Low Temperature Physics/Fizika Nizkikh Temperatur, 2021, vol. 47, No. 7, pp. 626–632

# Bose systems in linear traps: Exact calculations versus effective space dimensionality

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Received January 28, 2021, published online May 26, 2021

Systems of noninteracting bosons trapped by linear potentials $V(r)=\alpha r$, where $r=|\mathbf{r}|$, are studied in one and three dimensions. For the latter problem, an interpolation formula is suggested for energy levels between $n,\ell\sim 10$ and the WKB limit. Thermodynamic functions are calculated for $N=10,\ \dots,\ 10^4$ particles using discrete energy spectrum. The specific heat and fugacity are compared to the results of the quasiclassical approach, in which the external potential effectively increases the space dimensionality. As expected, the comparison demonstrates that the thermodynamic functions obtained using the discrete spectra rapidly approach the quasiclassical ones in a space with the effectively tripled space dimensionality as $N$ increases.

Keywords: Bose systems, linear traps, effective space dimensionality.

## 1. Introduction

As early as four centuries ago, Johannes Kepler was perhaps the first person to assume the mechanical action of light [1] when discussing the possibility of Sun rays to shape tails of comets in his 1619 book [2]. A lot of time had passed before this effect was introduced into the world of microparticles [3] and ultimately allowed trapping and cooling of atoms [4].

The development of techniques for cooling and trapping of neutral atoms played a key role in obtaining Bose–Einstein condensates of alkali atoms in 1995 [5, 6]. In subsequent years, Bose condensation was achieved for other atom species [7] as well as for other systems, like exciton-polaritons [8, 9] and light in microcavities [10]. Practical applications of trapped Bose condensates envisage such fields as quantum computations [11, 12] and high-precision interferometry [13, 14]. Studies of trapped bosons remain thus a topical subject in the field of quantum many-body physics.

The aim of the present paper is two-fold. First, we would like to demonstrate, using exact calculations involving discrete spectrum, how an external trapping potential influences thermodynamics of bosons and to compare the respective results with those obtained within the quasiclassical approach. We consider this external potential $V(r)=\alpha r$, where $r=|\mathbf{r}|$, corresponding thus to a linear trap. Such a problem triggers the second task, namely, obtaining the spectrum in space dimensions $D>1$. In particular, using numerical treatment of the respective eigenvalue problem, we propose an approximation for the spectrum applicable in a wide range of quantum numbers.

Linear potentials of various types appear in magnetic quadrupole traps [15] or in problems involving Bose–Einstein condensate surfaces [16]. Time-dependent linear terms in the external potential of the Gross–Pitaevskii equation can be used to study problems with energy dissipation [17, 18]. The so-called Airy gas model is suitable for the description of the electron gas near edge regions [19, 20]. We, therefore, expect our results to be applicable in a set of related problems.

The paper is organized as follows. Section 2 summarizes the general calculation procedure. In Sec. 3, obtaining energy levels in the one-dimensional $|x|$ potential is briefly recalled and the three-dimensional linear trap is analyzed in more detail. The quasiclassical treatment of external potentials is presented in Sec. 4. Results of numerical calculations are given in Sec. 5. Finally, Sec. 6 contains conclusions.

## 2. Calculation scheme

For a Bose system with excitation spectrum $\varepsilon_k$, occupation numbers are given by

$$n_k=\frac{1}{z^{-1}e^{\varepsilon_k/T}-1}, \tag{1}$$

where $T$ is temperature and $z$ is fugacity related to the chemical potential $\mu$ as $z=e^{\mu/T}$. The total number of particles is

$$N = \sum_k n_k . \quad (2)$$

Note that the summation index $k$ runs over the set of all possible quantum numbers. In specific cases, level degeneracies should be taken into consideration.

In fact, the above equation, namely,

$$N = \sum_k \frac{1}{z^{-1} e^{\varepsilon_k / T} - 1} \quad (3)$$

can be considered a transcendental equation for $z$ as a function of $T$ and $N$. Energy of the system is then calculated as

$$E = \sum_k \frac{\varepsilon_k}{z^{-1} e^{\varepsilon_k / T} - 1}, \quad (4)$$

yielding the specific heat as follows

$$\frac{C}{N} = \frac{1}{N} \frac{dE}{dT}. \quad (5)$$

For interlevel separations $\Delta\varepsilon_k = \varepsilon_{k+1} - \varepsilon_k$ small comparing to temperature, the summations in Eqs. (3)–(4) can be replaced by integration using the density of state function $g(\varepsilon)$:

$$N = n_0 + \int_0^\infty \frac{g(\varepsilon) d\varepsilon}{z^{-1} e^{\varepsilon/T} - 1}, \quad (6)$$

and

$$E = \int_0^\infty \frac{\varepsilon g(\varepsilon) d\varepsilon}{z^{-1} e^{\varepsilon/T} - 1}. \quad (7)$$

The occupation of the ground state, $n_0$ (the number of particles in the Bose condensate), should be written explicitly in this case.

Note that the condition $\Delta\varepsilon_k \ll T$ holds in most typical experimental setups up to very low temperatures, significantly lower that the critical temperature $T_c$, at which the Bose condensation occurs. For instance, a $D$-dimensional system of $N$ bosons trapped by the harmonic potential with frequency $\omega$ has

$$T_c = \hbar\omega \left[ \frac{N}{\zeta(D)} \right]^{1/D}, \quad (8)$$

where $\zeta(D)$ is Riemann's zeta function. The interlevel separation $\hbar\omega$ becomes thus much smaller than $T_c$ already for $N \sim 10^3$–$10^4$.

## 3. Energy levels in linear traps

Energy levels for particles in potentials $V(r) \propto \mathrm{sgn}(q) r^q$ are obtained from the eigenvalues $E_{n\ell}(q)$ corresponding to

$$\left( -\Delta + \mathrm{sgn}(q) r^q \right) \psi_{n\ell}(r) = E_{n\ell}(q) \psi_{n\ell}(r) \quad (9)$$

using simple relations [21]

$$-\xi\Delta + \alpha\, \mathrm{sgn}(q) r^q \to \xi \left( \frac{\alpha}{\xi} \right)^{\frac{2}{2+q}} E_{n\ell}(q), \quad (10)$$

where the coupling constant $\alpha > 0$ and $\xi = \hbar^2/(2m)$ for particles of mass $m$.

Further, we consider the case of linear trapping potentials ($q = 1$). For linear potentials $V(r) = \alpha r$ we thus have eigenvalues

$$\frac{\hbar^2}{2m} \left( \frac{2m\alpha}{\hbar^2} \right)^{2/3} E_{n\ell}, \quad (11)$$

where $E_{n\ell}$ correspond to the dimensionless problem (9).

### 3.1. One-dimensional case

The Schrödinger equation reads

$$\left( -\frac{d^2}{dx^2} + |x| \right) \psi_n(x) = E_n \psi_n(x). \quad (12)$$

The eigenvalues $E_n$ are obtained as zeros of the Airy function

$$\mathrm{Ai}(z) = \frac{1}{\pi} \int_0^\infty \cos\left( \frac{t^3}{3} + zt \right) dt \quad (13)$$

and its derivative $\mathrm{Ai}'(z)$ [22–24]. Namely,

$$\mathrm{Ai}(-E_{2p+1}) = 0, \quad \mathrm{Ai}'(-E_{2p}) = 0, \quad \text{where } p = 0, 1, 2, \ldots . \quad (14)$$

The asymptotic expression within the WKB approximation is as follows:

$$E_n^{\text{asymp}} = \left( \frac{3\pi}{4} \right)^{2/3} \left( n + \frac{1}{2} \right)^{2/3}. \quad (15)$$

The exact and asymptotic values are given in Table 1.

In future calculations of thermodynamic functions, we shift the spectrum so that the ground state energy is zero, namely:

$$\varepsilon_n = E_n - E_0, \quad (16)$$

where $(-E_0)$ is the first zero of the Airy function derivative, $E_0 = 1.01879297\ldots$.

### 3.2. Three-dimensional case

In higher dimensions, angular and radial variables in the Schrödinger equation can be separated and the radial equation inherits an additional term from the angular part yielding an effective potential

$$V_{\text{eff}}(r) = r + \frac{\gamma}{r^2}, \quad (17)$$

where $\gamma = m^2$ in two dimensions and $\gamma = \ell(\ell+1)$ in three dimensions.

Table 1. The first eleven and some higher eigenvalues compared to the asymptotic expression (15)

| $n$ | $E_n$ | $E_n^{\text{asymp}}$ | $\lvert E_n - E_n^{\text{asymp}} \rvert / E_n$ |
|---|---|---|---|
| 0 | 1.01879 | 1.115461 | $9.5\cdot10^{-2}$ |
| 1 | 2.33811 | 2.320251 | $7.6\cdot10^{-3}$ |
| 2 | 3.24820 | 3.261626 | $4.1\cdot10^{-3}$ |
| 3 | 4.08795 | 4.081811 | $15\cdot10^{-3}$ |
| 4 | 4.82010 | 4.826317 | $1.3\cdot10^{-3}$ |
| 5 | 5.52056 | 5.517165 | $6.2\cdot10^{-4}$ |
| 6 | 6.16331 | 6.167129 | $6.2\cdot10^{-4}$ |
| 7 | 6.78671 | 6.784455 | $3.3\cdot10^{-4}$ |
| 8 | 7.37218 | 7.374854 | $3.6\cdot10^{-4}$ |
| 9 | 7.94413 | 7.942488 | $2.1\cdot10^{-4}$ |
| 10 | 8.488493 | 8.218782 | $2.4\cdot10^{-4}$ |
| 20 | 13.26222 | 13.26305 | $6.2\cdot10^{-5}$ |
| 50 | 24.19156 | 24.19181 | $1.0\cdot10^{-5}$ |
| 100 | 38.27516 | 38.27526 | $2.6\cdot10^{-6}$ |
| 200 | 60.65734 | 60.65738 | $6.5\cdot10^{-7}$ |

No closed-form expressions are known for $m>0$ and $\ell>0$, only the $s$ states are given by the Airy functions:

$$\mathrm{Ai}(-E_{n0}) = 0, \quad \text{where} \quad n = 0, 1, 2, \ldots \,. \tag{18}$$

Note that the radial coordinate $r \geq 0$, while in the one-dimensional case we had $-\infty < x < \infty$, so that the zeros of the Airy function derivative $\mathrm{Ai}'(z)$ do not survive in higher dimensions.

Further we will focus on the three-dimensional case only. Analytical expressions for $\ell > 0$ are not known, so the respective eigenvalue problem should be treated numerically. One of possible approaches is the Numerov method [25, 26], which we will use for the respective calculations in the present work.

The general scheme of our approach is as follows. We first solve the eigenvalue problem for low-lying $n$ and $\ell$ quantum numbers and compare the obtained results with those available in the literature [26–30]. The most complete data we were able to discover are given in [29] for $n = 0, \ldots, 19$ and $\ell = 0, \ldots, 10$.

We solve the problem on the $r \in [0; L]$ segment evenly discretized into a $K$-sized grid. With $L = 50$ and $K = 8000$ still permitting reasonable-time-consuming computations on accessible computers, we are able to achieve the relative accuracy within $10^{-5}$. Note that eigenvalues very close to or higher than $L$ cannot be calculated reliably already.

On the other hand, the quasiclassical limit for the spectrum is also known [31]:

$$E_{n\ell}^{\text{asymp}} = \left(\frac{3\pi}{4}\right)^{2/3} \left(2n + \ell + \frac{3}{2}\right)^{2/3} . \tag{19}$$

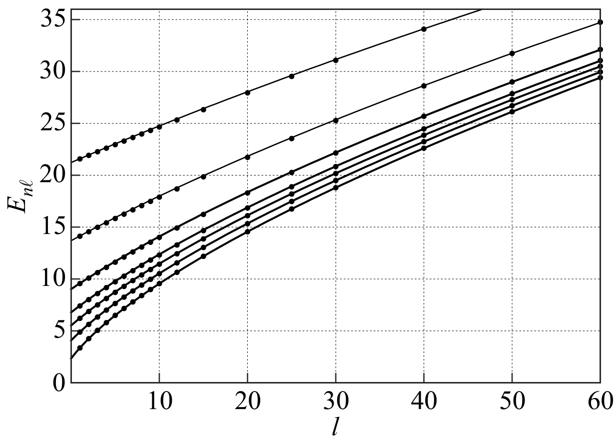


*Fig. 1.* Energy levels $E_{n\ell}$ in the three-dimensional linear trap (circles) compared to function (20) (solid lines) for several values of $n$, bottom to top, $n = 0, 1, 2, 3, 5, 10, 20$.

Our analysis shows that the following expression yields proper results for eigenvalues:

$$E_{n\ell} = \left(E_{n0}^{3/2} + b(n)\ell\right)^{2/3} , \tag{20}$$

where the values of coefficient $b(n)$ are obtained by fitting function (20) to the calculated eigenvalues $E_{n\ell}$, see Fig. 1.

Comparing the asymptotic expression

$$E_{n0}^{\text{asymp}} = \left(\frac{3\pi}{4}\right)^{2/3} \left(2n + \frac{3}{2}\right)^{2/3} \tag{21}$$

with (19) and (20), we immediately obtain the limiting value $b(n \to \infty) = 3\pi/4$. The fitting of the calculated $b(n)$ values for $n$ = 3–50 can be done using

$$b(n) = \frac{3\pi}{4} + A\exp\left(-Bn^{4/3}\right) \tag{22}$$

with $A = 0.233 \pm 0.003$, $B = 0.0049 \pm 0.0002$. For illustration, see Fig. 2. Actually, we have tested the powers of $n$

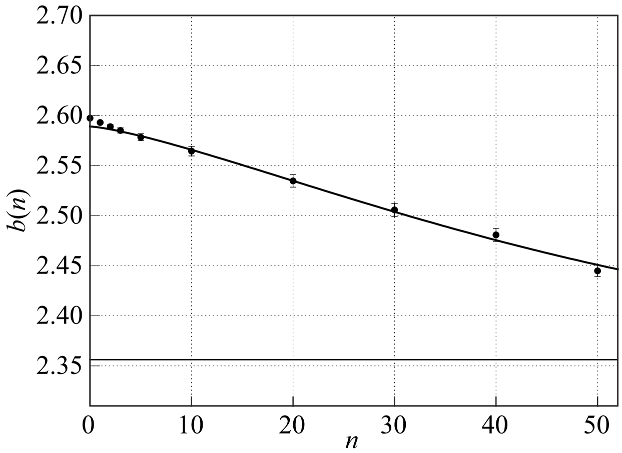


*Fig. 2.* Coefficient $b(n)$ (circles with errorbars) compared to function (22) (solid line). The horizontal line at $3\pi/4 = 2.356\ldots$ is the asymptotic value as $n \to \infty$.

within the range from 1 to 2 and the best fit has been achieved for $n \simeq 1.33$, with the determination coefficient $R^2 > 0.995$, so the rational fraction $4/3$ is chosen.

Similarly to the one-dimensional case, in our further calculations of thermodynamic functions, we shift the energy levels by $(-E_{00})$ to ensure the zero energy of the ground state:

$$\varepsilon_{n\ell} = E_{n\ell} - E_{00}, \tag{23}$$

where $(-E_{00})$ is the first zero of the Airy function, $E_{00} = 2.33810741\ldots$ .

### 4. Quasiclassical approximation

Following Bagnato *et al.* [32, 33], we can obtain the expression for the density of states corresponding to particles in power law potentials. The underlying idea is simple: the space region accessible to a particle with energy $\varepsilon$ is limited by classical turning points.

Let us briefly recall the derivation chain for the respective $D$-dimensional problem [34]. Let the particles of mass $m$ be placed in the isotropic external potential (for simplicity)

$$V(r) = V_0 \left(\frac{r}{a}\right)^{\eta}, \quad \text{where} \quad V_0, \eta > 0, \tag{24}$$

and $a$ is a parameter having the dimension of length. The single-particle spectrum is

$$\varepsilon(p, r) = \frac{p^2}{2m} + V(r). \tag{25}$$

In these formulas, $p = \sqrt{p_1^2 + \ldots + p_D^2}$ and $r = \sqrt{x_1^2 + \ldots + x_D^2}$. The summation over energy levels is changed to the integration over the phase space, and, consequently, over energies, as follows:

$$\sum_n (\ldots) = \int \frac{dp_1 \ldots dp_D dx_1 \ldots dx_D}{(2\pi\hbar)^D} (\ldots) = \int d\varepsilon g(\varepsilon)(\ldots). \tag{26}$$

For the isotropic problem,

$$dp_1 \ldots dp_D = \Omega_D p^{D-1} dp, \quad dx_1 \ldots dx_D = \Omega_D r^{D-1} dr, \tag{27}$$

where the $D$-dimensional solid angle can be written using Euler's gamma-function as follows:

$$\Omega_D = \frac{2\pi^{D/2}}{\Gamma(D/2)}. \tag{28}$$

So, the number of particles (3), (6) is given by

$$N = N_0 + \frac{\Omega_D^2}{(2\pi\hbar)^D} \frac{(2m)^{D/2}}{2} \times$$

$$\times \int_0^{\infty} \frac{d\varepsilon}{z^{-1} e^{\varepsilon/T} - 1} \int_{V(r)=\varepsilon} dr r^{D-1} \left[\varepsilon - V(r)\right]^{D/2-1}, \tag{29}$$

where momentum and energy are related as

$$p = \sqrt{2m[\varepsilon - V(r)]}, \tag{30}$$

and the classical turning points are defined by the condition $p = 0$, hence $V(r) = \varepsilon$. For the potential given by (24) the integral over $r$ evaluates to the beta-function yielding the following expression for the density of states:

$$g(\varepsilon) = \frac{\Omega_D^2}{(2\pi\hbar)^D} \frac{(2m)^{D/2}}{2} \frac{a^D}{\eta V_0^{D/\eta}} \mathrm{B}\left(\frac{D}{\eta}, \frac{D}{2}\right) \varepsilon^{D/2 + D/\eta - 1}. \tag{31}$$

Comparing this expression to the density of states of the $D$-dimensional ideal Bose gas placed in a box of volume $\mathcal{V}_D$ [35, 36],

$$g(\varepsilon) = \mathcal{V}_D \frac{\pi^{D/2}}{(2\pi\hbar)^D} \frac{(2m)^{D/2}}{\Gamma(D/2)} \varepsilon^{D/2-1}, \tag{32}$$

one can easily notice that external potential effectively increases the space dimensionality to some

$$D_{\text{eff}} = D\left(1 + \frac{2}{\eta}\right), \tag{33}$$

and also that some effective volume $\mathcal{V}_{\text{eff}}$ can be defined using the parameters of the potential $a$ and $V_0$. The critical temperature (Bose condensation point) is defined by

$$T_c = \frac{2\pi\hbar^2}{m} \left(\frac{N}{\mathcal{V}_{\text{eff}}} \frac{1}{\zeta(D_{\text{eff}}/2)}\right)^{2/D_{\text{eff}}}; \tag{34}$$

after simple transformations this yields for linear traps ($\eta = 1$):

$$T_c = \left(\frac{\hbar^2}{2m}\right)^{1/3} \left(\frac{2V_0}{a}\right)^{2/3} \left(\frac{\Gamma(D/2)}{2\Gamma(D)} \frac{N}{\zeta(3D/2)}\right)^{2/(3D)}, \tag{35}$$

while the effective space dimensionality $D_{\text{eff}} = 3D$.

### 5. Results for the thermodynamic functions

In the one-dimensional case, there is no level degeneracy, so

$$N = \sum_{n=0}^{\infty} \frac{1}{z^{-1} e^{\varepsilon_n/T} - 1}, \tag{36}$$

where spectrum $\varepsilon_n$ is given by (16) and (14). Solving this transcendental equation numerically we obtain $z = z(T, N)$, which is used in the calculation of energy and the specific heat

$$E = \sum_{n=0}^{\infty} \frac{\varepsilon_n}{z^{-1} e^{\varepsilon_n/T} - 1}, \quad \frac{C}{N} = \frac{1}{N} \frac{dE}{dT}. \tag{37}$$

The results of calculations are shown in Figs. 3 and 4. In these figures, comparison is made for several values of the number of particles $N$ with the ideal three-dimensional Bose gas. The latter corresponds to the system with effective space dimensionality $D_{\text{eff}} = 3$, see Eq. (33).

Note that for a $D$-dimensional ideal Bose gas of particles with mass $m$ the critical temperature is given by

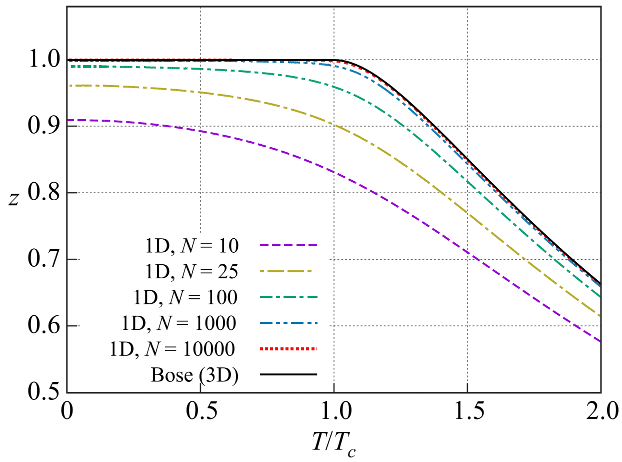


*Fig. 3.* Fugacity 1D compared to the 3D ideal Bose gas.

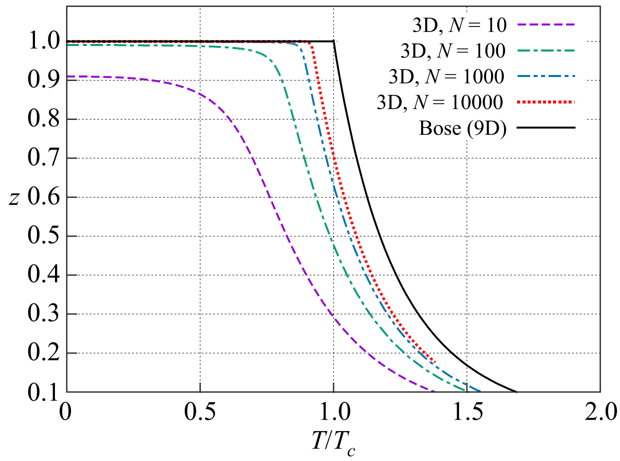


*Fig. 5.* Fugacity 3D compared to the 9D ideal Bose gas.

$$T_c = \frac{2\pi\hbar^2}{m}\left(\frac{\rho_D}{\zeta(D/2)}\right)^{2/D}, \qquad (38)$$

where concentration $\rho_D = N/V_D$ is fixed in the thermodynamic limit as both the number of particles $N \to \infty$ and the $D$-dimensional volume $V_D \to \infty$.

For $T > T_c$, fugacity $z$ is defined from Eq. (6) yielding after some transformation

$$1 = \frac{1}{\Gamma(D/2)\zeta(D/2)}\left(\frac{T}{T_c}\right)^{D/2}\int_0^\infty \frac{x^{D/2-1}\,dx}{z^{-1}e^x - 1}, \qquad (39)$$

while $z = 1$ for $T \le T_c$. In the same fashion, for energy from Eq. (7) one gets

$$E = \frac{NT}{\Gamma(D/2)\zeta(D/2)}\left(\frac{T}{T_c}\right)^{D/2}. \qquad (40)$$

As we can observe in Fig. 4, for finite $N$ specific heat is a smooth curve having a maximum at some $T_{\max}^{(N)}$ such that $T_{\max}^{(N)}/T_c > 1$, where $T_c$ is given by (35). These maxima tend to $T_c$ as the number of particles $N$ increases. In the latter case, the specific heat curve approaches that of the ideal three-dimensional Bose gas as expected. The difference is already barely noticeable for $N = 10^4$ and is the most pronounced in the vicinity of $T_c$ only, where the 3D system exhibits a cusp corresponding to the phase transition, which cannot be obtained for a finite system.

We also see in Fig. 3 that as the temperature increases, the value of $z$ decreases (tending in fact to zero), and for high temperatures the Bose distribution turns into the Boltzmann distribution, and the specific heat tends to the classical limit 3/2 (Fig. 4).

Similarly, one can obtain results in the three-dimensional case. Upon taking into account the level degeneracy of $2\ell+1$, we have

$$N = \sum_{n=0}^{\infty}\sum_{\ell=0}^{\infty}\frac{(2\ell+1)}{z^{-1}e^{\varepsilon_{n\ell}/T} - 1}, \qquad (41)$$

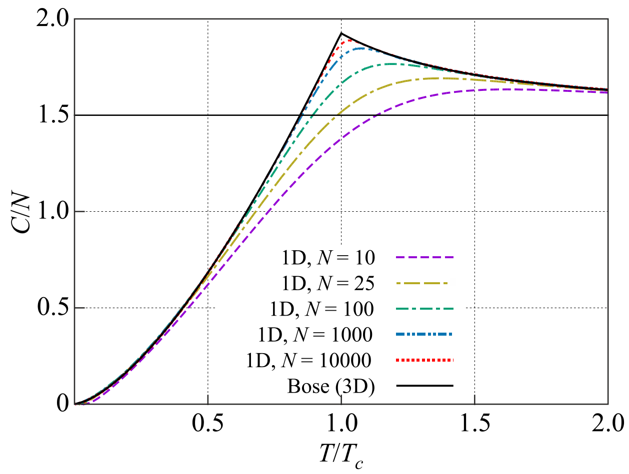


*Fig. 4.* Specific heat in 1D compared to the 3D ideal Bose gas.

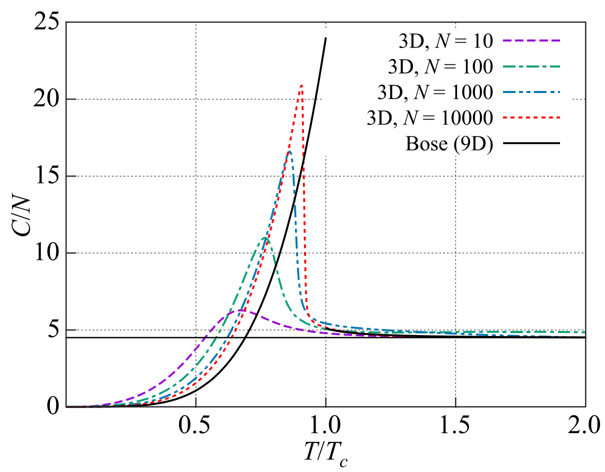


*Fig. 6.* Specific heat in 3D compared to the 9D ideal Bose gas.

where spectrum $\varepsilon_{n\ell}$ is given by (18)–(23). The numerical solution $z = z(T, N)$ is inserted in the expression for energy allowing then to calculate the specific heat, as above:

$$E = \sum_{n=0}^{\infty}\sum_{\ell=0}^{\infty}\frac{(2\ell+1)\varepsilon_{n\ell}}{z^{-1}e^{\varepsilon_{n\ell}/T}-1}, \qquad \frac{C}{N} = \frac{1}{N}\frac{dE}{dT}. \tag{42}$$

The results of calculations are shown in Figs. 5 and 6. Comparison is shown for several values of the number of particles $N$ with the ideal nine-dimensional Bose gas corresponding to the effective space dimensionality (33).

Note that for $D > 3$ the specific heat of the ideal Bose gas has a discontinuity at the critical temperature, cf. [34, 37, 38]. Contrary to the one-dimensional case, here we have specific heat curve maxima at some $T_{\max}^{(N)}$ such that $T_{\max}^{(N)} / T_c < 1$. The shape of the maxima rapidly becomes rather spiky predicting a gap observed in the thermodynamic limit of the nine-dimensional ideal Bose gas. At high temperatures, $C / N \to 9/2$ as expected.

## 6. Conclusions

In the present work, we have used numerical calculations to directly obtain thermodynamic functions based on the discrete energy spectrum of bosons trapped in the linear potential. After performing the analysis of the one-dimensional system, where the spectrum is known to be defined by zeros of the Airy function and its derivative, we have also studied the three-dimensional problem in detail. For the latter case, interpolating expressions have been obtained to describe the spectrum for intermediate values of quantum numbers between $n, \ell \sim 10$ and the WKB limit.

The results of the calculations with discrete spectra have been compared to those within the quasiclassical treatment of an external potential. In the latter approach, particles are confined in the space limited by classical turning points that yields a change in the density of states, hence, the effective rise in the space dimensionality compared to the real one. In the case of a linear external potential, it triples. So, the one-dimensional system confined by $V(x) = \alpha |x|$ would behave like a three-dimensional system in a box, while the three-dimensional system with $V(r) = \alpha r$ is effectively a nine-dimensional one. Our calculations have confirmed these facts. Namely, the specific heat calculated for finite systems of $N = 10, \ldots, 10^4$ particles with the discrete spectrum rapidly approaches to the quasiclassical result in the thermodynamic limit.

We hope our results explicitly confirming the validity of the notion of effective space dimensionality to be useful in studies of trapped Bose systems. The obtained interpolation for the spectrum in the three-dimensional linear trap is of interest on its own as well.

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## Бозе-системи в лінійних пастках: точні розрахунки в порівнянні з ефективною вимірністю простору

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Системи невзаємодіючих бозонів, захоплених лінійними потенціалами $V(r) = \alpha r$, де $r = |\mathbf{r}|$, вивчаються у випадку одновимірного та тривимірного просторів. Для останнього запропоновано інтерполяційну формулу для рівнів енергії між $n, \ell \sim 10$ та квазікласичною границею. Термодинамічні функції розраховано для $N = 10, \ldots, 10^4$ частинок з використанням дискретного енергетичного спектра. Питома теплоємність та фугативність порівнюються з результатами квазікласичного підходу, при якому зовнішній потенціал ефективно збільшує вимірність простору. Як і слід очікувати, це порівняння показує, що термодинамічні функції, отримані з використанням дискретних спектрів, зі збільшенням $N$ швидко наближаються до квазікласичних у просторі з ефективною потроєною вимірністю.

Ключові слова: бозе-системи, лінійні пастки, ефективна вимірність простору.