

1-A

The energy of the eigenstate is $E_n = \frac{(n_x^2 + n_y^2 + n_z^2)\pi^2 \hbar^2}{2mL^2}$. Let $n^2 = n_x^2 + n_y^2 + n_z^2$. For $T > T_C$, the total particle number N equals

$$N = \sum_{n_x, n_y, n_z} \frac{1}{z^{-1}e^{\beta\epsilon} - 1} \quad (1)$$

$$\approx \frac{\pi}{2} \left(\frac{2mL^2 kT}{\pi^2 \hbar^2} \right)^{3/2} \int_0^\infty \frac{x^2 dx}{z^{-1}e^{x^2} - 1} \quad (2)$$

$$= \frac{2L^3}{\sqrt{\pi}\lambda_T^3} \Gamma(3/2) g_{3/2}(z), \quad (3)$$

where $g_{3/2}(z) = \sum_{n=1}^\infty \frac{z^n}{n^{3/2}}$. From the above, $g_{3/2}(z) = n\lambda_T^3 \ll 1$, thus $z \approx n\lambda_T^3$. The population in the ground state is

$$N_0 = \frac{3}{z^{-1}e^{\beta\epsilon_1} - 1} \approx 3n\lambda_T^3 \ll 1. \quad (4)$$

1-B

The Bose distribution function is ill defined for the ground state population when $z^{-1}e^{\beta\epsilon_0} \approx 1$. Let's define the critical temperature T_c to be the temperature when the potential energy equals the ground state energy and take $\epsilon_0 \approx 0$. That is $\mu = 0$ or $z^{-1} = 1$. Thus, the phase space density $n\lambda_{T_c}^3 = g_{3/2}(1) = \zeta(3/2) \approx 2.612$, and the critical temperature is

$$T_c = \left(\frac{n}{2.612} \right)^{2/3} \frac{2\pi\hbar^2}{mk_B} \quad (5)$$

$$\approx 3.31 \frac{\hbar^2 n^{2/3}}{mk_B} \quad (6)$$

Below this temperature, the maximum number of atoms the excited states can accommodate is fixed assuming that the temperature is fixed. Thus, a macroscopic number of atoms can occupy the ground state.

1-C

In the harmonic trap, $\epsilon_n = (n_x + n_y + n_z + 3/2)\hbar\omega = (n + 3/2)\hbar\omega$. The total number N is

$$N \approx N_{ex} = \sum_{n_x, n_y, n_z} \frac{1}{e^{\beta\epsilon_n} - 1} \quad (7)$$

$$\approx \frac{1}{2} \int_0^\infty \frac{x^2 dx}{z^{-1}e^{\beta x \hbar\omega} - 1} \quad (8)$$

$$= g_3(z) \left(\frac{k_B T_c}{\hbar\omega} \right)^3. \quad (9)$$

At critical temperature, $z = 1$ and $g_3(1) = \zeta(3) = 1.202$. Thus,

$$T_c = \left(\frac{N}{1.202} \right)^{1/3} \frac{\hbar\omega}{k_B} \quad (10)$$

$$= 0.941 \frac{\hbar\omega}{k_B} N^{1/3} \quad (11)$$

1-D

Treat the Bose distribution function semi-classically, then at the center of the trap, $r = 0$ and $H = p^2/2m$

$$n\lambda_{T_c}^3 = \frac{\lambda_{T_c}^3}{2\pi\hbar^3} \int \frac{d^3p}{e^{p^2/2m} - 1} \quad (12)$$

$$= \frac{(2mk_B T_c \lambda_{T_c}^2)^{3/2}}{4\pi^2 \hbar^3} \Gamma(3/2) \zeta(3/2) \quad (13)$$

$$= 2.612 \quad (14)$$

The same as atoms in free space.

1-E

Oxygen in the air, $n = \frac{0.2atm}{k_B \times 300K} = 4.89 \times 10^{24} m^{-3}$. $\lambda_T = 1.77 \times 10^{-11} m$. Thus, phase space density $n\lambda_T^3$ is 2.7×10^{-8} .

2-A

Solve GP equation. when $a = 0$,

$$-\frac{\hbar^2}{2m}\nabla^2\psi = \mu\psi \quad (15)$$

The ground state wavefunction is,

$$\psi(\vec{r}) \propto \left(\frac{2}{L}\right)^{3/2} \sin \frac{\pi x}{L} \sin \frac{\pi y}{L} \sin \frac{\pi z}{L} \quad (16)$$

Thus

$$\begin{aligned} n(\vec{r}) &= |\psi(\vec{r})|^2 & (17) \\ &= 8n \sin^2 \frac{\pi x}{L} \sin^2 \frac{\pi y}{L} \sin^2 \frac{\pi z}{L}. & (18) \end{aligned}$$

2-B

Taking r as the distance from the wall, GP equation is,

$$-\frac{\hbar^2}{2m}\psi(r)'' + u_0\psi(r)^3 = \mu\psi(r). \quad (19)$$

As $r \rightarrow \infty$, ψ approaches the free space wavefunction, $\psi = \text{constant} = \sqrt{n}$, where n is the mean density. Thus, $\mu = u_0|\psi|^2 = 4\pi\hbar^2 an/m$. Near the box, let $\xi = \sqrt{8\pi na}$ and, by changing variable $x =$, we can rewrite GP equation as

$$-\psi(x)'' + (\psi(x)^2 - n)\psi(x) = 0. \quad (20)$$

The solution to the above equation together with the boundary condition $\psi(0) = 0$ and $\psi(\infty) = \sqrt{n}$ is just

$$\psi(x) = \sqrt{n} \tanh(x/\sqrt{2}). \quad (21)$$

Thus, the density is $n(r) = n \tanh^2(r/\sqrt{2}\xi)$

2-C

To deform the box actually means to change the form of the "potential box" (but not the physical size) such that the wavefunction of a single particle approaches a constant. Just use the potential to simulate the mean field term in GP equation. That is, $V(r) = n \tanh^2(r/\sqrt{2}\xi)$ lead the solution of single particle Schrödinger equation to $\psi(r) = \sqrt{n} \tanh(r/\sqrt{2}\xi)$. By making ξ larger, the wavefunction approaches constant faster when moving away from the wall.

3-**A**

If we put in any test function and try to estimate the upper bound of the ground state energy, we immediately find that it diverges if the two ions overlap. Thus, to minimize the energy, each of the two ions behaves like one particle in each half of the box and is perturbed by the Coulomb interaction from the other ion in another half of the box.

The unperturbed ground state energy is just $E_0 = \frac{4\pi^2\hbar^2}{mL^2}$ and the first order perturbation energy term is of the order $\Delta E \approx e^2/L$. If the box ranges from $-L/2$ to $L/2$, the unperturbed wavefunction for ion 1 is $\psi_{left,right}^0(x_1) = \frac{2}{\sqrt{L}} \sin \frac{2\pi x_1}{L}$ for $x_1 \leq 0$ and 0 for $x_1 \geq 0$. And the first order perturbation is

$$\psi^1(x_1) = \sum_{n=1}^{\infty} \frac{\psi_n(x_1) \langle \psi_n(x_1) | \frac{e^2}{|x_1 + \langle x_2 \rangle}| | \psi_0(x_1) \rangle}{E_0 - E_n} \quad (22)$$

from the sign in the above equation, we see that close to the center of the box, the perturbation term tends to have destructive interference on the unperturbed wavefunction, i.e. pushes the ion away from each other. Since the ions are bosons, the ground state wave function is

$$\psi(x_1, x_2) = 1/\sqrt{2}(\psi_{left}(x_1)\psi_{right}(x_2) + \psi_{left}(x_2)\psi_{right}(x_1)). \quad (23)$$

Notice that in the Schrödinger equation, the kinetic energy term is proportional to L^{-2} while the Coulomb term is proportional to L^{-1} . When the box is small, the kinetic energy dominates and the ions stay close to the center of the half-box. When the box becomes larger, the Coulomb term dominates and the ions are pushed away toward the wall. In either case, the wavefunction of the two ions won't overlap.

3-**B**

The ground state energy remains the same as helium with two fermionic electrons.

3-**C**

From A, the Coulomb interaction prevents any overlap of the ionic wavefunctions. Thus, it is not possible to condense the bosonic ions in 1D. In 3D, the Coulomb potential will not lead to the divergence of the energy if the ions overlap. However, if the ions are in the continuum, i.e. in the large box limit, according to 3-A, the Coulomb potential still dominates and the ions are pushed away from each other. They will still not be condensed. But if L is small such that the kinetic energy term takes over. The ions can still be sufficiently close to each other such that $n\lambda_T$ reaches the order of unity. The ions might be condensed under this condition.

4-A

Right after the potential is switched off, the density distribution is still the same as $t = 0^-$,

$$\rho(r_0, z_0, 0) = |\psi|^2 = \frac{\mu - V}{g} = \frac{\mu - 1/2m(\omega_r^2 r_0^2 + \omega_z^2 z_0^2)}{g}. \quad (24)$$

However, in free space, the condensate feels the mean field potential created by itself. Thus for atoms at (r_0, z_0) , it senses the acceleration

$$\vec{a} = \vec{F}/m = -\vec{\nabla}g\rho(r_0, z_0, 0)/m \quad (25)$$

$$= \omega_r^2 r_0 \hat{r} + \omega_z^2 z_0 \hat{z}. \quad (26)$$

4-B

At $t = 0^+$,

$$\ddot{r} = \omega_r^2 r_0, \quad \ddot{z} = \omega_z^2 z_0. \quad (27)$$

After an infinitesimal time dt , the velocity and new position, in r or z direction, of the atoms will still be proportional to r or z . The distribution still remains the same except for that the coordinate scales a little bit according to Newton's equation of motion. Thus, as t increases, the acceleration is always proportional to r and z and the coordinate scales accordingly. Hence, we have a dilatation of the wavefunction.

Let the new position of the atoms at time t be $r = R(t)r_0$ and $z = Z(t)z_0$. Since the total number N of the atoms conserves, we have

$$N = \int dr dz d\phi r \rho(r, z, t) \quad (28)$$

$$= \int dr_0 dz_0 d\phi r_0 \rho(r_0, z_0, 0) \quad (29)$$

That is

$$\int dr_0 dz_0 r_0 R^2(t) Z(t) \rho(r, z, t) = \int dr_0 dz_0 r_0 \rho(r_0, z_0, 0). \quad (30)$$

Thus, we get

$$R^2(t) Z(t) \rho(r, z, t) = \rho(r/R(t), z/Z(t), 0). \quad (31)$$

4-C

From Newton's law,

$$\ddot{\vec{a}} = \ddot{R}r_0 \hat{r} + \ddot{Z}z_0 \hat{z} \quad (32)$$

$$= -g\vec{\nabla}\rho(r, z, t)/m \quad (33)$$

$$= -R^{-2}(t)Z^{-1}(t)\vec{\nabla}\rho(r/R(t), z/Z(t), 0)/m \quad (34)$$

$$= \frac{\omega_r^2 r_0}{R^3 Z} \hat{r} + \frac{\omega_z^2 z_0}{R^2 Z^2} \hat{z}. \quad (35)$$

4-D

(i) $\omega_r = \omega_z$

This is an isotropic case, $R = Z$. Solve for $\ddot{R} = \omega_r^2/R^4$. First, time \dot{R} on each side and integrate. We get

$$\dot{R}^2 = \frac{2\omega_r^2}{3}(1 - R^{-3}), \quad (36)$$

where we have used the initial condition of $\dot{R}(0) = 0$. The time dependence of R on t can be obtained by performing the integral

$$\sqrt{\frac{2}{3}}\omega t = \int_1^R \frac{dR}{\sqrt{1 - 1/R^3}} \quad (37)$$

(ii) $\omega_r \gg \omega_z = \epsilon_r$

In this case, the expansion rate in r will be much faster than z, we can treat $Z(t)$ as a constant ($Z(t) = 1 + O(\epsilon^2) \approx 1$) while calculating $R(t)$. Hence, we get

$$R(t) = \sqrt{1 + \omega_r^2 t^2} + O(\epsilon^2). \quad (38)$$

Now, turn to $Z(t)$, since $\ddot{Z} = \omega_z^2/R^2 Z^2 \approx \omega_z^2/R^2 + O(\epsilon^4)$. We take the approximation $\ddot{Z} \approx \omega_z^2/(1 + \omega_r^2 t^2)$ and solve for $Z(t)$.

$$Z(t) = 1 + \epsilon^2(\omega_r t \tan^{-1}(\omega_r t) - \frac{1}{2} \ln(1 + \omega_r^2 t^2)) + O(\epsilon^4)$$

5-A-1: Coarse estimation

The Gross-Pitaevskii equation is

$$\mu\Psi = \left(-\frac{\hbar^2\nabla^2}{2m} + \frac{1}{2}m\omega_r^2 r^2 + g|\Psi|^2 \right) \Psi \quad (1)$$

where

$$\int |\Psi|^2 d^3r = N \quad (2)$$

and N is the particle number. The interaction strength is proportional to the scattering length:

$$g = \frac{4\pi\hbar^2 a}{m} \quad (3)$$

We are not going to solve the GP equation numerically. Rather, we start from the dependence of the energy terms on the particle number N and the effective size R of BEC:

(1) kinetic energy:

$$E_k \sim \frac{N\hbar^2}{2mR^2} \quad (4)$$

(2) potential energy:

$$E_p \sim \frac{Nm\omega_r^2 R^2}{2} \quad (5)$$

(3) interaction energy:

$$E_i \sim -\frac{|g|N^2}{R^3} \quad (6)$$

Thus the total energy per particle is

$$\begin{aligned} \frac{E}{N} &\sim \frac{\hbar^2}{2mR^2} + \frac{m\omega_r^2 R^2}{2} - \frac{|g|N}{R^3} \\ &= \frac{\hbar\omega_r}{2} \left(\frac{1}{x^2} + x^2 - \frac{8N\pi|a|}{a_{\text{ho}}x^3} \right) \\ &\equiv \frac{\hbar\omega_r}{2} \left(\frac{1}{x^2} + x^2 - \frac{\alpha}{x^3} \right) \end{aligned} \quad (7)$$

where $\alpha \equiv 8N\pi|a|/a_{\text{ho}}$; $a_{\text{ho}} \equiv \sqrt{\hbar/(m\omega_r)}$; $x \equiv R/a_{\text{ho}}$ is the dimensionless effective size of BEC.

Numerical calculations show that for $\alpha > \alpha_c = 0.4$, the **derivative** of E/N with respect to x is always positive. This means the system would collapse when

$$\begin{aligned} N > N_c &= \frac{\alpha_c a_{\text{ho}}}{8\pi |a|} \\ &= \left[0.02 \frac{a_{\text{ho}}}{|a|} \right] + 1 \end{aligned} \quad (8)$$

where the '[]' in the last step means 'taking the integer part'.

5-A-2 Gaussian trial wave function

Define the Gaussian trial wave function

$$\Psi_t = \sqrt{N} \frac{1}{(\sqrt{\pi}R)^{3/2}} \exp[-r^2/2R^2] \quad (9)$$

and use the Energy functional

$$E[\Psi] = \int d^3r \Psi^* \left(-\frac{\hbar^2\nabla^2}{2m} + \frac{1}{2}m\omega_r^2 r^2 \right) \Psi - \int d^3r \frac{1}{2} |g| |\Psi|^4 \quad (10)$$

we get

$$\begin{aligned}\frac{E[\Psi_t]}{N} &= \frac{1}{N} \left[N \frac{3\hbar^2}{4mR^2} + N \frac{3m\omega_r^2 R^2}{4} - N^2 \frac{|g|}{2^{5/2}\pi^{3/2}R^3} \right] \\ &= \hbar\omega_r \left(\frac{3}{4x^2} + \frac{3x^2}{4} - N \frac{|a|}{a_{\text{ho}}} \frac{1}{\sqrt{2\pi}x^3} \right)\end{aligned}\quad (11)$$

where x , etc. have the same definitions as in **5-A-1**. Similar calculation gives

$$\frac{\partial(E[\Psi_t]/N)}{\partial x} = \hbar\omega_r \left(-\frac{3}{2x^3} + \frac{3x}{2} + N \frac{|a|}{a_{\text{ho}}} \frac{3}{\sqrt{2\pi}x^4} \right)\quad (12)$$

and the collapsing range as $N > 0.67a_{\text{ho}}/|a|$.

5-B

The gravitational energy estimated as

$$E_g \sim -Gm^2 N^2/R\quad (13)$$

where G is Newton's gravitational constant. The total energy per particle is ($|a| = 0$)

$$\begin{aligned}\frac{E'}{N} &\sim \frac{\hbar^2}{2mR^2} + \frac{m\omega_r^2 R^2}{2} - Gm^2 N/R \\ &= \frac{\hbar\omega_r}{2} \left(\frac{1}{x^2} + x^2 - \beta/x \right)\end{aligned}\quad (14)$$

where $\beta \equiv 2NGm^2/(a_{\text{ho}}\hbar\omega_r)$. Thus we always have a finite energy minimum. There is no collapse.

Note: We know from general relativity that there exists black holes. When the mass of a system is large enough, it will collapse into a black hole. However, the above argument does not seem to support the collapse. There are two reasons: (1) We didn't consider the effect of general relativity. (2) Before the system collapses into a black hole, it will go through processes like 'electron + proton \rightarrow neutron', etc. During these processes, the concept of 'atom', 'electrons', etc. are no longer present, and the Hamiltonian we used for the above calculation already becomes invalid.

6

6-A

Let two beams be counter-propagating along the x-axis, and two along the y-axis. The polarizations of the two x-propagating beams are along the z-direction, while those of the two y-propagating beams are along the x-direction. The purpose of this arrangement is to eliminate interference between beams propagating along different axes.

Let the amplitude of the electric field be $E_0 = 1$ for each beam, and use the convention $k = 2\pi/\lambda = 1$ and $\omega = 2\pi/T = 1$. We get the total intensity as

$$\begin{aligned} I &= \langle (\cos(x-t) + \cos(-x-t))^2 \rangle + \langle (\cos(y-t) + \cos(-y-t))^2 \rangle \\ &= 2(\cos^2 x + \cos^2 y) \end{aligned} \quad (15)$$

where the average in the first step is with respect to time.

6-B

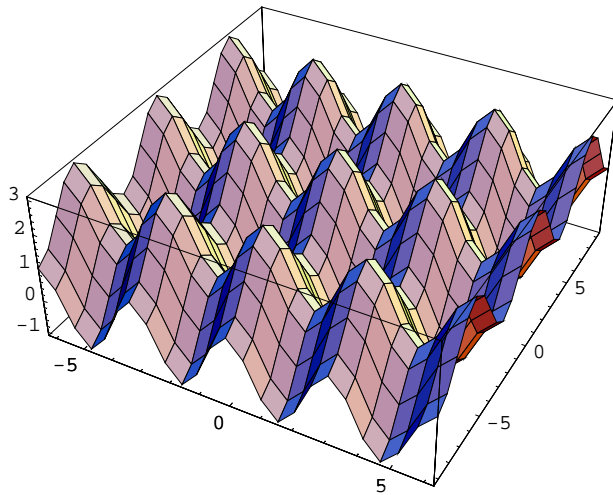
We choose the polarization to be along the z-direction. The three beams propagate along $(0, -1, 0)$, $(\sqrt{3}/2, 1/2, 0)$, and $(-\sqrt{3}/2, 1/2, 0)$. The total intensity is (with the same convention)

$$\begin{aligned} I &= \langle (\cos(-\sqrt{3}x/2 + y/2 - t) + \cos(\sqrt{3}x/2 + y/2 - t) + \cos(-y - t))^2 \rangle \\ &= 3/2 + \cos(\sqrt{3}x) + \cos(\sqrt{3}x/2 + 3y/2) + \cos(-\sqrt{3}x/2 + 3y/2) \end{aligned} \quad (16)$$

The mathematica graphs are attached at the end of this problem.

In[8]:=

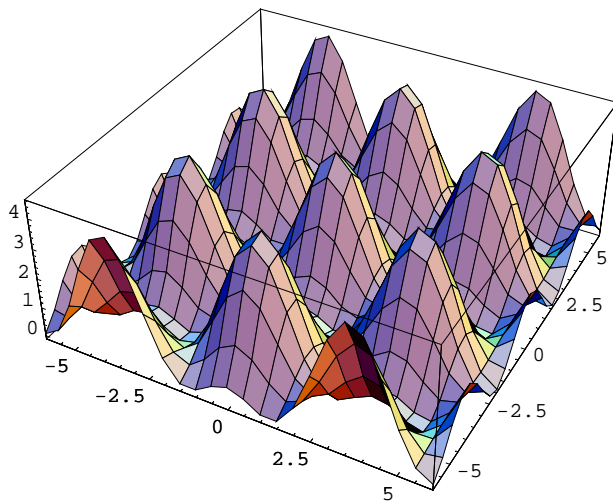
```
Plot3D[(0.5 * (Exp[I * x] + Exp[-I * x]) * Conjugate[(Exp[I * x] + Exp[-I * x])] +
  0.5 * (Exp[I * y] + Exp[-I * y]) * Conjugate[(Exp[I * y] * Exp[-I * y])]),
  {x, -2 * Pi, 2 * Pi}, {y, -3 * Pi, 3 * Pi}]
```



Out[8]= - SurfaceGraphics -

In[12]:= Plot3D[

```
0.5 * (Exp[I * (-Sqrt[3] / 2 * x + y / 2)] + Exp[I * (Sqrt[3] / 2 * x + y / 2)] + Exp[-I * y]) *
  Conjugate[(Exp[I * (-Sqrt[3] / 2 * x + y / 2)] +
  Exp[I * (Sqrt[3] / 2 * x + y / 2)] + Exp[-I * y])], {x, -6, 6}, {y, -6, 6}]
```



Out[12]= - SurfaceGraphics -

7

7-A Suppose there are L lattice sites (i.e., the $(L + 1)$ th site is the 1st site), with spacing a . The potential, for small x , can be expanded as

$$\begin{aligned} V &\approx V_0 k^2 x^2 \\ &\equiv \frac{1}{2} m \omega^2 x^2 \end{aligned} \quad (17)$$

where $\omega = \sqrt{2V_0/mk}$

In the tight-binding regime, the ground energy is equal to

$$\hbar\omega/2 = \hbar\sqrt{2V_0/mk}/2 \quad (18)$$

The ground state is

$$\Psi_1 = \frac{1}{\sqrt{L}} \sum_{l=0}^{L-1} f(x + la) \quad (19)$$

where

$$f(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right) \quad (20)$$

, $\omega = \sqrt{2V_0/mk}$, and we define $\Psi(x + La) \equiv \Psi(x)$. The normalization factor $1/\sqrt{L}$ comes from that $f(x + l_1 a)$ and $f(x + l_2 a)$ are orthogonal for $0 \neq (l_1 - l_2) \pmod{L}$

7-B,C

Suppose N ($N \geq 2$) atoms are in the ground state. In the zero-interaction case, the effective wave-function is characterized by

$$\begin{aligned} \Psi_N &= \sqrt{N} \Psi_1 \\ &= \frac{\sqrt{N}}{\sqrt{L}} \sum_{l=0}^{L-1} f(x + la) \end{aligned} \quad (21)$$

and the 0th order energy is

$$\begin{aligned} E_0 &= \int dx \Psi^* \left(-\frac{\hbar^2 \nabla^2}{2m} + V_0 \sin^2(kx)\right) \Psi \\ &= N \hbar \sqrt{2V_0/mk}/2 \\ &\equiv N \hbar \omega / 2 \end{aligned} \quad (22)$$

Taking interaction into account, the Hamiltonian for perturbation is

$$H_i = \frac{1}{2} g |\Psi|^2 \quad (23)$$

and the perturbation energy is

$$\begin{aligned} E_i &= \int dx \Psi^* H_i \Psi \\ &= \int dx \frac{1}{2} g |\Psi|^4 \\ &= \frac{g N^2}{2 L^2} \times L \sqrt{m\omega/(2\pi\hbar)} \\ &= \frac{g N^2}{2 L} \sqrt{m\omega/(2\pi\hbar)} \end{aligned} \quad (24)$$

The total ground energy is

$$\begin{aligned} E &= E_0 + E_i \\ &= \frac{1}{2} \hbar \omega \left(N + \frac{N^2 g}{L \hbar} \sqrt{m/(2\pi\hbar\omega)} \right) \end{aligned} \quad (25)$$

The energy per site is

$$E/L = \frac{1}{2}\hbar\omega \left(\frac{N}{L} + \frac{N^2g}{L^2\hbar} \sqrt{m/(2\pi\hbar\omega)} \right) \quad (26)$$

where $\omega \equiv \sqrt{2V_0/mk}$, and L is the number of lattice sites.

8 Let's consider the 1-D case first. The Hamiltonian for the system should not be understood as just $p^2/2m + V_0 \sin^2(kx)$, but as

$$H = \int dx \Psi^\dagger(x) \left(-\frac{\hbar^2 \partial_x^2}{2m} + V_0 \sin^2(kx) \right) \Psi(x) + \frac{g}{2} \int dx \Psi^\dagger(x) \Psi^\dagger(x) \Psi(x) \Psi(x) \quad (27)$$

If we are in the tight binding regime and the temperature is zero, the wave operator (previously 'wave function') can be expanded as

$$\Psi(x) = \sum_{l=0}^L b_l \phi(x - la) \quad (28)$$

where the sum is over the L lattice sites: $0, \pi/k, \dots, (L-1)\pi/k$; $\phi(x)$ is the single particle ground state of a harmonic trap ($V_0 k^2 x^2$) centered at the origin:

$$\phi(x) = \left(\frac{m\Omega}{\pi\hbar} \right)^{1/4} \exp \left[-\frac{m\Omega}{2\hbar} x^2 \right] \quad (29)$$

Thus

$$\begin{aligned} H &= -\sum_{i \neq j} t_{i,j} b_i^\dagger b_j + \frac{\hbar\Omega}{2} \sum_l b_l^\dagger b_l + \frac{g}{2} \sum_l b_l^\dagger b_l^\dagger b_l b_l \times \int dx \left(\left(\frac{m\Omega}{\pi\hbar} \right)^{1/4} \exp \left[-\frac{m\Omega}{2\hbar} x^2 \right] \right)^4 \\ &= -\sum_{i \neq j} t_{i,j} b_i^\dagger b_j + \frac{\hbar\Omega}{2} \sum_l n_l + \frac{g}{2} \sum_l n_l(n_l - 1) \times \sqrt{\frac{m\Omega}{2\pi\hbar}} \end{aligned} \quad (30)$$

where $n_l = b_l^\dagger b_l$; the coefficient

$$t_{ij} = -\int dx \phi^*(x - i\pi/k) \left(-\frac{\hbar^2 \partial_x^2}{2m} + V_0 \sin^2(kx) \right) \phi(x - j\pi/k) \quad (31)$$

We see that $t_{ij} = t_{ji} \equiv t_{(|i-j|)}$ and that the larger $|i-j|$ is, the smaller $t_{(|i-j|)}$ is. As a first-order approximation, we only consider the nearest neighbor interaction:

$$t \equiv t_{01} \quad (32)$$

$$= -\int dx \phi^*(x) \left(-\frac{\hbar^2 \partial_x^2}{2m} + V_0 \sin^2(kx) \right) \phi(x - \pi/k) \quad (33)$$

The Hamiltonian is approximated as

$$H = -t \sum_{l=0}^{L-1} \left(b_l^\dagger b_{l+1} + b_{l+1}^\dagger b_l \right) + \frac{U}{2} \sum_l n_l(n_l - 1) - \mu \sum_l n_l \quad (34)$$

where

$$U = g \sqrt{\frac{m\Omega}{2\pi\hbar}} \quad (35)$$

$$-\mu = \hbar\Omega/2 \quad (36)$$

9 9-A

Let's correct the definition of $|S\rangle$ to make it normalized:

$$|S\rangle = \frac{1}{2\sqrt{2}} (b_R^\dagger + b_L^\dagger)^2 |\text{vacuum}\rangle \quad (37)$$

$$\begin{aligned} |S\rangle &= \frac{1}{2\sqrt{2}} \left(\sqrt{2}|L, L\rangle + 2\frac{1}{\sqrt{2}}(|L, R\rangle + |R, L\rangle) + \sqrt{2}|R, R\rangle \right) \\ &= \frac{1}{2}|L, L\rangle + \frac{1}{2}(|L, R\rangle + |R, L\rangle) + \frac{1}{2}|R, R\rangle \end{aligned} \quad (38)$$

$$|M\rangle = \frac{1}{\sqrt{2}} (|L, R\rangle + |R, L\rangle) \quad (39)$$

We see that the $|S\rangle$ state is not normalized.

9-B

$$H = -t(b_L^\dagger b_R + b_R^\dagger b_L) + \frac{U}{2} \sum_{i=R,L} n_i(n_i - 1) - \mu \sum_{i=R,L} n_i \quad (40)$$

The energy is given by

$$\begin{aligned} E_S &= \frac{\langle S|H|S\rangle}{\langle S|S\rangle} \\ &= \frac{U - 4\mu - 4t}{2} \end{aligned} \quad (41)$$

and

$$\begin{aligned} E_M &= \frac{\langle M|H|M\rangle}{\langle M|M\rangle} \\ &= -2\mu \end{aligned} \quad (42)$$

Thus

$$E_S - E_M = \frac{U - 4t}{2} \quad (43)$$

It depends on t/U to determine which state has a higher energy: when $t/U > 1/4$ the superfluid state has lower energy; when $t/U < 1/4$ the Mott insulator state has lower energy.

9-C The critical $t/U = 1/4$ for $E_M = E_S$.

9-D: Only consider the nearest neighbor hopping in the 3-Dim case

For the N particle - N lattice sites case, the two states are defined as

$$\begin{aligned} |S\rangle &= \frac{1}{\sqrt{N!N^N}} (b_1^\dagger + \dots + b_N^\dagger)^N |\text{vacuum}\rangle \\ |M\rangle &= b_1^\dagger \dots b_N^\dagger |\text{vacuum}\rangle \end{aligned} \quad (44)$$

we have $\langle M|M\rangle = 1$ and $\langle S|S\rangle = 1$. In calculating the normalization constant for $|S\rangle$ we used

$$[b_1 + \dots + b_N, (b_1^\dagger + \dots + b_N^\dagger)^M] = MN(b_1^\dagger + \dots + b_N^\dagger)^{M-1} \quad (45)$$

and

$$\langle \text{vacuum} | (b_1 + \dots + b_N)^M (b_1^\dagger + \dots + b_N^\dagger)^M | \text{vacuum} \rangle = M!N^M \quad (46)$$

The energies are

$$\begin{aligned}
E_S &= \langle S|H|S \rangle \\
&= \frac{-t6NN!N^N + \frac{U(N-1)}{2}N!N^N - \mu NN!N^N}{N!N^N} \\
&= -t6N + \frac{U(N-1)}{2} - \mu N
\end{aligned} \tag{47}$$

and

$$\begin{aligned}
E_M &= \frac{\langle M|H|M \rangle}{\langle M|M \rangle} \\
&= \frac{-N\mu}{1} \\
&= -N\mu
\end{aligned} \tag{48}$$

where we used

$$[b_1, (b_1^\dagger + \dots + b_N^\dagger)^M] = M(b_1^\dagger + \dots + b_N^\dagger)^{M-1} \tag{49}$$

and

$$[(b_1 + \dots + b_N)^M, n_1] = Mb_1(b_1 + \dots + b_N)^{M-1} \tag{50}$$

Thus

$$E_S - E_M = -6Nt + \frac{U(N-1)}{2} \tag{51}$$

and the critical point is

$$\frac{t}{U} = \frac{N-1}{12N} \tag{52}$$

i.e. $t < \frac{N-1}{12N}$ for Mott insulator phase and $t > \frac{N-1}{12N}$ for superfluid phase.

10**10-A****10-A-1: Fourier analysis**

The wave-function would be of the following form, due to the Bloch theorem

$$\Psi(x) = e^{ipx} u(x) \quad (53)$$

where $u(x)$ has the same periodicity as $\sin^2(kx)$, i.e. with period of π/k

Let's expand the wave-function as

$$\Psi(x) = e^{ipx} \sum_{n=-\infty}^{\infty} u_n e^{in \cdot 2kx} \quad (54)$$

The Schrödinger's equation is equivalent to

$$u_n \left(\frac{\hbar^2(p + 2nk)^2}{2m} + \frac{V_0}{2} \right) = \frac{V_0}{4}(u_{n-1} + u_{n+1}) \quad (55)$$

$$u = -\infty, \dots, -1, 0, 1, \dots, \infty$$

Subsequently one can get the exact formula for the u_n 's.

10-A-2

Let's attack this problem by intuition. In the tight-binding regime, without self-interaction,

$$\Psi = \sqrt{\frac{1}{L}} \sum_{l=0}^{L-1} \phi(x - l\pi/k) \quad (56)$$

where L is total number of lattice sites; ϕ is the ground state of the single harmonic potential:

$$\phi(x) = \left(\frac{m\Omega}{\pi\hbar} \right)^{1/4} \exp \left[-\frac{m\Omega}{2\hbar} x^2 \right] \quad (57)$$

where $\Omega = \sqrt{2V_0/mk}$.

10-B

The wave-function in momentum space is

$$\begin{aligned} \Psi_q &= \int \Psi(x) e^{-iqx} dx \\ &= \sqrt{\frac{1}{L}} \sum_{l=0}^{L-1} \int dx e^{-iqx} \left(\frac{m\Omega}{\pi\hbar} \right)^{1/4} \exp \left[-\frac{m\Omega}{2\hbar} (x - l\pi/k)^2 \right] \\ &= \left(\frac{m\Omega}{\pi\hbar} \right)^{1/4} \sqrt{\frac{1}{L}} \sum_{l=0}^{L-1} \exp[-iql\pi/k] \int dx' e^{-iqx'} \exp \left[-\frac{m\Omega}{2\hbar} (x')^2 \right] \\ &= \left(\frac{\pi\hbar}{m\Omega} \right)^{1/4} \exp \left[-\frac{\hbar^2 q^2}{2m} / (\hbar\Omega) \right] \sqrt{\frac{2}{L}} \sum_{l=0}^{L-1} \exp[-iql\pi/k] \\ &= \left(\frac{\pi\hbar}{m\Omega} \right)^{1/4} \exp \left[-\frac{\hbar^2 q^2}{2m} / (\hbar\Omega) \right] \sqrt{\frac{2}{L}} \frac{1 - e^{-iqL\pi/k}}{1 - e^{-iq\pi/k}} \end{aligned}$$

As an example, for $L \rightarrow \infty$, the factor

$$\frac{1 - e^{-iqL\pi/k}}{1 - e^{-iq\pi/k}} \quad (58)$$

approaches – in the sense of averaging – 0 for $q \neq 2k \cdot \text{Integer}$; it is proportional to $\delta(q - 2k \cdot \text{Integer})$ for $q = 2k \cdot \text{Integer}$.

10-C

When V_0 increases, Ω increases. This means the gaussian pre-factor of the wave-function in momentum space becomes 'fatter' (variance larger) and 'flatter' (peak value smaller).