บทความวิจัย

ขอบเขตบนของพลังงานที่สถานะพื้นของสสารประเภทเฟอร์มิออนในสองมิติ

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บทคัดย่อ

ในการคำนวณหาพลังงานสถานะพื้นของสสารประเภทเฟอร์มิออนได้กำหนดให้อิเล็กตรอนจำนวน N ตัวถูกวางแบบไม่ซ้อนทับกันบนพื้นที่สี่เหลี่ยม กว้าง $2L$ ยาว $2L$ ที่เรียงตัวอยู่ในทิศทาง (1,1) จำนวน k พื้นที่สี่เหลี่ยม โดยมีนิวเคลียสวางอยู่ตำแหน่งกึ่งกลางของแต่ละพื้นที่สี่เหลี่ยม ขอบเขตบนของพลังงานสถานะพื้นอันเนื่องมาจากฟังก์ชันคลื่นทดลองที่คำนวณได้จะขึ้นกับ N ของอิเล็กตรอน

คำสำคัญ: ขอบเขตบนของพลังงานสถานะพื้น เสถียรภาพของสสาร

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Upper Bound for the Ground State Energy of fermionic Matter in 2D

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ABSTRACT

We derive the upper bound for the exact ground-state energy involving a single power of the number of electrons in matter, N. The bound is based on the following construction. We consider the N electrons localized in k non-overlapping ordered squares size $2L \times 2L$, with the k nuclei placed at the centers of each square area with appropriate choices of trial wavefunctions for the N electrons.

Keywords: upper bound for the ground-state energy, stability of matter

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1. Introduction

Undoubtedly, one of the most important and serious problems that quantum physics has faced over the years, since its birth over a three-quarter of a century ago, is that of the stability of matter. This is of consistently demonstrating as to why matter in our world consisting of a large number of electrons, in spite of their mutual repulsions, but with increasing attractions to its nuclei, as their number increase, and continuously accelerating around them, does not eventually lead to its collapse, as expected on classical grounds, and a perfect balance between these phenomenae occurs and matter remains stable. The so-called Pauli exclusion principle turns out to be not only sufficient for stability but also necessary. That is, if one invokes the exclusion principle then stability may be established.

The relevant papers which led to modern developments of the fundamental problem of stability were due to Dyson and Lenard [1, 2], Leib and Thirring [3], Leib [4, 5], Manoukian and Sirininlakul [6, 7, 8], Sripirom Sirininlakul and Sirininlakul [9], covering essentially the history of which is relevant to the problem of the stability of matter. In addition to the earlier investigations of Dyson and Lenard mentioned above, the contribution of Leib and Thirring [1] has embodied the central result of this problem, in which they bound the ground-state energy from below, as Dyson and Lenard, by a single power of N (the number of electrons in a piece of matter) multiplied by a negative constant whose magnitude is much smaller than that found by Dyson and Lenard. It is expected that an ultimate treatment of stability of matter should involve the full machinery of quantum electrodynamics [10]. Thus the actual demonstration of a single power of N for matter is essential.

The Hamiltonian under consideration for the stability of matter is taken to be the $N-$electron one

$$H=\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m}+\sum_{i<j}^{N}\frac{e^2}{\left|\mathbf{x}_i-\mathbf{x}_j\right|}-\sum_{i=1}^{N}\sum_{j=1}^{k}\frac{Z_j e^2}{\left|\mathbf{x}_i-\mathbf{R}_j\right|}+\sum_{i<j}^{k}\frac{Z_i Z_j e^2}{\left|\mathbf{R}_i-\mathbf{R}_j\right|} \tag{1}$$

where m denotes the mass of the electron and the x_i, R_j correspond, respectively, to positions of the electrons and nuclei. Also we consider neutral matter, i.e.,

$$\sum_{i=1}^{k}Z_i=N\,. \tag{2}$$

The Hamiltonian in (1) is a typical one in that it corresponds to motionless (i.e., infinitely massive) fixed point-like nuclei. This is non-academic. By doing so, one does not dwell on the fate and the dynamics of the positive background, and one is looking at, and monitoring the fate of, the electrons through the “eye” of the former system. The key result in the problem of the stability of matter, with the exclusion principle, is the single power law behaviour $-E_N/N$ of the ground-state energy, and the physically expected result that the ground-state energy per electron $|E_N/N|$ remains bounded for all N

The purpose of this paper is to carry a mathematically rigorous analysis of the problem of stability of matter in area (two dimensions) by involving, in the process, the fundamental Pauli exclusion principle which, as mentioned above, has far reaching consequences in nature relevant directly to our world.

2. Upper Bound for the Ground-State Energy of Matter

We consider the anti-symmetric normalized functions $\Psi(x_1\sigma_1,...,x_N\sigma_N)$ of N electrons, we then have for the expectation value of the Hamiltonian H in (1)

$$\langle\Psi|H|\Psi\rangle = \sum_{i=1}^{N}\left\langle\Psi\left|\frac{\mathbf{p}_i^2}{2m}\right|\Psi\right\rangle - \sum_{i=1}^{N}\sum_{j=1}^{k} Z_j e^2\left\langle\Psi\left|\frac{1}{|\mathbf{x}_i-\mathbf{R}_j|}\right|\Psi\right\rangle + \sum_{i<j}^{N} e^2\left\langle\Psi\left|\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}\right|\Psi\right\rangle + \sum_{i<j}^{k} e^2\frac{Z_i Z_j}{|\mathbf{R}_i-\mathbf{R}_j|}. \tag{3}$$

To derive an upper bound to this expectation value, we recall the definition of electron density

$$\rho(\mathbf{x}) = N\sum_{\sigma_1,\ldots,\sigma_N}\int d^2\mathbf{x}_2\ldots d^2\mathbf{x}_N\left|\Psi(\mathbf{x}\,\sigma_1,\mathbf{x}_2\,\sigma_2,\ldots,\mathbf{x}_N\,\sigma_N)\right|^2 \tag{4}$$

normalized to $\int d^2\mathbf{x}\;\rho(\mathbf{x}) = N$

A quick and rather conservative upper bound for E_N may be derived by considering the following determinantal function

$$\Psi(\mathbf{x}_1\,\sigma_1,\ldots,\mathbf{x}_N\,\sigma_N) = \frac{1}{\sqrt{N!}}\det\left[\varphi_j(\mathbf{x}_k,\sigma_k)\right] \tag{5}$$

(j, k = 1,..., N), where

$$\varphi_j(\mathbf{x},\sigma) = \varphi\left(\mathbf{x}-\mathbf{L}^{(j)}\right)\chi_j(\sigma) \tag{6}$$

with normalized spin functions $\chi_j(\sigma)$, which for simplicity may be taken to be all the same, and

$$\varphi(\mathbf{x}) = \prod_i\left(\frac{1}{\sqrt{L}}\cos\left(\frac{\pi x_i}{2L}\right)\right),\quad |x_i|\le L \tag{7}$$

$i = 1,2$, and is zero otherwise, $\mathbf{x} = (x_1, x_2)$. We choose the vectors $\mathbf{L}^{(1)},...,\mathbf{L}^{(k)}$ as follows

$$\mathbf{L}^{(j)} = j\,D\big(1,1\big), \quad j = 1,..., k \tag{8}$$

and we may choose

$$3L \le D. \tag{9}$$

It is easy to see that the intervals : $\{jD - L \le x_i \le jD + L\}$, for $j = 1,...,k$, are disjoint, for each $i = 1,2$, and the functions $\varphi(\mathbf{x}-\mathbf{L}^{(j)})$ are then non-overlapping, and orthogonal with respect to *each* of the components x_i of $\mathbf{x}$.

We choose

$$\mathbf{R}_j = \mathbf{L}^{(j)}, \quad j = 1,...,k. \tag{10}$$

The above construction (Figure 1) consists of conveniently placing the k nuclei at $\mathbf{L}^{(1)},...,\mathbf{L}^{(k)}$ and one electron in each one of the k squares with centers at $\mathbf{L}^{(1)},...,\mathbf{L}^{(k)}$. One electron is also placed in each of the remaining $(N-k)$ nuclei-free squares with center at $\mathbf{L}^{(k+1)},...,\mathbf{L}^{(N)}$. Because the Coulomb potential is of long range, the interactions occur between particles in the different squares as well.

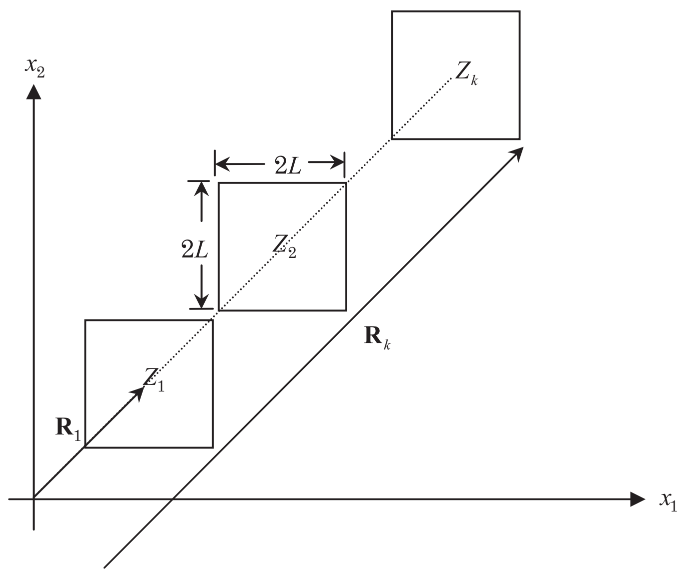

Figure 1 The construction of non-overlapping k squares align in direction (1,1)

Due to the localizations of the functions $\varphi_j(\mathbf{x},\sigma)$, as described above, the electrons are well separated, and we may write

$$\left|\mathbf{x}_i - \mathbf{x}_j\right| \geq \frac{D\sqrt{2}}{3}, \ \ i \neq j \tag{11}$$

and bound the repulsive $e-e$ interaction term as

$$\sum_{i<j}^{N} \frac{e^2}{\left|\mathbf{x}_i - \mathbf{x}_j\right|} \leq \frac{3}{D\sqrt{2}} \ \ e^2 \ \sum_{i<j}^{N}(1)\,. \tag{12}$$

From (10), (8), $|\mathbf{R}_i - \mathbf{R}_j| \geq D$ for $i \neq j$, then we have the inequality

$$\sum_{i<j}^{k} \frac{Z_i Z_j e^2}{\left|\mathbf{R}_i - \mathbf{R}_j\right|} \leq \frac{e^2}{D\sqrt{2}} \ \sum_{i<j}^{k} Z_i Z_j\,. \tag{13}$$

Finally, we use the conservative bound

$$\begin{aligned} -\sum_{i=1}^{N}\sum_{j=1}^{k} \frac{Z_j e^2}{\left|\mathbf{x}_i - \mathbf{R}_j\right|} &\leq -\sum_{i=1}^{k}\sum_{j=1}^{k} \frac{Z_j e^2}{\left|\mathbf{x}_i - \mathbf{R}_j\right|} \\ &\leq -\sum_{i=1}^{k} \frac{Z_i e^2}{\left|\mathbf{x}_i - \mathbf{R}_i\right|} \\ &= -\sum_{i=1}^{k} \frac{Z_i e^2}{\left|\mathbf{x}_i - \mathbf{L}^{(i)}\right|} \end{aligned} \tag{14}$$

to obtain

$$\begin{aligned} \langle \Psi | H | \Psi \rangle \leq \left\langle \Psi \left| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} \right| \Psi \right\rangle - \sum_{i=1}^{k} Z_i e^2 \int \frac{d^2\mathbf{x}}{\left|\mathbf{x} - \mathbf{L}^{(i)}\right|} \varphi_i^2(\mathbf{x}) \\ + \frac{e^2}{D}\left[\frac{3}{\sqrt{2}} \sum_{i<j}^{N}(1) + \sum_{i<j}^{k} Z_i Z_j\right]. \end{aligned} \tag{15}$$

The kinetic energy part is explicitly given by

$$\left\langle \Psi \left| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} \right| \Psi \right\rangle = N \, \frac{\hbar^2}{m}\left(\frac{\pi}{2L}\right)^2 \tag{16}$$

and

$$\int \frac{d^3\mathbf{x}}{\left|\mathbf{x}-\mathbf{L}^{(i)}\right|}\,\varphi_i^2\left(\mathbf{x}\right) = \int \frac{d^3\mathbf{x}}{\left|\mathbf{x}\right|}\,\varphi^2\left(\mathbf{x}\right) \geq \frac{1}{\sqrt{2}\,L}. \tag{17}$$

Since $|\mathbf{x}| \leq \sqrt{2}\,L$ in the latter integral.

All told, we obtain

$$\left\langle\Psi\middle|H\middle|\Psi\right\rangle \leq \frac{\hbar^2\pi^2}{4m}\frac{N}{L^2} - \frac{e^2}{\sqrt{2}\,L}N + \frac{e^2}{D\sqrt{2}}\left[3\sum_{i<j}^{N}(1) + \sum_{i<j}^{k} Z_i Z_j\right]. \tag{18}$$

Optimization over L gives

$$L = \left(\frac{\hbar^2\pi^2}{me^2\sqrt{2}}\right) \tag{19}$$

and leads to the bound

$$\left\langle\Psi\middle|H\middle|\Psi\right\rangle \leq -\frac{1}{\pi^2}\left(\frac{me^4}{2\hbar^2}\right)N + \frac{e^2}{D\sqrt{2}}\left[3\sum_{i<j}^{N}(1) + \sum_{i<j}^{k} Z_i Z_j\right]. \tag{20}$$

We may choose D large enough to make the second term as small as we please in comparison to the first one to obtain

$$\left\langle\Psi\middle|H\middle|\Psi\right\rangle \leq -\frac{1}{\pi^2}\left(\frac{me^4}{2\hbar^2}\right)N \tag{21}$$

Since Ψ does not necessarily coincide with the ground-state wavefunction, and the configuration positions of the nuclei does not necessarily correspond to the lowest possible energy, (21) leads to an upper bound for E_N:

$$E_N \leq -\,0.101321\left(\frac{me^4}{2\hbar^2}\right)N \tag{22}$$

with the upper bound having the single power of N.

Conclusion and Discussion

From the main result of this paper, (22), it leads to the conclusion that necessity for fermionic matter, the rigorous upper bound for the exact ground state energy types with Coulomb interactions in two dimensions with fixed positive charges depend on a single power of N, the number of electrons in matter. If we combine this upper bound with the lower bound of ground state energy which is derived by [9], we obtain $-c_{lower}N \leq E_N \leq -c_{upper}N$ where c_{lower}, c_{upper} are constant. This bounds give the range of the ground state energy of fermionic matter which makes the system stable.

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