

Chapter 1

Imaginary-Time Propagation Method

The technique of the imaginary-time propagation method on solving a Schrödinger-like equation is based on the idea of the eigenvalue problem of it while the eigensolutions with higher eigenvalues decay faster in the imaginary time. In the following, we are going to introduce the basic idea and implementation on solving Schrödinger equations for single-particle problems and then implement this technique for a non-linear Schrödinger equation.

1.1 Schrödinger equation

In the quantum mechanics, the motion of a single particle can be described by the Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{x}, t) = \hat{H} \Psi(\mathbf{x}, t), \quad (1.1)$$

where the Hamiltonian of the system is given by

$$\hat{H} = -\frac{\hbar^2 \nabla^2}{2M} + V(\mathbf{r}) \quad (1.2)$$

with the kinetic energy operator and the potential $V(\mathbf{r})$. The time-independent Schrödinger equation is an eigen-value problem of \hat{H} ,

$$\hat{H} \phi_n(\mathbf{r}) = E_n \phi_n(\mathbf{r}) \quad (1.3)$$

where $\phi_n(\mathbf{r})$ is the eigen-wavefunction with n -th eigen-energy E_n . While the Hamiltonian of a single particle is generally hermitian, E_n is real. Therefore, the time evolution of an eigen-wavefunction reads

$$\psi_n(\mathbf{r}, t) = e^{-iE_n t/\hbar} \phi_n(\mathbf{r}). \quad (1.4)$$

while $i\hbar\partial_t\psi_n = \hat{H}\psi_n = E_n\psi_n$.

While the eigen-wavefunction of a Hamiltonian normally forms a complete set, the evolution of an arbitrary wavefunction $\Psi(\mathbf{r}, t)$ can be expanded by the eigen-wavefunction

$$\Psi(\mathbf{r}, t) = \sum_n A_n e^{iE_n t/\hbar} \phi_n(\mathbf{r}) \quad (1.5)$$

with

$$A_n = \langle \phi_n | \Psi \rangle = \int d\mathbf{r} \Psi(\mathbf{r}, t=0) \phi_n^*(\mathbf{r}). \quad (1.6)$$

The bracket notation here would be useful for the following description. Eq. (1.5) gives us a useful direction on finding ϕ_n . The phase of ϕ_n oscillate in time with a frequency E_n/\hbar in Eq. (1.5), and hence higher value of eigenenergy oscillate faster.

By replacing time into an imaginary time, $t \rightarrow -i\tau$, Eq. (1.5) becomes

$$\Psi(\mathbf{r}, \tau) = \sum_n A_n e^{-E_n \tau/\hbar} \phi_n(\mathbf{r}) \quad (1.7)$$

in which all mode of ϕ_n decay or growth in τ with corresponding rate E_n/\hbar for $E_n > 0$ or $E_n < 0$ respectively, except the case of $E_n = 0$ that fixes in time. If we are firstly interested in the lowest eigensolution, labelled as $n = 0$ for convenience, it decays slowest or growth fastest in the imaginary-time evolution. Hence if we re-normalize the wavefunction every time step with step size $\Delta\tau$ or every few of it by

$$\Psi_{m+1}(\mathbf{r}, t_m + \Delta\tau) = \frac{\Psi_m(\mathbf{r}, t_m + \Delta\tau)}{\sqrt{\langle \Psi | \Psi \rangle}} \quad (1.8)$$

with $\langle \Psi | \Psi \rangle = \int d\mathbf{r} |\Psi(\mathbf{r})|^2$; m denotes the number of iteration and $t_m = m\Delta\tau$, the lowest eigenmode, ϕ_0 , becomes the majority occupation of Ψ after sufficient large propagating time, namely,

$$\Psi \rightarrow \phi_0. \quad (1.9)$$

after many iterations of propagation and renormalization. Generally, the iteration of the process should be as much as possible, and it is useful to define the *local error* to examine the goodness of solution at every time step,

$$\delta\mathcal{E}(\mathbf{r}) = \frac{[\hat{H}\Psi(\mathbf{r}) - E\Psi(\mathbf{r})]}{\Psi(\mathbf{r})} \quad (1.10)$$

where

$$E = \langle \Psi | \hat{H} | \Psi \rangle \quad (1.11)$$

and Ψ is normalized already with $\langle \Psi | \Psi \rangle = 1$. For a converged solution, $\delta\mathcal{E}(\mathbf{r}) \sim 0$, and we will obtain the corresponding eigenvalue by Eq. (1.11).

1.2 Modified Imaginary-Time Propagation for Excited States

The imaginary time propagation method is a good way to search the lowest energy solution, and it can be extended to probe the excited states. When we are targeting to the higher excited states, let say the n_{max} -th mode, $\phi_{n_{max}}$, is the final target of the solutions we are interested in, the orthogonality of the eigenbasis provides a way to search them. The projectors, \hat{P}_n , are introduced to truncate the occupations for the modes lower than n_{max} before Ψ is re-normalized in every iteration. The construction of \hat{P}_n requires the solution of ϕ_n with $n < n_{max}$, and hence we can find all the solutions below n_{max} modes step by step when we gradually search to the target. This method has the advantages that when the exact diagonalization is not implementable for the matrix form of \hat{H} being too huge.

In the following, we take $n_{max} = 1$ to explain the detail of the process. The projector for $n = 0$ is defined as

$$\hat{P}_0 = 1 - |0\rangle\langle 0| \quad (1.12)$$

which operates as

$$\hat{P}_0\Psi(\mathbf{r}) = \int d\mathbf{r}' [\delta(\mathbf{r} - \mathbf{r}') - \phi_0(\mathbf{r})\phi_0^*(\mathbf{r}')] \Psi(\mathbf{r}') \quad (1.13)$$

During each iteration, an initial wavefunction is firstly evolved with $\Delta\tau$ and then the projector is applied on it to remove the occupation of ϕ_0 . After the normalization, the one decays slowest in the existed modes is the ϕ_1 , and thus after many iterations, it becomes the largest occupied mode in Ψ while ϕ_0 is projected.

With this, we can then construct $\hat{P}_1 = 1 - |\phi_0\rangle\langle\phi_0|$ for finding ϕ_2 , and so on. Besides, it is indeed useful to check the goodness of the solution by checking Eq. (1.26) for ϕ_n during the iterations.

1.2.1 Application to Quantum Harmonic Oscillators

Quantum harmonic oscillator (HO) in multi-dimensions is already well-studied due to its simplicity and exact solutions. The one-dimensional system is simple, but the problem of degeneracy shows up while the system is in a higher dimension. Therefore, we put both methods to measure the reliability of these two methods in one dimension, and then use imaginary-time propagation to see what problem degeneracy raises in two dimensions.

One-Dimensional Harmonic Oscillator

In one dimension, the dimensionless Schrödinger equation is considered, that

$$i\frac{\partial}{\partial t}\psi = \left[-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2\right]\psi \equiv \hat{H}\psi \quad (1.14)$$

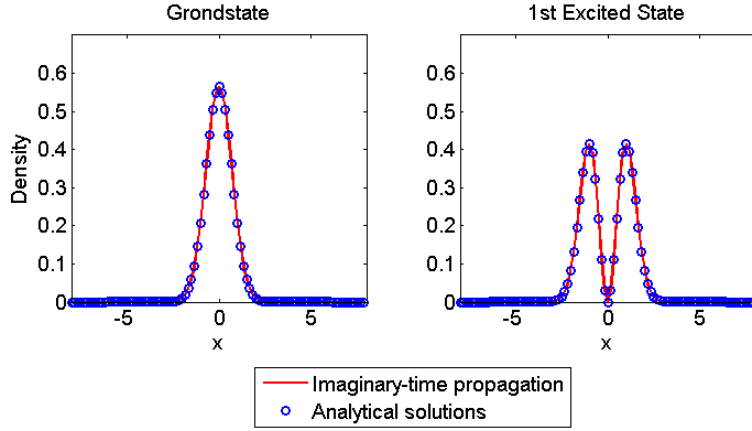


Figure 1.1: The ground state and first 5th excited state of Eq. (1.14) obtained by exact diagonalization.

The exact solution is

$$\phi_n(x) = \frac{\pi^{-1/4}}{\sqrt{2^n n!}} e^{-x^2/2} H_n(x) \quad (1.15)$$

where $H_n(x)$ is the n -th Hermite polynomial and the corresponding energy is $E_n = n + 1/2$.

First we use the exact diagonalization to solve Eq. (1.14) by using plane-wave basis, the results are shown in Figure 1.1. One thing is worth to mention that the more basis you apply to construct the matrix of Hamiltonian, the more precise solution you would get, especially for higher excited state.

Now we put imaginary-time propagation into test, and we only considered to 1st excited state. As shown in Fig. 1.2 (a) and (b), the results once again are perfect match with the analytical solutions of Eq. (1.14).

Two-Dimensional Harmonic Oscillator

In two dimension, the Schrödinger equation is

$$i \frac{\partial}{\partial t} \psi = \left[-\frac{1}{2} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) + \frac{1}{2} (x^2 + y^2) \right] \psi \equiv \hat{H} \psi \quad (1.16)$$

and the n -th solution is

$$\phi_{n_x n_y}(x, y) = \phi_{n_x}(x) \phi_{n_y}(y) \quad (1.17)$$

with the eigen-energy $E_{n_x, n_y} = (n_x + n_y) + 1$ with $n_{x,y} \in \mathbb{Z}$. It is clear that there is a degeneracy of the solutions.

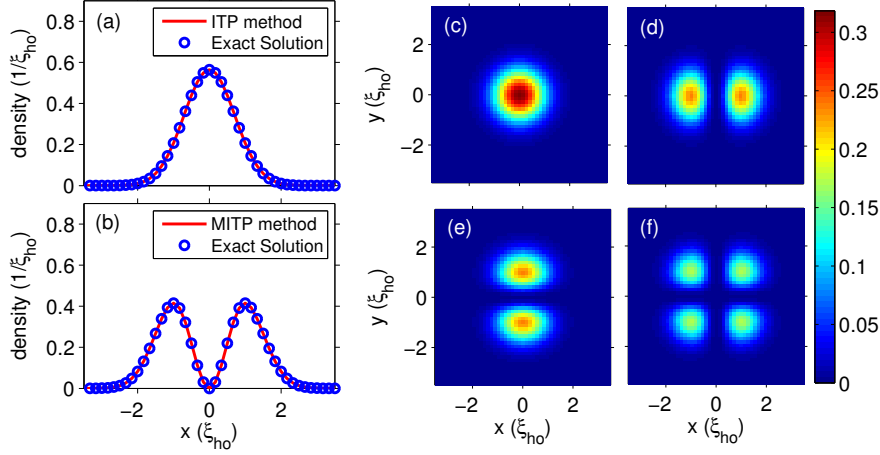


Figure 1.2: (a) and (b) shows the groundstate and first excited state of the one-dimensional quantum harmonic oscillator obtained by the exact diagonalization and the imaginary-time propagation method. (c) to (f) show the ground state and first 3 excited state of Eq. (1.16) obtained by the imaginary-time propagation method.

Fig. 1.2 (c) to (f) plot the numerical results of the ground state and first 3 excited state which are calculated by imaginary-time propagations. There is no noticeable numerical error of the eigen-energies, and clearly the degeneracies of the modes are also well captured.

1.3 Non-linear Schrödinger equation

In the following we are going to solve a nonlinear Schrödinger equation, which corresponds to the well-know Gross-Pitaevskii equation (GPE),

$$i\hbar\partial_t\Psi(\mathbf{r},t) = \left[-\frac{\hbar^2\nabla^2}{2M} + V(\mathbf{r}) + g|\Psi(\mathbf{r},t)|^2 - \mu \right] \Psi(\mathbf{r},t) \quad (1.18)$$

with a non-linear coupling constant g and a Lagrange multiplier μ . The GPE is an equation for Bose-Einstein condensate (BEC) in which Ψ is condensate wavefunction normalized to its particle number and $|\Psi|^2$ is the particle number density rather than the probability density of the system. The particle number and density are determined by g and μ together and of course the profile of Ψ .

In spite of the time-independent form of Eq. (1.18) also gives an eigenvalue problem, the non-linear term in Eq. (1.18) breaks the orthogonality of the eigen-solution and hence the set of solutions is not a complete set anymore. Besides, the nonlinearity also extends the solution for the same μ . For example, in the

homogeneous BEC with $V = 0$, the ground state solution is

$$\Psi = \sqrt{n_0} \quad (1.19)$$

with $n_0 = \mu/g$, but there also exists another stationary solution

$$\Psi(\mathbf{r}) = \sqrt{n_0} \tanh(x/\xi_0) \quad (1.20)$$

with $\xi_0 = \hbar/\sqrt{M\mu}$ in the system and more. Therefore Eq. (1.7) is not perfectly valid for the GPE, but we may still adopt the imaginary-time propagation method on it.

We label the stationary solutions of GPE for a given set of μ and g by Φ_α satisfying

$$\mu\Phi_\alpha(\mathbf{r}) = \left[-\frac{\hbar^2\nabla^2}{2M} + V(\mathbf{r}) + g|\Phi_\alpha(\mathbf{r})|^2 \right] \Phi_\alpha(\mathbf{r}) \quad (1.21)$$

with α labeling the type of solution. Rather than an oscillating global phase of Φ_α , the Lagrange multiplier makes the whole solution stationary in time, namely,

$$\Psi_\alpha(\mathbf{r}, t) = \Phi_\alpha(\mathbf{r}). \quad (1.22)$$

The other solutions of eigen-value higher than μ by Φ_n are written by

$$\mu_n\Phi_n(\mathbf{r}) = \left[-\frac{\hbar^2\nabla^2}{2M} + V(\mathbf{r}) + g|\Phi_n(\mathbf{r})|^2 \right] \Phi_n(\mathbf{r}) \quad (1.23)$$

with $\mu_n > \mu$ and arbitrary Ψ , and its time evolution reads

$$\Psi_n(\mathbf{r}, t) = \Phi_n(\mathbf{r})e^{-i(\mu_n-\mu)t/\hbar} \quad (1.24)$$

Similar to the concept of imaginary-time propagation for a Schrödinger equation discussed in previous sections, the imaginary-time propagation gives the decay of Φ_n in τ with,

$$\Psi_n(\mathbf{r}, t) = \Phi_n(\mathbf{r})e^{-(\mu_n-\mu)\tau/\hbar} \quad (1.25)$$

and only leave the solution of Φ_α remained when $\tau \rightarrow \infty$. The whole evolution can not be simplified to Eq. (1.7) while the non-linearity results complicate dynamics that the eigensolutions are changing in time. Nevertheless, by a properly choose of the initial condition, we may start with an initial condition closed to Φ_α which we are interested in to reaches the numerical solution of Φ_α while the residual of Φ_n will be damped away in imaginary-time evolution. Therefore we have to particularly understand the property of the target state Φ_α , such as the corresponding boundary condition.

During the imaginary-time evolution, the numerical solution should also be examined by the local error

$$\delta\mathcal{E}(\mathbf{r}, \tau) = \frac{[\hat{\mathcal{L}}_{GP}\Psi(\mathbf{r}, \tau) - \mu\Psi(\mathbf{r})]}{\Psi(\mathbf{r}, \tau)} \quad (1.26)$$

where

$$\hat{\mathcal{L}}_{GP} = \hat{\mathcal{L}}_{GP}[\Psi(\mathbf{r})] = \left[-\frac{\hbar^2 \nabla^2}{2M} + V(\mathbf{r}) + g |\Psi(\mathbf{r})|^2 \right] \quad (1.27)$$

and the error of the temporal chemical potential $\Delta\mu \equiv \mu' - \mu$ with

$$\mu(\tau)' = \int d\mathbf{r} \Psi^*(\mathbf{r}, \tau) \hat{\mathcal{L}}_{GP} \Psi(\mathbf{r}, \tau). \quad (1.28)$$

When Ψ is sufficiently closed to Φ_α for sufficiently long imaginary-time evolution, $\delta\mathcal{E}(\mathbf{r}, \tau) \sim 0$ and $\Delta\mu(\tau) \sim 0$.

In some case, the normalization of the wavefunction would be requested to be fixed, and μ can be changed during the imaginary-time evolution by

$$\mu(\tau + \Delta\tau) = \frac{\mu(\tau)}{\int d\mathbf{r} \Psi^*(\mathbf{r}, \tau) \Psi(\mathbf{r}, \tau)}. \quad (1.29)$$

This will allow one to probe the target normalization but, while every time step of the evolution the solution is evolved in different directions of the imaginary-time, it would normally take a longer time to converge.

Furthermore, it is also worth to check the eigenvalue and eigen-solution of the effective Hamiltonian after the imaginary-time propagation via exact diagonalization,

$$\hat{\mathcal{L}}_{GP}[\Psi(\mathbf{r})] \phi_n = E \phi_n, \quad (1.30)$$

in which the criteria must be satisfied

$$\phi_0 = \Phi_\alpha \quad (1.31)$$

and

$$\langle \phi_n | \Phi_\alpha \rangle = 0 \text{ for } n > 0, \quad (1.32)$$

otherwise, the propagating time is not long enough. The correct outcome can be regarded as the GPE eigenbasis and is very useful for computing Bogoliubov-de-Gennes equation with spectrum method which may requires high accuracy of the solution. For a accurate solution, Eq. (1.26) should reach numerical limit, the order of 10^{-15} , and fluctuate in space.

It is important to note that the normalization is set by μ , g and Φ_α . Hence we should NOT implement Eq. (1.8) during the imaginary-time evolution. The normalization breaks Eq. (1.30) and the corresponding solution does not satisfy Eq. (1.31).

There are also other methods on solving Φ_α , such as conjugate gradient method and the Newton method. The latter one is useful in searching many kinds of Φ_α while the former is also a kind of imaginary-time propagation.

1.4 Two-component condensate

The two-component GPE is written by

$$i\hbar\partial_t\Psi_j = \left[-\frac{\hbar^2\nabla^2}{2M_j} + V_j(\mathbf{r}) + g_{jj}|\Psi_j|^2 + g_{j,3-j}|\Psi_{3-j}|^2 - \mu_j \right] \Psi_j(\mathbf{r}) \quad (1.33)$$

where $j = 1, 2$ denotes the j -th component. The coupled equations for Ψ_j would lead a complexity on determine the chemical potentials, and hence in this note we consider the case that each componetn has a fixed particle number N_j . It is convenience to write the wavefunctions by

$$\Psi_j = \sqrt{N_j}\psi_j(\mathbf{r}) \quad (1.34)$$

with the normalized ψ_j ,

$$\int d\mathbf{r}|\psi_j|^2 \approx 1 \quad (1.35)$$

in the following self-consistent imaginary-time propagation. The GPEs becomes

$$i\hbar\partial_t\psi_j = \left[-\frac{\hbar^2\nabla^2}{2M_j} + V_j(\mathbf{r}) + g'_{jj}|\psi_j|^2 + g'_{j,3-j}|\psi_{3-j}|^2 - \mu_j \right] \psi_j(\mathbf{r}) \quad (1.36)$$

where

$$g'_{jk} = g_{jk}N_k. \quad (1.37)$$

Similar to the single-component case, we solve Eq. (1.36) with imaginary time propagation method with self-consistent determination μ_j ,

$$\mu_j(\tau + \Delta\tau) = \frac{\mu_j(\tau)}{\int d\mathbf{r}\psi_j^*(\mathbf{r}, \tau)\psi_j(\mathbf{r}, \tau)}. \quad (1.38)$$