Ground state energy of the two-dimensional weakly interacting Bose gas: First correction beyond Bogoliubov theory

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We consider the grand potential \(\Omega\) of a two-dimensional weakly interacting homogeneous Bose gas at zero temperature. Building on a number-conserving Bogoliubov method for a lattice model in the grand canonical ensemble, we calculate the next order term as compared to the Bogoliubov prediction, in a systematic expansion of \(\Omega\) in powers of the parameter measuring the weakness of the interaction. Our prediction is in very good agreement with recent Monte Carlo calculations.

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Recent experimental progress with ultracold atoms has renewed the interest in the two-dimensional weakly interacting Bose gas \([1,2]\). In view of a comparison to future experimental results on the equation of state of the gas at low temperatures, this raises the question of the accuracy of existing theoretical work \([3,4]\). Since the pioneering works of Schick \([5]\) and Popov \([6]\) on the energy of the weakly interacting Bose gas in two dimensions, several recent predictions have been proposed. In mathematical physics, it was proved that Schick’s formula for the ground state energy is asymptotically exact in the limit of vanishing density \([7]\). Numerically, very precise Monte Carlo calculations of the ground state energy have been performed \([8,9]\). Analytically, Popov’s result was confirmed by a Bogoliubov-type theory \([10]\) (and by Monte Carlo calculations \([9]\)) but several attempts to calculate analytically the energy beyond Popov’s result have led to non-identical predictions \([11,12,13]\).

The most systematic among the theoretical approaches are those relying on an expansion of the energy in powers of a small parameter. This is the case of the approaches \([6,10]\), which have led to the equation of state \([14]\)

\[
\rho \simeq \frac{m\mu}{4\pi\hbar^2} \ln \left( \frac{4\hbar^2}{m\mu a^2 e^{2\gamma+1}} \right) \tag{1}
\]

where \(m\) is the mass of a boson, \(a > 0\) is the two-dimensional scattering length among the particles, \(\mu\) is the chemical potential and \(\gamma = 0.57721566\ldots\) is Euler’s constant. Remarkably Eq. (1) is universal, i.e. it depends on the interaction potential through the scattering length only. One obtains from (1) the grand potential \(\Omega = E - \mu N\) in the thermodynamic limit, where \(E\) is the gas energy and \(N\) the atom number, by a simple integration over \(\mu\) since \(N = -\partial_\mu \Omega\):

\[
L^{-2}\Omega(\mu) \simeq -\frac{m\mu^2}{8\pi\hbar^2} \ln \left( \frac{4\hbar^2}{m\mu a^2 e^{2\gamma+1}} \right) \tag{2}
\]

where \(L^2\) is the surface of the gas. The small parameter

\[
\epsilon(\mu) = \frac{1}{\ln[4\hbar^2/(\mu ma^2 e^{2\gamma+1})]} \tag{3}
\]

is apparent in (2).

In the vanishing density (or chemical potential) limit, the prediction (1) can be checked to be asymptotically equivalent to Schick’s formula, as it should be. In a further expansion of the energy in terms of the density, the precise value of the constant under the logarithm in (1) eventually matters. In particular, a careful account of the low-energy two-body \(T\)-matrix is essential to derive this constant \([14]\). Its value turns out to agree with recent Monte Carlo results \([8,9]\), see in Fig. 1 the fact that the symbols significantly deviate from unity. Furthermore, this deviation is not accounted for by the beyond-Bogoliubov theories of Refs. \([11,14]\), see in Fig. 1 the fact that the symbols significantly deviate from the dashed and dotted lines.

In the present work we extend the Bogoliubov method \([10]\) as in \([15]\) and we go one step further than Eq. (2) in the expansion of the grand potential in powers of \(\epsilon(\mu)\). We obtain in the thermodynamic limit:

\[
L^{-2}\Omega(\mu) = -\frac{m\mu^2}{8\pi\hbar^2} \left[ \frac{1}{\epsilon(\mu) + \frac{1}{2} + \frac{8I(\epsilon(\mu))}{\pi} + \ldots} \right] \tag{4}
\]

where the numerical constant \(I\) is given by a multiple integral that we have evaluated numerically:

\[
I \simeq 1.0005\ldots \tag{5}
\]

Since the extra term that we have found with respect to (2) is indeed \(o(1)\), this analytically confirms that the numerical constant inside the logarithm in (1) is the correct one. Furthermore, the inclusion of the extra term leads to a now satisfactory agreement with the numerical results of \([8,9]\), see in Fig. 1 the agreement of the solid line with the plotting symbols.

**Our model:** In a first stage we still consider a general value \(d\) of the space dimension. As a regularization scheme to treat ultraviolet divergences, we use a lattice model \([10]\) to represent the interacting Bose gas, with the
The microscopic details of our model, the fact that it is a lattice model or that Catalan’s constant $G = 0.91596\ldots$ appears in \cite{3}, are thus not relevant in this limit. 

Elimination of the condensate mode: We now assume that the ground state of $H$ in the thermodynamic limit is a condensate, so that we take $d = 2$ \cite{5,6} or $d = 3$. We then use Bogoliubov method to eliminate the condensate mode and obtain a Hamiltonian for the field of non-condensed particles. We use here a $U(1)$ symmetry preserving approach in the spirit of \cite{13,19}, adjusted to the case of the grand canonical ensemble. We split the field operator as the sum of the condensate field and the field of the non-condensed modes:

$$
\hat{\psi}(\mathbf{r}) = \phi(\mathbf{r})\hat{a}_0 + \hat{\psi}_{nc}(\mathbf{r}),
$$

where $\hat{a}_0$ is the annihilation operator in the condensate mode $\phi(\mathbf{r}) = 1/L^{d/2}$. We eliminate the condensate particle number $\hat{n}_{k=0} = \hat{a}^\dagger_0 \hat{a}_0$ using

$$
\hat{n}_{k=0} = \hat{N} - \hat{N}_{nc},
$$

where $\hat{N}$ is the total number of particles and

$$
\hat{N}_{nc} = \sum_r \ell^d \hat{\psi}_{nc}^\dagger \hat{\psi}_{nc}
$$

is the number of non-condensed particles. To complete the elimination of the condensate mode, we introduce the representation \cite{20}

$$
\hat{a}_0 = \hat{A} \hat{n}_{k=0}^{1/2} \quad \text{with} \quad \hat{A} \equiv (1 + \hat{n}_{k=0})^{-1/2} \hat{a}_0.
$$

As shown in Eq.\,(5.40) of \cite{20} one has the exact relations $\hat{A} \hat{A}^\dagger = 1$ and $\hat{A}^\dagger \hat{A} = 1 - |\langle \text{vac} | \psi_{nc} \rangle|^2$, where $|\text{vac}\rangle$ is the vacuum state for the condensate mode. The condensate mode elimination is completed by inclusion of $\hat{A}^\dagger$ in the non-condensed field, defining as in \cite{19} the field operator

$$
\hat{A}(\mathbf{r}) = \hat{A}^\dagger \hat{\psi}_{nc}(\mathbf{r}),
$$

which conserves the total particle number. In the thermodynamic limit, the condensate mode has a vanishing probability to be empty, so that $\hat{A}^\dagger \hat{A} \rightarrow \hat{A}^\dagger = 1$, and $\hat{A}$ and $\hat{A}^\dagger$ obey simple commutation relations in this limit.

In the canonical ensemble, it remains to inject the splitting (9) into $H$ and to eliminate the condensate mode, finally replacing the operator $\hat{N}$ by its known value $\hat{N}$. One obtains contributions of various degrees in $\hat{A}$, starting from degree two. The terms of degree two in $\hat{A}$ gives the Bogoliubov Hamiltonian, the terms of higher degrees may be treated by perturbation theory.

In the grand canonical ensemble, however, the chemical potential $\mu$ rather than the particle number is known; at zero temperature, $\hat{N}$ does not fluctuate but assumes
an a priori unknown value $N(\mu)$, a function of $\mu$ to be
determined order by order in the weakly interaction limit.
To zeroth order in $\hat{\Lambda}$, the gas is a pure condensate and one
obtains the mean-field type relation

$$N^{(0)}(\mu) = \frac{\mu L^d}{g_0}. \quad (14)$$

It is then convenient to split $N$ as

$$N(\mu) = N^{(0)}(\mu) + \delta N(\mu). \quad (15)$$

As we shall see, $\delta N(\mu)$ to leading order is second order in
$\hat{\Lambda}$, as the mean number of non-condensed particles $\langle \hat{N}_{nc} \rangle$.
After some calculation, neglecting unity as compared to the condensate atom number and replacing $\hat{N}$ with
$N(\mu)$, we obtain the desired rewriting of the Hamiltonian
with no reference to the condensate mode:

$$H \simeq - \frac{1}{2} \mu N^{(0)}(\mu)$$

$$+ \sum_r e^d \left[ \hat{\Lambda}^\dagger \left( \frac{\hbar^2}{2m} \Delta \right) \hat{\Lambda} + \mu \hat{\Lambda}^\dagger \hat{\Lambda} + \mu \left( \hat{\Lambda}^2 + \hat{\Lambda}^\dagger^2 \right) \right]$$

$$+ \frac{g_0}{2L^d/2} \sum_r e^d \left\{ \left[ N(\mu) - \hat{N}_{nc} \right]^{1/2} \hat{\Lambda}^\dagger \hat{\Lambda} + \text{h.c.} \right\}$$

$$+ \frac{\delta N(\mu) + \hat{N}_{nc}}{2} - 4 \hat{N}_{nc}^2 + \left[ \delta N(\mu) - \hat{N}_{nc} \right] \hat{X}$$

$$+ \hat{X}^\dagger \left[ \delta N(\mu) - \hat{N}_{nc} \right] + \frac{g_0}{2} \sum_r e^d \hat{\Lambda}^\dagger \hat{\Lambda} \hat{\Lambda} \hat{\Lambda}. \quad (16)$$

We have used the fact that, in the spatially homogeneous case, one exactly has $\sum_r e^d \hat{\Lambda}(r) = 0$, and we have set

$$\hat{X} = \sum_r e^d \hat{\Lambda}^2. \quad (17)$$

Perturbative expansion: We now expand in powers of $\hat{\Lambda}$. Keeping terms up to second order in $\hat{\Lambda}$ we obtain

$$H_{\leq 2} = - \frac{1}{2} \mu N^{(0)}(\mu) + \sum_r e^d \left[ \hat{\Lambda}^\dagger \left( \frac{\hbar^2}{2m} \Delta \right) \hat{\Lambda} + \mu \hat{\Lambda}^\dagger \hat{\Lambda}^\dagger \right]$$

$$+ \mu \hat{\Lambda}^\dagger \hat{\Lambda} + \mu \left( \hat{\Lambda}^2 + \hat{\Lambda}^\dagger^2 \right). \quad (18)$$

This plays the role of the Bogoliubov Hamiltonian in the usual theory. Its ground state energy we thus call the
Bogoliubov approximation for the grand potential:

$$\Omega_{\text{Bog}}(\mu) = -\frac{\mu^2 L^d}{2g_0} - \sum_{k \in D^*} \epsilon_k V_k^2 \quad (19)$$

where we have replaced $N^{(0)}(\mu)$ by its value and we have introduced the Bogoliubov modal amplitudes obeying

$$U_k + V_k = \frac{1}{U_k - V_k} = \left( \frac{\hbar^2 k^2/(2m)}{2\mu + \hbar^2 k^2/(2m)} \right)^{1/4} \equiv s_k \quad (20)$$

and the corresponding Bogoliubov energies

$$\epsilon_k = \left[ \frac{\hbar^2 k^2}{2m} \left( \frac{\hbar^2 k^2}{2m} + 2\mu \right) \right]^{1/2}. \quad (21)$$

Taking minus the derivative of $\Omega_{\text{Bog}}$ with respect to $\mu$ to obtain the atom number, and using

$$\partial_\mu (\epsilon_k V_k^2) = -V_k(U_k + V_k), \quad (22)$$

one recovers, in the thermodynamic limit, Eq.(152) in [10], and thus (1) in the limit $\ell \rightarrow 0$ as [22].

To go beyond Bogoliubov, we collect into $H_3$ the terms of degree three in $\hat{\Lambda}$ and into $H_4$ the terms of degree four in $\hat{\Lambda}$, keeping in mind that $\delta N(\mu)$ is to leading order of degree two, $\delta N(\mu) = N^{(2)}(\mu) + \ldots$, so that

$$H_3 = g_0 \left[ N^{(0)}(\mu) \right]^{1/2} \sum_r e^d \hat{\Lambda}^\dagger (\hat{\Lambda} + \hat{\Lambda}^\dagger) \hat{\Lambda} \quad (23)$$

$$H_4 = g_0 \left\{ \left[ N^{(2)}(\mu) + \hat{N}_{nc} \right]^2 - 4 \hat{N}_{nc}^2 + \left[ N^{(2)}(\mu) - \hat{N}_{nc} \right] \hat{X}$$

$$+ \hat{X}^\dagger \left[ N^{(2)}(\mu) - \hat{N}_{nc} \right] + \frac{g_0}{2} \sum_r e^d \hat{\Lambda}^\dagger \hat{\Lambda} \hat{\Lambda} \hat{\Lambda}. \quad (24)$$

We treat $H_4$ to first order in perturbation theory and $H_3$ to second order, to obtain the first correction to the Bogoliubov prediction for the grand potential:

$$\delta \Omega = \langle H_4 \rangle + \langle H_3 \rangle - \frac{1}{\Omega_{\text{Bog}} - H_{\leq 2}} H_3 \quad (25)$$

where the expectation value is taken in the ground state of $H_{\leq 2}$, that is in the vacuum of the operators $b_k$ appearing in the modal expansion

$$\hat{\Lambda}(r) = L^{-d/2} \sum_{k \in D^*} \hat{b}_k U_k e^{ik \cdot r} + \hat{b}_k^\dagger V_k e^{-ik \cdot r}. \quad (26)$$

To find the value of $N^{(2)}(\mu)$, we minimize $\langle H_4 \rangle$ over $N^{(2)}$, keeping in mind that $H_{\leq 2}$ and $H_3$ do not depend on $N^{(2)}$. In the thermodynamic limit, one has $\langle \hat{N}_{nc}^2 \rangle \simeq \langle \hat{N}_{nc} \rangle^2$ and $\langle \hat{N}_{nc} \hat{X} \rangle \simeq \langle \hat{N}_{nc} \rangle \langle \hat{X} \rangle$, so that

$$N^{(2)}(\mu) \simeq -\langle \hat{N}_{nc} + \frac{\hat{X} + \hat{X}^\dagger}{2} \rangle = -\sum_{k \in D^*} V_k (U_k + V_k). \quad (27)$$

The divergence of $N^{(0)}(\mu)$ when $\ell \rightarrow 0$ is removed in the combination $N^{(0)}(\mu) + N^{(2)}(\mu)$. The resulting density is in agreement with Eq. (1). One is then left with

$$\langle H_4 \rangle \simeq -\frac{g_0}{L^d} \langle \hat{N}_{nc} \rangle \left[ \langle \hat{N}_{nc} \rangle + 2 \langle \hat{X} \rangle \right]. \quad (28)$$

Using the modal expansion (26) and Wick’s theorem we finally obtain after some calculation

$$\delta \Omega \simeq -\frac{\mu^2}{N^{(0)}(\mu) + N^{(2)}(\mu)} \sum_{k_1, k_2 \in D^*} \left\{ \frac{V^2_k V_{k_1} (U_{k_1} + s_{k_1})}{\mu} \right\}$$

$$+ (1 - \delta_{k_2,0}) \frac{U_{k_1} s_3 V_3}{s_1 + \epsilon_2 + \epsilon_3} \sum_{\sigma \in D} U_{(1)\sigma} s_{(2)\sigma} V_{(3)\sigma} \right\}. \quad (29)$$
We have introduced the vector $k_2 \in D$ such that $k_1 + k_2 + k_3 \in (2\pi/\ell)\mathbb{Z}^d$. The notation $U_{ij}, i, j \in \{1, 2, 3\}$, stands for $U_{k_i}$. The sum over $\sigma$ runs over the permutation group $S_3$. For convenience we have added $N^{(2)}(\mu)$ to $N^{(0)}(\mu)$ in the denominator of the overall factor in (29), which is allowed at the present order of the calculation.

Absence of divergences in 2D: We now take the thermodynamic limit, replacing sums over $k$ by integrals over the domain $D$ in (29). We also take the zero lattice spacing limit $\ell \to 0$ so that the integration domain over $k$ is now $\mathbb{R}^d$. Since $k_0 = -(k_1 + k_3)$ and the integrand depends only on the moduli $k_1, k_2$ and $k_3$, see (29), we are left with a triple integral over $k_1, k_3$ and the angle between the vectors $k_1$ and $k_3$. In 2D, we show below that this integral converges, that is it has neither an infrared nor an ultraviolet divergence. The first correction beyond the Bogoliubov energy is thus universal in 2D. Since convergence is established, we can resort to numerical integration. After the change of variables $q_i = h k_i/(2m \mu)^{1/2}$ and pulling out a factor $\pi (2m \mu)^{1/2} L/(2\pi h)^{1/2}$, we get [5]. Summing $\Omega_{\text{Bog}}$ to $\delta \Omega$ we then obtain (1).

To show the infrared convergence, we replace the integrand by its leading low-$k_1$ behavior: $U_i$ and $V_i$ diverge as $1/\sqrt{k_1}$, $s_i$ vanishes as $1/\sqrt{k_1}$ and $\epsilon_i$ vanishes as $k_i$. Including the Jacobian factors $k_1$ and $k_3$ from 2D integration in polar coordinates, we see that the integral of the first term in the curly brackets of (29) converges. The contribution of the term due to permutation $\sigma$ scales as

$$\frac{k_1 k_3}{k_1 + k_2 + k_3} \left( \frac{k_2}{k_1 k_3} \right)^{1/2} \left( \frac{k_{\sigma(2)}}{k_{\sigma(1)} k_{\sigma(3)}} \right)^{1/2} < 1,$$

(30)

so its integral over $k_1$ and $k_3$ is also convergent.

For the ultraviolet convergence, the full reasoning is rather long [21], so we give a simplified explanation. We approximate each term in the integrand in (29) by its leading high-$k_1$ behavior, $U_i$ and $s_i$ tending to unity, $V_i$ vanishing as $1/k_1^2$ and $\epsilon_i$ diverging as $k_i^2$. In the sum over $\sigma$, the terms with $\sigma(3) \neq 3$ are not dangerous. E.g. for $\sigma(3) = 1$, a factor $V_1 V_3$ appears, and including the Jacobian factors, one obtains a contribution scaling as

$$\frac{k_1 k_3}{k_1^2 + k_2^2 + k_3^2} \times \frac{1}{k_1^2 k_3^2} \leq \frac{1}{2k_1^2 k_3^2},$$

(31)

so that the resulting double integral over $k_1$ and $k_3$ is convergent at infinity. The dangerous terms in the sum over $\sigma$ thus correspond to $\sigma(3) = 3$: the factor $V_3^2$ ensures convergence of the integral over $k_3$ over a $k_1$-independent range $\sim (m \mu/h^2)^{1/2}$. At large $k_1$, the energy denominator $\epsilon_1 + \epsilon_2 + \epsilon_3$ approaches $2\epsilon_1$. Then, from the asymptotic relation $V_1 \simeq -\mu/(2\epsilon_1)$, we see that the two dangerous contributions coming from the permutations with $\sigma(3) = 3$ exactly compensate with the first term $\simeq 2V_3^2 V_1/\mu$ in the curly brackets of (29), which avoids an ultraviolet divergence of $\delta \Omega$.

In conclusion, we have calculated analytically and in a systematic way the first correction to the Bogoliubov prediction for the ground state grand potential of a 2D weakly interacting Bose gas. We find that this correction is universal, depending on the interaction potential through the scattering length only. It allows to describe analytically the not extremely weakly interacting regime, and contrary to all analytical works, we obtain a prediction for the ground state energy in excellent agreement with the numerical results of [8,9] over the range where the results of [8,9] are model independent.

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[22] More precisely, in 2D, our expansion in powers of $A$ is an expansion in powers of $\epsilon(\mu)$ for a fixed value of $\eta(\mu) = \ln(\xi/\ell) \gg 1$, where $\xi^2/(m \mu^2) = \mu$. The Bogoliubov method indeed relies on a Born expansion [23] (here in powers of $g_0$) of the scattering amplitude $f_k$ for $k \simeq 1/\xi$. From Eq.(167) of [10] the small parameter for the Born expansion is $2\epsilon$. This small parameter is explicitly obtained in our approach, from the requirement $N^{(2)}(\xi) \ll N^{(0)}(\xi)$. Estimating from (27) $N^{(2)} \simeq \eta L^2 m \mu/(2\pi \hbar^2)$ for $\xi \ll \ell$, we get $N^{(2)}/N^{(0)} \approx 2\epsilon/(1 + 2\epsilon)$. One then takes the limit $\eta \to +\infty$ in each coefficient of the expansion of $\Omega$ in powers of $\epsilon$. This limit is exponentially fast approached in $\eta$: we find that $\eta = 7$ is more than large enough, it gives the value of $I$ in [3] at the $10^{-15}$ level.
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