The Ground State Energy of a Dilute Two-Dimensional Bose Gas

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The ground state energy per particle of a dilute, homogeneous, two-dimensional Bose gas, in the thermodynamic limit is shown rigorously to be $E_0/N = (2\pi\hbar^2\rho/m) |\ln(\rho a^2)|^{-1}$, to leading order, with a relative error at most $O(|\ln(\rho a^2)|^{-1/5})$. Here N is the number of particles, $\rho = N/V$ is the particle density and a is the scattering length of the two-body potential. We assume that the two-body potential is short range and nonnegative. The amusing feature of this result is that, in contrast to the three-dimensional case, the energy, E_0 is not simply $N(N-1)/2$ times the energy of two particles in a large box of volume (area, really) V. It is much larger.

KEY WORDS: Bose gas; two-dimensions; low density; scattering length; ground state energy.

Dedicated to the memory of J. M. Luttinger

1. INTRODUCTION

An ancient problem, going back to the 1950's, is the calculation of the ground state energy of a dilute Bose gas in the thermodynamic limit. The particles are assumed to interact only with a two-body potential and are enclosed in a box of side length L. A formula was derived for the energy $E_0(N, L)$ in three dimensions for a two-body potential v with scattering length a (see Appendix) and fixed particle density $\rho = N/V$, ($N =$ particle

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number and $V =$ volume $= L^3$ in three dimensions). In the thermodynamic limit, the energy/particle is

$$e(\rho) \equiv \lim_{N \to \infty} E_0(N, \rho^{-1/3} N^{1/3})/N \simeq 4\pi\mu\rho a \tag{1.1}$$

to lowest order in ρ. Here, $\mu = \hbar^2/2m$ with m the mass of a particle.

Our goal here is to derive the analogous low density formula for a two-dimensional Bose gas.

There were several approaches in the 50's and 60's to the derivation of the three-dimensional formula (1.1), but none of them were rigorous. Recently we were able to give a rigorous derivation of (1.1) and we refer the reader to ref. 1 for a physically motivated discussion of the essential difficulty in proving (1.1), which, basically, is the fact that at low density the mean interparticle spacing is much smaller than the mean de Broglie wavelength of the particles. Thus, Bose particles cannot be thought of as localized. Furthermore, in ref. 1, we explain rather carefully why the usual expression "perturbation theory" is not appropriate for (1.1)—especially in the hard core case. Indeed, Bogolubov's 1947 "perturbation theory[2]" yields an estimate, which is incorrect for the low density limit:

$$e(\rho) \simeq \tfrac{1}{2}\rho \int_{\mathbb{R}^3} v \tag{1.2}$$

It was only with a leap of faith that Bogolubov and Landau recognized that $\int v$ is the first Born approximation to $8\pi\mu a$ and thus were able to derive (1.1). Obviously this cannot be called perturbation theory. Moreover, depending on the nature of v, it is sometimes the potential energy and sometimes the kinetic energy that is the dominating quantity; for example, in the hard core case the kinetic energy is the perturbation, rather than the potential energy, as the Bogolubov method assumes.

The two-dimensional theory, in contrast, began to receive attention only much later. The first derivation of the correct asymptotic formula was, to our knowledge, done by Schick[3] for a gas of hard discs:

$$e(\rho) \simeq 4\pi\mu\rho \, |\ln(\rho a^2)|^{-1} \tag{1.3}$$

This was accomplished by an infinite summation of "perturbation series" diagrams. Subsequently, a corrected modification of ref. 3 was given in ref. 4. Positive temperature extensions were given in refs. 5 and 6. All this work involved an analysis in momentum space—as was the case for (1.1), with the exception of a method due to one of us that works directly in configuration space.[7] Ovchinnikov[8] derived (1.3) by using, basically, the method in ref. 7. Again, these derivations require several unproven assumptions and are not rigorous.

One of the intriguing facts about (1.3) is that the energy for N particles is *not equal* to $N(N-1)/2$ times the energy for two particles in the low density limit—as is the case in three dimensions. The latter quantity, $E_0(2, L)$, is, asymptotically for large L, equal to $8\pi\mu L^{-2}[\ln(L^2/a^2)]^{-1}$. Thus, if the $N(N-1)/2$ rule were to apply, (1.3) would have to be replaced by the much smaller quantity $4\pi\mu\rho[\ln(L^2/a^2)]^{-1}$. In other words, L, which tends to ∞ in the thermodynamic limit, has to be replaced by the mean particle separation, $\rho^{-1/2}$ in the logarithmic factor. Various poetic formulations of this curious fact have been given, but the fact remains that the nonlinearity is something that does not occur in more than two-dimensions and its precise nature is hardly obvious, physically. This anomaly is the main reason that the present investigation is not a trivial extension of ref. 1.

We will prove (1.3) for nonnegative, finite range two-body potentials by finding upper and lower bounds of the correct form. The restriction to finite range can be relaxed somewhat, as was done in ref. 9, but the restriction to nonnegative v cannot be removed in the current state of our methodology. The upper bounds will have relative remainder terms $O(|\ln(\rho a^2)|^{-1})$ while the lower bound will have remainder $O(|\ln(\rho a^2)|^{-1/5})$. It is claimed in ref. 4 that the relative error for a hard core gas is negative and $O(\ln|\ln(\rho a^2)| |\ln(\rho a^2)|^{-1})$, which is consistent with our bounds.

In the next section we shall give the upper bound (following Dyson's analysis for the three-dimensional hard core gas[10]). Then we shall recall our method in ref. 1 for the lower bound and show how it has to be modified. An important point concerns the definition of the scattering length in two dimensions (which will be discussed in detail in Appendix A) and how "Dyson's Lemma[10, 1]" has to be modified accordingly (Appendix B).

An obvious extension of the present work is the case of 2D bosons in a trap and this will be the subject of a forthcoming paper. Just as the passage from 3D to 2D for the homogeneous case presents some non-trivial issues that have to be resolved, so the correct generalization of the Gross–Pitaevskii equation[11] to the 2D dilute trapped gas presents some additional complications.

We thank P. Kevrekidis for drawing our attention to this problem.

2. UPPER BOUND FOR THE GROUND STATE ENERGY

We begin with the well known definition of the Hamiltonian under discussion:

$$H^{(N)} = -\mu \sum_{i=1}^{N} \nabla_i^2 + \sum_{i<j} v(|x_i - x_j|) \qquad (2.1)$$

We assume that $v(r) \geqslant 0$ and $v(r) = 0$ if $r > R_0$, for some $R_0 < \infty$. The Hamiltonian (2.1) acts on totally *symmetric*, square integrable wave functions of $(x_1,..., x_N)$ with $x_i \in \mathbb{R}^2$. Its ground state energy in a box (rectangle, actually) of side length L is

$$E_0(N, L) = \inf_{\Psi} \frac{\langle \Psi, H^{(N)}\Psi \rangle}{\langle \Psi, \Psi \rangle} \tag{2.2}$$

where the infimum is over all wave functions Ψ satisfying appropriate conditions on the boundary of the box. For the upper bound it is natural to use Dirichlet boundary conditions, which gives the largest energy, but for the actual calculations it is more convenient to use periodic boundary conditions and a periodic extension of the interaction potential. This can only raise the energy since $v \geqslant 0$. Localization of the wave functions on the length scale L to obtain Dirichlet boundary conditions costs an energy $\sim$ (const.) L^{-2} per particle, so in the thermodynamic limit our upper bound is also a valid upper bound for Dirichlet boundary conditions. For the lower bound, on the other hand, we shall use Neumann boundary conditions, which yields the smallest energy.

Following ref. 10 we make a variational ansatz for Ψ of the following form:

$$\Psi(x_1,..., x_N) = \prod_{i=2}^{N} f(t_i(x_1,..., x_i)) \tag{2.3}$$

where $t_i = \min\{|x_i - x_j|, 1 \leqslant j \leqslant i-1\}$ is the distance of x_i to its *nearest neighbor* among the points $x_1,..., x_{i-1}$ and f is a nondecreasing function of $t \geqslant 0$ with values between zero and 1.

We wish to calculate $\langle \Psi, H^{(N)}\Psi \rangle / \langle \Psi, \Psi \rangle$. Dyson[10] carried out this calculation for the hard core case, namely when $f(r) = 0$ for $r <$ the core radius. His formula has been generalized in ref. 9 in two directions: One is the inclusion of an external potential (which we do not need here) and the other (which we do need) is the extension to a non-hard core potential v. We refer to ref. 9 for details. The result involves the following three integrals

$$I = 2\pi \int_0^\infty (1 - f(r)^2) \, r \, dr \tag{2.4}$$

$$J = 2\pi \int_0^\infty (|f'(r)|^2 + \tfrac{1}{2}v(r) \, |f(r)|^2) \, r \, dr \tag{2.5}$$

$$K = 2\pi \int_0^\infty f(r) \, f'(r) \, r \, dr \tag{2.6}$$

In terms of these integrals the bound on the energy is

$$\langle \Psi, H^{(N)}\Psi \rangle / \langle \Psi, \Psi \rangle \leqslant N\left(\frac{\rho J}{1-\rho I} + \frac{2}{3}\frac{(\rho K)^2}{(1-\rho I)^2}\right) \qquad (2.7)$$

The form of this bound is the same as in ref. 10. Compared to Eq. (3.29) in ref. 9 there is a factor $(1-\rho I)^{-1}$ in the first term in place of $(1-\rho I)^{-2}$. This can be traced to the use of the Cauchy–Schwarz inequality in Eq. (3.19) in ref. 9 which is not necessary in the case of the homogeneous system treated here.

The next step is to make a choice for f, and this will involve the scattering length a and a variational parameter b. First, we have to define the scattering length.

Consider the Schrödinger equation

$$-\mu\Delta\phi_0 + \tfrac{1}{2}v\phi_0 = 0 \qquad (2.8)$$

We do *not* require ϕ_0 to be bounded. As shown in Appendix A, up to an overall factor there is a unique, nonnegative, spherically symmetric $\phi_0(x) = f_0(|x|)$ that satisfies (2.8) provided the Schrödinger operator $-\mu\Delta + \tfrac{1}{2}v(r)$ in $L^2(\mathbb{R}^2)$ has no bound states. For $r > R_0$, f_0 necessarily has the form (since ϕ_0 is a harmonic function outside the range of v)

$$f_0(r) = (\text{const.})\ln(r/a) \qquad (2.9)$$

The length a is called the *scattering length*. Note that it depends on both μ and on v. In the case that v is nonnegative, f_0 is necessarily a monotonically increasing function of r.

We now define our variational f to be

$$f(r) = \begin{cases} f_0(r)/f_0(b) & \text{for} \quad 0 \leqslant r \leqslant b \\ 1 & \text{for} \quad r > b \end{cases} \qquad (2.10)$$

with some $b > R_0 > a$ to be chosen in an optimal way. By Appendix A we have that f satisfies $f' \geqslant 0$ and $0 \leqslant f \leqslant 1$, for all b. Moreover,

$$f(r) \geqslant \begin{cases} \ln(r/a)/\ln(b/a) & \text{for} \quad a \leqslant r \leqslant b \\ 0 & \text{for} \quad r < a \end{cases} \qquad (2.11)$$

Using this information one computes

$$I \leqslant \pi a^2 + 2\pi \int_a^b \left(1 - \frac{[\ln(r/a)]^2}{[\ln(b/a)]^2} \right) r \, dr$$

$$= \frac{\pi b^2}{\ln(b/a)} (1 + O([\ln(b/a)]^{-1})) \tag{2.12}$$

$$J = 2\pi [f(r) f'(r) r]_0^b = \frac{2\pi}{\ln(b/a)} \tag{2.13}$$

$$K = \pi \int (f(r)^2)' r \, dr = \pi b - \pi \int f(r)^2 \, dr$$

$$\leqslant \pi b - \pi \int_a^b \frac{[\ln(r/a)]^2}{[\ln(b/a)]^2} \, dr = \frac{2\pi b}{\ln(b/a)} (1 + O([\ln(b/a)]^{-1})) \tag{2.14}$$

Inserted in (2.7) this leads to the upper bound

$$E_0(N, L)/N \leqslant \frac{2\pi\rho}{\ln(b/a) - \pi\rho b^2} (1 + O([\ln(b/a)]^{-1})) \tag{2.15}$$

The minimum over b of the leading term is obtained for $b = (2\pi\rho)^{-1/2}$. Inserting this in (2.15) we thus obtain

Theorem 2.1 (Upper Bound). *The ground state energy with periodic boundary conditions satisfies*

$$E_0(N, L)/N \leqslant \frac{4\pi\rho}{|\ln(\rho a^2)|} (1 + O(|\ln(\rho a^2)|^{-1})) \tag{2.16}$$

Dirichlet boundary conditions may introduce an additional relative error, but as already noted it is at most $\Delta E_0/N \propto L^{-2}$.

3. LOWER BOUND TO THE GROUND STATE ENERGY

The method of ref. 1 for obtaining a lower bound to $E_0(N, L)$ involves the following steps:

1. A generalization of a lemma due to Dyson[10] that allows the replacement of the interaction potential v by a "soft" potential U at the cost of sacrificing kinetic energy.

2. Division of the large box of side length L into small boxes of side length ℓ, which is kept *fixed* as $L \to \infty$, and a corresponding lowering of the energy by the use of *Neumann* boundary conditions on each box. It is necessary to minimize the total energy over all distributions of the particles among the small boxes; this is accomplished with the aid of the super-additivity of the ground state energy in each box (i.e., $E_0(N_1 + N_2, L) \geqslant E_0(N_1, L) + E_0(N_2, L)$, which follows from $v \geqslant 0$).

3. The use of a rigorous version of first order perturbation theory, known as Temple's inequality[12] to estimate from below the energy with the new potential U in the small boxes.

We follow the same strategy here, but there are several modifications to be made. The two dimensional version of the generalized Dyson Lemma is as follows.

Lemma 3.1. *Let* $v(r) \geqslant 0$ *and* $v(r) = 0$ *for* $r > R_0$. *Let* $U(r) \geqslant 0$ *be any function satisfying*

$$\int_0^\infty U(r) \ln(r/a)\, r\, dr \leqslant 1 \qquad and \qquad U(r) = 0 \quad for\ r < R_0 \qquad (3.1)$$

Let $\mathscr{B} \subset \mathbb{R}^2$ *be star-shaped with respect to* 0. *Then, for all functions* $\phi \in H^1(\mathscr{B})$,

$$\int_{\mathscr{B}} \mu\, |\nabla\phi(x)|^2 + \tfrac{1}{2}v(r)\, |\phi(x)|^2\, d^2x \geqslant \mu \int_{\mathscr{B}} U(r)\, |\phi(x)|^2\, d^2x \qquad (3.2)$$

A domain $\mathscr{B}$ is star-shaped with respect to a point p if the line segment $[p, x] \subset \mathscr{B}$ whenever $x \in \mathscr{B}$. A convex domain is star-shaped with respect to any point in it (and conversely). The three-dimensional version of the lemma replaces (3.1) with $\int_0^\infty U(r)\, r^2\, dr \leqslant a$. The proof is given in Appendix B.

As in ref. 1, Lemma 3.1 can be used to bound the many body Hamiltonian $H^{(N)}$ from below, as follows:

Corollary 3.1. *For any* U *as in Lemma* 3.1 *and any* $0 < \varepsilon < 1$

$$H^{(N)} \geqslant \varepsilon T^{(N)} + (1 - \varepsilon)\, \mu W \qquad (3.3)$$

with $T^{(N)} = -\mu \sum_{i=1}^N \Delta_i$ *and*

$$W(x_1,...,x_N) = \sum_{i=1}^N U(\min_{j,\, j \neq i} |x_i - x_j|) \qquad (3.4)$$

For U we choose the following functions, parameterized by $R > R_0$:

$$U_R(r) = \begin{cases} v(R)^{-1} & \text{for} \quad R_0 < r < R \\ 0 & \text{otherwise} \end{cases} \tag{3.5}$$

with $v(R)$ chosen so that

$$\int_{R_0}^{R} U_R(r) \ln(r/a) \, r \, dr = 1 \tag{3.6}$$

for all $R > R_0$, i.e.,

$$\begin{aligned} v(R) &= \int_{R_0}^{R} \ln(r/a) \, r \, dr \\ &= \tfrac{1}{4} \{ R^2(\ln(R^2/a^2) - 1) - R_0^2(\ln(R_0^2/a^2) - 1) \} \end{aligned} \tag{3.7}$$

The nearest neighbor interaction (3.4) corresponding to U_R will be denoted W_R.

As in ref. 1 we shall need estimates on the expectation value, $\langle W_R \rangle_0$, of W_R in the ground state of $\varepsilon T^{(N)}$ of (3.3) with Neumann boundary conditions.

This is just the average value of W_R in a hypercube in $\mathbb{R}^{2N}$. Besides the normalization factor $v(R)$, the computation involves the volume (area) of the support of U_R, which is

$$A(R) = \pi(R^2 - R_0^2) \tag{3.8}$$

In contrast to the three-dimensional situation the normalization factor $v(R)$ is not just a constant (R independent) multiple of $A(R)$; the factor $\ln(r/a)$ in (3.1) accounts for the more complicated expressions in the two-dimensional case. Taking into account that U_R is proportional to the characteristic function of a disc of radius R with a hole of radius R_0, the following inequalities for n particles in a box of side length ℓ are obtained by the same geometric reasoning as in ref. 1:

$$\langle W_R \rangle_0 \geqslant \frac{n}{v(R)} \left(1 - \frac{2R}{\ell} \right)^2 [1 - (1-Q)^{(n-1)}] \tag{3.9}$$

$$\langle W_R \rangle_0 \leqslant \frac{n}{v(R)} [1 - (1-Q)^{(n-1)}] \tag{3.10}$$

with

$$Q = A(R)/\ell^2 \tag{3.11}$$

being the relative volume occupied by the support of the potential U_R. Since $U_R^2 = v(R)^{-1} U_R$ we also have

$$\langle W_R^2 \rangle_0 \leqslant \frac{n}{v(R)} \langle W_R \rangle_0 \tag{3.12}$$

As in ref. 1 we estimate $[1 - (1-Q)^{(n-1)}]$ by

$$(n-1) Q \geqslant [1 - (1-Q)^{(n-1)}] \geqslant \frac{(n-1) Q}{1 + (n-1) Q} \tag{3.13}$$

This gives

$$\langle W_R \rangle_0 \geqslant \frac{n(n-1)}{v(R)} \cdot \left(1 - \frac{2R}{l}\right)^2 \frac{Q}{1 + (n-1) Q} \tag{3.14}$$

$$\langle W_R \rangle_0 \leqslant \frac{n(n-1)}{v(R)} \cdot Q \tag{3.15}$$

From Temple's inequality (see refs. 1, 9) we obtain the estimate

$$E_0(n, \ell) \geqslant (1-\varepsilon) \langle W_R \rangle_0 \left(1 - \frac{\mu(\langle W_R^2 \rangle_0 - \langle W_R \rangle_0^2)}{\langle W_R \rangle_0 (E_1^{(0)} - \mu \langle W_R \rangle_0)}\right) \tag{3.16}$$

where

$$E_1^{(0)} = \frac{\varepsilon \mu}{\ell^2} \tag{3.17}$$

is the energy of the lowest excited state of $\varepsilon T^{(n)}$. This estimate is valid for $E_1^{(0)}/\mu > \langle W_R \rangle_0$, i.e., it is important that ℓ is not too big.

Putting (3.14) and (3.16) together we obtain the estimate

$$E_0(n, \ell) \geqslant \frac{n(n-1)}{\ell^2} \frac{A(R)}{v(R)} K(n) \tag{3.18}$$

with

$$K(n) = (1-\varepsilon) \cdot \frac{(1 - 2R/\ell)^2}{1 + (n-1) Q} \cdot \left(1 - \frac{n}{(\varepsilon v(R)/\ell^2) - n(n-1) Q}\right) \tag{3.19}$$

Note that Q depends on ℓ and R, and K depends on ℓ, R and ε besides n. We have here dropped the term $\langle W_R \rangle_0^2$ in the numerator in (3.16), which is appropriate for the purpose of a lower bound.

We note that K is monotonically decreasing in n, so for a given n we may replace $K(n)$ by $K(p)$ provided $p \geqslant n$. As explained in ref. 1 convexity of $n \mapsto n(n-1)$ together with superadditivity of $E_0(n, \ell)$ in n leads, for $p = 4\rho\ell^2$, to an estimate for the energy of N particles in the large box when the side length L is an integer multiple of ℓ:

$$E_0(N, L)/N \geqslant \frac{\rho A(R)}{v(R)} \left(1 - \frac{1}{\rho\ell^2}\right) K(4\rho\ell^2) \tag{3.20}$$

with $\rho = N/L^3$.

Let us now look at the conditions on the parameters ε, R and ℓ that have to be met in order to obtain a lower bound with the same leading term as the upper bound (2.15).

From (3.7) we have

$$\frac{A(R)}{v(R)} = \frac{4\pi}{(\ln(R^2/a^2) - 1)} \left(1 - \mathrm{O}((R_0^2/R^2)\ln(R/R_0))\right) \tag{3.21}$$

We thus see that as long as $a < R < \rho^{-1/2}$ the logarithmic factor in the denominator in (3.20) has the right form for a lower bound. Moreover, for Temple's inequality the denominator in the second factor in (3.19) must be positive. With $n = 4\rho\ell^2$ and $v(R) \geqslant (\mathrm{const.}) R^2 \ln(R^2/a^2)$ for $R \gg R_0$, this condition amounts to

$$(\mathrm{const.})\, \varepsilon \ln(R^2/a^2)/\ell^2 > \rho^2\ell^4 \tag{3.22}$$

The relative error terms in (3.20) that have to be $\ll 1$ are

$$\varepsilon, \qquad \frac{1}{\rho\ell^2}, \qquad \frac{R}{\ell}, \qquad \rho R^2, \qquad \frac{\rho\ell^4}{\varepsilon R^2 \ln(R^2/a^2)} \tag{3.23}$$

We now choose

$$\varepsilon \sim |\ln(\rho a^2)|^{-1/5}, \qquad \ell \sim \rho^{-1/2} |\ln(\rho a^2)|^{1/10}, \qquad R \sim \rho^{-1/2} |\ln(\rho a^2)|^{-1/10} \tag{3.24}$$

Condition (3.22) is satisfied since the left side is $> (\mathrm{const.}) |\ln(\rho a^2)|^{3/5}$ and the right side is $\sim |\ln(\rho a^2)|^{2/5}$. The first three error terms in (3.23) are all of the same order, $|\ln(\rho a^2)|^{-1/5}$, the last is $\sim |\ln(\rho a^2)|^{-1/5} (\ln |\ln(\rho a^2)|)^{-1}$. With these choices, (3.20) thus leads to the following:

Theorem 3.1 (Lower Bound). *For all N and L large enough such that $L > (\mathrm{const.}) \rho^{-1/2} |\ln(\rho a^2)|^{1/10}$ and $N > (\mathrm{const.}) |\ln(\rho a^2)|^{1/5}$ with*

$\rho = N/L^2$, *the ground state energy with Neumann boundary condition satisfies*

$$E_0(N, L)/N \geqslant \frac{4\pi\mu\rho}{|\ln(\rho a^2)|} (1 - O(|\ln(\rho a^2)|^{-1/5})) \tag{3.25}$$

In combination with the upper bound of Theorem 2.1 this also proves

Theorem 3.2 (Energy at Low Density in the Thermodynamic Limit).

$$\lim_{\rho a^2 \to 0} \frac{e_0(\rho)}{4\pi\mu\rho \, |\ln(\rho a^2)|^{-1}} = 1 \tag{3.26}$$

where $e_0(\rho) = \lim_{N \to \infty} E_0(N, \rho^{-1/2} N^{1/2})/N$. This holds irrespective of boundary conditions.

Remarks. 1. It follows from the remark at the end of Appendix A that Theorem 3.2 is also valid for an infinite range potential v provided that $v \geqslant 0$ and that for some R we have $\int_R^\infty v(r) \, r \, dr < \infty$.

2. As in refs. 1, 9 we could derive explicit bounds for the error term in (3.25), but there is little reason to belabor this point.

APPENDIX A. DEFINITION AND PROPERTIES OF SCATTERING LENGTH

In this appendix we shall define and derive the scattering length and some of its properties. The reader is referred to ref. 13, especially Chaps. 9 and 11, for many of the concepts and facts we shall use here. While we are interested in two dimensions, much of the following is valid in all dimensions.

We start with a potential $\frac{1}{2}v(x)$ that depends only on the radius, $r = |x|$, with $x \in \mathbb{R}^n$. For simplicity, we assume that v has finite range; this condition can easily be relaxed, but we shall not do so here, except for a remark at the end that shows how to extend the concepts to infinite range, nonnegative potentials. Thus, we assume that

$$v(r) = 0 \qquad \text{for} \quad r > R_0 \tag{A.1}$$

We decompose v into its positive and negative parts, $v = v_+ - v_-$, with v_+, $v_- \geqslant 0$, and assume the following for v_- only (with $\varepsilon > 0$):

$$v_- \in \begin{cases} L^1(\mathbb{R}^1) & \text{for} \quad n = 1 \\ L^{1+\varepsilon}(\mathbb{R}^2) & \text{for} \quad n = 2 \\ L^{n/2}(\mathbb{R}^n) & \text{for} \quad n \geqslant 3 \end{cases} \tag{A.2}$$

In fact, v can even be a finite, spherically symmetric measure, e.g., a sum of delta functions.

We also make the important assumption that $\frac{1}{2}v(x)$ has no negative energy bound states in $L^2(\mathbb{R}^n)$, which is to say we assume that for all $\phi \in H^1(\mathbb{R}^n)$ (the space of L^2 functions with L^2 derivatives)

$$\int_{\mathbb{R}^n} \mu |\nabla\phi(x)|^2 + \tfrac{1}{2}v(x) |\phi(x)|^2 \, d^n x \geqslant 0 \tag{A.3}$$

Theorem A.1. *Let $R > R_0$ and let $B_R \subset \mathbb{R}^n$ denote the ball $\{x : 0 < |x| < R\}$ and S_R the sphere $\{x : |x| = R\}$. For $f \in H^1(B_R)$ we set*

$$\mathscr{E}_R[\phi] = \int_{B_R} \mu |\nabla\phi(x)|^2 + \tfrac{1}{2}v(x) |\phi(x)|^2 \, d^n x \tag{A.4}$$

Then, in the subclass of functions such that $\phi(x) = 1$ for all $x \in S_R$, there is a unique function ϕ_0 that minimizes $\mathscr{E}_R[\phi]$. This function is nonnegative and spherically symmetric, i.e.,

$$\phi_0(x) = f_0(|x|) \tag{A.5}$$

with a nonnegative function f_0 on the interval $(0, R]$, and it satisfies the equation

$$-\mu \, \Delta\phi_0(x) + \tfrac{1}{2}v(x) \, \phi_0(x) = 0 \tag{A.6}$$

in the sense of distributions on B_R, with boundary condition $f_0(R) = 1$.
For $R_0 < r < R$

$$f_0(r) = f_0^{\text{asymp}}(r) \equiv \begin{cases} (r-a)/(R-a) & \text{for} \quad n = 1 \\ \ln(r/a)/\ln(R/a) & \text{for} \quad n = 2 \\ (1 - ar^{2-n})/(1 - aR^{2-n}) & \text{for} \quad n \geqslant 3 \end{cases} \tag{A.7}$$

for some number a called the scattering length.

The minimum value of $\mathscr{E}_R[\phi]$ is

$$E = \begin{cases} 2\mu/(R-a) & \text{for} \quad n=1 \\ 2\pi\mu/\ln(R/a) & \text{for} \quad n=2 \\ 2\pi^{n/2}\mu a/[\Gamma(n/2)(1-aR^{2-n})] & \text{for} \quad n \geqslant 3 \end{cases} \quad (A.8)$$

Remarks. 1. Given that the minimizer is spherically symmetric for every R, it is then easy to see that the R dependence is trivial. There is really one function, F_0, defined on all of the positive half axis, such that $f_0(r) = F_0(r)/F_0(R)$. That is why we did not bother to indicate the explicit dependence of f_0 on R. The reason is a simple one: If $\tilde{R} > R$, take the minimizer $\tilde{f}_0$ for $\tilde{R}$ and replace its values for $r < R$ by $f_0(r)\,\tilde{f}_0(R)$, where f_0 is the minimizer for the B_R problem. This substitution cannot increase $\mathscr{E}_{\tilde{R}}$.

Thus, by uniqueness, we must have that $\tilde{f}_0(r) = f_0(r)\,\tilde{f}_0(R)$ for $r \leqslant R$.

2. From (A.7) we then see that $f_0^{\text{asymp}}(r) \geqslant 0$ for all $r > R_0$, which implies that $a \leqslant R_0$ for $n \leqslant 3$ and $a \leqslant R_0^{n-2}$ for $n > 3$.

3. According to our definition (A.7), a has the dimension of a length only when $n \leqslant 3$.

4. The variational principle (A.4), (A.8) allows us to discuss the connection between the scattering length and $\int v$. We recall Bogolubov's perturbation theory,[2] which says that to leading order in the density ρ, the energy per particle of a Bose gas is $e_0(\rho) \sim \frac{1}{2}\rho\int v$, whereas the correct formula in two-dimensions is $4\pi\mu\rho\,|\ln(\rho a^2)|^{-1}$. The Bogolubov formula is an upper bound (for all ρ) since it is the expectation value of $H^{(N)}$ in the non-interacting ground state $\Psi \equiv 1$. Thus, we must have $\frac{1}{2}\int v \geqslant 4\pi\mu\,|\ln(\rho a^2)|^{-1}$ when $\rho a^2 \ll 1$, which suggests that

$$\int_{\mathbb{R}^2} v \geqslant \frac{4\pi\mu}{\ln(R_0/a)} \quad (A.9)$$

Indeed, the truth of (A.9) can be verified by using the function $\phi(x) \equiv 1$ as a trial function in (A.4). Then, using (A.8), $\frac{1}{2}\int v \geqslant E = 2\pi\mu/\ln(R/a)$ for all $R \geqslant R_0$, which proves (A.9). As $a \to 0$, (A.9) becomes an equality, however, in the sense that $(\int_{\mathbb{R}^2} v)\ln(R_0/a) \to 4\pi\mu$.

In the same way, we can derive the inequality of Spruch and Rosenberg[14] for dimension 3 or more:

$$\int_{\mathbb{R}^n} v \geqslant \frac{4\pi^{n/2}\mu a}{\Gamma(n/2)} \quad (A.10)$$

(Here, we take the limit $R \to \infty$ in (A.8)).

In one-dimension we obtain (with $R = R_0$)

$$\int_{\mathbb{R}} v \geqslant \frac{4\mu}{R_0 - a} \tag{A.11}$$

Proof of Theorem A.1.   Given any $\phi \in H^1$ we can replace it by the square root of the spherical average of $|\phi|^2$. This preserves the boundary condition at $|x| = R$, while the v term in (A.4) is unchanged. It also lowers the gradient term in (A.4) because the map $\rho \mapsto \int(\nabla\sqrt{\rho})^2$ is convex.[13] Indeed, there is a strict decrease unless ϕ is already spherically symmetric and nonnegative.

Thus, without loss of generality, we may consider only nonnegative, spherically symmetric functions. We may also assume that in the annular region $\mathscr{A} = \{x : R_0 \leqslant |x| \leqslant R\}$ there is some a such that (A.7) is true because these are the only spherically symmetric, harmonic functions in $\mathscr{A}$. If we substitute for ϕ the harmonic function in $\mathscr{A}$ that agrees with ϕ at $|x| = R_0$ and $|x| = 1$ we will lower $\mathscr{E}_R$ unless ϕ is already harmonic in $\mathscr{A}$. (We allow the possibility $a = 0$ for $n \leqslant 2$, meaning that $\phi = \text{constant}$.)

Next, we note that $\mathscr{E}_R[\phi]$ is bounded below. If it were not bounded then (with R fixed) we could find a sequence ϕ^j such that $\mathscr{E}_R[\phi^j] \to -\infty$. However, if h is a smooth function on $\mathbb{R}_+$ with $h(r) = 1$ for $r < R + 1$ and $h(r) = 0$ for $r > 2R + 1$ then the function $\hat{\phi}^j(x) = \phi^j(x)$ for $|x| \leqslant R$ and $\hat{\phi}^j(x) = h(|x|)$ for $|x| > R$ is a legitimate variational function for the $L^2(\mathbb{R}^n)$ problem in (A.3). It is easy to see that $\mathscr{E}_R[\hat{\phi}^j] \leqslant \mathscr{E}_R[\phi^j] + (\text{const.}) R^{n-2}$, and this contradicts (A.3) (recall that R is fixed).

Now we take a minimizing sequence ϕ^j for $\mathscr{E}_R$ and corresponding $\hat{\phi}^j$ as above. By the assumptions on v_- we can see that the kinetic energy $T^j = \int |\nabla\phi^j|^2$ and $\int |\phi^j|^2$ are bounded. We can then find a subsequence of the $\hat{\phi}^j$ that converges weakly in H^1 to some spherically symmetric $\hat{\phi}_0(x) = \hat{f}_0(|x|)$. Correspondingly, $\phi^j(x)$ converges weakly in $H^1(B_R)$ to $\phi_0(x) = f_0(|x|)$. The important point is that the term $-\int v_-|\phi^j|^2$ is weakly continuous while the term $\int v_+|\phi^j|^2$ is weakly lower continuous.[13] We also note that $f_0(R) = 1$ since the functions $\hat{\phi}^j$ are identically equal to 1 for $R < |x| < R + 1$ and the limit $\hat{\phi}_0$ is continuous away from the origin since it is spherically symmetric and in H^1.

Thus, the limit function ϕ_0 is a minimizer for $\mathscr{E}[\phi]$ under the condition $\phi = 1$ on S_R. Since it is a minimizer, it must be harmonic in $\mathscr{A}$, so (A.7) is true. Eq. (A.6) is standard and is obtained by replacing ϕ_0 by $\phi_0 + \delta\psi$, where ψ is any infinitely differentiable function that is zero for $|x| \geqslant R$. The first variation in δ gives (A.6).

Equation (A.8) is obtained by using integration by parts to compute $\mathscr{E}_R[\phi_0]$.

The uniqueness of the minimizer can be proved in two ways. One way is to note that if $\phi_0 \neq \psi_0$ are two minimizers then, by the convexity noted above, $\mathscr{E}_R[\sqrt{\phi_0^2 + \psi_0^2}] < \mathscr{E}_R[\phi_0] + \mathscr{E}_R[\psi_0]$. The second way is to notice that all minimizers satisfy (A.6), which is a linear, ordinary differential equation for f_0 on $(0, R)$ since all minimizers are spherically symmetric, as we noted. But the solution of such equations, given the value at the end points, is unique. ∎

We thus see that if the Schrödinger operator on $\mathbb{R}^n$ with potential $\frac{1}{2}v(x)$ has no negative energy bound state then the scattering length in (A.7) is well defined by a variational principle. Our next task is to find some properties of the minimizer ϕ_0. For this purpose we shall henceforth assume that v is *nonnegative*, which guarantees (A.3), of course.

Lemma A.1. *If v is nonnegative then for all $0 < r \leqslant R$ the minimizer $\phi_0(x) = f_0(|x|)$ satisfies*

(A)

$$f_0(r) \geqslant f_0^{\mathrm{asymp}}(r) \tag{A.12}$$

where f_0^{asymp} is given in (A.7)

(B) *$f_0(r)$ is a monotonically nondecreasing function of r.*

(C) *If $v(r) \geqslant \tilde{v}(r) \geqslant 0$ for all r then the corresponding minimizers satisfy $f_0(r) \leqslant \tilde{f}_0(r)$ for all $r < R$. Hence, $a > \tilde{a} \geqslant 0$.*

Proof. Let us define $f_0^{\mathrm{asymp}}(r)$ for all $0 < r < \infty$ by (A.7), and let us extend $f_0(r)$ to all $0 < r < \infty$ by setting $f_0(r) = f_0^{\mathrm{asymp}}(r)$ when $r \geqslant R$.

To prove (A) note that $-\Delta\phi_0 = -\frac{1}{2}v\phi_0$, which implies that ϕ_0 is subharmonic (we use $v \geqslant 0$ and $\phi_0 \geqslant 0$, by Theorem A.1). Set $h_\varepsilon(r) = f_0(r) - (1 + \varepsilon) f_0^{\mathrm{asymp}}(r)$ with $\varepsilon > 0$ and small. Obviously, $x \mapsto h_\varepsilon(|x|)$ is subharmonic on the open set $\{x : 0 < |x| < \infty\}$ because $f_0^{\mathrm{asymp}}(|x|)$ is harmonic there. Clearly, $h_\varepsilon \to -\infty$ as $r \to \infty$ and $h_\varepsilon(R) = -\varepsilon$. Suppose that (A.12) is false at some radius $\rho < R$ and that $h_0(\rho) = -c < 0$. In the annulus $\rho < r < \infty$, $h_\varepsilon(r)$ has its maximum on the boundary, i.e., either at ρ or at ∞ (since $h(|x|)$ is subharmonic in x). By choosing ε sufficiently small and positive we can have that $h_\varepsilon(\rho) < -2\varepsilon$ and this contradicts the fact that the maximum (which is at least $-\varepsilon$) is on the boundary.

(B) is proved by noting (by subharmonicity again) that the maximum of f_0 in $(0, r)$ occurs on the boundary, i.e., $f_0(r) \geqslant f_0(r')$ for any $r' < r$.

(C) is proved by studying the function $g = f_0 - \tilde{f}_0$. Since f_0 and $\tilde{f}_0$ are continuous, the falsity of (C) implies the existence some open subset,

$\Omega \subset B_R$ on which $g(|x|) > 0$. On Ω we have that $g(|x|)$ is subharmonic (because $vf_0 > \tilde{v}\tilde{f}_0$). Hence, its maximum occurs on the boundary, but $g = 0$ there. This contradicts $g(|x|) > 0$ on Ω. ∎

Remark About Infinite Range Potentials. If $v(r)$ is infinite range and non-negative it is easy to extend the definition of the scattering length under the assumptions:

(1) $v(r) \geqslant 0$ for all r and

(2) For some R_1 we have $\int_{R_1}^{\infty} v(r)\, r^{n-1}\, dr < \infty$.

If we cut off the potential at some point $R_0 > R_1$ (i.e., set $v(r) = 0$ for $r > R_0$) then the scattering length is well defined but it will depend on R_0, of course. Denote it by $a(R_0)$. By part C of Lemma (A.1), $a(R_0)$ is an increasing function of R_0. However, the bounds (A.9) and (A.10) and assumption (2) above guarantee that $a(R_0)$ is bounded above. (More precisely, we need a simple modification of (A.9) and (A.10) to the potential $v(r) \equiv \infty$ for $r \leqslant R_1$ and $v(r) \equiv v(r)$ for $r > R_1$. This is accomplished by replacing the "trial function" $f(x) = 1$ by a smooth radial function that equals 0 for $r < R_1$ and equals 1 for $r > R_2$ for some $R_2 > R_1$.) Thus, a is well defined by

$$a = \lim_{R_0 \to \infty} a(R_0) \tag{A.13}$$

APPENDIX B. PROOF OF DYSON'S LEMMA 3.1 IN TWO DIMENSIONS

Proof. In polar coordinates, r, θ, one has $|\nabla \phi|^2 \geqslant |\partial \phi / \partial r|^2$. Therefore, it suffices to prove that for each angle $\theta \in [0, 2\pi)$, and with $\phi(r, \theta)$ denoted simply by $f(r)$,

$$\int_0^{R(\theta)} \left(\mu\, |\partial f(r)/\partial r|^2 + \tfrac{1}{2} v(r)\, |f(r)|^2 \right) r\, dr \geqslant \mu \int_0^{R(\theta)} U(r)\, |f(r)|^2\, r\, dr \tag{B.1}$$

where $R(\theta)$ denotes the distance of the origin to the boundary of $\mathscr{B}$ along the ray θ.

If $R(\theta) \leqslant R_0$ then (B.1) is trivial because the right side is zero while the left side is evidently nonnegative. (Here, $v \geqslant 0$ is used.)

If $R(\theta) > R_0$ for some given value of θ, consider the disc $\mathscr{D}(\theta) = \{x \in \mathbb{R}^2 : 0 \leqslant |x| \leqslant R(\theta)\}$ centered at the origin in $\mathbb{R}^2$ and of radius $R(\theta)$.

Our function f defines a spherically symmetric function, $x \mapsto f(|x|)$ on $\mathscr{D}(\theta)$, and (B.1) is equivalent to

$$\int_{\mathscr{D}(\theta)} \mu \, |\nabla f(|x|)|^2 + \tfrac{1}{2} v(r) \, |f(|x|)|^2 \, d^2 x \tag{B.2}$$

Now choose some $R \in (R_0, R(\theta))$ and note that the left side of (B.2) is not smaller than the same quantity with $\mathscr{D}(\theta)$ replaced by the smaller disc $\mathscr{D}_R = \{ x \in \mathbb{R}^2 : 0 \leqslant |x| \leqslant R \}$. (Again, $v \geqslant 0$ is used.) According to Appendix A, Theorem A.1, Eq. (A.8), and linearity in $|f|^2$, this integral over $\mathscr{D}_R$ is at least $E(R) \, |f(R)|^2$. Hence, for every $R_0 < R < R(\theta)$,

$$2\pi \int_0^{R(\theta)} \left(\mu \, |\partial f(r)/\partial r|^2 + \tfrac{1}{2} v(r) \, |f(r)|^2 \right) r \, dr \geqslant E(R) \, |f(R)|^2 \tag{B.3}$$

The proof is completed by noting that $E(R) = 2\pi\mu/\ln(R/a)$, by multiplying both sides of (B.3) by $U(R) \, R\ln(R/a)$ and, finally, integrating with respect to R from R_0 to $R(\theta)$. ∎

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