Upper bound for the ground state energy of a dilute 2D Bose gas

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1 Introduction

So far, there are few rigorous results about the ground state energy of a dilute Bose gas in two dimensions. For nonnegative potentials the ground state energy per particle in the thermodynamic limit has been shown to be

$$e_0(\rho) = 4\pi\rho b + o(\rho b)$$

for $\rho \to 0$, where $b = 1/|\ln \rho a^2|$ and a denotes the scattering length of the interaction potential [4]. For the next order, non-rigorous approximations [1] and Monte Carlo simulations [5] suggest the negative correction $4\pi\rho b^2 \ln(b)$. We calculate an upper bound on the ground state energy using the variational method with a quasi-free trial state. For a dilute Bose gas in 3D the same calculation has been done previously in [2]. We follow their computation and make the necessary adjustments for the 2D case.

The setup is as follows. First we consider a finite 2D box $\Lambda = [0, L]^2 \subset \mathbb{R}^2$ with periodic boundary conditions. The number of bosons in our system is N and we include only two-body interactions. The interactions are described by a rotationally symmetric potential V. We assume that $V \neq 0$ is nonnegative, continuous and has finite range, i.e. V(x) = 0 for $|x| \geq R_0$. The Hamiltonian is

$$H_N = -\sum_{i=1}^N \Delta_i + \frac{1}{2} \sum_{\substack{i,j=1\\i \neq j}}^N V(x_i - x_j),$$

where Δ_i is the Laplace operator with respect to the coordinates of the *i*th particle. For the Fourier transfom of any function f(x) on Λ we use the convention

$$\hat{f}_p = \int_{\Lambda} e^{-ip \cdot x} f(x) \mathrm{d}x, \qquad f(x) = \frac{1}{|\Lambda|} \sum_{p \in \Lambda^*} e^{ip \cdot x} \hat{f}_p,$$

where $p \in \Lambda^* := \left(\frac{2\pi}{L}\mathbb{Z}\right)^2$ and $|\Lambda| = L^2$ is the size of the box. For any continuous function f on \mathbb{R}^2 we have

$$\lim_{L \to \infty} \frac{1}{|\Lambda|} \sum_{p \in \Lambda^*} f(p) = \int_{\mathbb{R}^2} \frac{\mathrm{d}p}{(2\pi)^2} f(p).$$

After second quantization the Hamiltonian becomes

$$H = \sum_{p} p^2 a_p^{\dagger} a_p + \frac{1}{2|\Lambda|} \sum_{p,q,r} \hat{V}_r a_p^{\dagger} a_q^{\dagger} a_{p-r} a_{p+r}$$

for bosonic creation and annihilation operators a_p, a_p^{\dagger} and $p \in \Lambda^*$. The commutation relations are

$$[a_p, a_q^{\dagger}] = a_p a_q^{\dagger} - a_q^{\dagger} a_p = \begin{cases} 1 & \text{if } p = q \\ 0 & \text{otherwise.} \end{cases}$$

For the variational principle we pick the Ansatz

$$|\Psi\rangle = \exp\left(\frac{1}{2}\sum_{k\neq 0}c_k a_k^{\dagger} a_{-k}^{\dagger} + \sqrt{N_0}a_0^{\dagger}\right)|0\rangle,$$

where $|0\rangle$ denotes the vacuum, c_k are real numbers with $|c_k| < 1$ and $c_k = c_{-k}$ and N_0 is a positive real number. The goal is to minimize the energy

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

under the constraint of constant particle number

$$N = \frac{\langle \Psi | \sum_{m \in \Lambda^*} a_m^{\dagger} a_m | \Psi \rangle}{\langle \Psi | \Psi \rangle}.$$

This will motivate our choice of parameters c_k and N_0 . Then we take the limit $N, L \to \infty$ of the energy per particle $e(\rho) = E/N$ while keeping the density $\rho = N/L^2$ constant. We are interested in the dilute limit, i.e. small density ρ .

2 Computation

2.1 Energy

The Ansatz for $|\Psi\rangle$ looks precisely the same as the trial state in [2]. However, the bosonic creation operators and the vacuum have a different physical meaning since they describe a 2D instead of a 3D system. Their algebraic relations are the same though. This is why the functional expression for the energy is precisely the same as in the 3D case. From Lemma 2 and equations (46) and (47) in [2] we have $e(\rho) = e_M + \Omega_2 + \Omega_4$, where

$$e_{M} = \frac{1}{2}\hat{V}_{0}\rho + \frac{1}{\rho|\Lambda|}\sum_{p\neq0}\left[(p^{2}+\rho\hat{V}_{p})\frac{e_{p}^{2}}{1-2e_{p}} + \rho\hat{V}_{p}\frac{e_{p}(1-e_{p})}{1-2e_{p}} - \frac{\hat{V}_{p}}{|\Lambda|}\left(\sum_{r\neq0}\frac{e_{r}^{2}}{1-2e_{r}}\right)\frac{e_{p}(1-e_{p})}{1-2e_{p}} + \frac{1}{2|\Lambda|}\sum_{r\neq0,\pm p}\hat{V}_{p-r}\frac{e_{p}(1-e_{p})e_{r}(1-e_{r})}{(1-2e_{p})(1-2e_{r})}\right], \quad (1)$$

$$\begin{split} \Omega_2 + \Omega_4 &= \frac{1}{\rho|\Lambda|} \sum_{p \neq 0} \left[\frac{1}{2|\Lambda|} \sum_{r \neq 0, \pm p} (\hat{V}_0 + \hat{V}_{p-r}) \frac{e_r^2 e_p^2}{(1 - 2e_r)(1 - 2e_p)} - \frac{\hat{V}_p + \hat{V}_0}{|\Lambda|} \left(\sum_{r \neq 0} \frac{e_r^2}{1 - 2e_r} \right) \frac{e_p^2}{1 - 2e_p} \right. \\ &+ \frac{1}{2|\Lambda|} \left(\frac{e_p(1 - e_p)}{1 - 2e_p} \right)^2 \left(\hat{V}_0 \frac{1 - 2e_p + 4e_p^2}{(1 - e_p)^2} + \hat{V}_{2p} \frac{1 - 2e_p + 2e_p^2}{(1 - e_p)^2} \right) \right] + \frac{\hat{V}_0}{2|\Lambda|} \left(\sum_{p \neq 0} \frac{e_p^2}{1 - 2e_p} \right)^2 \end{split}$$

and $e_p = \frac{c_p}{1+c_p}$. The condition $|c_p| < 1$ translates to $e_p \in (-\infty, \frac{1}{2})$.

2.2 Choice of parameters

From the previous results [4] we know that the leading order term of $e(\rho)$ should only depend on the scattering length of the potential and not on other details of the potential. The scattering length is defined as follows. For every $R > R_0$ let us consider the zero energy scattering equation $-\Delta u + \frac{1}{2}Vu = 0$ on $B_R(0)$ with boundary condition u(x) = 1 for |x| = R. In Appendix C of [4] they show that a function $\beta : \mathbb{R} \to \mathbb{R}$ determines the solution u_R of the scattering equation for any R through

$$u_R(x) = \frac{\beta(|x|)}{\ln(R/a)},$$

where a is a constant depending only on the potential V. This constant a is the scattering length. The function β is nonnegative, monotonically increasing and for $r > R_0$ it is given by $\beta(r) = \ln(r/a)$. Therefore, the scattering length $a \leq R_0$ and the scattering solutions satisfy $0 \leq u_R(x) \leq 1$.

We want to pick a particular R and relate \hat{V}_0 to the scattering length using u_R . It turns out that the choice $R = R^* := (c\rho)^{-1/2} > R_0$ for some constant c > 0 will reproduce the correct leading order term for $e(\rho)$. Note that the average particle distance is of order $\rho^{-1/2}$. Intuitively, two-particle interactions should be important precisely up to this length scale. This gives a physical motivation for the choice of u_R . For $|x| \leq (c\rho)^{-1/2}$ let

$$u(x) = u_{R^*}(x) = \frac{2\beta(|x|)}{|\ln(c\rho a^2)|}.$$

We extend the domain of the scattering solution to the whole box. For $|x| > (c\rho)^{-1/2}$ we choose u(x) = 1.

This function u obeys the modified scattering equation

$$-\Delta u + \frac{1}{2}Vu = \frac{2(c\rho)^{1/2}}{|\ln(c\rho a^2)|}\delta(r - (c\rho)^{-1/2})$$
(2)

With

$$w = 1 - u$$
, $g = Vu$ and $f = Vw$

the Fourier transform of this equation is

$$-p^{2}\hat{w}_{p} + \frac{1}{2}\hat{g}_{p} = \frac{4\pi}{|\ln(c\rho a^{2})|}J_{0}\left(p(c\rho)^{-1/2}\right),\tag{3}$$

where J_0 denotes the Bessel function of the first kind. An important expansion parameter will be $b = 1/|\ln \rho a^2|$. Let $\tilde{b} = 1/|\ln(c\rho a^2)| = b + \ln(c)b^2 + \ln(c)^2b^3 + O(b^4)$. Note that $\hat{g}_0 = 8\pi \tilde{b}$ by eq. (3). Since $0 \le w(x), u(x) \le 1$ we have $0 < \hat{f}_0 \le \hat{V}_0$ and $0 \le \hat{g}_0 < \hat{V}_0$. Moreover, thanks to rotational symmetry \hat{g}_p, \hat{V}_p and \hat{f}_p only depend on |p|.

The full energy is very difficult to minimize. However, it is possible to minimize certain terms in the energy explicitly. This motivates our choice of e_p as will become clear later. We choose the e_p like in [2] as minimizer of

$$m_p(e_p) = p^2 \frac{e_p}{1 - 2e_p} + \rho \hat{V}_p \frac{e_p}{1 - 2e_p} - \rho \hat{f}_p e_p$$

This results in

$$e_p = \frac{1}{2} \left[1 - \left(1 + 2 \frac{\rho \hat{g}_p}{p^2 + 2\rho \hat{f}_p} \right)^{1/2} \right] \le 0.$$
(4)

The minimal value of m_p is

$$m_p = \frac{1}{2} \left[\sqrt{(p^2 + 2\rho \hat{V}_p)(p^2 + 2\rho \hat{f}_p)} - (p^2 + \rho (\hat{V}_p + \hat{f}_p) \right].$$

2.3 Estimates

Proposition 2.1. The Fourier transforms of V, f and g are uniformly Lipschitz continuous, *i.e.* there is a constant C depending only on V such that for all p, r in Λ^*

$$\hat{V}_p - \hat{V}_{p-r} \leq C|r|, \quad |\hat{f}_p - \hat{f}_{p-r}| \leq C|r|, \quad |\hat{g}_p - \hat{g}_{p-r}| \leq C|r|\tilde{b}.$$
(5)

Therefore, there is a small δ depending on V such that for $|p| \leq \delta$

$$\frac{\hat{V}_0}{2} \le \hat{V}_p \le \hat{V}_0, \quad \frac{\hat{f}_0}{2} \le \hat{f}_p \le \hat{f}_0, \quad \frac{\hat{g}_0}{2} \le \hat{g}_p \le \hat{g}_0.$$
 (6)

Proof. We have $|\hat{g}_p - \hat{g}_{p-r}| = |\int_{B_{R_0}} V(x)u(x)e^{ip\cdot x}(e^{ir\cdot x} - 1)dx|$, where B_{R_0} is the disk with radius R_0 centered at zero. Since $|(e^{ir\cdot x} - 1)| \le |r||x|$ and $u(x) \le 2\tilde{b} \max_{x \in B_{R_0}} \beta(|x|)$ the bound follows. For \hat{V} and \hat{f} in the above equation we replace u by 1 or $w \le 1$, respectively.

Now we want to prove the analogon of Lemma 5 in [2].

Lemma 2.2. For $\rho \to 0$ the energy per particle is $e(\rho) = e_M + \Omega_2 + \Omega_4 = e_M + O(\rho \tilde{b}^4)$, where

$$e_M = 4\pi\rho\tilde{b} + \frac{1}{\rho|\Lambda|} \sum_{p\neq 0} \left[(p^2 e_p + \rho\hat{V}_p) \frac{e_p}{1 - 2e_p} + \frac{1}{2|\Lambda|} \sum_{r\neq 0} \hat{V}_{p-r} e_p e_r + \frac{\rho^2}{2} \hat{V}_p \hat{w}_p \right] + O(\rho\tilde{b}^4).$$

Proof. First of all we rewrite \hat{V}_0 in the first term of (1) as $\hat{V}_0 = \hat{g}_0 + \frac{1}{|\Lambda|} \sum_p \hat{V}_p \hat{w}_p = 8\pi \tilde{b} + \frac{1}{|\Lambda|} \sum_{p \neq 0} \hat{V}_p \hat{w}_p + \frac{\hat{V}_0 \hat{w}_0}{|\Lambda|}$. The last term is negligible in the thermodynamic limit $|\Lambda| \to \infty$, because \hat{V}_0 and $\hat{w}_0 \leq \pi (c\rho)^{-1}$ are finite.

The functional expression for e_p is the same as in 3D. The upper bounds for $|e_p|$ in equation (49) in [2] rely only on uniform Lipschitz continuity of \hat{V}, \hat{g} and $\hat{f}, 0 < \hat{f}_0 \leq \hat{V}_0$ and $0 \leq \hat{g}_0 < \hat{V}_0$. Since these conditions hold in 2D, we can use the upper bounds in (49). Also equations (50) and (51) go through unchanged. In order to estimate $\Omega_2 + \Omega_4$ we follow the procedure in [2]. To calculate the estimates for expressions (53) - (55) in 2D, we use that $|\hat{g}_p| \leq \hat{g}_0 = 8\pi \tilde{b}, \hat{f}_0 \leq \hat{V}_0$ and $\int_{|p|\geq\delta} \hat{g}_p \frac{dp}{(2\pi)^2} \leq g(0) = 2V(0)\beta(0)\tilde{b}$. For the quantities in (53) - (55) this results in new bounds

$$(53) \le C\rho\tilde{b}^2, \qquad (54) \le C\rho\tilde{b}, \qquad (55) \le C\rho\tilde{b}^2.$$

The 2D analogon of bounds (58) - (62) therefore is

$$(58) \le CN\rho\tilde{b}^4, \quad (59) \le CN\rho\tilde{b}^4, \quad (60) \le CN\rho\tilde{b}^4, \quad (61) \le C\rho\tilde{b}^2, \quad (62) \le C\rho\tilde{b}^2.$$

Thus, there is a constant C such that $\Omega_2 + \Omega_4 \leq C\rho b^4$.

The next step is to replace the \hat{V}_p by \hat{V}_{p-r} in the second last term of (1). The difference can be estimated as in eq. (63) in [2]. It adds a negligible error of $O(\rho^{3/2}\tilde{b}^3)$ to e_M . Following the calculation after (63) in [2], the last two terms in (1) combine to give the term $\frac{1}{2\rho|\Lambda|^2}\sum_{r,p\neq 0}\hat{V}_{p-r}e_pe_r$ at expense of an error $O(\rho\tilde{b}^4)$.

Like in the proof of Theorem 1 in [2] we use the identity

$$\frac{1}{2}(e, \hat{V} * e) = \frac{1}{2}(e + \rho\hat{w}, \hat{V} * (e + \rho\hat{w})) - \rho(e, \hat{V} * \hat{w}) - \frac{\rho^2}{2}(\hat{w}, \hat{V} * \hat{w})$$

and (3) to arrive at the analogon of (65) in [2]:

$$e(\rho) = 4\pi\rho\tilde{b} + \frac{1}{\rho|\Lambda|} \sum_{p\neq0} \left[(p^2e_p + \rho\hat{V}_p) \frac{e_p}{1 - 2e_p} - \rho(\hat{V} * \hat{w})_p e_p + \frac{\rho^2 \hat{g}_p}{4p^2} \left(\hat{g}_p - 8\pi\tilde{b}J_0\left(p(c\rho)^{-1/2}\right) \right) \right] \\ + \frac{1}{2|\Lambda|} \sum_{r,p\neq0} \hat{V}_{p-r}(e_p + \rho\hat{w}_p)(e_r + \rho\hat{w}_r) + O(\rho b^4).$$
(7)

Calculating the first sum and estimating the second one, we obtain the following result.

Theorem 2.3. The energy per particle in the thermodynamic limit is

$$e(\rho) = 4\pi\rho b + 8\pi\rho b^2 (\Gamma + \frac{1}{2}(\ln\hat{V}_0 - \ln 2)) + R + O(\rho b^3),$$
(8)

where Γ denotes the Euler-Mascheroni constant and

$$R = \frac{1}{2(2\pi)^4 \rho} \int_{\mathbb{R}^2} dr \int_{\mathbb{R}^2} dp \ \hat{V}_{p-r}(e_p + \rho \hat{w}_p)(e_r + \rho \hat{w}_r) \le C\rho b^2.$$

Proof. Let us first estimate R. Since $|\hat{V}_{p-r}| \leq \hat{V}_0$, we have

$$R \le \frac{C}{\rho} \left(\int_{\mathbb{R}^2} e_p + \rho \hat{w}_p \mathrm{d}p \right)^2.$$

From equation (3) we get $\hat{w}_p = \frac{\hat{g}_p}{2p^2} - \frac{4\pi\tilde{b}}{p^2}J_0\left(p(c\rho)^{-1/2}\right)$. We will estimate the integral the following way:

$$\left| \int_{\mathbb{R}^{2}} e_{p} + \rho \hat{w}_{p} \mathrm{d}p \right| \leq \int_{p^{2} \leq 4\hat{V}_{0}\rho} |e_{p}| \,\mathrm{d}p + \int_{p^{2} \leq 4\hat{V}_{0}\rho} |\rho \hat{w}_{p}| \,\mathrm{d}p + \int_{p^{2} \geq 4\hat{V}_{0}\rho} \left| e_{p} + \frac{\rho \hat{g}_{p}}{2p^{2}} \right| \mathrm{d}p + \int_{p^{2} \geq 4\hat{V}_{0}\rho} \left| \frac{4\pi\rho \tilde{b}}{p^{2}} J_{0}\left(p(c\rho)^{-1/2}\right) \right| \mathrm{d}p.$$
(9)

Let us first take care of the terms with $p^2 \leq 4\hat{V}_0\rho$. Thanks to uniform Lipschitz continuity, for ρ small enough we have $\inf_p(p^2 + 2\rho\hat{f}_p) > \rho\hat{f}_0 > 0$ like in (45) in [2]. It follows that $\left|\frac{\rho\hat{g}_p}{p^2 + 2\rho\hat{f}_p}\right| \leq \frac{g_0}{f_0} = O(\tilde{b})$. Thus $|e_p| = O(\tilde{b})$ and the first term in (9) is bounded by $C\rho\tilde{b}$ for some constant C.

In the second term we replace \hat{g}_p by \hat{g}_0 using uniform Lipschitz continuity. This gives a negligible error of order $O(\rho^{3/2}\tilde{b})$. The rest is

$$\int_{p^2 \le 4\hat{V}_0\rho} \left| \rho \frac{\hat{g}_0}{2p^2} - \frac{4\pi\tilde{b}}{p^2} J_0\left(p(c\rho)^{-1/2}\right) \right| \mathrm{d}p = 8\pi^2 \rho \tilde{b} \int_0^{2\sqrt{\hat{V}_0/c}} \frac{1 - J_0(x)}{x} \mathrm{d}x = C\rho \tilde{b}.$$

For $p^2 > 4\hat{V}_0\rho$ we expand e_p in $\rho \hat{g}_p/p^2$ to obtain

$$e_p = -\frac{\rho \hat{g}_p}{2(p^2 + 2\rho \hat{V}_p)} + O\left(\left(\frac{\rho \hat{g}_p}{p^2}\right)^2\right).$$

Then

$$\int_{p^2 \ge 4\hat{V}_0\rho} \left| e_p + \frac{\rho \hat{g}_p}{2p^2} \right| \mathrm{d}p \le \int_{p^2 \ge 4\hat{V}_0\rho} \frac{\rho \hat{g}_0}{2p^2} \sum_{k=1}^{\infty} \left(\frac{2\rho \hat{V}_0}{p^2} \right)^k \mathrm{d}p + O(\rho \tilde{b}^2) = C\rho \tilde{b} + O(\rho \tilde{b}^2)$$

where we were able to swap integration and summation by Tonelli's theorem. The last summand in (9) is equal to $8\pi^2 \rho \tilde{b} \int_{2\sqrt{\hat{V}_0/c}}^{\infty} \frac{J_0(x)}{x} dx = C\rho \tilde{b}$. Therefore, we can bound (9) with $C\rho \tilde{b}$ and $R \leq C\rho \tilde{b}^2$. Note that the next order error terms are $O(\rho \tilde{b}^3)$.

Let us now compute the second sum in (7). Note that the choice of e_p minimizes this term. Using (2.2) and substituting $|p| = \sqrt{x\rho}$ the term is equal to

$$Q = \frac{\rho}{8\pi} \int_0^\infty \mathrm{d}x \left[F(x, \sqrt{x\rho}) - \frac{8\pi \tilde{b}\hat{g}_p}{2x} J_0\left(\sqrt{x/c}\right) \right],$$

where

$$F(x,p) = \sqrt{(x+2\hat{f}_p)(x+2\hat{V}_p)} - (x+\hat{f}_p+\hat{V}_p) + \frac{\hat{g}_p^2}{2x}$$

The first step is to replace all the Fourier transforms at p by their respective values at 0. The error I can be estimated with

$$I \le C\rho \int_0^\infty |F(x,\sqrt{x\rho}) - F(x,0)| \,\mathrm{d}x + C\rho\tilde{b} \int_0^\infty \frac{|\hat{g}_p - \hat{g}_0|}{x} \left| J_0\left(\sqrt{x/c}\right) \right| \,\mathrm{d}x,$$

To bound the second integral, we use $|\hat{g}_p - g_0| \leq C\tilde{b}\sqrt{x\rho}$ for $x \leq \rho^{-1}$ and $|\hat{g}_p - g_0| \leq C\tilde{b}$ for $x \geq \rho^{-1}$. Moreover, for $x \leq c$ we estimate $\left|J_0\left(\sqrt{x/c}\right)\right| \leq 1$, while for $x \geq c$ we use $\left|J_0\left(\sqrt{x/c}\right)\right| \leq Cx^{-1/4}$. With this the second integral is $O(\rho^{1/4}\tilde{b})$.

 $\left| J_0\left(\sqrt{x/c}\right) \right| \leq Cx^{-1/4}.$ With this the second integral is $O(\rho^{1/4}\tilde{b})$. For the first integral we proceed as in [2] after (70). The same argument as in 3D shows there is a constant ϵ such that for $x \leq \epsilon \rho^{-1}$ we have $\left| F(x, \sqrt{x\rho}) - F(x, 0) \right| \leq C |p| x^{-1} (1+x)^{-1}.$ Hence,

$$\int_0^{\epsilon \rho^{-1}} |F(x, \sqrt{x\rho}) - F(x, 0)| \, \mathrm{d}x \le C\sqrt{\rho} \arctan\left(\epsilon \rho^{-1/2}\right) \le C\sqrt{\rho}.$$

Moreover, the same expansion as in 3D shows that for small enough ρ we have $F(x, p) \leq Cx^{-2}$ for $x \geq \epsilon \rho^{-1}$ and all p. Hence,

$$\int_{\epsilon\rho^{-1}}^{\infty} |F(x,\sqrt{x\rho}) - F(x,0)| \, \mathrm{d}x \le C\rho.$$

In total we have that I is of negligible order $O(\rho^{5/4}\tilde{b}^2)$.

Next, we substitute $y = x/8\pi \tilde{b}$ and obtain $Q = 8\pi \rho \tilde{b}^2 \int_0^\infty h(y,\rho) dy + O(\rho^{5/4} \tilde{b}^2)$, where

$$h(y,\rho) = \sqrt{\left(y + \frac{2\hat{V}_0}{8\pi\tilde{b}}\right)\left(y + \frac{2\hat{V}_0}{8\pi\tilde{b}} - 2\right) - \left(y + \frac{2\hat{V}_0}{8\pi\tilde{b}} - 1\right) + \frac{1}{2y}\left(1 - J_0\left(\sqrt{8\pi\tilde{b}y/c}\right)\right)}.$$

Computing the integral and expanding yields

$$Q = 8\pi\rho \tilde{b}^2 \left(\Gamma + \frac{1}{2} (\ln \hat{V}_0 - \ln 2 - \ln c) + O(\tilde{b}) \right).$$

Combining $e(p) = 4\pi\rho\tilde{b} + Q + R + O(\rho\tilde{b}^3)$ and using $\tilde{b} = b + \ln(c)b^2 + O(b^3)$ we arrive at the result (8).

3 Conclusion

Our result gives an upper bound on the ground state energy of a dilute Bose gas in 2D. To leading order the bound is tight. However, our bound does not provide the expected negative correction of order $\rho b^2 \ln(b)$ and directly gives a smaller correction of order $O(\rho b^2)$. The main difference between the computations in 2D and 3D comes from the different scattering solutions.

Remark 3.1. In our computation, we did not specify the constant c. The choice of this constant may affect the result at order $O(\rho b^2)$ through the term R.

Remark 3.2. With the additional assumption that $\hat{V}_0 = \nu b$ for $\nu = O(1)$ in ρ we obtain $e(\rho) = 4\pi\rho b + 4\pi\rho b^2 \ln b + O(\rho b^2)$. The same assumption is made in [3], where they also obtain the $4\pi\rho b^2 \ln(b)$ correction with a calcuation similar to ours.

In our derivation, we chose the e_p in such a way that we could find explicit expressions for them. However, they do not minimize the full energy functional. It remains an open question whether this method definitely fails in finding the negative correction of order $\rho b^2 \ln(b)$. Maybe minimizing the full functional would give us the desired term.

4 References

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