Study miscible and immiscible in the two species BEC

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Outline

1. Overviews of Bose-Einstein Condensation
   - Properties of Bose-Einstein Condensation
   - Derivative Gross–Pitaevskii equation
     - Low energy scatter theory
     - Partial wave method
     - Pseudo potential
     - Meanfield Theory
     - Variational principle

2. Two species atom of coupled GP equation
   - Dimensionless coupled GP equation
   - Time evolution of coupled GP equations
     - Real time evolution
     - Imaginary time evolution

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Diluted Bose gas I

In the GP equation, it describes diluted bose gas, Let us recap the definition of diluted gas.

1. weak interaction between the atoms.
2. the thermal wavelength is larger than the effective interaction distance.
3. the density of the atom is low.

Because the thermal wavelength is larger than the interaction distance, we consider the two bodies interaction as low energy scatter, then using the S wave theory in quantum scattering to describe the properties diluted gas system.

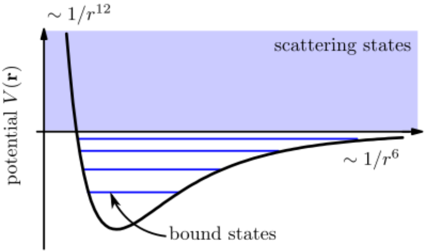


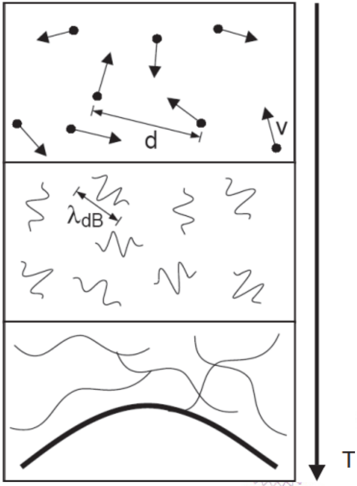
Figure: Lennard-Jones potential

$$\lambda_{dB} = \sqrt{\frac{2\pi\hbar^2}{mk_b T}} \tag{1}$$

$$V_{L-J}(r) = (\frac{A}{r})^{12} - (\frac{B}{r})^{6} \tag{2}$$

Diluted Bose gas II

1. At temperatures $\geq T_c$ (top), the separation d between particles is much greater than their size and atoms can be treated as point particles.
2. As the sample is cooled (middle), the wave nature of the particles becomes more apparent. At $T \approx T_c$,
3. and a condensate forms (bottom).



Low energy scatter theory

Let us consider a two-body system with interaction, we use the center of mass and relative coordinate to describe the Hamiltonian:

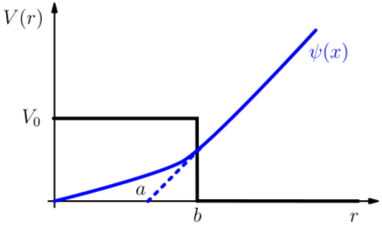
$$\hat{H} = \frac{\hat{\vec{p}}_1^2}{2m_1} + \frac{\hat{\vec{p}}_2^2}{2m_2} + V(|\vec{r}_1 - \vec{r}_2|) = \frac{\vec{p}_{cm}^2}{2M} + \frac{\vec{p}_{rel}^2}{2m_\mu} + V(|\vec{r}_{rel}|) \tag{3}$$

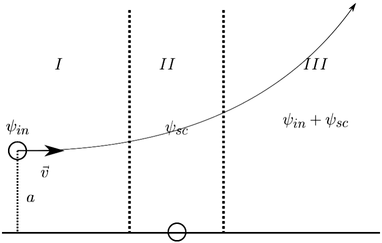
where $\hat{\vec{p}}_\alpha$, $\vec{r}_\alpha$ $(\alpha = 1, 2)$ are momentum and position on the lab frame. $M = m_1 + m_2$ is total mass, $m_\mu = \frac{m_1 m_2}{m_1 + m_2}$ is reduced mass. $\hat{\vec{p}}_\beta$, $\vec{r}_{rel}$ $(\beta = cm, rel)$ is momentum and position in central or relative coordinate. After coordinate transform, the stationary equation is $\hat{H}\Psi(\vec{r}_{cm}, \vec{r}_{rel}) = E\Psi(\vec{r}_{cm}, \vec{r}_\beta)$ we can do the separation variables on $\Psi(\vec{r}_{cm}, \vec{r}_{rel}) = \phi(\vec{r}_{cm})\psi(\vec{r}_{rel})$. Hence, we treat the two-body problems to simplify to a single particle on the potential problem. where $E = E_{rel} + E_{cm}$.

$$\left[\frac{\vec{p}_{rel}^2}{2m_\mu} + V(|\vec{r}_{rel}|)\right]\psi(\vec{r}_{rel}) = E_{rel}\psi(\vec{r}_{rel}) \tag{4a}$$

$$\left[\frac{\vec{p}_{cm}^2}{2M}\right]\phi(\vec{r}_{cm}) = E_{cm}\phi(\vec{r}_{cm}) \tag{4b}$$

Partial wave in low energy scatter theory I





1. we reduce the scattering amplitude to a single number with the scattering length: $\lim_{\vec{k}\to 0} f(\vec{k}, \vec{r}) = -a$.
2. In Region II, we use the spherical harmonic (l=0, s wave) function expand wave function: $\psi_{\vec{r}} \approx Y_{0,0} R(\vec{r})$, where $R(\vec{r}) = u_k(\vec{r})/r$.

Figure: scattering process. In region I(incident region), we set the matter wave like a plane wave, it is described by $\psi_{in} = e^{i\vec{p}\cdot\vec{r}}$. In region II(scattering region), two-particle is scattering, and the scattering wave (spherical wave) is given by $\psi_{sc} = f(\vec{k}, \vec{r})\frac{e^{i\vec{p}\cdot\vec{r}}}{r}$. In region III (after scattering), it is a superposition of the $\psi_{in} + \psi_{sc}$.

Partial wave in low energy scatter theory II

The radius part is given by

$$\left[\frac{\partial^2}{\partial r^2} + k^2 - \frac{2m_\mu V(r)}{\hbar^2}\right] u_k(r) = 0 \tag{5}$$

In the following, we are solving the equation for the two kind of potentials to approach further insight into the Lennard-Jones potential. The only constraint is that the $u_k(r)$ must be vanished on $r \to 0$ because of $V_{LJ}(r \to 0) \to \infty$.

$$V_{barrier}(x) = \begin{cases} V_0 > 0, & r < b, \\ 0, & r > b. \end{cases} \quad V_{well}(x) = \begin{cases} -V_0 < 0, & r < b, \\ 0, & r > b. \end{cases} \tag{6}$$

Solving partial wave I

1. $r > b, k \to 0 : \partial_r^2 u(r) = 0$, then $u(r) = \chi(r - a)$ in the barrier potential.
2. $r < b, k \to 0 : \partial_r^2 u(r) = \kappa^2 u(r)$, where $\kappa^2 = 2mV_0/\hbar^2$ then $u(r) = \xi \sinh(\kappa r)$ in the barrier potential. we take the odd function because of $u_k(r \to 0) \to 0$.
3. Makes the wave function smoothly at the connection point. it means $u(k = r_l) = u(r = b_r)$ and $u'(r = b_l) = u'(r = b_r)$. This condition leads to $a = b - \tanh(\kappa b)/\kappa$.

1. $r > b, k \to 0 : \partial_r^2 u(r) = 0$, then $u(r) = \chi(r - a)$ in the well potential.
2. $r < b, k \to 0 :$ $\partial_r^2 u(r) = -\kappa^2 u(r)$, where $\kappa^2 = 2mV_0/\hbar^2$ then $u(r) = \xi \sin(\kappa r)$ in the well potential. we take the odd function because of $u_k(r \to 0) \to 0$.
3. Makes the wave function smoothly at the connection point. it means $u(k = r_l) = u(r = b_r)$ and $u'(r = b_l) = u'(r = b_r)$. This condition lead to $a = b - \tan(\kappa b)/\kappa$.

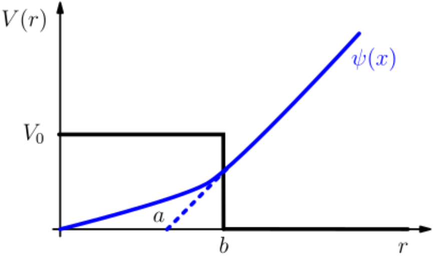


Figure: Repulsive potential lead to the positive value of the scattering length *a*. We can see that the small potential depth κ, *a* tends to zero. i.g: if V_0 is zero, then two-particle is not interaction so *a* must be zero.

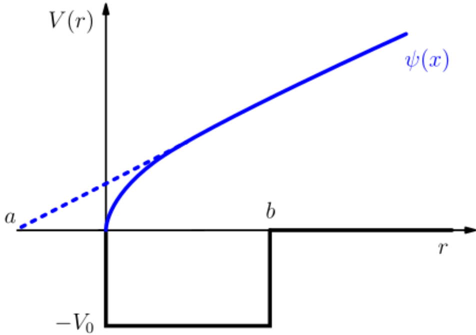


Figure: Attractive potential makes the negative value of scattering length *a*. The *a* is smaller than 0 in this case.

Solving partial wave III

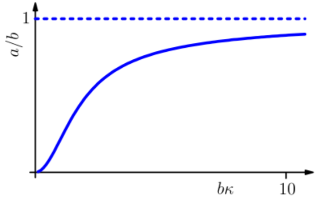


Figure: Evolution of the scattering length a of a repulsive barrier potential as a function of the depth κ by fixing b. In this case, the scattering length is an increasing function.

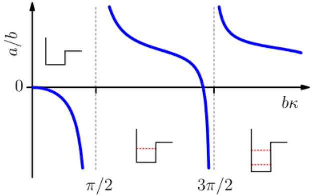


Figure: Evolution of the scattering length a of an attractive barrier potential as a function of the depth κ by fixing b. There is some interesting points that we figure out. One is $b\kappa = \pi/2$, the a goes through a resonance such that the value of a from $-\infty$ to ∞, the other is each point of $b\kappa = (n + 1/2)\pi$, a new bound state will be added in the square well. Now we know a can be positive (repulsive) and negative(attractive) in attractive potential, depending on the how depth of the attractive potential.

Pseudo potential I

In BEC problem, we don't need to deal with the L-J potential because the L-J potential can give the crystal structure, there is no crystal structure in the BEC system, the better way is that use a pseudo potential to approximate the L-J potential to avoid the crystal structure. We construct the pseudo potential $V_p(r)$ with the same scattering length a as the L-J potential $V_{L-J}(r)$. We deal with the scattering problem so we ignore the bound state part in the $V_{L-J}(r)$. In the repulsive barrier potential, we have the scattering solution at region $r \in (b, \infty)$:

$$u(r) = \chi(r - a) \rightarrow R(r) = \chi(1 - a/r) \tag{7}$$

We hope the pseudo potential exist the property $V_p(r) = p\delta(r)$ because of $V_{L-J}(r \rightarrow 0) = \infty$, where p is function of scattering length a. How do we find the radius part of wave function exact form? we use the following trick:

Pseudo potential II

$$\partial_r u(r) = \partial_r(rR(r)) = \chi, \quad \nabla^2(1/r) = -4\pi\delta(r) \tag{8}$$

We plug (7) of $R(r)$ in the Schrodinger equation of radius part:

$$\nabla^2 R(r) = 4\pi a\chi\delta(r) = 4\pi a\delta(r)\partial_r(rR(r)) \tag{9}$$

We count the left of (9) the result is $\nabla^2 R(r) = u''(r)/r$ and right part $4\pi a\delta(r)\partial_r u(r)$, then the (9) can be rewritten as:

$$u''(r) - 4\pi ar\delta(r)\partial_r u(r) = 0 \tag{10}$$

Using the $r\partial_r u(r) = r\chi \approx (\partial_r r)u_r = \chi(r-a)$, where $r \in (b, +\infty), b \gg a$

$$\left[\partial_r^2 - 4\pi a\delta(r)\right] u(r) = 0 \tag{11}$$

Compare (11) with (5) at $k \to 0$, we have $V_p(r) = \frac{4\pi\hbar^2 a}{2m_\mu}\delta(r)$.

Meanfield Theory I

We defined the single particle state $\phi_{k_i}(\vec{r}_i)$ with the normalization condition: $\int |\phi_{k_i}(\vec{r}_i)|^2 \, d^3 r_i = 1$, we use the Hatree Fork approximation to describe the BEC system with the Hamiltonian:

$$\hat{H} = \sum_{i=1}^{N} \frac{\vec{p}_i^2}{2m_i} + V(\vec{r}_i) + U_0 \sum_{i<j}^{N} \delta(\vec{r}_i - \vec{r}_j) \tag{12}$$

where $U_0 = \frac{4\pi\hbar^2 a}{2m_\mu}$, obviously, we need create a many-body ground wave function by the tensor product state with single body wave function.

$$\Psi(\vec{r}_1, \vec{r}_2 ... \vec{r}_N) = \Pi_{i=1}^{N} \phi(\vec{r}_i) \tag{13}$$

The many-body wave function also respect to the normalization condition: $\int |\Psi(\vec{r}_1, \vec{r}_2 ... \vec{r}_N)|^2 d\vec{r}_1 ... d\vec{r}_N = N$. We assume that the ground state wave function can be replaced by
$\Psi(\vec{r}_1, \vec{r}_2 ... \vec{r}_N) = \sqrt{N} \Pi_{i=1}^{N} \phi(\vec{r}_i) = \sqrt{N} \phi(\vec{R})$.

Meanfield Theory II

$$
\begin{aligned}
E =\ & N\sum_{i=1}^{N}\Pi_{q=1}^{N}\int d^3r_q\phi^*(\vec{r}_q)\left[\frac{\vec{p}_i^2}{2m_i}+V(\vec{r}_i)\right]\phi(\vec{r}_q)\\
&+N^2U_0\Pi_{n=1}^{N}\Pi_{m=1}^{N}\sum_{i<j}^{N}\int\int d^3r_nd^3r_m\phi^*(\vec{r}_n)\phi^*(\vec{r}_m)\delta(\vec{r}_i-\vec{r}_j)\phi(\vec{r}_n)\phi(\vec{r}_m)\\
=\ & N\Pi_{q=1}^{N}\int d^3r_q\phi^*(\vec{r}_q)\left[\frac{\vec{p}_q^2}{2m_q}+V(\vec{r}_q)\right]\phi(\vec{r}_q)\\
&+\frac{1}{2}N^2\sum_{i\neq j}^{N}\sum_{j\neq i}^{N}\Pi_{n=1}^{N}\Pi_{m=1}^{N}\int\int d^3r_nd^3r_m\phi^*(\vec{r}_n)\phi^*(\vec{r}_m)\delta(\vec{r}_i-\vec{r}_j)\phi(\vec{r}_n)\phi(\vec{r}_m)\\
=\ & N\Pi_{q=1}^{N}\int d^3r_q\phi^*(\vec{r}_q)\left[\frac{\vec{p}_q^2}{2m_q}+V(\vec{r}_q)\right]\phi(\vec{r}_q)\\
&+\frac{1}{2}N^2\Pi_{n=1}^{N}\Pi_{m=1}^{N}\int\int d^3r_nd^3r_m\phi^*(\vec{r}_n)\phi^*(\vec{r}_m)\delta(\vec{r}_n-\vec{r}_m)\phi(\vec{r}_n)\phi(\vec{r}_m)\\
=\ & N\Pi_{q=1}^{N}\int d^3r_q\phi^*(\vec{r}_q)\left[\frac{\vec{p}_q^2}{2m_q}+V(\vec{r}_q)\right]\phi(\vec{r}_q)+\frac{1}{2}N^2\Pi_{n=1}^{N}\int d^3r_n\phi^*(\vec{r}_n)\phi^*(\vec{r}_n)\phi(\vec{r}_n)\phi(\vec{r}_n)\\
=\ & N\Pi_{q=1}^{N}\int d^3r_q\left[\frac{\hbar^2}{2m_q}\left[\nabla_q\phi(\vec{r}_q)\right]^2+V(\vec{r}_q)\left[\phi(\vec{r}_q)\right]^2+\frac{1}{2}NU_0\left[\phi(\vec{r}_q)\right]^4\right]\\
=\ & N\int d^3R\left[\frac{\hbar^2}{2m}\left[\nabla\phi(\vec{R})\right]^2+V(\vec{R})\left[\phi(\vec{R})\right]^2+\frac{1}{2}NU_0\left[\phi(\vec{R})\right]^4\right]
\end{aligned}
\tag{14}
$$

Meanfield Theory III

In last two equations of (14), the $\phi(\vec{r_q}) = \phi(\vec{r_n})$ because the position r_q, r_n is dummy variables in the meanfield approximation, we can remove the subscripts q.
Once we have the Engergy function, doing the Variation method on this functional to find the equation of motion. This method also called minimizing energy functional, it satisfy the equilibrium state in theomodynamics. I give a time-independent case with the constraint : $\int d^3R \left|\phi(\vec{R})\right|^2 = 1$, then the total functional:

$$X(\phi^*, \phi) = E(\phi^*, \phi) - \mu N \int d^3R \left|\phi(\vec{R})\right|^2 \tag{15}$$

where μ is Lagrangian multiplier(chemical potential). we treat $\delta X = 0$ with two independent variables ϕ and ϕ^*.

Gross–Pitaevskii equation I

For the convenience of calculation, we replace $\left[\frac{\vec{R}^2}{2m} + V(\vec{R})\right]$ to H_s Now we find the δX:

$$\delta X = N \int d^3R \left(\delta\phi^*(H_s - \mu)\phi + \phi^*(H_s - \mu)\delta\phi + NU_0(|\phi|^2 \phi\delta\phi + |\phi^*|^2 \phi\delta\phi^*)\right) = 0 \tag{16}$$

Then we have complex conjugate equations of motion:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{R}) + NU_0 |\phi(\vec{r})|^2\right] \phi(\vec{R}) = \mu\phi(\vec{R}) \tag{17a}$$

$$\phi^*(\vec{R}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{R}) + NU_0 \left|\phi(\vec{R})\right|^2\right] = \phi^*(\vec{R})\mu \tag{17b}$$

Gross–Pitaevskii equation II

Let us consider the time-dependent $\phi(R,t)$, We know the schrodinger equation of many body system as:

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r}_1,\vec{r}_2...\vec{r}_N,t)=\hat{H}\Psi(\vec{r}_1,\vec{r}_2...\vec{r}_N,t) \tag{18}$$

Then, we construct the Lagrangian density functional as:

$$\mathcal{L}=\Psi^*(i\hbar\frac{\partial}{\partial t}-\hat{H})\Psi^* \tag{19}$$

The full form of Lagrangian density is :

$$\mathcal{L}=\phi^*(i\hbar\frac{\partial}{\partial t}-H_s-\frac{1}{2}NU_0\left|\phi\right|^2)\phi^* \tag{20}$$

This Lagrangian density lead to equation of motion is given by

$$i\hbar\frac{\partial}{\partial t}\phi=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\vec{r})+NU_0\left|\phi(\vec{R})\right|^2\right]\phi(\vec{R}) \tag{21}$$

Now, we need to deal with the two species (A and B) coupled GP equations, We can write down total Hamiltonian intuitively.

$$
\begin{aligned}
\hat{H} = \sum_{i=1}^{N_A} \frac{\vec{p}_{i,A}^{2}}{2m_i} + V_A(\vec{r}_{i,A}) + U_A \sum_{i<j}^{N_A} \delta(\vec{r}_{i,A} - \vec{r}_{j,A}) \\
+ \sum_{k=1}^{N_B} \frac{\vec{p}_{i,B}^{2}}{2m_{k,B}} + V_B(\vec{r}_{k,B}) + U_B \sum_{k<l}^{N_B} \delta(\vec{r}_{k,B} - \vec{r}_{l,B}) + U_{AB} \sum_{i<k}^{N_A,N_B} \delta(\vec{r}_{i,A} - \vec{r}_{k,B})
\end{aligned}
\tag{22}
$$

where $U_\alpha = \frac{4\pi\hbar^2 a_\alpha}{2m_{\mu,\alpha}}, \alpha = A, B, AB$. We just do the variational method on the Hamiltonian (22) with two constraints: $\int d^3R_\alpha \left|\phi(\vec{R}_\alpha)\right|^2 = 1$ where $\alpha = A, B$. then we have coupled GP equations:

$$
\left[-\frac{\hbar^2}{2m_A}\nabla_A^2 + V_A(\vec{R}) + N_A U_A \left|\phi_A(\vec{R})\right|^2 + N_B U_{AB} \left|\phi_B(\vec{r})\right|^2\right] \phi_A(\vec{r}) = \mu_A \phi_A(\vec{R}) \tag{23a}
$$

$$
\left[-\frac{\hbar^2}{2m_B}\nabla_B^2 + V_B(\vec{R}) + N_B U_B \left|\phi_B(\vec{R})\right|^2 + N_A U_{AB} \left|\phi_A(\vec{R})\right|^2\right] \phi_B(\vec{R}) = \mu_B \phi_B(\vec{R}) \tag{23b}
$$

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Two species GP equation

For two spices coupled GP equation in cylindrical coordinate:

$$\left[\frac{\hbar^2}{2m_A}\nabla_A^2 + \frac{1}{2}m_A(\omega_{A,r}^2 r^2 + \omega_{A,z}^2 z^2) + \frac{4\pi\hbar^2 a_A N_A}{m_A}|\psi_A(r,z)|^2 + \frac{m_A+m_B}{m_A m_B}2\pi\hbar^2 a_{AB} N_B|\psi_B(r,z)|^2\right]\psi_A(r,z) = \mathbf{i}\hbar\frac{\partial}{\partial t}\psi_A(r,z) \tag{24a}$$

$$\left[\frac{\hbar^2}{2m_B}\nabla_B^2 + \frac{1}{2}m_B(\omega_{B,r}^2 r^2 + \omega_{B,z}^2 z^2) + \frac{4\pi\hbar^2 a_B N_B}{m_B}|\psi_B(r,z)|^2 + \frac{m_A+m_B}{m_A m_B}2\pi\hbar^2 a_{AB} N_A|\psi_A(r,z)|^2\right]\psi_B(r,z) = \mathbf{i}\hbar\frac{\partial}{\partial t}\psi_B(r,z) \tag{24b}$$

We need to find the ground state of these coupled differential equations. Let us remove the unit(dimension) first. For detail, I will show it step by step.

- Remove the energy dimension by divided by $\hbar\omega_{A,r}$ in (24a) and (24b)

Two species GP equation

For two spices coupled GP equation in cylindrical coordinate:

$$\left[\frac{\hbar^2}{2m_A}\nabla_A^2 + \frac{1}{2}m_A(\omega_{A,r}^2 r^2 + \omega_{A,z}^2 z^2) + \frac{4\pi\hbar^2 a_A N_A}{m_A}|\psi_A(r,z)|^2 + \frac{m_A+m_B}{m_A m_B}2\pi\hbar^2 a_{AB} N_B|\psi_B(r,z)|^2\right]\psi_A(r,z) = \mathbf{i}\hbar\frac{\partial}{\partial t}\psi_A(r,z) \tag{24a}$$

$$\left[\frac{\hbar^2}{2m_B}\nabla_B^2 + \frac{1}{2}m_B(\omega_{B,r}^2 r^2 + \omega_{B,z}^2 z^2) + \frac{4\pi\hbar^2 a_B N_B}{m_B}|\psi_B(r,z)|^2 + \frac{m_A+m_B}{m_A m_B}2\pi\hbar^2 a_{AB} N_A|\psi_A(r,z)|^2\right]\psi_B(r,z) = \mathbf{i}\hbar\frac{\partial}{\partial t}\psi_B(r,z) \tag{24b}$$

We need to find the ground state of these coupled differential equations. Let us remove the unit(dimension) first. For detail, I will show it step by step.

- Remove the energy dimension by divided by $\hbar\omega_{A,r}$ in (24a) and (24b)
- Setting the unit length : $\frac{\hbar}{2m_A\omega_{A,r}} := l^2$ to remove dimension of a_A, a_B, a_{AB} and ψ_i

Two species GP equation

For two spices coupled GP equation in cylindrical coordinate:

$$\left[\frac{\hbar^2}{2m_A}\nabla_A^2 + \frac{1}{2}m_A(\omega_{A,r}^2 r^2 + \omega_{A,z}^2 z^2) + \frac{4\pi\hbar^2 a_A N_A}{m_A}|\psi_A(r,z)|^2 + \frac{m_A+m_B}{m_A m_B}2\pi\hbar^2 a_{AB} N_B |\psi_B(r,z)|^2\right]\psi_A(r,z) = \mathbf{i}\hbar\frac{\partial}{\partial t}\psi_A(r,z) \tag{24a}$$

$$\left[\frac{\hbar^2}{2m_B}\nabla_B^2 + \frac{1}{2}m_B(\omega_{B,r}^2 r^2 + \omega_{B,z}^2 z^2) + \frac{4\pi\hbar^2 a_B N_B}{m_B}|\psi_B(r,z)|^2 + \frac{m_A+m_B}{m_A m_B}2\pi\hbar^2 a_{AB} N_A |\psi_A(r,z)|^2\right]\psi_B(r,z) = \mathbf{i}\hbar\frac{\partial}{\partial t}\psi_B(r,z) \tag{24b}$$

We need to find the ground state of these coupled differential equations. Let us remove the unit(dimension) first. For detail, I will show it step by step.

- Remove the energy dimension by divided by $\hbar\omega_{A,r}$ in (24a) and (24b)
- Setting the unit length : $\frac{\hbar}{2m_A\omega_{A,r}} := l^2$ to remove dimension of a_A, a_B, a_{AB} and ψ_i
- define the dimensionless constants κ_i, λ_i, G_i and $G_{i,j}$ to get the dimensionless coupled equations of (24a) and (24b).

Remove dimension of coupled GP equations

$$\left[\frac{\hbar}{2m_A\omega_{A,r}}\nabla_A^2+\frac{1}{2}m_A(\frac{\omega_{A,r}}{\hbar}r^2+\frac{\omega_{A,z}^2}{\hbar\omega_{A,r}}z^2)+\frac{4\pi\hbar a_A N_A}{m_A\omega_{A,r}}|\psi_A(r,z)|^2+\frac{m_A+m_B}{m_A m_B\omega_{A,r}}2\pi\hbar a_{AB}N_B|\psi_B(r,z)|^2\right]\psi_A(r,z)=\mathbf{i}\frac{\partial}{\omega_{A,r}\partial t}\psi_A(r,z) \tag{25a}$$

$$\left[\frac{\hbar m_A}{2m_B m_A\omega_{A,r}}\nabla_B^2+\frac{1}{2}m_B(\frac{\omega_{B,r}^2}{\hbar\omega_{A,r}}r^2+\frac{\omega_{B,z}^2}{\hbar\omega_{A,r}}z^2)+\frac{4\pi\hbar a_B N_B}{m_B\omega_{A,r}}|\psi_B(r,z)|^2+\frac{m_A+m_B}{m_A m_B\omega_{A,r}}2\pi\hbar a_{AB}N_A|\psi_A(r,z)|^2\right]\psi_B(r,z)=\mathbf{i}\frac{\partial}{\omega_{A,r}\partial t}\psi_B(r,z) \tag{25b}$$

Setting $\frac{\hbar}{2m_A\omega_{A,r}} := l^2$, then the coupled equations will be dimensionless. I list these dimensionless variables: $l^{-1}r=\bar{r}$, $z^{-1}z=\bar{z}$, $l^{-1}a_i=\bar{a}_i$, $l^{-1}a_{ij}=\bar{a}_{ij}$, $\omega_{1,r}t=\bar{t}$, $l^{3/2}\psi(r,z)=\bar{\psi}(\bar{r},\bar{z})$.
Defining the dimensionless coefficents: $k_1=\frac{m_A}{m_B}$, $k_2=\frac{m_B}{m_A}$, $k_3=k_1\bar{a}_B$, $k_4=\bar{a}_{AB}(k_1+1)$, $\kappa_1=1$, $\lambda_1=\frac{\omega_{A,z}^2}{\omega_{A,r}^2}$, $\kappa_2=\frac{\omega_{B,r}^2}{\omega_{A,r}^2}$, $\lambda_2=\frac{\omega_{B,z}^2}{\omega_{A,r}^2}$, $G_A=8\pi\bar{a}_A$, $G_{AB}=8\pi k_4$, $G_B=8\pi k_3$. And then we can get the coupled dimensionless GP equations.

Remove dimension of coupled GP equations

$$\left[\bar{\nabla}_A^2 + \frac{1}{4}(\kappa_1\bar{r}^2 + \lambda_1\bar{z}^2) + N_A G_A|\bar{\psi}_A(\bar{r},\bar{z})|^2 + N_B G_{AB}|\bar{\psi}_B(\bar{r},\bar{z})|^2\right]\bar{\psi}_A(\bar{r},\bar{z}) = \mathbf{i}\frac{\partial}{\partial\bar{t}}\bar{\psi}_A(\bar{r},\bar{z}) \tag{26a}$$

$$\left[k_1\bar{\nabla}_B^2 + \frac{1}{4}k_2(\kappa_2\bar{r}^2 + \lambda_2\bar{z}^2) + N_B G_B|\bar{\psi}_B(\bar{r},\bar{z})|^2 + N_A G_{AB}|\bar{\psi}_A(\bar{r},\bar{z})|^2\right]\psi_B(r,z) = \mathbf{i}\frac{\partial}{\partial\bar{t}}\bar{\psi}_B(\bar{r},\bar{z}) \tag{26b}$$

with the normalization conditions:

$$2\pi\int_{-\infty}^{\infty}\bar{r}|\bar{\psi}_A(\bar{r},\bar{z})|^2 d\bar{r}d\bar{z} \tag{27a}$$

$$2\pi\int_{-\infty}^{\infty}\bar{r}|\bar{\psi}_B(\bar{r},\bar{z})|^2 d\bar{r}d\bar{z} \tag{27b}$$

Now we can "Crank-Nicolson" method to find the time evolution of the coupling GP equation, we also can use the imaginary time algorithm to find the ground state.

Hamiltonian From (26a), we can split the Hamiltonian to two part: $\hat{H} = \hat{T} + \hat{V}_{tot}$, where $V_{tot} = V_{ext} + V_{non}$, and the commutation relation $:\left[\hat{T}, \hat{V}_{tot}\right] \neq 0$. The time evolution operation $\hat{U}(t + \delta t, t)$:

$$\hat{U}(t + \delta t, t) = e^{-i \int_t^{t+\delta t} \left(\hat{T} + \hat{V}_{tot}(t')\right) dt'} \tag{28}$$

A better way to do the approximation is:

$$\hat{U}(t + \delta t, t) = e^{-\frac{it}{2}\hat{T}} e^{-i \int_t^{t+\delta t} \hat{V}_{tot}(t') dt'} e^{-\frac{it}{2}\hat{T}} e^{O(\delta t'^3)} \tag{29a}$$

$$\int_t^{t+\delta t} \hat{V}_{tot}(t') dt' = \hat{V}(t + \delta t/2)\delta t + O(\delta t^3) \tag{29b}$$

It can be proven by the BCH formula. For the simplest case, We can treat the time evolution operator by the Zassenhaus formula, it also works well under small δt:

$$e^{-i\delta t(\hat{T} + \hat{V}_{tot})} = e^{-i\delta t \hat{T}} e^{-i\delta t \hat{V}_{tot}} \cancel{e^{\frac{-\delta t^2}{2}[\hat{T}, \hat{V}_{tot}]}} \ldots \tag{30}$$

Real-time propagation of GP equations I

Dividing $\hat{H}_\alpha$ of (26a) and (26b) into two part: $\hat{T}_\alpha + \hat{V}_\alpha, \alpha = A, B$:

$$\hat{V}_A = \frac{1}{4}(\kappa_1 \bar{r}^2 + \lambda_1 \bar{z}^2) + N_A G_A |\bar{\psi}_A(\bar{r}, \bar{z})|^2 + N_B G_{AB} |\bar{\psi}_B(\bar{r}, \bar{z})|^2 \quad (31a)$$

$$\hat{T}_A = \bar{\nabla}_A^2 \quad (31b)$$

$$\hat{V}_B = \frac{1}{4} k_2 (\kappa_2 \bar{r}^2 + \lambda_2 \bar{z}^2) + N_B G_B |\bar{\psi}_B(\bar{r}, \bar{z})|^2 + N_A G_{AB} |\bar{\psi}_A(\bar{r}, \bar{z})|^2 \quad (31c)$$

$$\hat{T}_B = k_1 \bar{\nabla}_B^2 \quad (31d)$$

We apply the (30) on the wave function $\bar{\psi}_\alpha(\bar{t} = 0)$:

$$\bar{\psi}_\alpha(\delta \bar{t}) = e^{-i\delta t \hat{T}_\alpha} \left[e^{-i\delta t \hat{V}_\alpha} \bar{\psi}_\alpha(\bar{t} = 0) \right] \quad (32)$$

Definding $\left[e^{-i\delta t \hat{V}_\alpha} \bar{\psi}_\alpha(\bar{t} = 0) \right] = \bar{\psi}_\alpha(\delta \bar{t}/2)$, here, the $\bar{\psi}_\alpha(\delta \bar{t}/2)$ is a abitrary solution not $\bar{\psi}_\alpha(\bar{t} = \delta \bar{t}/2)$ in physical meanning.

Real-time propagation of GP equations II

Expanding the right-hand size of exponent of (32) and decreasing the time and space.

$$\frac{\bar{\psi}_\alpha(\delta\bar{t}) - \bar{\psi}_\alpha(\delta\bar{t}/2)}{-i\delta t} = \frac{1}{2}\hat{T}_\alpha(\bar{\psi}_\alpha(\delta\bar{t}) + \bar{\psi}_\alpha(\delta\bar{t}/2)) \tag{33}$$

Finally, we have the formal solution:

$$\bar{\psi}_\alpha(\delta\bar{t}) = \frac{1 - i\hat{T}_\alpha\delta\bar{t}/2}{1 + i\hat{T}_\alpha\delta\bar{t}/2}\bar{\psi}_\alpha(\delta\bar{t}/2) \tag{34}$$

I write the pseudocode for the process of the program:

- 1. $\left[e^{-i\delta t\hat{V}_A}\bar{\psi}_A(\bar{t}=0)\right] = \bar{\psi}_A(\delta\bar{t}/2)$, $\left[e^{-i\delta t\hat{V}_B}\bar{\psi}_B(\bar{t}=0)\right] = \bar{\psi}_B(\delta\bar{t}/2)$
- 2. $\bar{\psi}_A(\delta\bar{t}) = \frac{1-i\hat{T}_A\delta\bar{t}/2}{1+i\hat{T}_A\delta\bar{t}/2}\bar{\psi}_A(\delta\bar{t}/2)$, $\bar{\psi}_B(\delta\bar{t}) = \frac{1-i\hat{T}_B\delta\bar{t}/2}{1+i\hat{T}_B\delta\bar{t}/2}\bar{\psi}_B(\delta\bar{t}/2)$
- 3. Doing iteration, we replaced the $\bar{\psi}_A(\delta\bar{t}/2)$ with $\bar{\psi}_A(\delta\bar{t})$, and $\bar{\psi}_B(\delta\bar{t}/2)$ with $\bar{\psi}_B(\delta\bar{t})$.
- 4. repeat steps 1,2,3.

Imaginary-time propagation of GP equations I

Use the imaginary time method to find the ground state. we give a trial wavefunction: $\psi(t=0)$:

$$\psi(\delta t) \approx \sum_{i=1}^{\infty} c_{i,t=0} e^{-i\delta t \hat{H}} \phi_i(t=0) \tag{35}$$

where ϕ_i is the eigenstate of $\hat{H}$, $i=1$ is ground state, $i=2$ is the first excited state. we set the $i\delta t$ to $\delta\tau$. As the imaginary time evolves, the ground state will be dominant.

$$\psi(\tau) \approx \sum_{i=1}^{\infty} c_{i,t=0} e^{-\tau E_i} \phi_i(t=0) \approx c_{i,t=0}\phi_0(t=0), \quad \tau \to \infty \tag{36}$$