic energy and potential energy

$$
\begin{aligned}
&\int \prod_k d\boldsymbol{r}_k \Psi^* \{ \sum_{i=1}^{N} H_0(\boldsymbol{r}_i) \} \Psi \\
=&\int \prod_{i=1}^{N} d\boldsymbol{r}_i \phi^*(\boldsymbol{r}_i) \sum_{j=1}^{N} H_0(\boldsymbol{r}_j) \phi(\boldsymbol{r}_i) \\
=&\sum_{j=1}^{N} \int d\boldsymbol{r}_j \phi^*(\boldsymbol{r}_i) H_0(\boldsymbol{r}_i) \phi(\boldsymbol{r}_i) \prod_{i \neq j} \int d\boldsymbol{r}_i |\phi(\boldsymbol{r}_i)|^2 \\
=&N \int d\boldsymbol{r} \phi^*(\boldsymbol{r}) H_0(\boldsymbol{r}) \phi(\boldsymbol{r})
\end{aligned}
$$

where $H_0 = -\frac{\hbar^2 \nabla_{\boldsymbol{r}}^2}{2m} + V(\boldsymbol{r})$.

- Interaction energy,

$$\int \prod_{i=1}^{N} d\boldsymbol{r}_i |\phi(\boldsymbol{r}_i)|^4 U_0 \sum_{i<j} \delta(\boldsymbol{r}_i - \boldsymbol{r}_j)$$
$$= \quad C_N^2 U_0 \int d\boldsymbol{r} |\phi(\boldsymbol{r})|^4$$

- The total energy functional is

$$\frac{E(\phi(\boldsymbol{r}))}{N} = \int d\boldsymbol{r} \Big[\frac{\hbar^2}{2m} |\nabla\phi(\boldsymbol{r})|^2 + V(\boldsymbol{r})|\phi(\boldsymbol{r})|^2 + \frac{N-1}{2} U_0 |\phi(\boldsymbol{r})|^4\Big]$$

Note,

$$\int d\boldsymbol{r} \phi^*(\boldsymbol{r}) \nabla^2 \phi(\boldsymbol{r}) = -\int d\boldsymbol{r} |\nabla\phi|^2 + \int d\boldsymbol{r} \nabla \cdot [\phi^*(\boldsymbol{r}) \nabla\phi(\boldsymbol{r})]$$
$$= -\int d\boldsymbol{r} |\nabla\phi|^2 + \oint d\boldsymbol{n} [\phi^*(\boldsymbol{r}) \nabla\phi(\boldsymbol{r})].$$

Surface integral vanished, and we used
$\nabla \cdot (f\nabla g) = \nabla f \cdot \nabla g + f\nabla^2 g$.

- Defined the condensate wavefunction,

$$\psi(\boldsymbol{r}) = N^{\frac{1}{2}}\phi(\boldsymbol{r}), \quad \int d\boldsymbol{r}|\psi(\boldsymbol{r})|^2 = N.$$

  With this, the energy functional becomes,

$$E(\psi(\boldsymbol{r})) = \int d\boldsymbol{r}[\frac{\hbar^2}{2m}|\nabla\psi(\boldsymbol{r})|^2 + V(\boldsymbol{r})|\psi(\boldsymbol{r})|^2 + \frac{1}{2}U_0|\psi(\boldsymbol{r})|^2].$$

  where we used $N - 1 \approx N$ for large N.
- Minimize the energy functional with respect to ψ , ψ^*. Conservation condition $\int d\boldsymbol{r}|\psi(\boldsymbol{r})|^2 = N$.
- Lagrange multiplier. Chemical potential μ , and minimize $E - \mu N$

Minimizing the energy functional $\frac{\delta E[\psi]}{\delta \psi^*} = 0$,

$$-\frac{\hbar}{2m}\nabla^2\psi(\boldsymbol{r}) + V(\boldsymbol{r})\psi(\boldsymbol{r}) + U_0|\psi(\boldsymbol{r})|^2\psi(\boldsymbol{r}) = \mu\psi(\boldsymbol{r}).$$

- Time independent Gross-Pitaevskii equation (GPE).
- The potential is given by the external potential and a non-linear mean field term $U_0|\psi(\boldsymbol{r})|^2$.

GPE from second quantized Hamiltonian

Second quantized Hamiltonian,

$$\hat{H} = \int d^3\mathbf{r}\hat{\Psi}^\dagger(\mathbf{r},t)\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t)\right]\hat{\Psi}(\mathbf{r},t)$$
$$+\frac{1}{2}\int \hat{\Psi}^\dagger(\mathbf{r}',t)\,\hat{\Psi}^\dagger(\mathbf{r},t)U(\mathbf{r}-\mathbf{r}')\,\hat{\Psi}(\mathbf{r},t)\hat{\Psi}(\mathbf{r}',t)\,d^3\mathbf{r}d^3\mathbf{r}'.$$

- Heisenberg equation for the field operator,

$$i\hbar\frac{\partial}{\partial t}\hat{\Psi}(\mathbf{r},t) = [\hat{\Psi}(\mathbf{r},t),\hat{H}]$$
$$= \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t) + \int d^3\mathbf{r}'\hat{\Psi}^\dagger(\mathbf{r}',t)\,U(\mathbf{r}-\mathbf{r}')\,\hat{\Psi}(\mathbf{r}',t)\right]\hat{\Psi}(\mathbf{r},t).$$

- Bogoliubov mean field expansion, $\hat{\Psi} = \langle\hat{\Psi}\rangle + \delta\hat{\Psi}$. have left out the fluctuation, Bogoliubov approximation $\hat{\Psi} \approx \langle\hat{\Psi}\rangle = \psi$.

- Contact interaction, $U(\mathbf{r}-\mathbf{r}') = \frac{4\pi\hbar^2 a_s}{m}\delta(\mathbf{r}-\mathbf{r}')$.
- Time-Dependent Gross-Pitaevskii Equation,

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t) + U_0|\psi(\mathbf{r},t)|^2\right]\psi(\mathbf{r},t).$$

- $\psi(\mathbf{r},t) = \psi(\mathbf{r})e^{-i\mu t}$, $V(\boldsymbol{r},t) \equiv V(\boldsymbol{r})$,

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) + U_0|\psi(\mathbf{r})|^2\psi(\mathbf{r}) = \mu\psi(\mathbf{r})$$

Split-Step Fourier Method

In one-dimension,

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

- $\hat{H} = T(x) + V(x),\ T = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

Time-evolution equation,

$$\psi(x, t+\Delta t) = e^{-i\Delta t H/\hbar}\psi(x,t)$$

- In position space V is diagonal, T is diagonal in momentum space.
- $e^{-i\Delta t H/\hbar} \neq e^{-i\Delta t T/\hbar}e^{-i\Delta t V/\hbar}$

  $$e^{-i\Delta t H/\hbar} \approx e^{-i\Delta t V/(2\hbar)}e^{-i\Delta t T/\hbar}e^{-i\Delta t V/2\hbar}\psi$$

  holds the error($\mathcal{O}(\Delta t^3)$).
- Conversion to momentum space is achieved by taking the Fourier transform $\mathcal{F}$

  $$\psi(x, t+\Delta t) \approx e^{\frac{-i}{2\hbar}V(x)\Delta t}\cdot\mathcal{F}^{-1}\left[e^{\frac{-i\hbar k^2}{2m}\Delta t}\cdot\mathcal{F}\left[e^{-\frac{i}{2\hbar}V(x)\Delta t}\cdot\psi(x,t)\right]\right]$$

Fast Fourier transformation

Discrete Fourier transformation

$$f_k = \sum_{n=0}^{N-1} f_n e^{-i2\pi kn/N}$$

- 在一个周期内，实空间坐标离散化成 N 个点
- 时间复杂度：$\mathcal{O}(N^2)$
- 周期性

$$f_{N+k} = f_k$$

$x = e^{-2i\pi k/N}$，有

$$\begin{aligned} A(x) &= a_0 + a_1 x + a_2 x^2 + \cdots + a_{N-1} x^{N-1} \\ &= \left(a_0 + a_2 x^2 + \cdots + a_{N-2} x^{N-2}\right) + \left(a_1 x + a_3 x^3 + \cdots + a_{N-1} x^{N-1}\right) \\ &= \left(a_0 + a_2 x^2 + \cdots + a_{N-2} x^{N-2}\right) + x\left(a_1 + a_3 x^2 + \cdots + a_{N-1} x^{N-2}\right) \\ &\equiv F_{N/2}(x^2) + x\, G_{N/2}(x^2) \end{aligned}$$

- 设 $\omega_N^k = e^{-2i\pi k/N}$

$$\left(\omega_N^k\right)^2 = x^2 = e^{-\frac{4\pi k}{N}} = e^{-\frac{2\pi k}{N/2}} = \omega_{N/2}^k$$

- $A(x)$ 分成奇偶两部分，可以看成

两个 $N/2$ 个点的离散傅立叶变换 相加

- $k \in [0, N/2)$ 时

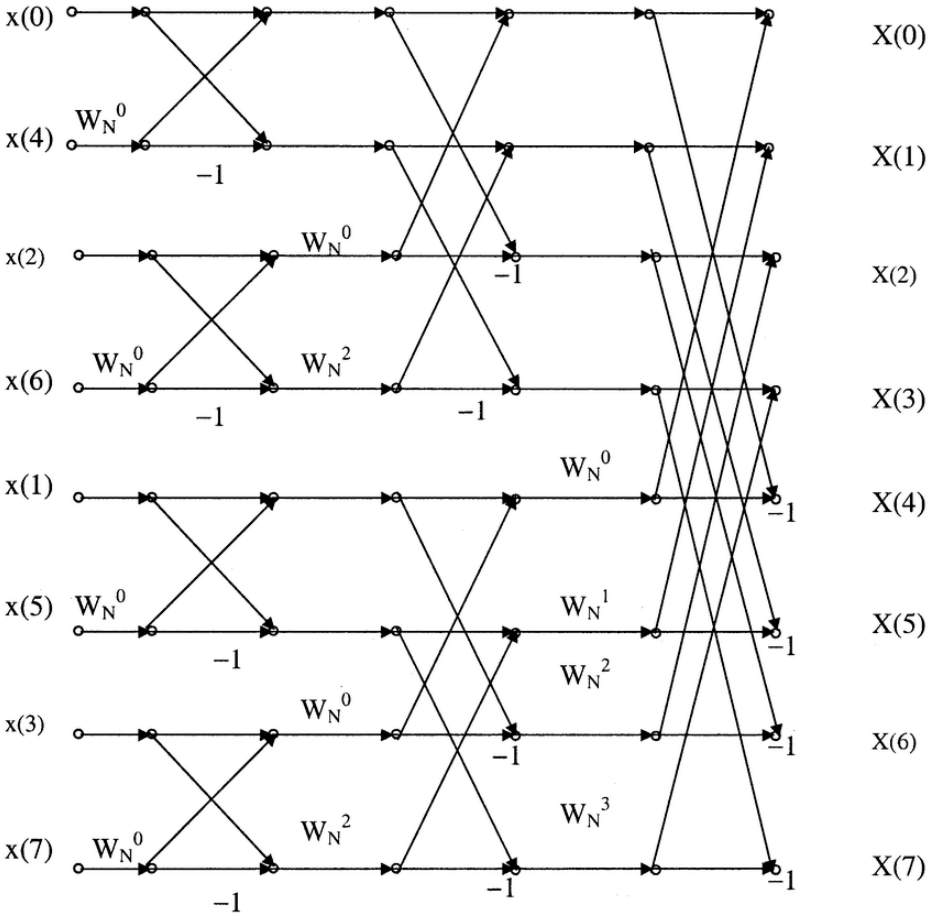
$$A(\omega_N^k) = F_{N/2}(\omega_{N/2}^k) + \omega_N^k G_{N/2}(\omega_{N/2}^k)$$

- $k \in [N/2, N]$ 时

$$A(\omega_N^k) = F_{N/2}(\omega_{N/2}^k) - \omega_N^k G_{N/2}(\omega_{N/2}^k)$$

- $N/2$ 个点的变换再分成两个 $N/4$ 个点的傅立叶变换 $\cdots$，$\cdots$

$N = 8$



- 利用频域上的对称性不断把变换分解，实现快速傅立叶变换

$$\mathcal{O}(N^2) \to \mathcal{O}(N \log N)$$

Imaginary Time Method

- $\psi(x,t)$ expressed as a superposition of eigenstates $\phi_m(x)$,

$$\psi(x,t) = \sum_m a_m(t)\phi_m(x).$$

- substitution $\Delta t \to -i\Delta t$,

$$\psi(t+\Delta t) = e^{-\Delta t\hat{H}/\hbar}\psi(x,t) = \sum_m a_m(t)\phi_m(x)e^{-\Delta t E_m/\hbar}.$$

  The ground state (with lowest E_m) decaying the slowes.
- Renormalizing ψ after each iteration (to ensure $\int |\psi(x)|^2 = N$ or 1), will evolve towards the ground state.
- Convergent condition$e^{-iH\Delta t}|\psi(t)\rangle = e^{-i\mu\Delta t}|\psi(t)\rangle = |\psi(t+\Delta t)\rangle$

$$\mu = (\hbar/\Delta t)\ln|\psi(x,t)/\psi(x,t+\Delta t)|$$

Dimensionless

Gross–Pitaevskii equation in one-dimension,

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2 x}\psi(x) + g_{1d}|\psi(x)|^2 + \frac{1}{2}mx^2\omega^2\psi(x) = i\hbar\frac{\partial}{\partial t}\psi(x).$$

In the unit of recoil energy. $E_R = \frac{\hbar^2 k_R^2}{2m}$, $k = \tilde{k}k_R$, $x = \tilde{x}\frac{1}{k_R}$.

- Kinetic term $\frac{\hbar^2 k^2}{2m}/E_R = E_R\tilde{k}^2/E_R = \tilde{k}^2$.
- Trap potential, $\frac{1}{2}mx^2\omega^2/E_R = \frac{\hbar^2 \mathrm{Hz}^2}{4E_R^2}\tilde{r}^2\tilde{\omega}^2$.
  For ^{87}Rb: $E_R = 2\pi\hbar \cdot 3632.5\mathrm{Hz}$. $\omega = 500\mathrm{Hz}$, $\tilde{\omega} \approx 0.02$.

- Interaction. The ground state of Harmonic wavefunction of y (z) component,

$$\psi(y)\psi(z) = \sqrt{\frac{m\sqrt{\omega_y\omega_z}}{\hbar\pi}} e^{-\frac{1}{2}\frac{m}{\hbar}(\omega_y y^2+\omega_z z^2)}.$$

- Integrate out $\psi(y)$ and $\psi(z)$, And the interaction coefficient is $g_{3d} = \frac{4\hbar^2\pi a_s}{m}$. Then,

$$\begin{aligned} g_{1d} &= g_{3d}\int\int dydz|\psi(y)\psi(z)|^2 = \frac{4\hbar^2\pi a_s}{m}\frac{m\mathrm{Hz}\sqrt{\tilde{\omega}_y\tilde{\omega}_z}}{2\hbar\pi} \\ &= 2\hbar a_B \cdot \mathrm{Hz} \cdot \sqrt{\tilde{\omega}_y\tilde{\omega}_z}\tilde{a}_s. \end{aligned}$$

- In consideration of $\int |\psi(\frac{\tilde{x}}{k_R})|^2 \frac{d\tilde{x}}{k_R} = N$, the dimension of the wavefunction is $\sqrt{k_R}$, $\psi(\frac{\tilde{x}}{k_R}) = \sqrt{k_R}\tilde{\psi}(\frac{\tilde{x}}{k_R})$.

$$g_{1d}|\psi(x)|^2 \to 2\hbar a_B \cdot \mathrm{Hz} \cdot k_R \cdot N\sqrt{\tilde{\omega}_y\tilde{\omega}_z}\tilde{a}_s|\tilde{\psi}|^2$$

- Dimensionless equation,

$$\tilde{k}^2\tilde{\psi} + \frac{\hbar^2 \cdot \mathrm{Hz}^2}{4E_R^2}\tilde{x}^2\tilde{\omega}_x^2\tilde{\psi} + \frac{2\hbar \cdot \mathrm{Hz} \cdot a_B k_R}{E_R} N\sqrt{\tilde{\omega}_y\tilde{\omega}_z}\tilde{a}_s|\tilde{\psi}|^2\tilde{\psi} = i\frac{\hbar}{E_R}\frac{\partial}{\partial t}\tilde{\psi}$$

^{87}Rb: $a_s = 100a_B$, $\omega_y = \omega_z = 2000\mathrm{Hz}$, $g_{1d} \approx 0.004N$.

Characteristic length, $a_0 = \sqrt{\frac{\hbar}{m\omega}}$,

$$(\frac{\hbar\omega_0}{2}\tilde{k}^2 + \frac{\hbar\omega_0}{2}\tilde{x}^2\tilde{\omega}^2 + g_{1d}N|\psi|^2)\psi = i\hbar\omega_0\frac{\partial}{\partial t}\psi$$

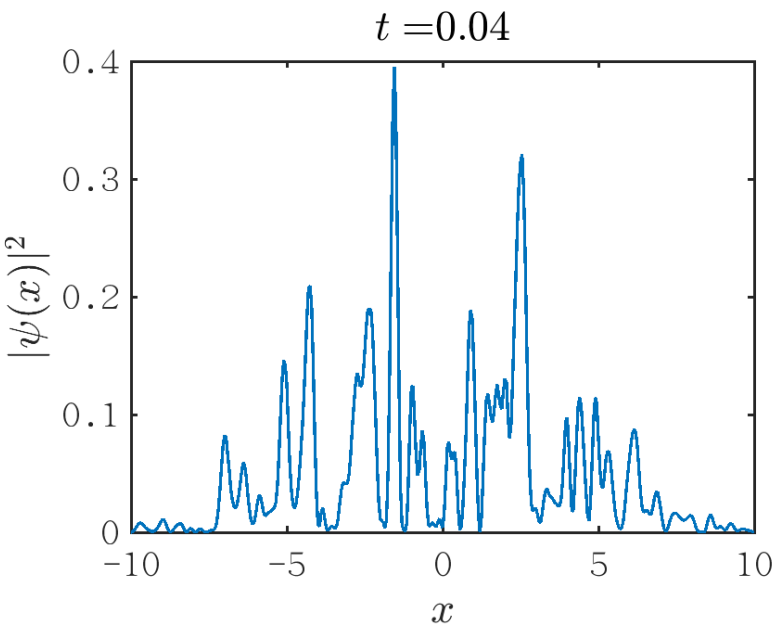
- Interaction,

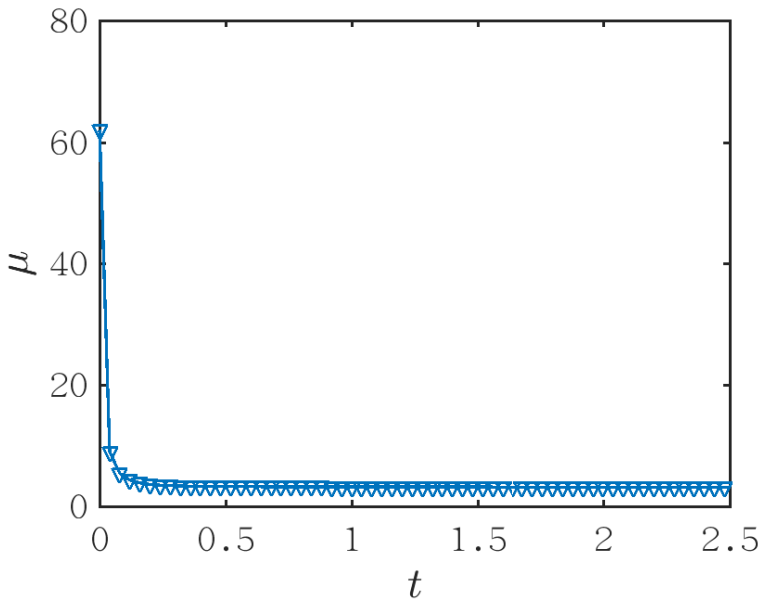
$$\begin{aligned} g_{1d}N|\phi(x)|^2 &= g_{3d}\Big(\int\int dydz|\psi(y)\psi(z)|^4\Big)N|\phi(x)|^2 \\ &= g_{3d}\sqrt{\frac{m^2\omega_z\omega_y}{(2\hbar\pi)^2}}N|\phi(x)|^2 \\ &= 4\tilde{a}_s\hbar\omega\sqrt{\tilde{\omega}_z\tilde{\omega}_y}N|\tilde{\phi}(\tilde{x})|^2 \end{aligned}$$

Dimensionless equation,

$$(\frac{\tilde{k}^2}{2} + \frac{\tilde{x}^2\tilde{\omega}^2}{2} + 4\tilde{a}_s\sqrt{\tilde{\omega}_z\tilde{\omega}_y}N|\tilde{\phi}(\tilde{x})|^2)\psi = i\frac{\partial}{\partial t}\psi$$

$a_s = 100a_B \approx 5.3 \times 10^{-3}\mu\text{m}$

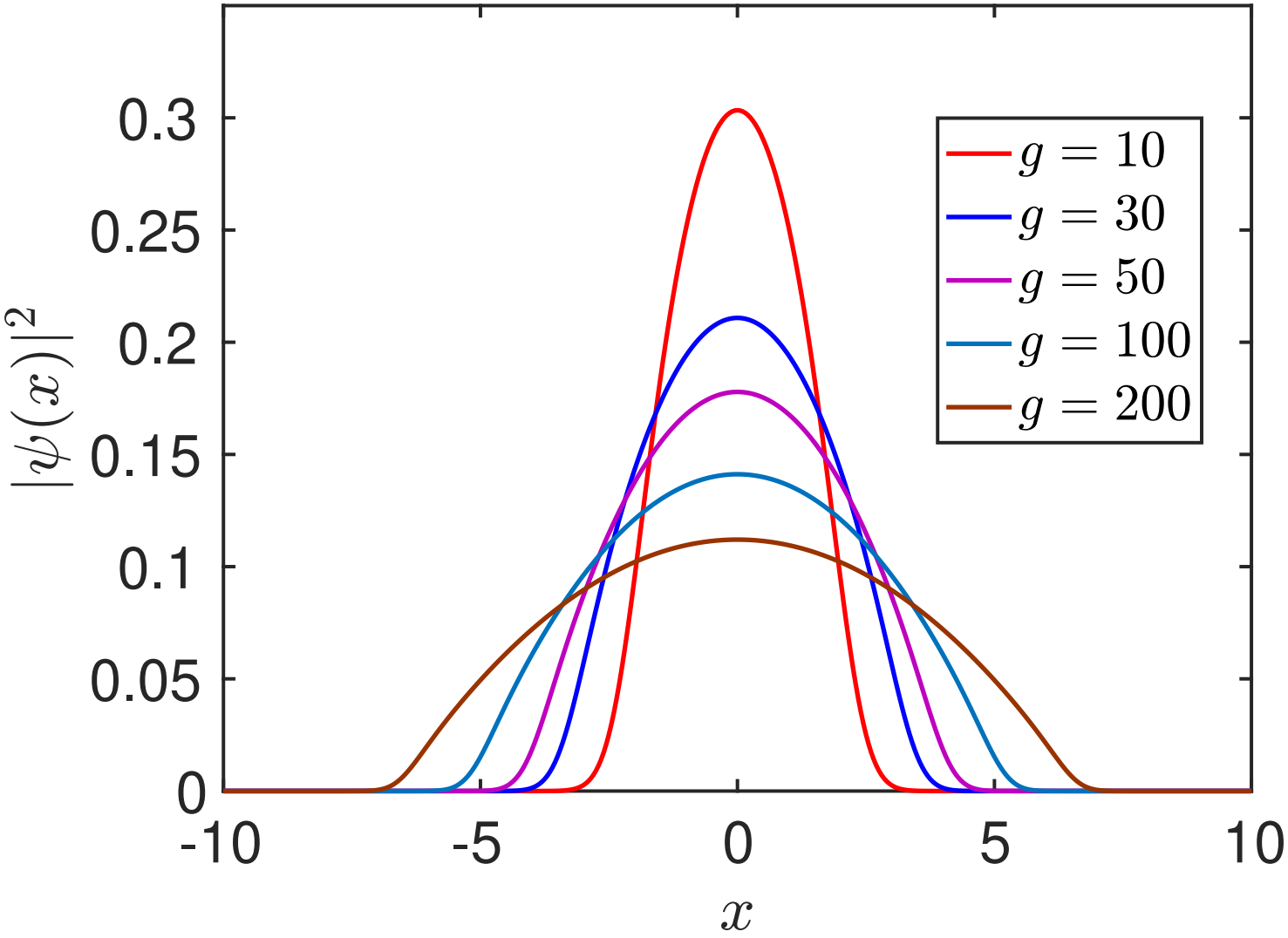




$$dt = 0.04, \quad g = 10.$$

- Evolution of the wave function and chemical potential with $g = 10$.

- Ground state with different interaction coefficient g.



Code

$$\psi(x,t+\Delta t) \approx e^{\frac{-i}{2\hbar}V(x)\Delta t} \cdot \mathcal{F}^{-1}\left[e^{\frac{-i\hbar k^2}{2m}\Delta t} \cdot \mathcal{F}\left[e^{-\frac{i}{2\hbar}U(x)\Delta t} \cdot \psi(x,t)\right]\right]$$

```
tic
M=1.0; %%mass
w=1;    %%trap
g=10; %%interaction
dt=0.04;
t=0:dt:20000;
bound=10;
dx=bound/200;
x=-bound:dx:bound;

nu=0;
accuracy=1.0e-7;
Nx=length(x);

%%%initial wave function
phi0=rand(1,Nx)+1i*rand(1,Nx)-0.5-0.5*1i;
%phi0=exp(rand(1,Nx)+1i*rand(1,Nx)-0.5-0.5*1i);
nor=sum(abs(phi0).^2)*dx;
phi0=phi0/sqrt(nor);
phi_initial=phi0;

dkx=2*pi/((Nx-1)*dx);
kx=-pi/dx:dkx:pi/dx;%Define k-space grid
```

```
chemical_mu=zeros(length(t),1);
%%
Ek=(kx).^2/(2*M);
Uk=exp(-0.5.*Ek.*dt);
Vtrap=0.5*M*x.^2*w.^2;
%%
for it=0:length(t)
    if mod(it,1000)==0
        it
        toc
    end
    Vint=g*abs(phi0).^2;
    V=Vint+Vtrap;
    U=exp(-0.5*V*dt);

    phi1=U.*phi0;       %%%第一步演化
    phi1k=fftshift(fft(phi1)); %%%转到k空间
    phi2k=Uk.*phi1k;       %%%第二步演化
    phi2=ifft(ifftshift(phi2k));    %%%转到实空间
    phi3=U.*phi2;       %%%第三步演化

    mu=-log(abs(sum(conj(phi0).*phi3)*dx))/dt; %%%化学势
    nor=dx*sum(abs(phi3).^2);
    phi3=phi3/(sqrt(nor));

    if abs(mu-nu)<accuracy    %%%%判断精度
        'mu_nu'
        break
    end
    nu=mu;
    chemical_mu(it+1)=mu;
    phi0=phi3;
end
```

Summary

- Gross–Pitaevskii equation
- Split-Step Fourier Method
- Fast Fourier Method
- Dimensionless
- Imaginary Time Method