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LETTER TO THE EDITOR

Microcanonical ensemble for Bose-condensed gas in optical lattices

Hongwei Xiong[1], Shujuan Liu[1] and Guoxiang Huang[2]

[1] Department of Applied Physics, Zhejiang University of Technology, Hangzhou, 310032, China
[2] Department of Physics, East China Normal University, Shanghai, 200062, China

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Abstract
The statistical properties of Bose-condensed gas in a magnetic trap and an optical lattice are investigated within the microcanonical ensemble. It is found that, due to the unique statistical behaviour of the thermal atoms in different lattice sites, we cannot describe the thermodynamics of the system by the usual boson statistics. The number of states for a fixed energy and number of atoms is given, and is used to investigate the distribution of the thermal atoms in different lattice sites.

The realization of Bose-condensed gas in a magnetic trap and an optical lattice [1] has opened up many new opportunities to develop a general theory to interpret the unique property of the ultra-low atomic gas [2]. In contrast to the BEC (Bose–Einstein condensation) in a magnetic trap, due to the presence of the optical lattice potential, there are a lot of condensates confined in the lattice sites. Especially, one can control the coherent properties of the condensates in different lattice sites by increasing the depth of the optical lattice. This sort of manipulation has led to the experimental realization of the quantum transition from a superfluid to a Mott insulator [3]. Statistical behaviour is a fundamental problem for the Bose-condensed gas in the combined potentials. The statistical properties of the ideal and weakly interacting Bose-condensed gases in a magnetic trap have been studied in a lot of theoretical works [4–17]. As far as we know, there is still no theoretical research on the statistical properties of Bose-condensed gas in the combined potentials. In particular, it is found that we cannot describe the statistical properties of Bose-condensed gas in the combined potentials by the usual boson statistics due to the different statistical behaviour of the thermal atoms and condensates.

For the Bose-condensed gas in an optical lattice, if the depth of the optical lattice is chosen so that the condensates are in a superfluid state and the tunnel effect for the thermal atoms in different wells can be omitted, the statistical properties in this case cannot be described by the usual boson statistics. For this situation, which has been realized in the experiments for the Bose-condensed gas in 1D (one-dimensional) [18, 19], 2D [20] and 3D [3, 21] optical lattices, the thermal atoms in different lattice sites are *distinguishable*, due to the fact that the overlap between the wavefunction of the thermal atoms in different lattice sites can be omitted safely. Note that, due to the superfluid behaviour of the condensates, through the exchanges between thermal atoms and condensates, there are still exchanges between the thermal atoms in different lattice sites. Thus the distribution of the thermal atoms in different lattice sites can be investigated by regarding the system as an equilibrium state. In addition, it is worth pointing out that the thermal atoms in a lattice site are *indistinguishable*.

Assuming that the overall number of atoms in the system is N and the overall number of atoms in the condensates is N_0, the overall number of thermal atoms is then $N_T = N - N_0$. Assuming further that N_{Ti} is the number of thermal atoms in the ith lattice site, we have $N_T = \Sigma_i N_{Ti}$. For the thermal atoms in the lattice site, assuming that n_{Ti}^j is the number of thermal atoms in the energy level indexed by j and the ith lattice site indexed by i, we have $N_{Ti} = \Sigma_j n_{Ti}^j$. In the microcanonical ensemble, based on the above analysis, the number of states of the system described by the distribution set $\{n_{Ti}^j, N_0\}$ is given by

$$W\{n_{Ti}^j, N_0\} = \frac{\Gamma N_T!}{\Pi_i N_{Ti}!}, \tag{1}$$

where Γ is a constant factor which should be investigated carefully. The factor $N_{Ti}!$ in the above expression is due to the *indistinguishable* behaviour for the thermal atoms in a lattice site. In the case of $N_T \to 0$, all the atoms are in the condensates (this is a system that can be investigated by boson statistics) and therefore are indistinguishable, thus $W\{n_{Ti}^j, N_0\} \to 1$. Under this consideration, we have $\Gamma = 1$. Note that, although the form of $W\{n_{Ti}^j, N_0\}$ is similar to the case of Boltzmann statistics, it is in fact different from Boltzmann statistics in essence. In the usual Boltzmann statistics, all the particles are regarded as distinguishable. In the problem discussed here, however, only the thermal atoms in different lattice sites are distinguishable.

In the microscopic ensemble, the overall number of atoms N and the overall energy E are fixed. The number of states for N and E is then

$$W\{N, E\} = \sum_{n_{Ti}^j}{}' \frac{N_T!}{\Pi_i N_{Ti}!}, \tag{2}$$

where the prime in the sum denotes the following confinement conditions in the summation of the above equation:

$$N = N_0 + \sum_{i,j} n_{Ti}^j, \tag{3}$$

and

$$E = E_0 + \sum_{i,j} \varepsilon_i^j n_{Ti}^j. \tag{4}$$

In equation (4), E_0 denotes the overall energy of the condensates, while ε_i^j represents energy level j of the thermal atoms in the ith lattice site. For this confinement condition about E, we have omitted the interaction energy between thermal atoms and the interaction energy between thermal atoms and condensates.

Now we turn to calculate the most probable distribution set $\{n_{Ti}^j, N_0\}$ by investigating $W\{n_{Ti}^j, N_0\}$. For equation (1), we have

$$\ln W\{n_{Ti}^j, N_0\} = N_T(\ln N_T - 1) - \sum_i N_{Ti}(\ln N_{Ti} - 1). \tag{5}$$

In deriving the above equation, we have used the well known Stirling formula $\ln x! = x(\ln x - 1)$. Because N_{Ti} is the overall number of atoms in the ith well, we have $N_{Ti} \gg 1$

for finite temperatures. This means that the Stirling formula can be used in the problem discussed here. Let $\{\tilde{n}^j_{Ti}, \tilde{N}_0\}$ denote the distribution of the atoms that maximizes $\ln W\{n^j_{Ti}, N_0\}$. By using the well known method of Lagrange multipliers we have

$$\delta \ln W\{n^j_{Ti}, N_0\} - \alpha\left(\delta N_0 + \sum_{i,j} \delta n^j_{Ti}\right) - \beta\left(\frac{\partial E_0}{\partial \tilde{N}_0}\delta N_0 + \sum_{i,j} \varepsilon^j_i \delta n^j_{Ti}\right) = 0, \quad (6)$$

where

$$\delta \ln W\{n^j_{Ti}, N_0\} = \ln \tilde{N}_T \sum_{i,j} \delta n^j_{Ti} - \sum_{i,j} \ln(\tilde{N}_{Ti})\delta n^j_{Ti}. \quad (7)$$

In addition, α and β are Lagrangian multipliers which will be determined by the confinement conditions given by equations (3) and (4). The overall energy of the condensates $E_0 = E_{int} + N_0\varepsilon_0$, with E_{int} the interaction energy and $N_0\varepsilon_0$ the energy due to the presence of the optical lattice potential. In this situation, $\partial E_0/\partial \tilde{N}_0 = \mu + \varepsilon_0$, with $\mu = \partial E_{int}/\partial \tilde{N}_0$ (i.e., the chemical potential of the system) and ε_0 the ground state energy level due to the presence of the optical lattice potential. For equation (6), since δn^j_{Ti} and δN_0 are independent variations when the method of Lagrangian multipliers is used, we have

$$\alpha + \beta(\mu + \varepsilon_0) = 0, \quad (8)$$

and

$$\ln(\tilde{N}_{Ti}) = \ln \tilde{N}_T - \beta(\varepsilon^j_i - \varepsilon_0 - \mu). \quad (9)$$

The most probable value of the number of atoms in the condensates is then

$$\tilde{N}_0 = N - \sum_i \tilde{N}_{Ti}. \quad (10)$$

Generally speaking, the constants $\tilde{N}_0$ and β can be obtained by using the confinement conditions given by equations (3) and (4).

From equation (9), one gets

$$\tilde{N}_{Ti} = \tilde{N}_T \mathrm{e}^{-\beta(\varepsilon^j_i - \varepsilon_0 - \mu)}. \quad (11)$$

From this form, we have $\beta = 1/k_B T$, with k_B the Boltzmann constant and T the temperature. In equation (11), ε^j_i is j-dependent, while $\tilde{N}_{Ti}$ is j-independent. For this formula to have physical significance, we must request that the thermal atoms can only exist in the first excited state. Assuming ε^{first}_i denotes the energy level of the first excited state, we have

$$\tilde{N}_{Ti} = \tilde{N}_T \mathrm{e}^{-(\varepsilon^{first}_i - \varepsilon_0 - \mu)/k_B T}. \quad (12)$$

Due to the unique statistical property for the Bose-condensed gas in an optical lattice, within the microcanonical ensemble, the high excited states of thermal atoms are frozen out. Nevertheless, there is still the possibility that the thermal atoms can exist in the high excited states when the fluctuations are considered, and especially when there is an energy exchange between the system and the external environment, where the canonical ensemble should be used. For the Bose-condensed gas in optical lattices, the thermal atoms can exist in different lattice sites. Assuming $(2k_{TM}+1)$ is the number of lattice sites that have thermal atoms, k_{TM} can be obtained by the normalization condition $\Sigma_i \tilde{N}_{Ti} = \tilde{N}_T$, i.e.,

$$\sum_{i=-k_{TM}}^{k_{TM}} \mathrm{e}^{-(\varepsilon^{first}_i - \varepsilon_0 - \mu)/k_B T} = 1. \quad (13)$$

Now we turn to discuss the experiment of the Bose-condensed gas in a 1D optical lattice by using the theory developed here. For the Bose-condensed gas in 1D optical lattices, μ can be regarded as the chemical potential of the system, and is given by [19, 22]

$$\mu = \tfrac{1}{2} m\omega_x^2 k_M^2 d^2, \tag{14}$$

where $(2k_M + 1)$ is the total number of condensates in the optical lattice potential. Note that k_M is different from k_{TM}. When the harmonic potential of the magnetic trap is considered, we have $\varepsilon_i^{first} - \varepsilon_0 = \hbar\tilde{\omega}_x + m\omega_x^2 \mathrm{i}^2 d^2/2$. The normalization condition is then

$$\sum_{i=-k_{TM}}^{k_{TM}} \mathrm{e}^{-(\hbar\tilde{\omega}_x + m\omega_x^2 d^2(\mathrm{i}^2 - k_M^2)/2)/k_B T} = 1. \tag{15}$$

By using the experimental parameters $\omega_x = 2\pi \times 9$ Hz, $\tilde{\omega}_x \approx 2\pi \times 14$ kHz and $k_M \approx 100$, $T \approx 200$ nk [19], we have $k_{TM} = 12$. This shows that $k_{TM} \ll k_M$, i.e., the thermal atoms exist mainly in the central lattice sites in the thermal equilibrium. When the overall number of thermal atoms N_T is approximated as 5×10^3, the number of thermal atoms in each lattice site is estimated to be 21, which shows that the Stirling formula can be used safely. For the experimental parameters used in [19], the result of $k_{TM} \ll k_M$ makes it possible to test the effect obtained here, i.e., the thermal cloud would exist mainly in the centre of the one-dimensional optical lattice.

In conclusion, the statistical property of the Bose-condensed gas in a magnetic trap and a 1D optical lattice is investigated within the microcanonical ensemble. It is obvious that the theory proposed here can be developed to investigate the case of 2D and 3D optical lattices. When 2D and 3D optical lattices are used, one expects that there will be some new effects due to the different confinement conditions of the lattice sites. For example, for a 2D optical lattice whose radial trapping angular frequency is much larger than the angular frequency of the magnetic trap, the subcondensate in each lattice site would be a quasi-1D case. When canonical and grand canonical ensembles are used to investigate the thermodynamics of the system, we should also consider the distinguishable behaviour of the thermal atoms in different lattice sites.

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References

[1] Morsch O and Arimondo E 2002 *Preprint* cond-mat/0209034
Burger S *et al* 2001 *Preprint* cond-mat/0111235
[2] Dalfovo F, Giorgini S, Pitaevskii L P and Stringari S 1999 *Rev. Mod. Phys.* **71** 463
[3] Greiner M *et al* 2002 *Nature* **415** 39
[4] Kirsten K and Toms D J 1996 *Phys. Rev.* A **54** 4188
[5] Borrmann P *et al* 1999 *Phys. Rev.* A **60** 1519
[6] Wilkens M and Weiss C 1997 *J. Mod. Opt.* **44** 1801
[7] Gajda M and Rzążewski K 1997 *Phys. Rev. Lett.* **78** 2686
[8] Grossmann S and Holthaus M 1997 *Phys. Rev. Lett.* **79** 3557
[9] Navez P *et al* 1997 *Phys. Rev. Lett.* **79** 1789
[10] Holthaus M, Kalinowski E and Kirsten K 1998 *Ann. Phys., NY* **270** 198
[11] Giorgini S, Pitaevskii L P and Stringari S 1998 *Phys. Rev. Lett.* **80** 5040
[12] Idziaszek Z *et al* 1999 *Phys. Rev. Lett.* **82** 4376
[13] Illuminati F, Navez P and Wilkens M 1999 *J. Phys. B: At. Mol. Opt. Phys.* **32** L461
[14] Kocharovsky V V, Kocharovsky Vl V and Scully M O 2000 *Phys. Rev. Lett.* **84** 2306
[15] Jaksch D *et al* 1998 *Phys. Rev.* A **58** 1450

[16] Bhaduri R K, Murthy M V N and Tran M N 2002 *J. Phys. B: At. Mol. Opt. Phys.* **35** 2817
[17] Xiong H W *et al* 2001 *J. Phys. B: At. Mol. Opt. Phys.* **34** 4203
Xiong H W *et al* 2002 *Phys. Rev.* A **65** 033609
Xiong H W *et al* 2001 *J. Phys. B: At. Mol. Opt. Phys.* **34** 3013
Xiong H W, Liu S J and Huang G X 2002 *J. Phys. B: At. Mol. Opt. Phys.* **35** 2105
[18] Orzel C *et al* 2001 *Science* **291** 2386
Cataliotti F S *et al* 2001 *Science* **293** 843
Burger S *et al* 2002 *Europhys. Lett.* **57** 1
Müller J H *et al* 2002 *Preprint* cond-mat/0211079
[19] Pedri P *et al* 2001 *Phys. Rev. Lett.* **87** 220401
[20] Greiner M *et al* 2001 *Phys. Rev. Lett.* **87** 160405
[21] Greiner M *et al* 2002 *Nature* **419** 51
[22] Xiong H W, Liu S J, Huang G X and Xu Z J 2002 *J. Phys. B: At. Mol. Opt. Phys.* **35** 4863