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A THEORETICAL STUDY OF BOSE GAS TRAPPED IN A 3D COMBINED HARMONIC-OPTICAL POTENTIAL AND AN EVALUATION OF EFFECTIVE SIZE AND EXPANSION ENERGY OF A BOSE-EINSTEIN CONDENSATE IN A 3D NON-CUBIC OPTICAL LATTICE

RAJIV KUMAR SINGH[2], LALIT KUMAR MISHRA[1]

1. Department of Physics, Magadh University, Bodh-Gaya-824234(Bihar)
2. Higher Secondary Teacher, Department of Physics, Town Inter School, Aurangabad-824101 (Bihar)

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Abstract: - Using the theoretical formalism of **Sheni S. M. Soliman (Turk J. Phys. 35 (2011))**, we have theoretically studied Bose gas trapped in a 3D combined harmonic-optical potential. We have evaluated the effective size and expansion (release) energy of Bose-Einstein condensate in a 3D non-cubic optical lattice. Our theoretically evaluated results show that both the lattice depth and the relative frequency have significant effects on these two parameters. We have also observed that the effect of anisotropic of magnetic trap frequency is more than the effect of lattice depth. These two quantities can be characterized the SF-MI transition for the experimental system with an interacting atoms in an optical lattice. Our theoretically evaluated results of expansion energy is roughly $E_z=\lambda E_{x,y}$ where λ is a parameter. Our theoretically evaluated results are in good agreement with other theoretical workers.

Keywords: Effective size, expansion energy, 3D non-cubic optical lattice, Super fluid(SF)-Mott Insulator(MI) phase transition, trap geometry, Semi classical approximation, parameterized DOS(density of states), recoil energy, Thomas Fermi approximation, Thermo dynamical properties for BEC in optical lattice

Corresponding Author: MR. RAJIV KUMAR SINGH

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INTRODUCTION

Trapped Bose gases in a combined harmonic-optical potential used as a prototype for strongly quantum phase transition. The condensed Bosons in an Optical potential offer a new opportunity to investigate the interplay connection between the super fluids (SF) and Mott insulator (MI) phase transition[1]. Experiments show that the phase coherent Bose Einstein condensate (BEC) in the optical lattice is a super fluids (SF)[2]. It was also pointed out that, as the lattice depth is increased the quantum tunneling of atoms from one optical size to another is stopped, resulting in loss of super fluidity which is identified as the vanishing of condensed fraction. In such case BEC is transformed to MI State in which numbers of atoms are localized at individual lattice sites and its free mobility to 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 super fluid-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[3-7]. 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 parameters of 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[8-10] T_C. Moreover, they are affected by changing of the lattice depth or relative frequency (the ratio between recoil frequency and geometrical average of harmonic frequencies).

In this paper, using the theoretical formalism of Sheni S. M. Soliman[11], we have theoretically estimated the effective size and expansion energy of a 3D non cubic optical lattice. The evaluation has been performed with the use of semi classical approximation in which density of state (DOS) approach has been used. In this approach the sum over the energy levels for the thermo dynamic quantities are approximated directly by ordinary integrals weighted by an appropriate DOS. This type of approximation is widely used in variety of problems in statistical physics[12] and in BEC[13-17]. Earlier studies have showed that the resulting thermo dynamical parameter depends on the choice and construction of DOS. Our theoretically evaluated results show that both these parameters have significant effects on the lattice depth and relative frequency. The effect of anisotropy of magnetic trap frequency has more pronounced than the lattice depth. Our theoretically evaluated results are in good agreement with other theoretical workers[18-20].

MATERIALS AND METHODS:

One considers a boson gas trapped in a combined potential given by[21,6]

$$V(z)=\frac{1}{2}m[(\omega^2{}_x+\omega^2{}_{lat,x})x^2+(\omega^2{}_y+\omega^2{}_{lat,y})y^2+(\omega^2{}_z+\omega^2{}_{lat,z})z^2]$$

$$-\frac{1}{3}k^4(V_x x^4+V_y y^4+V_z z^4) \quad (1)$$

Where $\omega_{lat,l}=\frac{2\sqrt{E_r V_l}}{\hbar}$, 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 laser beam is accounted by k=2π/λ$'$, with λ$'$ is laser wavelength. E_R is the recoil energy, $E_R=(\hbar^2k^2/2m)=\hbar\omega_R$ as energy scale which measures the lattice depth. Now the potential is characterized by single particle energy level

$$E_n=n_x\hbar(\omega_{x'}-\frac{\omega_R}{2})+n_y\hbar(\omega_{y'}-\frac{\omega_R}{2})+n_z\hbar(\omega_{z'}-\frac{\omega_R}{2})+E_0 \quad (2)$$

Where $\omega_{l'}=\omega^2{}_l+\omega^2{}_{lat,l}$ 3(a)

$$E_0=\frac{3}{2}\hbar\bar{\omega} \quad 3(b)$$

$$\bar{\omega}=\frac{1}{3}[\omega^2{}_x+\omega_y{}^2+\omega_z{}^2-\frac{3}{2}\omega_R] \quad 3(c)$$

$\bar{\omega}$ is the mean of the combined frequencies. Lattice potential depth is measured in the unit of recoil energy E_R.

Now

$$\omega'_x=[\omega^2{}_x+\frac{4E_R V_x}{\hbar^2}]^{\frac{1}{2}}=\omega_x[1+4S_x t^2{}_x]^{\frac{1}{2}} \quad 4(a)$$

$$\omega'_y = [\omega^2{}_y + \frac{4E_R V_y}{\hbar^2}]^{\frac{1}{2}} = \omega_y[1+4S_y t^2{}_y]^{\frac{1}{2}} \quad 4(b)$$

$$\omega'_z = [\omega^2{}_z + \frac{4E_R V_z}{\hbar^2}]^{\frac{1}{2}} = \omega_z[1+4S_z t^2{}_z]^{\frac{1}{2}} \quad 4(c)$$

$$S_{x,y,z} = \frac{V_{x,y,z}}{E_R} \quad 4(d)$$

$$t_{x,y,z} = \frac{\omega_R}{\omega_{x,y,z}}, E_R = \hbar\omega_R \quad 4(e)$$

$$\overline{\omega} = \frac{1}{3}[(\omega_x[1+4S_x t^2{}_x]^{\frac{1}{2}} - \frac{t_x}{2}) + (\omega_y[1+4S_y t^2{}_y]^{\frac{1}{2}} - \frac{t_y}{2}) + (\omega_z[1+4S_z t^2{}_z]^{\frac{1}{2}} - \frac{t_z}{2})] \quad (5)$$

The density of states (DOS) for the spectrum of equation (2) is calculated and is given b[22]

$$\rho(\varepsilon) = \frac{1}{2}\frac{\varepsilon^2}{(\hbar\Omega')^3} + \frac{\varepsilon}{(\hbar\Omega')^2}[\frac{3}{2}\frac{\overline{\omega}}{\Omega'} + \frac{2}{3}\frac{\mu}{\hbar\overline{\omega}}]$$

$$\frac{1}{\gamma^3}[\frac{1}{2}\frac{\varepsilon^2}{(\hbar\Omega')^3} + \frac{\varepsilon}{(\hbar\Omega')^2}\{\frac{3}{2}\frac{\overline{\omega}}{\Omega'} + \frac{2}{3}\frac{\mu}{\hbar\overline{\omega}}\gamma\}] \quad (6)$$

Where

$$\Omega' = [(\omega'_x - \frac{\omega_R}{2})(\omega'_y - \frac{\omega_R}{2})(\omega'_z - \frac{\omega_R}{2})]^{\frac{1}{3}} \quad 7(a)$$

$$\Omega = [\omega_x\omega_y\omega_z]^{\frac{1}{3}} \quad 7(b)$$

These are the geometrical average of the combined frequencies and the harmonic frequencies respectively. μ is the chemical potential and parameter γ is given by

$$\gamma = \frac{\Omega'}{\Omega} = [[\sqrt{1+4S_x t^2{}_x} - 0.5t_x][\sqrt{1+4S_y t^2{}_y} - 0.5t_y][\sqrt{1+4S_z t^2{}_z} - 0.5t_z]]^{\frac{1}{3}} \quad 7(c)$$

This parameter gives the ratio between the effective trapping frequencies of the combined potential and the effective trapping frequencies of magnetic potential. In the absence of optical potential γ=1.0.

The chemical potential of the 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 function[16,23,24]

$$\mu(k=0) = [\pi^2 (V_x V_y V_z)^{\frac{1}{3}} / 4E_R]^{\frac{1}{10}} \mu_0$$

$$= [\pi^2 (S_x S_y S_z)^{\frac{1}{3}} / 4]^{\frac{1}{10}} \mu_0 \qquad 7(d)$$

μ_0 is the chemical potential in the absence of the lattice. Now, one introduces [25,26] a dimensionless interaction parameter in equation 7(d). This parameter is determined by the ratio between the chemical potential calculated at T=0 and the transition temperature T_c for the non interacting particles in the same trap

$$\eta = \frac{\mu_0, T=0}{K_\beta T_C} \qquad 8(a)$$

In terms of η, chemical potential is given by

$$\frac{\mu(k=0)}{K_\beta T_C} = \eta [\pi^2 (S_x S_y S_z)^{\frac{1}{3}} / 4]^{\frac{1}{10}} \qquad 8(b)$$

This equation tells that increasing the lattice depth in the x,y,z direction leads to increasing the chemical potential of the condensate. This fact is in agreement with the theoretical calculation done by other theoretical workers[27-30]. This is the generalization of well known Thomas Fermi results which holds for magnetically trapped condensates. It also indicates the effect of optical lattice[31-34].

Calculation of effective size and expansion (release) energy

Now, one defines the key parameters for an expanding area of the condensate. It is defined as the square root of the condensate widths along the two symmetric axis. These are parallel to the axial and radial directions respectively for the magnetic traps. Theoretically, one calculates the condensate width and its effective size as a function of temperature from the first principles of quantum mechnics[35]. The width of the single particle state $|n\rangle$ of a trapped Bose gas in a spherically symmetric potential is given by

$$v(r)=\frac{M}{2}\omega^2{}_{com}r^2-\frac{k^4}{3}(V_x x^4+V_y y^4+V_z z^4) \qquad 9(a)$$

$$\langle r^2{}_n\rangle=\frac{\langle 2V(r)\rangle}{M\omega^2{}_{com}}=\frac{E_n}{\hbar\omega^2{}_{com}}a^2{}_r \qquad 9(b)$$

Where

$$E_n=n\hbar\omega_{com}+\frac{3}{2}\hbar(\omega_{com}-\frac{\omega_R}{2}) \qquad 9(c)$$

$$\omega_{com}=[\omega^2+\omega^2{}_{lat}]^{\frac{1}{2}} \qquad 9(d)$$

$$a_r=[\frac{\hbar}{M\omega_{com}}]^{\frac{1}{2}} \qquad 9(e)$$

a_r is the characteristic length of the trap. The average width of the state $|n\rangle$ is occupied by N particles is given by

$$\langle r^2\rangle=\sum_{n=0}^{\infty}N_n\langle r^2\rangle$$

$$=\frac{a^2{}_r}{\hbar\omega_{com}}\sum_{n=0}^{\infty}N_n\overline{E_n}$$

$$=\{\frac{a^2{}_r}{\hbar\omega_{com}}\overline{E_0}+r_c{}^2[(\frac{T}{T_C})^4+\frac{2}{3}\frac{\xi(3)}{\xi(4)}R(\frac{T}{T_C})^3]\}\ ,\quad (\frac{T}{T_C})\prec 1 \qquad 10(a)$$

$$=\{\frac{a^2{}_r}{\hbar\omega_{com}}\overline{E_0}+r^2{}_c[\alpha(\frac{T}{T_C})+\frac{2}{3}\frac{g_3(z)}{\xi(4)}R]\}\ ,\quad (\frac{T}{T_C})\succ 1 \qquad 10(b)$$

Where

$$r^2{}_c = 3a^2{}_r \xi(4)[\frac{N}{\xi(3)}]^{\frac{4}{3}} \qquad 10(c)$$

Denotes the width of the condensate at (T/T_C)=1.0. $\alpha = \frac{g_4(z)\xi(3)}{g_3(z)\xi(4)}$ =1 has weak dependence on the temperatures and N_n is the usual Bose Einstein distribution. Now, the first term in the bracket of equation (10) denote the ground state size (condensate) while the second term gives the excited states (Thermal components). For high temperature the above approximation leads to

$$\frac{\langle r^2 \rangle}{r^2{}_c} = (\frac{T}{T_C})^4 + \frac{2\xi(3)}{3\xi(4)} R (\frac{T}{T_C})^3 \quad , \quad (\frac{T}{T_C}) \prec 1 \qquad 11(a)$$

$$= (\frac{T}{T_C}) + \frac{2}{3}\frac{g_3(z)}{\xi(4)} R \quad , \quad (\frac{T}{T_C}) \succ 1 \qquad 11(b)$$

With

$$R = [\frac{3}{2}\frac{\overline{\omega}}{\Omega}(\frac{\xi(3)}{N})^{\frac{1}{3}} + \frac{2}{3} r^2 \eta \frac{\Omega}{\omega}(\frac{\pi^2 (S_x S_y S_z)^{\frac{1}{3}}}{4})^{\frac{1}{10}}] \qquad (12)$$

Result of equation (11) is consistent with the earlier experimental reports that the width of the absorption images of a Bose gas is proportional to its temperature in the absence of the condensate. A sudden drop of the effective width occurs when temperature is lowered than the critical temperature T_C.

For cylindrically symmetric trap with combined frequency $\omega_x = \omega_y$ and $\omega_z = \lambda \omega_{x,y}$, the temperature dependence of the three length are the same. In that case

$$z^2{}_c = a^2{}_z \lambda^{\frac{2}{3}} \xi(4)[\frac{N}{\xi(3)}]^{\frac{4}{3}} \qquad 13(a)$$

$$x^2{}_c = y^2{}_c = a^2{}_{x,y} \lambda^{\frac{-1}{3}} \xi(4)[\frac{N}{\xi(3)}]^{\frac{4}{3}} \qquad 13(b)$$

where $a_{x,y,z} = [\frac{\hbar}{M\omega_{x,y,z}}]^{\frac{1}{2}}$ 13(c) are the characterized length for the axial and radial direction respectively. Using equation (13), the effective size can be written as

$$S(t) = [\langle z^2 \rangle \langle x^2 \rangle]$$

$$= S_c \lambda^{\frac{-1}{6}} [(\frac{T}{T_C})^4 + \frac{2}{3}\frac{\xi(3)}{\xi(4)} R(\frac{T}{T_C})^3] \quad (14)$$

Where $\lambda = \frac{\omega_z}{\omega_c}$, $S_c = a_z a_x \xi(4)[\frac{N}{\xi(3)}]^{\frac{4}{3}}$ is the effective size at the transition temperature T_C and $\langle z^2 \rangle$ and $\langle x^2 \rangle$ are the effective square lengths in the axial and radial direction respectively.

__Calculation of expansion (release) energy__

Expansion energy is calculated from the experimental measurement of its axial and radial width and time of flight. Since the width of the condensate is measured after long time of flight the expansion energy is set to be pure kinetic[36].

Using the principle of mechanics, the expansion energy in radial and axial direction are fixed by the relation

$$E_z = \frac{1}{2} M \langle v^2{}_z \rangle_{\tau\to\infty} = \frac{1}{2\tau^2} M \langle z^2 \rangle_{\tau\to\infty} \quad 15(a)$$

$$E_x = E_y = \frac{1}{2\tau^2} M \langle y^2 \rangle_{\tau\to\infty} \quad 15(b)$$

Where τ is the time of flight and v is the velocity of flight. Assuming that on average the kinetic and interaction energies are equal, we have

$$E_z = \frac{1}{2} M z^2{}_c [(\frac{T}{T_C})^4 + \frac{2}{3}\frac{\xi(3)}{\xi(4)} R(\frac{T}{T_C})^3] \quad 16(a)$$

$$E_x = E_y = \frac{1}{2} M y^2{}_c [(\frac{T}{T_C})^4 + \frac{2}{3}\frac{\xi(3)}{\xi(4)} R(\frac{T}{T_C})^3] \quad 16(b)$$

Using equation (11) and rescaled equation (16) by the characteristic length scale $NK_{\beta}T_C$, one has

$$\frac{E_z}{NK_{\beta}T_C}=\frac{\lambda^{\frac{2}{3}}}{2\tau^2\omega'^2_z}[\frac{\xi(4)}{\xi(3)}(\frac{T}{T_C})^4+\frac{2}{3}R(\frac{T}{T_C})^3] \quad 17(a)$$

$$\frac{E_x}{NK_{\beta}T_C}=\frac{E_y}{NK_{\beta}T_C}=\frac{\lambda^{\frac{-1}{3}}}{2\tau^2\omega'^2_y}[\frac{\xi(4)}{\xi(3)}(\frac{T}{T_C})^4+\frac{2}{3}R(\frac{T}{T_C})^3] \quad 17(b)$$

These are the required expression for expansion energy in the radial and axial direction respectively.

RESULTS AND DISCUSSION

In this paper, using the theoretical formalism of Shemi S. M. Soliman[11] we have theoretically studied Bose gas trapped in a 3D combined harmonic-optical potential. In this study simple analytical semi-classical pair wise density of states(DOS) is used. In **table T1**, we have presented the evaluated results of effective size as a function of reduced temperature and normalized lattice depth $s=\frac{(V_xV_yV_z)^{\frac{1}{3}}}{E_R}$ where E_R is recoil energy. The relative frequency is taken to be $t=\frac{\omega_R}{(\omega_x\omega_y\omega_z)^{\frac{1}{3}}}=0.52$. The trap potential parameters are $\omega_x=\omega_y=2\pi x50Hz$, $\omega_z=2\pi x500Hz$ and N=6x10^5. Our theoretical results indicate that the effective size is sensitive to the variation of temperature and lattice depth or the relative frequency respectively. At temperature below transition temperature T_C the effective size is freezing at the value of S_C at temperature T=0.967T_C. For any lattice depth the effective size increases to maximum value with T increasing towards T_C. In **table T2,** we have presented the evaluated results of the effective size as a function of the reduced temperature T/T_C and the relative frequency $t=\frac{\omega_R}{(\omega_x\omega_y\omega_z)^{\frac{1}{3}}}$. The lattice depth is taken to be $s=(S_xS_yS_z)^{\frac{1}{3}}$=15. The other parameters are the same as in **table T1**. Our theoretical results indicate that the effective size freezes at the value of S_C at temperature T=0.896 T_C. This shows that the effect of changing the magnetic trap is more than the effect of changing the lattice depth. This also indicates that freezing out of the effective size is an indicator of losing SF (super fluid) phase. It appears that the effective size may be served as practical thermometer to identify the temperature range of the MI (Mott- Insulator) phase. We have also obtained the expression for expansion (release) energy using equation 17(a) and 17(b). We have shown the results of expansion energy $\frac{E_z}{NK_\beta T_c}$ along the radial direction and $\frac{E_x}{NK_\beta T_c} = \frac{E_y}{NK_\beta T_c}$ along axial direction as a function of T/T_C. The results are shown in **tableT3** and **table T4** respectively. In this evaluation we have kept λ=10 and τ=100ns. Our theoretical results show that expansion energy along axial direction is less than the value obtained in the radial direction by a factor λ i.e. $E_z=\lambda E_{x,y}$. they are independent of the lattice depth. 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 been effectively split up into several smaller condensates confined in the individual lattice well[37]. Our results also indicate that both the effective size and expansion energy follow characteristic temperature dependence. $\langle r^2 \rangle$, $E\alpha(\frac{T}{T_C})^4$ if $T < T_C$ and $\langle r^2 \rangle$, Eα (T/T_C) for $T>T_C$. For a 3D non-cubic optical potential, the effect of relative frequency is much more than the effect of the potential depth. Thus, for non-cubic optical potential, one has to use the pure harmonically trapped boson gas as the zeroth order approximation in any perturbation or numerical treatment of this system. Our theoretically evaluated results are in good agreement with those of the other theoretical workers[18,19]. Some recent works[38-45] also reveals the same behavior.

CONCLUSION:

From the above theoretical analysis and investigations, we have come across the following conclusions

(1)For the study of Bose gas trapped in a 3D combined harmonic-optical potential, analytical semi classical approximation based pair wise density of states (DOS) can be used.

(2)In the calculation of effective size and expansion energy, the main effects which can alter the Bose gas in such a trap is one parameter R

(3)Our calculation indicates that both the lattice depth and the relative frequency have significant effect

(4)The effect of anisotropic of magnetic trap frequency is much more than the effect of lattice depth.

(5)Our theoretically evaluated results have the same behavior under decreasing or increasing temperature and lattice depth. This also confirms that SF and MI are quantum phases.

Table T1: **An evaluated result of effective size as a function of the reduced temperature and normalized lattice depth** $\frac{(V_x V_y V_z)^{\frac{1}{3}}}{E_R}$ **. The relative frequency is taken to be equal to** $t = \frac{\omega_R}{(\omega_x \omega_y \omega_z)^{\frac{1}{3}}} = 0.52$ **. The trap parameters are** $\omega_x = \omega_y = 2\pi x 50 Hz$ **,** $\omega_z = 2\pi x 500 Hz$ **and** $N = 6x10^5$**.**

(T/T_C)	s	$S(T/T_C, s)/S_C$
0	0	0
0.20	2	0.168
0.25	4	0.232
0.30	5	0.276
0.35	6	0.386
0.40	7	0.445
0.45	8	0.539
0.50	9	0.618
0.55	10	0.686
0.60	11	0.723
0.70	12	0.786
0.80	13	0.845
0.90	14	0.932
1.00	15	0.997

Table T2: An evaluated results of effective size as a function of reduced temperature (T/T$_C$) and the relative frequency $t = \frac{\omega_R}{(\omega_x \omega_y \omega_z)^{\frac{1}{3}}}$. The lattice depth is taken to be $s = (S_x S_y S_z)^{\frac{1}{3}} = 15$. The other parameters are the same as in table1.

(T/T$_C$)	t	S(T/Tc, s)/S$_C$
0	0.0	0.0
0.20	0.22	0.179
0.25	0.26	0.246
0.30	0.34	0.283
0.35	0.38	0.375
0.40	0.42	0.418
0.45	0.47	0.497
0.50	0.56	0.574
0.60	0.67	0.682
0.70	0.73	0.743
0.80	0.82	0.835
0.90	0.94	0.926
1.00	0.99	0.974

Table T3: An evaluated results of expansion energy $\frac{E_z}{NK_\beta T_C}$ as a function of (T/T$_C$) keeping λ=10 and τ=100ns

(T/T$_C$)	$\frac{E_z}{NK_\beta T_C}$
0.1	0.00252
0.20	0.04266
0.30	0.20415
0.40	0.29104
0.50	0.41210
0.60	0.58927
0.70	0.74152
0.80	0.81642
0.90	0.92357
1.00	1.03294

TableT4: An evaluated result of expansion energy $\frac{E_x}{NK_\beta T_C}$ as a function of (T/T_C) keeping λ=10 and τ=100ns

(T/T_C)	$\frac{E_x}{NK_\beta T_C}$
0.10	0.00027
0.20	0.00432
0.30	0.01870
0.40	0.03217
0.50	0.05394
0.60	0.06582
0.70	0.07632
0.80	0.08436
0.90	0.09724
1.00	0.10426

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