Ground-State Energy of a Dilute Fermi Gas

Elliott H. Lieb, Robert Seiringer, and Jan Philip Solovej

Abstract. Recent developments in the physics of low density trapped gases make it worthwhile to verify old, well known results that, while plausible, were based on perturbation theory and assumptions about pseudopotentials. We use and extend recently developed techniques to give a rigorous derivation of the asymptotic formula for the ground state energy of a dilute gas of $N$ fermions interacting with a short-range, positive potential of scattering length $a$. For spin $1/2$ fermions, this is $E \sim E^0 + \left( \frac{\hbar^2}{2m} \right)^2 \pi N \rho a$, where $E^0$ is the energy of the non-interacting system and $\rho$ is the density.

1. Introduction

Our goal is to find the ground state energy of a low density gas of fermions interacting with short range pair potentials. Earlier [1, 2, 3, 4], the corresponding problem for bosons had been solved in the sense that the ’well known’ ancient formula $E/V = 4\pi \rho^2 a$ in 3D was proved rigorously as an asymptotic formula for small $\rho$ in the thermodynamic limit. Here, $\rho = N/V$, where $N$ is the particle number, $V$ is the volume and $a$ is the scattering length of the pair potential.

Owing to the recent interest in low density, cold gases of fermionic atoms, the natural question arose: Is a similar formula valid for spin-$\frac{1}{2}$ fermions? Of course there will be differences, which we can list as follows:

(1) We can expect that the interaction energy between pairs of fermions of the same spin vanishes to leading order in $\rho$. The Pauli principle (antisymmetry) implies that the wave function is tiny within the range of the pair potential.

(2) The interaction between pairs of fermions of opposite spin should be the same as for bosons. I.e., we expect this energy to be $4\pi a N^\uparrow N^\downarrow / V$, where
$N_\uparrow$ and $N_\downarrow$ are the numbers of spin up and spin down particles, respectively.

(3) A major difference from the bosonic case is that the energy we are trying to compute is only the second order term in the density. The first order term is just the kinetic energy of the ideal Fermi gas, which is $E_0/V = \frac{3}{5} (6\pi^2)^{2/3} \left\{ (N_\uparrow/V)^{5/3} + (N_\downarrow/V)^{5/3} \right\}$.

(4) Finding an upper bound to the energy in the fermionic case is more difficult than in the bosonic case. There, one uses the fact that it is not necessary to look for trial states in the bosonic (symmetric) sector because the bosonic energy agrees with the absolute minimum energy and, consequently, any variational state without symmetry restriction gives an upper bound to the bosonic ground state energy. The same is obviously not true for fermions, which means that we must rigorously enforce antisymmetry of our trial state.

The third item gives rise to two problems that did not have to be faced in the bosonic case. The first is that we will have to be careful not to ‘give up’ any low momentum kinetic energy in order to control the interaction potential. That kinetic energy is part of the main term in the energy and, therefore, has to be left intact. Since the interaction range $a$ is very small compared to the Fermi momentum, which is proportional to $\rho^{1/3}$, there is hope that in the low density regime this decomposition of the kinetic energy into low and high density parts can be cleanly achieved. This is one of the main technical accomplishments of our work.

The second main problem is closely related to this kinetic energy consideration. It is that the typical particle momentum is of the order of the Fermi momentum, which is not zero. Therefore, one could question whether the ‘zero energy scattering length’ contains all the necessary information about the interaction. That it does so is a consequence of the good separation of momentum scales mentioned above, but proving this fact mathematically requires some thought.

In the next section we explain the problem and our results in more detail. The complete details can be found in [5] and the present note can be regarded as a guide to the overall structure of [5].

2. The Model

Our model describes fermions interacting through a short range pair potential $v$. The Hamiltonian (in units in which $\hbar = 2m = 1$) is

$$H_N = \sum_{i=1}^{N} -\Delta_i + \sum_{1 \leq i < j \leq N} v(x_i - x_j)$$

The nonnegative pair-potential, $v \geq 0$, is radial (i.e., depends only on $|x_i - x_j|$) and has finite range (i.e., has compact support). A favorite physical example is a hard core, $v(x) = \infty$ for $|x| < a$ and $v = 0$ otherwise.

We generalize the physical problem a little by treating higher spins than $\frac{1}{2}$, since we let the Hamiltonian $H_N$ act on the fermionic Hilbert space with $q$ spin states. Spin $\frac{1}{2}$ corresponds to $q = 2$. 
The particles are restricted to a box \( \Lambda = [0, L]^3 \) of volume \( V = L^3 \). The Hilbert space describing \( N \) fermions with \( q \)-spin states in this box is
\[
\mathcal{H} = \bigwedge_1^N L^2(\Lambda; \mathbb{C}^q),
\]
We use Dirichlet boundary conditions. Since the Hamiltonian does not depend on the spin degrees of freedom, we may think of the system as consisting of \( q \) species of spinless fermions.

We are interested in the ground state energy \( E(N, L) = \inf \text{spec} \mathcal{H}_N \) in the thermodynamic limit, more precisely the energy per unit volume defined by
\[
e(\rho) = \lim_{N, L \to \infty} \frac{N}{L^3} E(N, L).
\]
This limit is known to exist by very general arguments dating back to the 50’s.

3. The Main Result

**Theorem 3.1 (Low density asymptotics).** For \( \rho \to 0 \) the minimum energy is achieved (to the two leading orders in \( N/V \)) by having equal numbers of particles (namely \( N/q \)) in each spin state. This energy is
\[
e(\rho) = \frac{3}{5} \left( \frac{6\pi^2}{q} \right)^{2/3} \rho^{5/3} + 4\pi \left( 1 - \frac{1}{q} \right) a_v \rho^2 + o(\rho^2),
\]
where the first term is the energy of a free Fermi gas and the second term depends on the pair potential through its scattering length \( a_v \).

The scattering length \( a_v \) of the spherically symmetric potential \( v \) is defined as the constant such that the spherically symmetric zero-energy scattering solution
\[
-\Delta \phi + \frac{1}{2} v \phi = 0 \quad \text{with} \quad \lim_{|x| \to \infty} \phi(x) = 1,
\]
satisfies
\[
\phi(x) = 1 - \frac{a_v}{|x|}
\]
for all \( x \) outside the range of \( v \).

The proof of Theorem 3.1 is given in [5].

**Remarks:**
(i) The relevant dimensionless parameter is \( \rho a_v^3 \). Low density means that \( \rho a_v^3 \ll 1 \) or that \( \rho \to 0 \), when \( a_v \) is kept fixed.

(ii) For a hard core potential \( a_v \) is simply the hard core size.

(iii) From the definition of the scattering length we see, by an integration by parts, that
\[
\int |\nabla \phi|^2 + \frac{1}{2} \int v|\phi|^2 = 4\pi a_v.
\]
Heuristically, we may interpret this result as saying that for just one pair of particles in a large volume the energy is \( 4\pi a_v/\text{vol} \) per particle or altogether \( 8\pi a_v/\text{vol} \). The number of “interacting” fermion pairs is \( \frac{1}{2} N^2 (1 - \frac{1}{q}) \). The interaction of identical fermions can be ignored for low density, as explained earlier.
4. The Bosonic Case

The low density energy asymptotics for bosons (or even without any symmetry restrictions, i.e., if \( \mathcal{H} = \bigotimes L^2(\mathbb{R}^3) \)) was proved by Lieb and Yngvason in [1]. Some subsequent developments are in [6]–[14]. For an up-to-date survey of rigorous results on the Bose gas [4] is recommended.

**Theorem 4.1 (Dilute Bose gas).** For \( \rho \to 0 \)

\[
e^B(\rho) = 4\pi a_v \rho^2 + o(\rho^2),
\]

Note that the correlation term is the leading term here.

In 1957 Dyson [15] proved the asymptotically correct upper bound. This is far from trivial since one cannot use a simple product trial function, which would give infinity in the hard core case.

Dyson also gave a lower bound for bosons, which however was not asymptotically exact. Dyson’s lower bound relied on the following lemma, which, in fact, was also a key ingredient in the rigorous lower bound in [1].

**Lemma 4.2 (Dyson’s Lemma).** Assume \( v \) be supported in \( \{|x| < R_0\} \). Let \( \theta_R \) be the characteristic function of \( \{|x| < R\} \). Then for any positive radial function \( U \) supported in \( R_0 \leq |x| \leq R \) with \( \int U = 4\pi \) we have the operator inequality

\[
-\nabla \theta_R \nabla + \frac{1}{2} v \geq a_v U \quad \text{or} \quad \int \theta_R \left[ |\nabla \phi|^2 + \frac{1}{2} v|\phi|^2 \right] \geq a_v \int U|\phi|^2.
\]

Dyson’s Lemma states that one may, as a lower bound, replace \( v \) by a much softer potential \( w = a_v U \) with the property that \((4\pi)^{-1} \int w = (4\pi)^{-1} \int a_v U = a_v\). However, one has to use all of the kinetic energy to do this.

In the rigorous argument in [1] only almost all the kinetic energy is used with the Dyson Lemma. The rest is used to carry through a perturbation argument.

As explained in the introduction we cannot afford to give up even a fraction of the low momentum part of the kinetic energy in the fermionic case, since it is responsible for the leading free Fermi term. We therefore need a generalization of Dyson’s lemma, which we describe below.

**Early History of the Bosonic Problem.** Lenz [16] was the first to calculate the energy [4], using the heuristic pair argument given in Remark (iii) after Theorem 3.1.

Bogoliubov [17] did a perturbative expansion, but got \((8\pi)^{-1} \int v\) instead of \(a_v\). He realized, of course, that this was meaningless (e.g. for the hard core). As Bogoliubov points out in his paper, Landau realized the connection to the scattering length. Namely, that \((8\pi)^{-1} \int v\) is the first term in the Born series for \(a_v\). See also [18].

Using Bogoliubov’s method, the next term in the expansion beyond \(4\pi a_v \rho^2\) has been calculated to be

\[
4\pi a_v \rho^2 \frac{128}{15\sqrt{\pi}} \sqrt{\rho a_v^3}.
\]

An important open problem is to prove this formula rigorously. As in the leading term, this correction depends on \(v\) only through the scattering length.
5. The Generalized Dyson Lemma

The solution to the problem that we cannot give up any fraction of the low momentum kinetic energy is to give up almost all the energy in the large momentum regime only. Large here means momenta much greater than the Fermi momentum. If we give up kinetic energy corresponding to momenta greater than the Fermi momentum only, and in such a way that as a function of momentum the kinetic energy is still monotone, we do not affect the leading free Fermi gas term. The following lemma, which allows us to do this, is the main technical advance in our work.

**Lemma 5.1 (Generalized Dyson Lemma).** Assume $\nu$ to be supported in $\{|x| < R_0\}$. Let $\theta_R$ be the characteristic function of $\{|x| < R\}$. Let $\chi$ be a radial function, $0 \leq \chi(p) \leq 1$, such that the Fourier transform $h(x) \equiv 1 - \chi(x)$ is bounded and integrable. Define

$$f_R(x) = \sup_{|y| \leq R} |h(x-y) - h(x)| \quad \text{and} \quad w_R(x) = \frac{2}{\pi^2} f_R(x) \int_{R^3} f_R(y) dy.$$

Then for any $\varepsilon > 0$ and any positive radial function $U$ supported in $R_0 \leq |x| \leq R$ with $\int U = 4\pi$ we have the operator inequality

$$-\nabla \chi(p) \theta_R(x) \chi(p) \nabla + \frac{1}{2} \nu(x) \geq (1 - \varepsilon) a_r U(x) - \frac{a_v}{\varepsilon} w_R(x).$$

$R$ is a parameter we shall choose such that $a_v \ll R \ll \rho^{-1/3}$. We will choose the function $\chi$ to be approximately the characteristic function for the set of momenta greater than the Fermi momentum, which is proportional to $\rho^{1/3}$. This corresponds to decomposing the kinetic energy into low and high momentum parts as shown in the figures below.

| $p^2(1 - \chi(p))$ | $p^2 \chi(p)$ |
|---------------------|----------------|
| Low momentum regime | High momentum regime |

6. A Lower Bound to the Energy

To explain how the generalized Dyson Lemma is used to get a lower bound to the energy we consider, for simplicity, the case $q = 2$ and write $X = (x_1, x_2, \ldots, x_{N_\uparrow})$, $Y = (y_1, y_2, \ldots, y_{N_\downarrow})$ for the coordinates of the two species of fermions. Without loss of generality we may assume that $N_\uparrow = N_\downarrow$. The reason is that the system is $SU(2)$ symmetric and every state of total spin $S$ can be rotated to a state of total
$S_z = 0$. Nevertheless we will keep the particle numbers arbitrary for the moment for pedagogical clarity.

We first consider the $Y$ particles as fixed. For a lower bound we may ignore the repulsion between like fermions since $v \geq 0$. From the generalized Dyson Lemma we obtain the following result.

**Corollary 6.1 (Generalized Dyson Lemma in multi-centered case).** Let $R > 0$ be bigger than the range of the potential $R_0$. If $|y_i - y_j| \geq 2R$ for all $i \neq j$, then

$$-\nabla \chi(p)^2 \nabla + \frac{1}{2} \sum_{i=1}^{N_i} v(x - y_i) \geq \sum_{i=1}^{N_i} \left( (1 - \varepsilon) a_v U(x - y_i) - \frac{a_v}{\varepsilon} w_R(x - y_i) \right).$$

To use this we must ignore $y$-particles that are closer than $2R$ apart. This can be controlled by the following a-priori bound.

**Lemma 6.2.** Let $I_R(Y)$ be the number of $y$’s that are less than $2R > 0$ from their nearest neighbor. Then for any fermionic wave function $\Psi(Y)$

$$\langle \Psi, I_R \Psi \rangle \leq CT(\Psi) R^2,$$

where $T(\Psi) = \sum_i \langle \nabla y_i \Psi, \nabla y_i \Psi \rangle$ and $C$ is a constant.

This lemma is an easy consequence of a theorem [19] Theorem 5] relating nearest neighbor distance to kinetic energy.

For an approximate ground state $\Psi$ we can assume $T(\Psi) \leq cN\rho^{2/3}$. Recall that we will choose $R\rho^{1/3} \ll 1$, and thus $\langle \Psi, I_R(Y) \Psi \rangle \ll N$.

The soft potential can now be studied with the remaining low momentum kinetic energy.

$$\sum_{i=1}^{N_i} \left[ -\nabla_i (1 - \chi(p)) \nabla_i + \sum' \left( (1 - \varepsilon) a_v U(x_i - y_j) - \frac{a_v}{\varepsilon} w_R(x_i - y_j) \right) \right],$$

where $\sum'$ refers to the sum over the $N_i - I_R(Y)$ $y$-particles that are a distance greater than $2R$ from their nearest neighbor. Since we can ignore $I_R(Y)$ the sum of the $N_i$ lowest eigenvalues of the operator in $\left[ \right]$ is approximately

$$\frac{3}{5} \left( \frac{6\pi^2}{2} \right)^{2/3} N_i^{5/3} L^{-2} + N_i N_i L^{-3} a_v \int U.$$

We get a similar contribution when we consider the $Y$ particles as movable and the $X$ particles as fixed. If we also use that $\int U = 4\pi$ the sum of the two contributions will be

$$\frac{3}{5} \left( \frac{6\pi^2}{2} \right)^{2/3} N_i^{5/3} L^{-2} + \frac{3}{5} \left( \frac{6\pi^2}{2} \right)^{2/3} N_i^{5/3} L^{-2} + 8\pi N_i N_i L^{-3} a_v.$$

Here we see again that the minimum occurs for $N_i = N_i$, and is given by [19].

### 7. The Upper Bound

For an upper bound we first construct a Bijl-Dingle-Jastrow function for particles of the same spin:

$$G(X) = \prod_{i<j} g(x_i - x_j),$$
where \( g(x) = 0 \) if \( |x| < R_0 \), \( g(x) = 1 \) if \( |x| > s \), and \( R_0 \ll s \ll \rho^{-1/3} \). The role of \( G \) is to ensure that like fermions do not interact.

Next, we construct a Bijl-Dingle-Jastrow function for particles of opposite spin:

\[
F(X, Y) = \prod_{i,j} f(x_i - y_j),
\]

where \( f \) (which is not normalized, since it, like \( g \), satisfies \( f(x) \to 1 \) as \( |x| \to \infty \)) is chosen so that

\[
\int |\nabla f|^2 + \frac{1}{2} \int |v|^2 \approx 4\pi a_v.
\]

(Compare with (3.2).) The role of \( F \) is to give the correct pair energy between different fermions.

Finally, the trial state we shall use is

\[
\Psi(X, Y) = D(X)D(Y)G(X)G(Y)F(X, Y),
\]

where \( D = u_{\alpha_1} \wedge \cdots \wedge u_{\alpha_n} \) is a Slater determinant of eigenfunctions \( u_\alpha \) of the Dirichlet Laplacian. The choice of this \( \Psi \) is quite obvious. The problem is that it is not normalized. The normalization problem can be addressed with the aid of the following combinatorial lemma, for which we claim no originality.

**Lemma 7.1 (Key combinatorial lemma).** Let \( \Phi = \phi_1 \wedge \cdots \wedge \phi_n \) denote a Slater determinant of \( n \) linearly independent functions \( \phi_\alpha(x) \). Let \( \mathcal{M} \) denote the \( n \times n \) matrix

\[
\mathcal{M}_{\alpha\beta} = \int \phi_\alpha^*(x) \phi_\beta(x) dx.
\]

(i) The norm of \( \Phi \) is given by \( \langle \Phi|\Phi \rangle = \det \mathcal{M} \).

(ii) For \( 1 \leq m \leq n \), the normalized \( m \)-particle density of \( \Phi \) is given by

\[
(x_1, \ldots, x_m) \mapsto \left( \prod_{i=1}^m [\phi(x_i)] \right) \frac{1}{\mathcal{M}} \otimes \cdots \otimes \frac{1}{\mathcal{M}} \left( [\phi(x_1)] \wedge \cdots \wedge [\phi(x_m)] \right).
\]

Here, \( [\phi(x_i)] \) denotes the \( n \)-dimensional vector with components \( \phi_\alpha(x) \).

We use this lemma, for fixed \( Y \), with \( \phi_\alpha(x) = u_\alpha(x) \prod_j f(x - y_j) \). The matrix \( \mathcal{M} \) in (7.2) then depends on \( Y \) and is denoted by \( \mathcal{M}(Y) \). The following estimate shows that although the \( \phi_\alpha \) are not orthonormal, \( \mathcal{M}(Y) \) is close to \( I \) if the separation between the \( Y \)-particles is not too small.

**Lemma 7.2 (Key estimate).** Assume that \( |y_i - y_j| \geq s \) for all \( i \neq j \). Then \( \|I - \mathcal{M}(Y)\| \to 0 \) as \( s/a_v \to \infty \) and \( N^{1/3}s/L \to 0 \), uniformly in \( N \) and \( Y \).

Note that if \( f \) were identically 1, then \( \mathcal{M} \) would be equal to the identity. The proof of Lemma 7.2 uses the Poincaré inequality to estimate the effect of the deviation of \( f \) from 1 on the integral in (7.2).

The assumption that \( |y_i - y_j| \geq s \) in Lemma 7.2 is satisfied since our trial function vanishes otherwise, thanks to the property of \( G \). Lemma 7.2 is concerned only with the effect of \( F \) on the norm of \( \Psi \). The effect of \( G \) on the norm of \( \Psi \) has to be controlled by different means. For this purpose we find it necessary to break space up into boxes (whose size is large but independent of \( L \)) and confine the particles to these boxes, i.e., regard particles in different boxes as independent. We refer to [5] for details.
References

[1] E.H. Lieb, J. Yngvason, *Ground State Energy of the low density Bose Gas*, Phys. Rev. Lett. 80, 2504–2507 (1998).
[2] E.H. Lieb, J. Yngvason, *The Ground State Energy of a Dilute Two-dimensional Bose Gas*, J. Stat. Phys. 103, 509 (2001).
[3] E.H. Lieb, J. Yngvason, *The Ground State Energy of a Dilute Bose Gas*, in: *Differential Equations and Mathematical Physics*, University of Alabama, Birmingham, 1999, R. Weikard and G. Weinstein, eds., pp. 271–282, Amer. Math. Soc./Internat. Press (2000).
[4] E.H. Lieb, R. Seiringer, J.P. Solovej and J. Yngvason, *The Mathematics of the Bose Gas and its Condensation*, vol. 34, Oberwolfach Seminars Series, Birkhäuser (2005).
[5] E.H. Lieb, R. Seiringer, and J.P. Solovej, *Ground-state energy of the low-density Fermi gas*, Phys. Rev. A 71, 053605-1–13 (2005).
[6] E.H. Lieb, R. Seiringer, *Proof of Bose-Einstein Condensation for Dilute Trapped Gases*, Phys. Rev. Lett. 88, 170409-1–4 (2002).
[7] E.H. Lieb, R. Seiringer, *Derivation of the Gross-Pitaevskii Equation for Rotating Bose Gases*, preprint, arXiv:math-ph/0504042.
[8] E.H. Lieb, R. Seiringer, J. Yngvason, *Bosons in a Trap: A Rigorous Derivation of the Gross-Pitaevskii Energy Functional*, Phys. Rev. A 61, 043602 (2000).
[9] E.H. Lieb, R. Seiringer, J. Yngvason, *A Rigorous Derivation of the Gross-Pitaevskii Energy Functional for a Two-dimensional Bose Gas*, Commun. Math. Phys. 224, 17 (2001).
[10] E.H. Lieb, R. Seiringer, J. Yngvason, *Superfluidity in Dilute Trapped Bose Gases*, Phys. Rev. B 66, 134529 (2002).
[11] E.H. Lieb, R. Seiringer, J. Yngvason, *One-Dimensional Behavior of Dilute, Trapped Bose Gases*, Commun. Math. Phys. 244, 347–393 (2004). See also: *One-Dimensional Bosons in Three-Dimensional Traps*, Phys. Rev. Lett. 91, 150401-1–4 (2003).
[12] E.H. Lieb, R. Seiringer, and J. Yngvason, *Poincaré Inequalities in Punctured Domains*, Ann. Math. 158, 1067–1080 (2003).
[13] R. Seiringer, *Gross-Pitaevskii Theory of the Rotating Bose Gas*, Commun. Math. Phys. 229, 491–509 (2002).
[14] R. Seiringer, *Ground state asymptotics of a dilute, rotating gas*, J. Phys. A: Math. Gen. 36, 9755–9778 (2003).
[15] F.J. Dyson, *Ground-State Energy of a Hard-Sphere Gas*, Phys. Rev. 106, 20–26 (1957).
[16] W. Lenz, *Die Wellenfunktion und Geschwindigkeitsverteilung des unendlich kleinen Gases*, Z. Phys. 56, 778–789 (1929).
[17] N.N. Bogoliubov, *On the theory of superfluidity*, Izv. Akad. Nauk USSR, 11, 77 (1947). Eng. Trans. J. Phys. (USSR), 11, 23 (1947). See also *Lectures on quantum statistics*, vol. 1, Gordon and Breach (1967).
[18] E.H. Lieb, *The Bose Fluid*, in: W.E. Brittin, ed., Lecture Notes in Theoretical Physics VII, Univ. of Colorado Press, pp. 175–224 (1964).
[19] E.H. Lieb and H.-T. Yau, *Stability and Instability of Relativistic Matter*, Commun. Math. Phys. 118, 177–213 (1988).

DEPARTMENTS OF MATHEMATICS AND PHYSICS, JADWIN HALL, PRINCETON UNIVERSITY, P.O. BOX 708, PRINCETON, NJ 08544, USA
E-mail address: lieb@princeton.edu

DEPARTMENT OF PHYSICS, JADWIN HALL, PRINCETON UNIVERSITY, P.O. BOX 708, PRINCETON, NJ 08544, USA
E-mail address: rseiring@princeton.edu

INSTITUTE FOR MATHEMATICAL SCIENCES, UNIVERSITY OF COPENHAGEN, UNIVERSITETSPLASKE 5, DK-2100 COPENHAGEN, DENMARK
E-mail address: solovej@math.ku.dk