Effective size and expansion energy of a Bose-Einstein condensate in a 3D non-cubic optical lattice

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Abstract

This work is devoted to study the temperature dependence of the effective size $\langle r^2 \rangle$ and expansion energy $E_{x,z}$ of a Bose-Einstein condensate in a 3D non-cubic optical lattice. Correction due to the finite size, interatomic interaction and the deepness of the lattice potential are given simultaneously. The calculated results show that these two parameters increase with the lattice depth or the relative frequency at temperature less than the transition temperature, $(T < T_o)$; yet it has little effect at temperatures higher than the transition temperature $(T > T_o)$. Both the effective size and expansion energy follow a characteristic temperature dependence, i.e. $\langle r^2 \rangle$, $E \propto (T/T_0)^4$ if $T < T_0$ and $\langle r^2 \rangle$, $E \propto (T/T_0)$ if $T > T_0$. For a 3D non cubic optical potential the effect of relative frequency is much more than the effect of the optical potential depth. Thus for a non-cubic optical potential one has to use the pure harmonically trapped boson gas as the zeroth order approximation in any perturbation or numerically treatment for this system.

Key Words: Thermodynamical properties for BEC in optical lattice, semiclassical theories and applications

1. Introduction

Recently, trapped Bose gases in a combined harmonic-optical potential is used as a prototype for strongly quantum phase transition. Indeed, the condensate Boson in optical potential offer a new opportunity to investigate the interplay connection between the superfluid (SF) and Mott insulator (MI) phase transition [1]. Experiments in this area show that the phase-coherent Bose-Einstein condensate (BEC) in the optical lattice is a SF [2]. Greiner et al. [1] pointed out that, as the lattice depth is increased, the quantum tunneling of atoms from one optical site to another is stopped, resulting in loss of superfluidity, which is identified by vanishing of the condensed fraction. In such case BEC is transformed to a MI state in which exact numbers of atoms are localized at individual lattice sites and its free mobility to a nearly site by tunneling is stopped as insulator. Consequently, no interference pattern is formed upon free expansion of such a BEC. This phenomenon represents a superfluid-Mott insulator quantum phase transition. The SF to MI transition can be accessed by changing the depth of the optical potential and has been observed in different trap geometry [3, 4, 5, 6, 7].

One way of obtaining information about the properties of this phase transition is to investigate its behavior after it is released from the trap. The most important thermodynamical parameters for this investigation are the effective size and the expansion energy. These two parameters have special behavior at temperature greater or less than the transition temperature T_0 [8, 9, 10]. Moreover, they are affected by changing of the lattice depth or relative frequency (the ratio between recoil frequency and geometrical average of the harmonic frequencies).

In this paper, an expression for the effective size and expansion energy of the condensate Bose gas in a 3D non-cubic optical lattice is calculated. The semiclassical approximation, which is the density of state (DOS) approach is used. In this approach the sums over the energy levels for the thermodynamical quantities are approximated directly by ordinary integrals weighted by an appropriate DOS. This approximation has been widely used in variety of problems in statistical physics [11] and in BEC [12, 13, 14, 15]. Previous studies have showed that the resulting thermodynamical parameters depend crucially on the choice and construction of the DOS. The calculation techniques are extension for that given in our previous work [16, 17, 18, 19]. The parametrized DOS here providing a consistent way for treating the main effects which can be altering the harmonically trapped Bose gas in a non-cubic optical lattice. I have undertaken this study in an effort to provide some theoretical support for the experiment. The calculated results show that, for high temperature ($K_{\mathrm{B}}T >> \hbar\omega$), and ignoring the contribution from the condensate, the effective size and expansion energy are proportional to T for $T > T_0$, and proportional to T^4 for $T < T_0$. This temperature dependence behavior agrees with the measured experimental data [6, 7, 8]. Changing the depth of the optical potential or changing the magnetic potential frequencies led to significant change in the effective size or expansion energy.

This paper is organized as follows. The present section provides a brief introduction. Section two provides the theoretical model. The calculation of the effective size and expansion energy is outlined in section three. Section four presents a short conclusion.

2. Theoretical model for BEC in a combined potential

Let us consider a Boson gas trapped in a combined potential given by [20, 6]

$$V(\mathbf{r}) = \frac{1}{2}m \left[(\omega_x^2 + \omega_{\mathrm{lat},x}^2)x^2 + (\omega_y^2 + \omega_{\mathrm{lat},y}^2)y^2 + (\omega_z^2 + \omega_{\mathrm{lat},z}^2)z^2\right] - \frac{1}{3}\,k^4\,(V_x x^4 + V_y y^4 + V_z z^4). \qquad (1)$$

Here, $\omega_{\mathrm{lat},l} = \frac{2\sqrt{E_{\mathrm{R}}V_l}}{\hbar}$ with l stands for x, y and z, $\{\omega_x, \omega_y, \omega_z\}$ are the effective trapping frequencies of the external harmonic confinement and $\{V_x, V_y, V_z\}$ are the potential depths of the three superimposed 1D laser beam standing waves. The wave vector of the laser beam is accounted by $k = 2\pi/\lambda'$, with λ' is the laser wavelength. In terms of k, we have to introduce the recoil energy $E_{\mathrm{R}} = (\hbar^2 k^2/2m)\,\{\equiv \hbar\omega_{\mathrm{R}}\}$ as an energy scale which measures the lattice depth.

In order to use the density of states approach, the single particle spectrum for this system is needed. For the potential (1) it is impossible to find an exact analytical expression for these energy levels. However, this potential is characterized by a single particle energy level is given by [16]

$$E_n = n_x \hbar(\omega_x' - \frac{\omega_{\mathrm{R}}}{2}) + n_y \hbar(\omega_y' - \frac{\omega_{\mathrm{R}}}{2}) + n_z \hbar(\omega_z' - \frac{\omega_{\mathrm{R}}}{2}) + E_0, \qquad (2)$$

where $\omega_l' = \omega_l^2 + \omega_{\mathrm{lat},l}^2$, and $E_0 = \frac{3}{2}\hbar\bar{\omega}$ with $\bar{\omega} = \frac{1}{3}(\omega_x' + \omega_y' + \omega_z' - \frac{3}{2}\omega_{\mathrm{R}})$ is the mean of the combined frequencies. Mainly the lattice potential depth is measured in units of the recoil energy E_{R}. Thus one has to

write $V_{x,y,z} = integer \times E_{\mathrm{R}}$, and rewrite $\omega'_{x,y,z}$ in the form

$$
\begin{aligned}
\omega'_x &= \sqrt{(\omega_x^2 + 4E_{\mathrm{R}}V_x/\hbar^2)} = \omega_x\sqrt{1 + 4s_x t_x^2}, \\
\omega'_y &= \sqrt{(\omega_y^2 + 4E_{\mathrm{R}}V_y/\hbar^2)} = \omega_y\sqrt{1 + 4s_y t_y^2}, \\
\omega'_z &= \sqrt{(\omega_z^2 + 4E_{\mathrm{R}}V_z/\hbar^2)} = \omega_z\sqrt{1 + 4s_z t_z^2},
\end{aligned}
\tag{3}
$$

where $s_{x,y,z} = \frac{V_{x,y,z}}{E_{\mathrm{R}}}$, $t_{x,y,z} = \frac{\omega_{\mathrm{R}}}{\omega_{x,y,z}}$ and $E_{\mathrm{R}} = \hbar\omega_{\mathrm{R}}$ is used. Moreover in terms of ω_{R} the mean of the combined frequencies $\bar{\omega}$ is given by $\bar{\omega} = \frac{1}{3}(\omega_x[\sqrt{1 + 4s_x t_x^2} - t_x/2] + \omega_y[\sqrt{1 + 4s_y t_y^2} - t_y/2] + \omega_z[\sqrt{1 + 4s_z t_z^2} - t_z/2])$.

The accurate DOS for the spectrum (2) is calculated in [19] and is given by

$$
\begin{aligned}
\rho(\epsilon) &= \frac{1}{2}\frac{\epsilon^2}{(\hbar\Omega')^3} + \frac{\epsilon}{(\hbar\Omega')^2}\left[\frac{3}{2}\frac{\bar{\omega}}{\Omega'} + \frac{2}{3}\frac{\mu}{\hbar\bar{\omega}}\right] \\
&= \frac{1}{\gamma^3}\left[\frac{1}{2}\frac{\epsilon^2}{(\hbar\Omega)^3} + \frac{\epsilon}{(\hbar\Omega)^2}\left[\frac{3}{2}\frac{\bar{\omega}}{\Omega} + \frac{2}{3}\frac{\mu}{\hbar\bar{\omega}}\gamma\right]\right],
\end{aligned}
\tag{4}
$$

where $\Omega' = [(\omega'_x - \frac{\omega_{\mathrm{R}}}{2})(\omega'_y - \frac{\omega_{\mathrm{R}}}{2})(\omega'_z - \frac{\omega_{\mathrm{R}}}{2})]^{1/3}$ and $\Omega = [\omega_x\omega_y\omega_z]^{1/3}$ are the geometrical average of the combined frequencies and the harmonic frequencies respectively, μ is the chemical potential, and the parameter γ is given by

$$
\gamma = \frac{\Omega'}{\Omega} = \left[[\sqrt{1 + 4s_x t_x^2} - 0.5t_x][\sqrt{1 + 4s_y t_y^2} - 0.5t_y][\sqrt{1 + 4s_z t_z^2} - 0.5t_z]\right]^{1/3}.
\tag{5}
$$

This parameter gives the ratio between the effective trapping frequencies of the combined potential and the effective trapping frequencies of the magnetic potential. Moreover, it includes the effect of the depth of the optical potential. In the absence of the optical potential $\gamma = 1$.

The chemical potential for this system is a local potential and it is dependent on the lattice site k. For the system under consideration the chemical potential can be approximated by the functions [16, 21, 22]

$$
\mu_{k=0} = \left(\frac{\pi^2(V_x V_y V_z)^{1/3}}{4E_{\mathrm{R}}}\right)^{1/10}\mu_0 = \left(\frac{\pi^2(s_x s_y s_z)^{1/3}}{4}\right)^{1/10}\mu_0,
\tag{6}
$$

where μ_0 is the chemical potential in the absence of the lattice. For simplicity, one has to use a dimensionless interaction parameter η in equation (6), first introduced by Dalfovo et al. and Naraschewski [23, 24]. This parameter is determined by the ratio between the chemical potential calculated at $T = 0$ and the transition temperature T_0 for the noninteracting particles in the same trap,

$$
\eta = \frac{\mu_{0,T=0}}{K_{\mathrm{B}}T_0}.
\tag{7}
$$

This scaling parameter vanishes when the thermodynamic limit is taken [17]. In terms of η the chemical potential is given by

$$
\frac{\mu_{k=0}}{K_{\mathrm{B}}T_0} = \eta\left(\frac{\pi^2(s_x s_y s_z)^{1/3}}{4}\right)^{1/10}
\tag{8}
$$

This equation shows that increasing the lattice depth in the x, y and z lead to increasing in the chemical potential of the condensate. This behavior is in agreement with the theoretical calculation given in [25] and it is generalization for the well known Thomas-Fermi results holding for magnetically trapped condensate [23] to include the effects of the optical lattice [19].

Mainly, the BEC is described within the grand canonical ensemble. Moreover, its relevant thermodynamic quantities are calculated from the partial derivative of the corresponding thermodynamical potential q. For a Boson trapped in a combined potential the thermodynamical potential q is given by the relation [11, 14, 15, 16]

$$
\begin{aligned}
q &= q_0 + \sum_{j=1}^{\infty} \frac{z^j}{j} \int_0^{\infty} \rho(\epsilon) e^{-j\beta\epsilon} d\epsilon, \\
&= q_0 + \gamma^{-3} \left[\left(\frac{K_B T}{\hbar\Omega} \right)^3 g_4(z) + \left(\frac{K_B T}{\hbar\Omega} \right)^2 g_3(z) \left\{ \frac{3}{2} \frac{\bar{\omega}}{\Omega} + \frac{2}{3} \frac{\mu_k}{\hbar\bar{\omega}} \gamma \right\} \right],
\end{aligned}
\tag{9}
$$

where $g_k(z) = \sum_{j=1}^{\infty} (z^j/j^k)$ is the usual Bose function.

3. Effective size and expansion energy

One of the key parameters for describing an expanding condensate is its effective area, which is normally defined as the square root of the condensate widths along the two symmetric axis. In general, for the magnetic traps that are used in the experiment the axis are parallel to the axial and the radial direction, respectively. Theoretically, the expansion of the condensate width and its effective size as a function of temperature, can be calculated from the first principal of quantum mechanics [9, 26]. In the following, for simplicity I will consider an isotropic harmonic potential. Generalization to an isotropic one is straightforward.

The width of a single particle state $|n\rangle$ of a trapped Bose gas in spherically symmetric potential

$$
V(r) = \frac{M}{2} \omega_{\text{com}}^2 r^2 - \frac{k^4}{3} \quad (V_x x^4 + V_y y^4 + V_z z^4)
$$

is given by [10],

$$
\langle r_n^2 \rangle = \frac{\langle 2V(r) \rangle}{M\omega_{\text{com}}^2} = \frac{E_n}{\hbar\omega_{\text{com}}^2} a_r^2,
\tag{10}
$$

where $\mathbf{E}_n = n\hbar\omega_{\text{com}} + \frac{3}{2}\hbar(\omega_{\text{com}} - \frac{\omega_R}{2})$, with $\omega_{\text{com}} = \sqrt{\omega^2 + \omega_{\text{lat}}^2}$ and $a_r = \sqrt{\frac{\hbar}{M\omega_{\text{com}}}}$ is the characteristic length

for the trap. The average width of a state $|n\rangle$ occupied by N particles is given by

$$
\begin{aligned}
\langle r^2 \rangle &= \sum_{n=0}^{\infty} N_n \langle r_n^2 \rangle \\
&= \frac{a_r^2}{\hbar\omega_{\text{com}}} \sum_{n=0}^{\infty} N_n \mathbf{E}_n \\
&= \frac{a_r^2}{\hbar\omega_{\text{com}}} (K_{\text{B}}T^2) \frac{\partial q}{\partial T}|_z \\
&= \left\{ \frac{a_r^2}{\hbar\omega_{\text{com}}} \mathbf{E}_0 + r_c^2 \left[\left(\frac{T}{T_0}\right)^4 + \frac{2}{3}\frac{\zeta(3)}{\zeta(4)} R \left(\frac{T}{T_0}\right)^3 \right] \right\}, \quad \left(\frac{T}{T_0}\right) < 1 \\
&= \left\{ \frac{a_r^2}{\hbar\omega_{\text{com}}} \mathbf{E}_0 + r_c^2 \left[\alpha\left(\frac{T}{T_0}\right) + \frac{2}{3}\frac{g_3(z)}{\zeta(4)} R \right] \right\}, \quad \left(\frac{T}{T_0}\right) \geq 1.
\end{aligned}
\tag{11}
$$

Here, $r_c^2 = 3a_r^2\zeta(4)[N/\zeta(3)]^{4/3}$ denotes the width of the condensate at $(\frac{T}{T_0}) = 1$, $\alpha = \frac{g_4(z)\zeta(3)}{g_3(z)\zeta(4)} \approx 1$ has a weak dependence on the temperature and N_n is the usual Bose-Einstein distribution. Bracket in equation (11) takes a familiar form with the first term denoting the ground state size (condensate), while the second term gives the excited states(thermal component). Zhang et al. [9] pointed that for high temperature $K_{\text{B}}T >> \hbar\omega_{\text{com}}$ the contribution from the condensate can be ignored. This approximation leads to the relations

$$
\begin{aligned}
\frac{\langle r^2 \rangle}{r_c^2} &= \left(\frac{T}{T_0}\right)^4 + \frac{2}{3}\frac{\zeta(3)}{\zeta(4)} R \left(\frac{T}{T_0}\right)^3, \quad \left(\frac{T}{T_0}\right) < 1 \\
&= \left(\frac{T}{T_0}\right) + \frac{2}{3}\frac{g_3(z)}{\zeta(4)} R, \quad \left(\frac{T}{T_0}\right) \geq 1
\end{aligned}
\tag{12}
$$

with

$$
R = \left[\frac{3}{2}\frac{\bar{\omega}}{\Omega}\left(\frac{\zeta(3)}{N}\right)^{1/3} + \frac{2}{3}\gamma^2 \eta \frac{\Omega}{\bar{\omega}}\left(\frac{\pi^2(s_x s_y s_z)^{1/3}}{4}\right)^{1/10} \right].
\tag{13}
$$

Results in equation (12) is consistent with the earlier experimental reports that the width of the absorption image of a Bose gas is proportional to its temperature in the absence of a condensate [4, 8]. A sudden drop for the effective width occurs when temperature is lowered than the transition temperature T_0. In the following, the condensate phase will be considered in detail, that is in the case of $(\frac{T}{T_0}) < 1$.

For cylindrically symmetric trap with combined frequencies $\omega_x = \omega_y$ and $\omega_z = \lambda\omega_{x,y}$ (for which the effective potential is defined in equation (1)), the temperature dependence of the three lengths are the same as in a spherically symmetric trap discussed above, except that the prefactors become

$$
\begin{aligned}
z_c^2 &= a_z^2 \lambda^{\frac{2}{3}} \zeta(4)[N/\zeta(3)]^{4/3} \\
x_c^2 &\equiv y_c^2 = a_{x,y}^2 \lambda^{-\frac{1}{3}} \zeta(4)[N/\zeta(3)]^{4/3},
\end{aligned}
\tag{14}
$$

where $a_{x,y,z} = \sqrt{\hbar/M\omega_{x,y,z}}$ are the characterized lengths for the axial and radial directions, respectively. The

effective size can be parametrized from equation (14) as

$$
\begin{aligned}
S(t) &= \sqrt{\langle z^2 \rangle \langle x^2 \rangle} \\
&= S_c \lambda^{-\frac{1}{6}} \left\{ \left(\frac{T}{T_0} \right)^4 + \frac{2}{3} \frac{\zeta(3)}{\zeta(4)} R \left(\frac{T}{T_0} \right)^3 \right\},
\end{aligned}
\tag{15}
$$

where $\lambda = \frac{\omega_z}{\omega_x}$, $S_c = a_z a_x \zeta(4)[N/\zeta(3)]^{4/3}$ is the effective size at the transition temperature and $\langle z^2 \rangle$ and $\langle x^2 \rangle$ are the effective square lengths in the axial and radial direction respectively, it is defined such that $\frac{\langle z^2 \rangle}{z_c^2} = \frac{\langle x^2 \rangle}{x_c^2} = \frac{\langle y^2 \rangle}{y_c^2} = \{ (\frac{T}{T_0})^4 + \frac{2}{3} \frac{\zeta(3)}{\zeta(4)} R (\frac{T}{T_0})^3 \}$.

The calculated results from equation (15) are represented in Figures 1 and 2. These two figures reveal

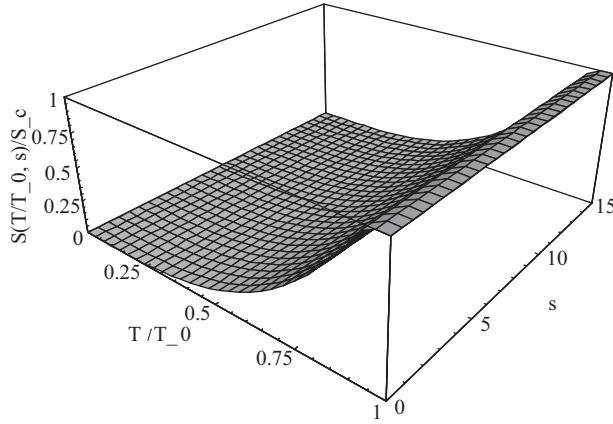**Figure 1**. Effective size as a function of the reduced temperature and the normalized lattice depth $s = (V_x V_y V_z)^{1/3}/E_{\mathrm{R}}$. The relative frequency is taken to be $t = \omega_{\mathrm{R}}/(\omega_x \omega_y \omega_z)^{1/3} = 0.1$. The trap parameters are: $\omega_x = \omega_y = 2\pi \times 50$ Hz, $\omega_z = 2\pi \times 500$ Hz, and $N = \times 10^5$.

that the effective size is sensitive to the variation of temperature and the lattice depth or the relative frequency, respectively. At temperature below BEC transition, Figure 1 reveals that the effective size is freezing at the value S_c at temperature $T = .95 T_0$. For any lattice depth the effective size increases monotonically to its maximum value with T increasing toward T_0.

Figure 2 shows that the effective size freezes at the value S_c at temperature $T = .85 T_0$. Thus, the effect of changing the magnetic trap is more than the effect of changing the lattice depth. However, freezing out of the effective size is used as an indicator of losing the SF [18, 19]. So, the effective size may be served as a practical thermometer to identify the temperature range of the MI phase. At this site, the obtained results provide a solid theoretical foundation for the experiment.

Another important quantity to discuss is the expansion energy (release energy) in the axial and redial direction. It can be calculated from the experimental measurements of its axial and redial width and the time of flight as has been done in [4, 27]. Since the width of the condensate is measured after a long time-of flight, the expansion energy is set to be a pure kinetic energy [8, 9]. From the first principal of mechanics, the expansion
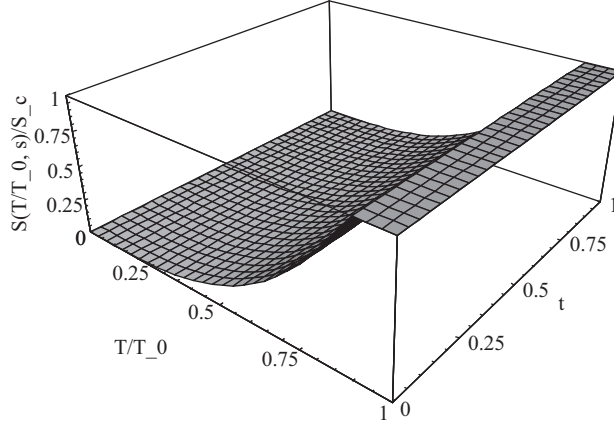
Figure 2. Effective size as a function of the reduced temperature T/T_0 and the relative frequency $t = \omega_{\mathrm{R}}/(\omega_x\omega_y\omega_z)^{1/3}$. The lattice depth is taken to be $s = (s_x s_y s_z)^{(1/3)} = 12$. The same trap parameters given in Figure 1 are used.

energy in radial and axial direction are fixed by the relations

$$
\begin{aligned}
E_z &= \frac{1}{2}M\left\langle v_z^2 \right\rangle_{\tau\to\infty} = \frac{1}{2\tau^2}M\left\langle z^2 \right\rangle_{\tau\to\infty} \\
E_x &\equiv E_y = \frac{1}{2\tau^2}M\left\langle y^2 \right\rangle_{\tau\to\infty},
\end{aligned}
\tag{16}
$$

where τ is the time of flight and v is velocity of flight. Assuming that, on average, the kinetic and interaction energy are equal, then

$$
\begin{aligned}
E_z &= \frac{1}{2\tau^2}M z_c^2 \left\{ \left(\frac{T}{T_0}\right)^4 + \frac{2}{3}\frac{\zeta(3)}{\zeta(4)}R\left(\frac{T}{T_0}\right)^3 \right\} \\
E_x &\equiv E_y = \frac{1}{2\tau^2}M y_c^2 \left\{ \left(\frac{T}{T_0}\right)^4 + \frac{2}{3}\frac{\zeta(3)}{\zeta(4)}R\left(\frac{T}{T_0}\right)^3 \right\}
\end{aligned}
\tag{17}
$$

Where equation (12) is used here. Rescaling equation (17) by the characteristic energy scale $NK_{\mathrm{B}}T_0$, one has

$$
\begin{aligned}
\frac{E_z}{NK_{\mathrm{B}}T_0} &= \frac{\lambda^{\frac{2}{3}}}{2\tau^2\omega_z'^2} \left\{ \frac{\zeta(4)}{\zeta(3)}\left(\frac{T}{T_0}\right)^4 + \frac{2}{3}R\left(\frac{T}{T_0}\right)^3 \right\} \\
\frac{E_x}{NK_{\mathrm{B}}T_0} &\equiv \frac{E_y}{NK_{\mathrm{B}}T_0} = \frac{\lambda^{-\frac{1}{3}}}{2\tau^2\omega_y'^2} \left\{ \frac{\zeta(4)}{\zeta(3)}\left(\frac{T}{T_0}\right)^4 + \frac{2}{3}R\left(\frac{T}{T_0}\right)^3 \right\}.
\end{aligned}
\tag{18}
$$

This equation provides a very important result; it shows that the expansion along the axial direction is less than the expansion in the radial direction by a factor λ, i.e. $E_z = \lambda E_{x,y}$, independent of both lattice depths. The difference in the expansion energy is attributed to the strong anisotropy of the trapping potential. The lack of expansion in the axial direction reflects the fact that the condensate has effectively been split up into several smaller condensates confined in the individual lattice wells [3].

4.   Conclusion

In this paper, a detailed study has been given of a Bose gas trapped in a 3D combined harmonic-optical potential. Simple analytical semiclassical approximation based on a piecewise density of states (DOS) is used in this study. The effective size and the expansion energy are investigated. The main effects which can alter the Bose gas in such trap are collected simultaneously in one parameter, R. Thus, for a non-cubic optical potential, one has to use the pure harmonically trapped boson gas as the zeroth order approximation in any perturbation for numerically treatment of this system. The obtained results show that both the lattice depth and the relative frequency have significant effects on this two parameters. The effect of anisotropic of the magnetic trap frequency is much more than the effect of lattice depth. The above mentioned quantities can be characterized the SF-MI transition for the experimental systems with interacting atoms in an optical lattice. Thus, the obtained results provide a solid theoretical foundation for the current experiments. Finally, the calculated parameters have the same behavior under decreasing or increasing temperature, and lattice depth. Thus they are fully reversible. This means that both SF and MI phases are quantum phases for any optical potential [28].

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