Theory of Critical Temperature Adiabatic Change for Ideal Gas Bose-Einstein Condensation in Optical Lattices

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Abstract

We present a scheme of analytical calculations determining the critical temperature and the number of condensed atoms of ideal gas Bose-Einstein condensation in external potentials with 1D, 2D or 3D periodicity. In particular we show that the width of the lowest energy band appears as the main parameter determining the critical temperature of condensation. Is obtained a very simple, proportional to 1/3 degree, regularity for this dependence. The fundamental role of tunneling in physics of condensate establishment is underscored.

1 Introduction

Degenerate Bose gases provide an excellent ground for the theoretical study of quantum fluids since their diluteness makes possible first-principles approaches[1]. Thanks to today’s atomic physics powerful experimental techniques their properties can be studied quantitatively through a wide range of temperature and densities. In the last few years Bose-Einstein condensates (BEC) and Fermi gases in optical lattices have been an extremely active area of research[2]. Periodic potentials have been used to examine the transport of Bose-condensed samples [3], to investigate effects correlated with the physics of strongly correlated many-body systems [4]. These systems can be possibly implemented in quantum information processing [5] and there are proposals on how to build quantum gates [6],[7] and qubit buses [8] for information exchange.

The presence of trapping potentials has a big impact on characteristics of the condensate, and in particular on the value of temperature at which the gas passes from normal into BEC state and a macroscopic order coherence starts to form. The predicted increase of critical temperature in a trap played a big role
in obtaining the BEC state with the help of laser cooling and evaporative cooling techniques. However presence of the external potential doesn’t always bring to the increase of critical temperature of condensation ($T_C$). In [9] was shown that if the external potential is periodic, $T_C$ decreases and for asymptotically deep potentials tends to 0. The decrease of critical temperature for relatively deep potentials, created as off-resonant standing waves, was observed experimentally in [10]. We also gave a descriptive physical interpretation for the dependence of $T_C$ on external trapping potential parameters [11], basing on behavior of the distance between the low-laying energy levels of translational atom. For strictly periodic potentials this role is naturally played by widths of the low energy bands, distances between them and most of all the width of the lowest energy band.

In this paper, using some nondrastic mathematical approximations, we derive an elementary analytic expression for critical temperature $T_C$ as a function of optical lattice parameters. The potential periodicity is assumed in one, two or three independent directions. The motion for the left directions in first two cases is assumed to be free. The analytical result justifies, in particular, our physical reasonings brought in [11] about the $T_C$ behavior relative to lattice depth adiabatic changes, and concretizes the form of that behavior. The obtained results, we hope, will help in experimentally more accurately determining the range of parameters, where the ultracold Bose gases behave as ideal.

2 The statistical problem of ideal Bose-gas in periodic potentials

The impact of laser radiation fields on translational motion of atoms is presented as a momentum exchange in photon absorption and emission processes. This means that, in general, the atom (molecule) translational state evolution is connected with the evolution of internal states, leading to notion of potential for each energy level. In the case of large resonance detunings, however, it becomes possible to introduce the idea of potential for the center of mass, as for unstructured particles. Just such a situation will be assumed later, taking the laser field in form of standing waves creating the periodic potential. The coordinate space in our calculations is ordinary, three dimensional, while the periodic potential is present on one, two, or in all three directions.

The principal grand canonical relation, relating the chemical potential $\mu$ with the number of atoms $N$ in a system of volume $V$ [12], in case of interest takes the form

$$\frac{k^3 V}{\pi^3} \int_{-\infty}^{+\infty} dP_x \int_{-\infty}^{+\infty} dP_y \int_{-\infty}^{+\infty} dP_z \frac{1}{\exp\left[\frac{\epsilon_X(P_x) + \epsilon_Y(P_y) + \epsilon_Z(P_z) - \mu}{k_B T}\right] - 1} = N.$$  

Here $P_j (j = X, Y, Z)$ is the atomic momentum for free motion directions and is the quasimomentum for the periodic potential directions. Momentum (quasimomentum) is scaled by the recoil momentum $2\hbar k$, where $k$ is the wavevector of
the counterpropagating waves forming the standing wave. The energies $\varepsilon_j(P_j)$, as well as the chemical potential $\mu$ and the thermal energy $\kappa B T$, are scaled in recoil energy units $E_R = (2\hbar k)^2/2M$, corresponding to momentum value $2\hbar k$. Formula (1) assumes an extended form for the dispersion relation between energy and quasimomentum.

2.1 1D periodic potential

After taking the elementary integrals over two free directions in (1), we get

$$-\frac{2k^3V\kappa B T}{\pi^2} \int_0^{+\infty} dP \ln \left[ 1 - \exp \left( \frac{\mu - \varepsilon(P)}{\kappa B T} \right) \right] = N, \quad (2)$$

where the integration over the total range of quasimomentum is replaced by two half-range integrals - from zero to infinity. To proceed, it is convenient to divide the whole range of integration into a sequence of Brillouin zones and expand the integrand logarithm into convergent Taylor series. Then the above relation takes the following form:

$$\frac{2k^3V\kappa B T}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n} \exp \left[ \frac{\mu}{\kappa B T} \right] \sum_{m=1}^{\infty} \int_{(m-1)/2}^{m/2} dP \exp \left( -\frac{n\varepsilon(P)}{\kappa B T} \right) = N. \quad (3)$$

Now let’s temporarily concentrate on the integral term and take a dispersion relation, for example, for a biparabolic form of the periodic potential, introduced in [11]:

$$\cos(2\pi P) = 1 + 2G_{11}(\varepsilon)G_{22}(\varepsilon), \quad (4)$$

(the explicit expressions of $G_{11}(\varepsilon)$ and $G_{22}(\varepsilon)$ are not necessary for our later presentation).

As is seen from Fig.1, the dependence of energy $\varepsilon$ on quasimomentum $P$, calculated by relation (4), is almost linear in frame of the first energy band and this linearity isn’t rapidly lost for higher energy bands. Such a behavior prompts us to introduce a new, main in context of this paper, approximation taking the $\varepsilon(P)$-dependence inside each energy band as linear. Here we come from the fact, that in assumed thermal equilibrium state of the Bose gas the population and respective contribution of upper energy bands into the left-side value of (3) decreases quite rapidly.

After denoting boundary energy values of the m-th zone by $\varepsilon_{m}\text{min}$ and $\varepsilon_{m}\text{max}$ and performing the mentioned linearization, the dispersion relation (4) will have the form

$$\varepsilon(P) = \frac{\varepsilon_{m}\text{max} + \varepsilon_{m}\text{min}}{2} + (-1)^m \frac{\varepsilon_{m}\text{max} - \varepsilon_{m}\text{min} \cos(2\pi P)}{2}, \quad (5)$$

and the integral in (3) is expressed by zero order modified Bessel function $I_0(x)$ with an exponential factor. As a result we obtain the following, more simple form for the main statistical relation:

$$\frac{k^3V\kappa B T}{\pi^2} \sum_{m=1}^{\infty} \left\{ \sum_{n=1}^{\infty} \frac{1}{n} \exp \left( \frac{\mu - \varepsilon_{m}\text{max} - \varepsilon_{m}\text{min}}{\kappa B T} \right) \right\} I_0 \left( \frac{n\delta_{m}\text{max} - \varepsilon_{m}\text{min}}{2\kappa B T} \right) = N, \quad (6)$$
where $\bar{\varepsilon}^{(m)} = \frac{\varepsilon^{(m)}_{\text{max}} + \varepsilon^{(m)}_{\text{min}}}{2}$ is the mean energy in the $m$-th band and the parameter $\delta^{(m)} = \varepsilon^{(m)}_{\text{max}} - \varepsilon^{(m)}_{\text{min}}$ in the argument of modified Bessel function is the width of that band. The contribution of each energy band in this relation is now determined by the expression in curve brackets and presents a single-variable convergent series, a very convenient form for numerical calculations.

To be convinced in convergent nature of the mentioned series, one would address to asymptotic formulae of the modified Bessel function for great values of argument:

$$I_0\left(n \frac{\delta^{(m)}}{2\kappa_B T}\right) \approx \frac{\sqrt{2\kappa_B T}}{\sqrt{2\pi n \delta^{(m)}}} \exp\left(n \frac{\delta^{(m)}}{2\kappa_B T}\right).$$

(7)

The asymptotic behavior of the mentioned sum is then determined by expression

$$\sum_{\text{large } n} \frac{1}{n^{3/2}} \exp\left[-\frac{n}{\kappa_B T} (\varepsilon^{(m)} - \mu)\right],$$

(8)

which evidently converges for any $\mu \leq \varepsilon^{(m)}_{\text{min}}$, as usual for bosonic systems.

Thus, from mathematical viewpoint relation (6) is reasonably defined and is convenient for calculating the functional dependence of $\mu$ on $T$ with any in advance prescribed accuracy. In particular the critical temperature will be decided by substituting $\mu = \varepsilon^{(1)}_{\text{min}}$:

$$\frac{k^3 V \kappa_B T}{\pi^2} \sum_{m=1}^{\infty} \left(\sum_{n=1}^{\infty} \frac{1}{n} \exp\left(-\frac{n}{\kappa_B T C} \right) I_0\left(n \frac{\delta^{(m)}}{2\kappa_B T C}\right)\right) = N.$$  

(9)

From general principles of the Bose -Einstein condensation theory directly follows that for $T < T_C$ in (6) we should interpret $N$ as the number of noncondensed atoms($N_{nc}$) and not as the total number, simultaneously taking $\mu = \varepsilon^{(1)}_{\text{min}}$ which corresponds to the critical temperature. The number of condensed atoms is determined by the complementary relation $N_{c} = N - N_{nc}$.

Now let’s go back to formulae (7) and use it not for showing the convergence of the series, but for getting a new, much more simple approximate form of problem solution. Really, the formulae (7) can be used for small values of $n$ too, if first of all $\kappa_B T < \frac{\delta^{(1)}}{2}$, that is if atom’s thermal energy is appreciably smaller than the half-width of the first, most narrow energy band (for critical and lower temperatures this condition is well satisfied in today’s experiments). Nevertheless, in general, the fulfillment of this condition is not mandatory and the use of (7) for the first addends too would be allowed approximation when the impact of these first members is small. Without going into details we will just mention that for the above mentioned replacement is enough to satisfy the condition

$$\frac{\pi^2 N}{k^3 V \kappa_B T} > 2 \frac{\kappa_B T}{\delta^{(m)}}.$$  

(10)

After substituting (7) into (6) the sum over $n$ can be calculated and expressed by confluent hypergeometric function $\Phi(a, 3/2; 1)$. Then the main statistical
relation takes the form

\[
\frac{k^3V}{\pi^{5/2}(\kappa_B T_c)^{3/2}} \sum_{m=1}^{\infty} \frac{1}{\delta^{(m)}} \exp \left(-\frac{\varepsilon^{(m)}_{\text{min}} - \mu}{\kappa_B T_c}\right) \Phi(e^{-\left(\varepsilon^{(m)}_{\text{min}} - \varepsilon^{(1)}_{\text{min}}\right)}/\kappa_B T_c, 3/2; 1) = N,
\]

from which the critical temperature is decided as before, substituting \(\mu = \varepsilon^{(1)}_{\text{min}}\):

\[
\frac{k^3V}{\pi^{5/2}(\kappa_B T_c)^{3/2}} \left\{ \Phi(1, 3/2; 1) + \sum_{m=2}^{\infty} \frac{1}{\delta^{(m)}} \exp \left(-\frac{\varepsilon^{(m)}_{\text{min}} - \varepsilon^{(1)}_{\text{min}}}{\kappa_B T_c}\right) \Phi(e^{-\left(\varepsilon^{(m)}_{\text{min}} - \varepsilon^{(1)}_{\text{min}}\right)}/\kappa_B T_c, 3/2; 1) \right\} = N.
\]

First term in curve brackets stands for the number of atoms in the first energy band. The number of atoms in any, higher laying energy band is determined by the respective addend of the series: \(m = 2\) for the second (first excited) one, and so on.

Often in experiments with optical lattices we can limit ourselves with the first energy band. For this cases we get elementary relation and for making its appearance more concise, it is appropriate to introduce a notion of the first energy band for free (when the energy gaps tend to zero) Bose gas. If we denote this width by \(\delta^{(1)}_0\) (in normalized units it is equal to 1/4), and the critical temperature of a free ideal gas \([12]\) by \(T_{C0}\), than we arrive at the following final form:

\[
T_{C} = \left(\frac{\pi}{2}\right)^{2/3} \left[\frac{\delta^{(1)}_0}{\delta^{(1)}}\right]^{1/3} T_{C0}.
\]

This formulae is one of the main results of the present paper. The width \(\delta^{(1)}\) is the only parameter depending on external potential. The deepening of the periodic potential, as is well known, compresses this width and, consequently, decreases \(T_C\), the critical temperature of condensation (such a result, based on numerical calculations and physical reasonings, we have presented in \([11]\)). The formulae shows that this decrease happens by a very simple law: proportional to 1/3 degree of the first energy band width.

The approximate character of formulae (13) is seen in fact, that in the limit of free gas \((\delta^{(1)} \to \delta^{(1)}_0)\) the critical temperature \(T_C\) tends not to \(T_{C0}\) but to \((\pi/2)^{2/3} \approx 1.35\) times higher value. For not very deep potentials (in \(E_v\) units smaller than one) the main approximation done here is the substitution of dispersion curves with straight lines. The deepening of the potential (decreasing \(\delta^{(m)}\)) straightens the dispersion curves, starting from the first energy band, and consequently softens the role of this approximation. But now grows the role of using the asymptotic formulae (7), as for the first members of series the condition \(n\delta^{(m)}/2\kappa_B T > 1\) fails. The single band approximation for ultracold gases has a minor impact whatever the case.
2.2 2D and 3D periodic potentials

Suppose that 2D (3D) periodic potential is a sum of two (three) periodic potentials, each one of which is periodic only in one direction. The calculation scheme doesn’t undergo any qualitative changes and we will write the final results straight away. Instead of (6), we come to relation

\[ k^3 V \kappa_B T \sum_{m,m' = 1}^{\infty} \left( \sum_{n=1}^{\infty} \frac{1}{\sqrt{n}} \exp \left( \frac{n\mu - \bar{\epsilon}(m,X) - \bar{\epsilon}(m',Y)}{k_B T} \right) \right) \times I_0 \left( n \frac{\bar{\epsilon}(m,X)}{2\kappa_B T} \right) I_0 \left( n \frac{\bar{\epsilon}(m',Y)}{2\kappa_B T} \right) = N \]

for 2D periodicity and

\[ k^3 V \kappa_B T \sum_{m,m',m'' = 1}^{\infty} \left( \sum_{n=1}^{\infty} \exp \left( \frac{n\mu - \bar{\epsilon}(m,X) - \bar{\epsilon}(m',Y) - \bar{\epsilon}(m'',Z)}{k_B T} \right) \right) \times I_0 \left( n \frac{\bar{\epsilon}(m,X)}{2\kappa_B T} \right) I_0 \left( n \frac{\bar{\epsilon}(m',Y)}{2\kappa_B T} \right) I_0 \left( n \frac{\bar{\epsilon}(m'',Z)}{2\kappa_B T} \right) = N \]

for 3D periodicity, where the new notations are the full analogies of the 1D case. After applying (7) these relations are simplified and take the forms

\[ k^3 V \kappa_B T \sum_{m,m = 1}^{\infty} \left( \sum_{n=1}^{\infty} \frac{1}{\sqrt{n}} \exp \left( \frac{n\mu - \bar{\epsilon}(m,X) - \bar{\epsilon}(m',Y)}{k_B T} \right) \right) \times \Phi \left( e^{-\epsilon_{\text{min}}(m,X) - \epsilon_{\text{min}}(m',Y) - \mu}/k_B T, \frac{3}{2}, 1 \right) = N \]

and

\[ k^3 V \kappa_B T \sum_{m,m',m'' = 1}^{\infty} \left( \sum_{n=1}^{\infty} \exp \left( \frac{n\mu - \bar{\epsilon}(m,X) - \bar{\epsilon}(m',Y) - \bar{\epsilon}(m'',Z)}{k_B T} \right) \right) \times \Phi \left( e^{-\epsilon_{\text{min}}(m,X) - \epsilon_{\text{min}}(m',Y) + \epsilon_{\text{min}}(m'',Z) - \mu}/k_B T, \frac{3}{2}, 1 \right) = N \]

correspondingly. For critical temperatures we get just as simple relations as was (13):

\[ T_C \approx \left( \frac{\pi}{2} \right)^{4/3} \left[ \frac{\delta(1,X)}{\delta_0} \right]^{1/3} \left[ \frac{\delta(1,Y)}{\delta_0} \right]^{1/3} T_{C_0} \quad (13) \]

for potentials with 2D and

\[ T_C \approx \left( \frac{\pi}{2} \right)^{2} \left[ \frac{\delta(1,X)}{\delta_0} \right]^{1/3} \left[ \frac{\delta(1,Y)}{\delta_0} \right]^{1/3} \left[ \frac{\delta(1,Z)}{\delta_0} \right]^{1/3} T_{C_0} \quad (14) \]

with 3D periodicity.
3 Conclusions

Formulas (12), (13), (14) and (15) represent the main results of this paper. They show that with good approximation the width of the first energy band is the only parameter determining the ideal gas Bose-Einstein condensation critical temperature in a field of periodic potentials. From the Bloch theory of periodic potentials is well known that the deepening of the potential rapidly narrows energy bands and especially the first one. Therefore even the $1/3$ degree proportionality in 1D case will be enough for decreasing the critical temperature twice for $2E_R - 3E_R$ potential depths. The comparison of the above mentioned formulas also shows that in a single-band approximation each direction of periodicity acts as though independent and by that speeds up the critical temperature dependence on the potential depth when the periodicity passes from 1D to 2D and 3D correspondingly.

The band structure of energy spectrum assumes the existence of Bloch-type wavefunctions, the modulus of which is periodically spread over the whole potential. For the states which are of interest, that is with energies smaller than the potential height, the only mechanism of the Bloch state realization is the quantum tunneling through the potential barriers. By this we conclude that the phenomena of tunneling has an exceptional role for the obtained BEC critical temperature behavior regularity. If we exclude the possibility of tunneling for quantum particles (in our case of atom), then each low-energy atom would’ve stay trapped and localized only in one well-type region of the potential, as for example in harmonic potential case. The atom translational motion energy spectrum would be discrete and the energy levels would move away as the potential depth increases. Then it would bring to an increase of the critical temperature, a result well known for isolated wells and just opposite to the above obtained ones.

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Figure 1: The dependence of the right hand side (RHS) of (4) from normalized energy $\varepsilon$. The optical lattice depth is taken $1E_R$. The bold intervals of the curve correspond to allowed energy bands.