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Asymptotics of Heavy Molecules in High Magnetic Fields

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Abstract. As the extention of the results of Lieb, Solovej and Yngvason[LSY1], we consider the Coulomb systems of large molecules in strong magnetic field and study the energy asymptotics.

1. Introduction

The aim of this paper is to consider the N electrons interacting each other by the Coulomb repulsion, attracted by K fixed nuclei in a strong uniform magnetic field.

The corresponding Hamiltonian of quantum mechanics is defined as:

$$(1.1)\quad H_N := \sum_{i=1}^{N}\{(\mathbf{p}^i + A(x^i))^2 + \sigma^i \cdot \mathbf{B}\} + \sum_{i=1}^{N} V(x^i) + \sum_{1\le k<l\le N} |x^k - x^l|^{-1}.$$

where $x^i = (x^i_1, x^i_2, x^i_3) \in \mathbf{R}^3$ is the coordinate of the i-th particle. We often write $x = (x_1, x_2, x_3) = (x_\perp, x_3)$ where $x_\perp = (x_1, x_2) \in \mathbf{R}^2$. $V(x) := \sum_{j=1}^{K} Z_j |x^i - R_j|^{-1}$, $Z_j > 0$ (resp. $R_j \in \mathbf{R}^3$) is the charge(resp. position) of the nuclei, $\mathbf{p} = -i\nabla$, σ is the Pauli spin matrix, and $\mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{x}$ is the vector potential associated to the uniform magnetic field $\mathbf{B} = (0, 0, B)$, $B > 0$. We consider H_N on $\mathcal{H}_N := \Lambda^N L^2(\mathbf{R}^3; \mathbf{C}^2)$ which is the space of the antisymmetric spinor valued functions on $\mathbf{R}^{3N}$(Λ^N means the exterior product).

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H_N is essentially self-adjoint on $\Lambda^N C_0^\infty(\mathbf{R}^3; \mathbf{C}^2)$ whose self-adjoint extension is also denoted by H_N. Our main object is to obtain the large field asymptotics of the ground state energy:

$$(1.2) \quad E^Q(N, \{Z_j\}, B, \{R_j\}) := \inf\{(\Psi, H_N\Psi) : \Psi \in \mathcal{D}(H_N), (\Psi, \Psi) = 1\},$$

where $(\cdot, \cdot)$ denotes the inner product of $L^2(\mathbf{R}^{3N})$. $\{Z_j\}$ and $\{R_j\}$ means $\{Z_1, \cdots, Z_K\}$ and $\{R_1, \cdots, R_K\}$ respectively. This model is arised from the investigation of the surface structure of neutron star. This has been studied by many physicists and mathematicians. Among the mathematical papers, Lieb, Solovej and Yngvason[1,2] have studied quite extensively. They divided the domain of the asymptotic parameter into five regions, namely, $1.B \ll Z^{4/3}$, $2.B \approx Z^{4/3}$, $3.Z^{4/3} \ll B \ll Z^3$, $4.B \approx Z^3$, $5.Z^3 \ll B$, and derive the leading asymptotics in each region ($B \ll Z^\alpha$ is meant by $B/Z^\alpha \to 0$ as $Z \to \infty$, and $B \approx Z^\alpha$ is meant by $0 < C < B/Z^\alpha < D < \infty$ where C, D are some constant). Briefly speaking, the magnetic Thomas Fermi theory is used in region 1,2,3, and the density matrix functional is used in region 3,4,5. They treated the one nuclear case($K = 1$ case), so we shall show that as for the density matrix functional theory, that is, in region 3,4,5, it is easily extended to K nuclei case.

Therefore, we want to obtain the leading asymptotics of E^Q when $Z_j = k_j Z$, k_j, $\lambda := N/Z$ are fixed, $B = O(Z^\alpha)$ $(\alpha \geq 4/3)$, and $Z \to \infty$. The motivation we extend to the K nuclei case is that, first, in the future we want to consider the atomic binding. If $B \ll Z^3$, no binding occurs which is proved using the magnetic Thomas Fermi theory[LSY2]. On the other hand, if $Z^3 \ll B$, the occurrence of binding is proved by the hyper strong theory[LSY1]. But when $B \approx Z^3$, whether binding occurs or not is the open problem. The author hope that the study of the K nuclei case will serve a little to approach this problem. Second, this paper will help us to consider infinitely many nuclei called "molecular chain" by physicists. In [NKL], by numerical calculations it is suggested that, as B is order $10^{12}G$, molecular chain is preferred by single atoms. But if B grows higher, no results have been showed up to the author's knowledge.

The first observation is that, if $\lambda(= N/Z)$ is fixed and $\beta := B/Z^{4/3} \to \infty$ as $Z \to \infty$, the leading order of the ground state energy is the same as the ground state energy restricted on the lowest Landau band. Before the precise statement, let us recall about the Landau band[LSY1,LL]. This is the eigenstate of the Pauli Hamiltonian $H_A := (\mathbf{p}+\mathbf{A}(x))^2+\sigma\cdot\mathbf{B}, \mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{x}$, whose spectrum is written formally by the sum of the spectrum of one-dimensional harmonic oscillator and that of the free particle moving along the magnetic field:

$$\varepsilon_{p\alpha\sigma} = 2(\alpha+\sigma+\frac{1}{2})B + p^2, \tag{1.3}$$

where α is a nonnegative integer, σ is the spin variable and p^2 is the energy of the one dimensional free particle. The eigenspace corresponding to (1.3) for fixed $\nu = \alpha+\sigma+\frac{1}{2}$ is called the ν-th Landau band. When $\nu = 0$(the lowest Landau band), that is, $\alpha = 0, \sigma = -1/2$, the remaining energy is only the kinetic energy along the magnetic field and spin is restricted to down($\sigma = -1/2$). Therefore if we write Π_0 to be the projection operator onto the lowest Landau band, the Pauli Hamiltonian is reduced to simple form:

$$\Pi_0 H_{\mathbf{A}} \Pi_0 = -\frac{\partial^2}{\partial x_3^2}\Pi_0. \tag{1.4}$$

Π_0 has the integral kernel

$$\Pi_0(x,x') = \frac{B}{2\pi}\exp\{\frac{i}{2}(x_\perp \times x'_\perp)\cdot\mathbf{B} - \frac{1}{4}|x_\perp - x'_\perp|^2 B\}\delta(x_3 - x'_3)P^{\downarrow}, \tag{1.5}$$

where $P^{\downarrow}$ is the projection in the vectors in $\mathbf{C}^2$ with spin $\sigma = -1/2[LSY1]$. Let $\Pi_0^N := \bigotimes_{i=1}^N \Pi_0$ which is the projection onto the subspace where all particles are in the lowest Landau band. We define the ground state energy within the lowest Landau band:

$$\begin{aligned} &E^Q_{conf}(N,\{Z_j\},B,\{R_j\}) \\ &\qquad := \inf\{(\Psi,H_N\Psi) : \Psi\in\mathcal{D}(H_N), \Pi_0^N\Psi = \Psi, (\Psi,\Psi) = 1\}. \end{aligned} \tag{1.6}$$

THEOREM 1.1. *If $\lambda = N/Z \le \Lambda, \Lambda > 0$ is fixed, then there exists some constant $\delta = \delta(\lambda^{2/3}\beta,\Lambda)$ such that $\delta\to 0$ as $\lambda^{2/3}\beta\to\infty$ and*

$$(1-\delta)E^Q(N,\{Z_j\},B,\{R_j\}) \le E^Q_{conf}(N,\{Z_j\},B,\{R_j\}).$$

REMARKS.

(1) In general, $E^Q < 0$ (theorem 5.3 of [LSY1]). Hence the above statement implies the upper bound of the modulus of E^Q in terms of E^Q_{conf}.

(2) By the definition, $E^Q \leq E^Q_{conf}$, hence in particular we obtain $E^Q/E^Q_{conf} \to 1$ as $\lambda^{2/3}\beta \to \infty$.

(3) The theorem does not say the ground state corresponding to E^Q lie in the lowest Landau band. It only shows that E^Q is asymptotically calculated as if all particles were in the lowest Landau band.

(4) Roughly speaking, the idea of its proof is to show that $E^Q \geq E^Q_{conf} - (error)$, where error term is estimated by Lieb-Thirring inequality as the order of $Z^{7/3}$(that is the leading order of N-electron systems when the magnetic field vanishes). On the other hand, E^Q_{conf} is estimated by variational inequality of Lieb[L] as the order of $N^{3/5}Z^{6/5}B^{2/5}$(in case of $B \ll Z^3$). The condition $B \gg Z^{4/3}$ comes from requiring that error term is lower order than E^Q_{conf}.

As stated before the theorem, in the lowest Landau band, all spins are down and the remaining kinetic energy is only that of the movement parallel to the field,i.e.,$(-\frac{\partial^2}{\partial x_3^2})$, so that the situation becomes quite simple.

The next step is, when $\Psi \in$ domain H_N satisfies $\Pi_0^N \Psi = \Psi$, to write the energy $(\Psi, H_N\Psi)$ in terms of the density matrix:

$$
\begin{aligned}
(1.7) \quad \Gamma^{\Psi}_{x_\perp}(x_3, x_3') := & \sum_{i=1}^{N} \int \cdots \int \Psi(x^1, \cdots, x^{i-1}; x_\perp, x_3; x^{i+1}, \cdots, x^N) \\
& \times \overline{\Psi(x^1, \cdots, x^{i-1}; x_\perp, x_3'; x^{i+1}, \cdots, x^N)} \\
& \times dx^1 \cdots dx^{i-1} dx^{i+1} \cdots dx^N, \\
= & N \int \cdots \int \Psi(x_\perp, x_3; x^2 \cdots x^N) \\
& \times \overline{\Psi(x_\perp, x_3'; x^2 \cdots x^N)} dx^2 \cdots dx^N.
\end{aligned}
$$

The second equality holds since Ψ is antisymmetric. $\int$ means the integration on $\mathbf{R}^3$ unless stated otherwise.

$\Gamma^{\Psi}_{x_\perp}(x_3, x_3')$ stands for the probability amplitude of the particles transferring from the point $(x_\perp, x_3)$ to $(x_\perp, x_3')$. For example, let $N = 2$ and we take $\phi_1, \phi_2 \in L^2(\mathbf{R}^3)$ such that $\Pi_0\phi_i = \phi_i (i = 1, 2)$ and $(\phi_i, \phi_j)_{L^2(\mathbf{R}^3)} = \delta_{ij}$. Set $\Phi := (2)^{-1/2}\{\phi_1(x_1)\phi_2(x_2) - \phi_1(x_2)\phi_2(x_1)\} \in \mathcal{H}_N$(that is the Slater determinant). Then, $\Gamma^{\Phi}_{x_\perp}(x_3, x_3') = \sum_{i=1}^{2} \phi_i(x_\perp, x_3)\overline{\phi_i(x_\perp, x_3')}$. We will be able to understand the density matrix theory easier if we keep this example in mind.

At first sight, it seems strange to let $N \to \infty$ because as it goes, $H_N, \mathcal{H}_N$,etc. would varies. But by reducing the Hamiltonian in terms of the one density matrix alone, it will become simple which we shall briefly see here.

The kinetic energy of H_N which is simpler in the lowest Landau band (1.4) is

$$\begin{aligned}
\sum_{i=1}^{N}(\Psi, \frac{\partial^2}{\partial x_3^{i2}}\Psi) &= N\int \left|\frac{\partial}{\partial x_3}\Psi(x_\perp, x_3'; x^2 \cdots x^N)\right|^2 dx dx^2 \cdots dx^N, \\
&= N\int \frac{\partial}{\partial x_3}\Psi(x_\perp, x_3; x^2 \cdots x^N) \\
&\quad \times \frac{\partial}{\partial x_3}\overline{\Psi(x_\perp, x_3'; x^2 \cdots x^N)}\big|_{x_3 = x_3'} dx dx^2 \cdots dx^N, \\
&= \int \frac{\partial}{\partial x_3}\frac{\partial}{\partial x_3'}\Gamma^{\Psi}_{x_\perp}\Big|_{x_3 = x_3'} dx_3 dx_\perp.
\end{aligned}$$

It has an easier interpretation by regarding $\Gamma^{\Psi}_{x_\perp}$ as the kernel of an operator on $L^2(\mathbf{R})$ parameterized by $x_\perp \in \mathbf{R}^2$. To do this, let $\{\phi_n\}_{n=1}^{\infty}$ by the complete orthonormal basis of $L^2(\mathbf{R})$

$$\begin{aligned}
&\frac{\partial}{\partial x_3}\frac{\partial}{\partial x_3'}\Gamma^{\Psi}_{x_\perp}(x_3, x_3') \\
&\quad = \sum_{n,m=1}^{\infty} \phi_n(x_3)\phi_m(x_3') \int_{\mathbf{R}}\int_{\mathbf{R}} \frac{\partial}{\partial y_3}\frac{\partial}{\partial y_3'}\Gamma^{\Psi}_{x_\perp}(y_3, y_3')\phi_n(y_3)\phi_m(y_3') dy_3 dy_3'.
\end{aligned}$$

Then,

$$\int \frac{\partial}{\partial x_3}\frac{\partial}{\partial x_3'}\Gamma^{\Psi}_{x_\perp}(x_3, x_3')|_{x_3 = x_3'} dx$$

$$= \sum_{n=1}^{\infty} \int_{\mathbf{R}} dy_3 \int_{\mathbf{R}} dy_3' \int_{\mathbf{R}^2} dx_\perp \frac{\partial \phi_n}{\partial y_3} \Gamma^{\Psi}_{x_\perp}(y_3, y_3') \frac{\partial \phi_n}{\partial y_3'},$$

$$= \int_{\mathbf{R}^2} \sum_{n=1}^{\infty} \left(\frac{\partial \phi}{\partial x_3}, \Gamma^{\Psi}_{x_\perp} \frac{\partial \phi}{\partial x_3} \right)_{L^2(\mathbf{R})} dx_\perp,$$

where $\Gamma^{\Psi}_{x_\perp}$ is the operator on $L^2(\mathbf{R})$ whose kernel is $\Gamma^{\Psi}_{x_\perp}(x_3, x_3')$.

We define :

$$Tr_{L^2(\mathbf{R})}[-\frac{\partial^2}{\partial x_3^2}\Gamma^{\Psi}_{x_\perp}] := \sum_{n=1}^{\infty} \left(\frac{\partial \phi}{\partial x_3}, \Gamma^{\Psi}_{x_\perp} \frac{\partial \phi}{\partial x_3} \right)_{L^2(\mathbf{R})}. \tag{1.8}$$

Hence the kinetic energy of H_N equals to $\int_{\mathbf{R}^2} Tr_{L^2(\mathbf{R})}[-\frac{\partial^2}{\partial x_3^2}\Gamma^{\Psi}_{x_\perp}]dx_\perp$ which is finite if $\Psi \in$ the domain of $\sum_{i=1}^{N} H_A^{(i)}$.

We turn to the attraction energy of the Coulomb force by nuclei.

$$\begin{aligned}(\Psi, \sum_{i=1}^{N} V(x^i)\Psi) = & \sum_{i=1}^{N} \int \Psi(x^1, \cdots, x^{i-1}, x^i, x^{i+1}, \cdots, x^N) V(x^i) \\ & \times \overline{\Psi(x^1, \cdots, x^{i-1}, x^i, x^{i+1}, \cdots, x^N)} \\ & \times dx^1 \cdots dx^{i-1} dx^{i+1} \cdots dx^N dx^i \\ = & \int V(x) \rho_\Psi(x) dx,\end{aligned}$$

where $\rho_\Psi(x) := \Gamma^{\Psi}_{x_\perp}(x_3, x_3)$ which is the diagonal part of $\Gamma^{\Psi}_{x_\perp}$. Note that $\rho_\Psi(x)$ is interpreted as the density of particles which satisfies $\int \rho_\Psi(x)dx = N$.

As for the repulsion term:$\sum_{i<j} |x^i - x^j|^{-1}$, we expect that exchange energy is lower order, so that we replace $(\Psi, \sum_{i<j} |x^i - x^j|^{-1}\Psi)$ by $D(\rho_\Psi, \rho_\Psi) := \frac{1}{2}\int\int |x-y|^{-1}\rho_\Psi(x)\rho_\Psi(y)dxdy$. The main error will arise from here whose estimation is the most difficult part of this theory.

Now we are in a position to establish the density matrix functional:

$$\mathcal{E}^{DM}[\Gamma] := \int_{\mathbf{R}^2} Tr_{L^2(\mathbf{R})} \left[-\frac{\partial^2}{\partial x_3^2} \Gamma_{x_\perp} \right] dx_\perp \tag{1.9}$$

$$+\int V(x)\rho_\Gamma(x)dx + D(\rho_\Gamma,\rho_\Gamma),$$

where $\rho_\Gamma(x) := \Gamma_{x_\perp}(x_3,x_3)$ is the diagonal part of Γ and $D(f,g) := \frac{1}{2}\int\int |x-y|^{-1}f(x)g(y)dxdy$. As the domain of Γ, we take

$$\text{(1.10)}\quad \mathcal{G}_B^{DM} := \{\Gamma_{x_\perp} : \Gamma_{x_\perp} \textit{ is a } L^2(\mathbf{R}) - \textit{operator valued function on } x_\perp \in \mathbf{R}^2 \textit{ which satisfies the following four conditions}\}$$

(1) For arbitrary $f \in \mathbf{L}^2(\mathbf{R})$, the map $x_\perp \mapsto (f, \Gamma_{x_\perp} f)$ is measurable
(2) $\Gamma_{x_\perp}$ is a positive semidefinite, trace class operator for almost all $x_\perp \in \mathbf{R}^2$
(3) $0 \le \Gamma_{x_\perp} \le B/2\pi$ for almost all $x_\perp \in \mathbf{R}^2$
(4) $\int_{\mathbf{R}^2} Tr_{\mathbf{L}^2(\mathbf{R})}[(1-\frac{\partial^2}{\partial x_3^2})\Gamma_{x_\perp}]dx_\perp < \infty$.

Remarks.

(1) Because of the condition(1), the integral of $Tr_{\mathbf{L}^2(\mathbf{R})}[(1-\frac{\partial^2}{\partial x_3^2})\Gamma]$ and $\rho_\Gamma(x)$ makes sense[LSY1].
(2) The condition (3) above comes from the fact that in the lowest Landau band, the density states per unit area perpendicular to the field is at most $B/2\pi$.
(3) If $\Psi \in$ the domain of $\sum_{i=1}^N H_A^i$, $(\Psi,\Psi) = 1$, and $\Pi_0^N\Psi = \Psi$, then $\Gamma_{x_\perp}^\Psi$ belongs to $\mathcal{G}_B^{DM}$(lemma 4.1 of [LSY1]).

We set the variational problem:

$$\text{(1.11)}\quad E^{DM}(N,\{Z_j\},B,\{R_j\}) := \inf\{\mathcal{E}^{DM}[\Gamma] : \Gamma \in \mathcal{G}_B^{DM}, \int_{\mathbf{R}^2} Tr_{L^2(\mathbf{R})}[\Gamma_{x_\perp}]dx_\perp \le N\}.$$

The last condition comes from the fact that, $N = \int \rho_\Gamma(x)dx = \int \Gamma_{x_\perp}(x_3,x_3)dx_3dx_\perp = \int_{\mathbf{R}^2} Tr_{L^2(\mathbf{R})}[\Gamma]dx_\perp$. $\mathcal{E}^{DM}$ has the unique minimizer Γ^{DM}(we can refer to theorem 4.3 of [LSY1] and confirm that it holds for K nuclei case).

We state the main theorem of this paper:

Theorem 1.2. *If* $\lambda := N/Z$, $Z_j = k_j Z$, $k_j > 0$ *are fixed and* $\beta := B/Z^{4/3} \to \infty$, *as* $Z \to \infty$, *then* $E^Q/E^{DM} \to 1$.

Finally, we prove the relation between $\rho^{DM} := \rho_{\Gamma^{DM}}$ and the density function ρ^Q corresponding to the true ground state Φ^Q, i.e., the minimizer of (1.2).

To do this, we must let the position of the each nuclear $R_j \in \mathbf{R}^3$ depend on Z, that is, $R_j(Z) = Z^{-1}\tilde{R}_j$ where each $\tilde{R}_j \in \mathbf{R}^3$ is fixed. This comes from the scaling property of $\mathcal{E}^{DM}$

$$E^{DM}(N, \{k_j Z\}, B, \{Z^{-1}R_j\}) = Z^3 E^{DM}(N/Z, \{k_j\}, B/Z^3, \{R_j\}). \tag{1.12}$$

We split E^{DM} into three terms

$$E^{DM} = K^{DM} - A^{DM} + R^{DM}, \tag{1.13}$$

where $K^{DM} = \int_{\mathbf{R}^2} Tr_{L^2(\mathbf{R})}\left[-\frac{\partial^2}{\partial x_3^2}\Gamma^{DM}_{x_\perp}\right] dx_\perp$, $-A^{DM} = \int V(x)\rho^{DM}(x)dx$ and $R^{DM} = D(\rho^{DM}, \rho^{DM})$. Similarly, we write

$$E^Q = K^Q - A^Q + R^Q. \tag{1.14}$$

To avoid confusion, we use the notation $\rho^{DM}(x; N, \{Z_j\}, B, \{R_j\})$ when the number of particles is N, the charge(resp. position) of j-th nuclear is $Z_j(resp.\ R_j)$ and the value of the magnetic field is B.

Theorem 1.3. *Let* $Z_j = k_j Z$, $R_j(Z) = Z^{-1}\tilde{R}_j$ *and* $k_j > 0$, $\lambda = N/Z$, $\eta := B/2\pi Z^3$ *and* $\tilde{R}_j \in \mathbf{R}^3$ *are all fixed. Then as* Z *tends to infinity, it holds that*

$$\begin{aligned}
&Z^{-4}\rho^Q(Z^{-1}x; N, \{Z_j\}, B, \{R_j\}) \\
&\qquad \to \rho(x; \lambda, \{k_j\}, 2\pi\eta, \{\tilde{R}_j\}) \text{ weakly in } L^1_{loc}(\mathbf{R}^3), \\
&Z^{-3}K^Q(N, \{Z_j\}, B, \{R_j\}) \to K^{DM}(\lambda, \{k_j\}, 2\pi\eta, \{\tilde{R}_j\}), \\
&Z^{-3}A^Q(N, \{Z_j\}, B, \{R_j\}) \to A^{DM}(\lambda, \{k_j\}, 2\pi\eta, \{\tilde{R}_j\}), \\
&Z^{-3}R^Q(N, \{Z_j\}, B, \{R_j\}) \to R^{DM}(\lambda, \{k_j\}, 2\pi\eta, \{\tilde{R}_j\}).
\end{aligned}$$

In the following sections, we will prove the above theorems. Since their proofs are based on the same argument as in [LSY1], we will only prove part of them. In section 2, we prove theorem 1.1, in section 3, we see various properties of the density matrix theory and in section 4, we will meet the proof of theorem 1.2 and 1.3 (though stated quite briefly).

Before leaving introduction, we comment on the extension of superstrong and hyperstrong theory in [LSY1] in the K nuclei case. We can easily see the existence and uniqueness of minimizers of them. But the main difference from the atom case is that it is difficult to derive the explicit form of the minimizer of $\mathcal{E}^{HS}$, the hyper strong functional(it seems to need the elliptic functions) and is also difficult to obtain the critical binding number of $\mathcal{E}^{HS}$, which seems to be essential in order to prove $E^{DM} = E^{SS}$(the superstrong energy E^{SS} can be defined as E^{DM}) for large η so their study for molecules is trusted to the future study.

2. Proof of Theorem 1.1

The proof of theorem 1.1 is almost the same as theorem 1.2 of [LSY1] which we see here.

Step 1.

In this section, we treat the wave functions in $\bigotimes^N L^2(\mathbf{R}^3;\mathbf{C}^2)$, that is, forget antisymmetry. Let α be the subset of $\{1,\cdots,N\}$. We want to define the projection Π^α whose eigenspace corresponds that if $i \in \alpha$, i-th particle lies in the lowest Landau band and $i \notin \alpha$ is not. To do this, at first we define Π_0^i which is the projection onto the subspace in which the i-th particle lies in the lowest Landau band(as for the other particles, it operates as the identity operator). Let $\Pi_>^i := I - \Pi_0^i$ that is the projection onto higher bands. We define

$$\Pi^\alpha := \prod_{i\in\alpha} \Pi_0^i \prod_{j\notin\alpha} \Pi_>^j. \tag{2.1}$$

It is clear that $\sum_\alpha \Pi^\alpha = I$. The plan of proof is to "expand" H_N in terms of Π^α and treat each $\Pi^\alpha H_N \Pi^\alpha$. We will divide $\Pi^\alpha H_N \Pi^\alpha$ into two terms. The first term contains $i \in \alpha$ particles and it is estimated from below by E^Q_{conf}. The second term including the variables $i \notin \alpha$ corresponds to the error term and we estimate it by Lieb-Thirring inequality.

Now we begin the proof. We decompose H_N with respect to Π^α

$$H_N \geq \sum_\alpha \Pi^\alpha H_\alpha \Pi^\alpha.$$

Where $\varepsilon > 0$ is arbitrary, and

$$\begin{aligned}(2.1)\quad H_\alpha = \sum_{i=1}^{N} H_A^i &- (1+\varepsilon)\sum_{j=1}^{K} Z_j \sum_{i\in\alpha} |x^i - R_j|^{-1} \\ &- (1+\varepsilon^{-1})\sum_{j=1}^{K} Z_j \sum_{i\notin\alpha} |x^i - R_j|^{-1} \\ &+ (1-3\varepsilon)\sum_{\substack{i<j\\ i,j\in\alpha}} |x^i - x^j|^{-1} - (3\varepsilon^{-1}-1)\sum_{\substack{i<j\\ i,j\notin\alpha}} |x^i - x^j|^{-1} \\ &- (\frac{3}{2}\varepsilon^{-1} + \frac{3}{2}\varepsilon - 1)\sum_{\substack{i\in\alpha\\ j\notin\alpha}} |x^i - x^j|^{-1}.\end{aligned}$$

To see this, we consider each term of H_N respectively. The first term of (2.2) $\sum_{i=1}^N H_A^i$ is obvious since H_A^i commutes Π^α for arbitrary α. For the second term we write

$$V(x^i) = (\Pi_0^i + \Pi_>^i)V(x^i)(\Pi_0^i + \Pi_>^i). \tag{2.3}$$

From it arises two diagonal terms, ($\Pi_0^i V(x^i)\Pi_0^i$ and $\Pi_>^i V(x^i)\Pi_>^i$) and two remaining non-diagonal terms. Diagonal terms of (2.3) corresponds respectively to $\sum_{i\in\alpha} V(x^i) = -\sum_{j=1}^K \sum_{i\in\alpha} Z_j|x^i - R_j|^{-1}$ and $-\sum_{j=1}^K \sum_{i\notin\alpha} Z_j|x^i - R_j|^{-1}$ of (2.2)(if $i \in \alpha$ (resp. $i \notin \alpha$), $\Pi_>^i V(x^i)\Pi_>^i$ (resp. $\Pi_0^i V(x^i)\Pi_0^i$) vanishes since Π^α is operated). Non-diagonal terms of (2.3) are estimated

$$\Pi_>^i V(x^i)\Pi_0^i + \Pi_0^i V(x^i)\Pi_>^i \geq \varepsilon\Pi_0^i V(x^i)\Pi_0^i + \varepsilon^{-1}\Pi_>^i V(x^i)\Pi_>^i, \tag{2.4}$$

which is derived by taking form of the left hand side of (2.4), apply Schwarz inequality, and use $ab \geq \frac{1}{2}(\varepsilon a^2 + \varepsilon^{-1}b^2)$. (2.4) says that "the non-diagonal terms become the diagonal terms" so that they become $\varepsilon\sum_{i\in\alpha} V(x^i) =$

$-\varepsilon \sum_{j=1}^{K} \sum_{i\in\alpha} Z_j |x^i - R_j|^{-1}$ and $-\varepsilon^{-1} \sum_{j=1}^{K} \sum_{i\notin\alpha} Z_j |x^i - R_j|^{-1}$ of (2.2) respectively. Thus we obtain (2.2) for the attraction term. The terms $\sum_{i<j} |x^i - x^j|^{-1}$ are treated similarly as (2.3) except that $|x^i - x^j|^{-1}$ is operated by $(\Pi_0^i + \Pi_>^i)(\Pi_0^j + \Pi_>^j)$ from both sides. There will be 16 terms but "non-diagonal terms become into diagonal terms" similarly as (2.4).

Step 2.

We estimate each term H^α respectively from below and thus estimate H_N from below. This is possible since

$$\inf \operatorname{spec}(A + B) \geq \inf \operatorname{spec} A + \inf \operatorname{spec} B, \tag{2.5}$$

for any operators A, B.

Fix α. We bound H^α below on functions Ψ which are antisymmetric with respect to $x^i (i \in \alpha)$ and also antisymmetric with respect to $x^i (i \notin \alpha)$. In addition, we impose that $\Pi_0^i \Psi = \Psi$ if $i \in \alpha$ and $\Pi_0^i \Psi = 0$ if $i \notin \alpha$. At first we consider three terms of (2.2) that depend on only $x^i (i \in \alpha)$'s. They are in the first, second and fourth terms

$$\hat{H}^\alpha := (1 - 3\varepsilon) H_{n_\alpha} + \varepsilon \sum_{i\in\alpha} \left(3H_A^i - 4 \sum_{j=1}^{K} Z_j |x^i - R_j|^{-1} \right), \tag{2.6}$$

where $n_\alpha := \sharp\alpha$ that is the number of elements of α and H_{n_α} is the Hamiltonian(1.1) of $x^i (i \in \alpha)$ particles where N is replaced by n_α. We shall estimate the second term of (2.6).

$$\begin{aligned} \sum_{i\in\alpha} \left[3H_A^i - 4 \sum_{j=1}^{K} |x^i - R_j|^{-1} \right] & \\ \geq 3 \sum_{j=1}^{K} \left[\sum_{i\in\alpha} \frac{1}{K} H_A^i - \frac{4}{3} Z_j |x^i - R_j|^{-1} \right]. \end{aligned} \tag{2.7}$$

We also treat each term of $\sum_{j=1}^{K}$ separately and use (2.5). By translation invariance, we can let $R_j = 0$ in each term. Let $\delta_j > 0$ which satisfies $\delta_j (\frac{Z_j}{K} - \frac{n_\alpha}{2K}) = \frac{4}{3} Z_j$(in fact, $\delta_j > 1$) so that we claim

$$\Pi_0^i \left(\frac{1}{K} H_A^i - \delta_j (\frac{Z_j}{K} - \frac{n_\alpha}{2K}) |x^i|^{-1} \right) \Pi_0^i \tag{2.8}$$

$$\geq \delta_j^2 \Pi_0^i \left(\frac{1}{K} H_A^i - (\frac{Z_j}{K} - \frac{n_\alpha}{2K}) |x^i|^{-1} \right) \Pi_0^i.$$

This can be seen as follows. Let $h(\delta) := \Pi_0(H_A - \delta Z/|x|)\Pi_0 = \Pi_0(p_3^2 - \delta Z/|x|)\Pi_0$. By scaling, $x_3 \to \delta^{-1} x_3$, we can show $h(\delta)$ is unitarily equivalent to $\delta^2 \Pi_0 [p_3^2 - Z(x_3^2 + \delta^2 x_\perp^2)^{-1/2}]\Pi_0$ and this operator is greater than $\delta^2 h(1)$. Thus (2.8) is obtained.

We forget the multiplication by Π_0 which is already contained in Π^α. By the method of theorem 5.3 of [LSY1], it holds that

$$\begin{aligned} &\sum_{i \in \alpha} \left[\frac{1}{K} H_A^i - (\frac{Z_j}{K} - \frac{n_\alpha}{2K}) |x^i|^{-1} \right] \\ &\qquad \geq \sum_{i \in \alpha} \left[\frac{1}{K} H_A^i - \frac{Z_j}{K} |x^i|^{-1} + \frac{1}{K} \sum_{i<j} |x^i - x^j|^{-1} \right]. \end{aligned} \tag{2.9}$$

By translation invariance, RHS of (2.9) is unitarily equivalent to

$$\sum_{i \in \alpha} \left[\frac{1}{K} H_A^i - \frac{Z_j}{K} |x^i - R_j|^{-1} + \frac{1}{K} \sum_{i<j} |x^i - x^j|^{-1} \right].$$

And this is estimated from below by

$$\begin{aligned} &\geq \sum_{i \in \alpha} \left[\frac{1}{K} H_A^i - \sum_{k=1}^{K} \frac{Z_k}{K} |x^i - R_k|^{-1} + \frac{1}{K} \sum_{i<j} |x^i - x^j|^{-1} \right], \\ &= \frac{1}{K} \sum_{i \in \alpha} \left[H_A^i - \sum_{k=1}^{K} Z_k |x^i - R_k|^{-1} + \sum_{i<j} |x^i - x^j|^{-1} \right]. \end{aligned} \tag{2.10}$$

Putting it into RHS of (2.7), we estimate that the second term of (2.6) is bounded below by $3 \sum_{j=1}^{K} \delta_j^2 E^Q(n_\alpha, \{Z_j\}, B, \{R_j\})$. Therefore, we arrive at the purpose for $\hat{H}^\alpha$:

$$\begin{aligned} \Pi^\alpha \hat{H}^\alpha \Pi^\alpha \geq \Pi^\alpha \{ &(1 - 3\varepsilon) E_{conf}^Q(n_\alpha, \{Z_j\}, B, \{R_j\}) \\ &+ (const.) \varepsilon E^Q(n_\alpha, \{Z_j\}, B, \{R_j\}) \} \Pi^\alpha. \end{aligned} \tag{2.11}$$

Step 3.

The remaining terms of (2.2) is bounded below for $\varepsilon > 0$ small by

$$\tag{2.12} \begin{aligned} \tilde{H}^\alpha := \tilde{T}^\alpha - (1+\varepsilon^{-1}) \sum_{j=1}^{K} Z_j \sum_{i \notin \alpha} |x^i - R_j|^{-1} \\ - 3\varepsilon^{-1} \sum_{i \notin \alpha} \sum_{j \in \alpha} |x^i - x^j|^{-1} - 3\varepsilon^{-1} \sum_{\substack{i<j \\ i,j \notin \alpha}} |x^i - x^j|^{-1}, \end{aligned}$$

where $\tilde{T}^\alpha := \sum_{i \notin \alpha} H_A^i$ is the kinetic energy operator of $i(i \notin \alpha)$-th particle. We shall employ two ways to estimate $\tilde{H}^\alpha$ and apply them at the same time.

The first is to consider the kinetic energy. Note that for one particle

$$2B\Pi_> \le \Pi_> H_A \Pi_> = \Pi_>[(\mathbf{p} + \mathbf{A})^2 + \sigma \cdot \mathbf{B}]\Pi_>.$$

Since on the higher Landau band, $\varepsilon_{p\alpha\sigma} \ge 2B$(see (1.3)). Thus, $\Pi_>(\mathbf{p} + \mathbf{A})^2\Pi_> \ge \Pi_>(2B - \sigma \cdot \mathbf{B})\Pi_>$. Hence

$$\tag{2.13} \begin{aligned} \Pi_> H_A \Pi_> &\ge \Pi_> \left[\frac{1}{2}(\mathbf{p} + \mathbf{A})^2 + \frac{1}{2}(2B - \sigma \cdot \mathbf{B}) + \sigma \cdot \mathbf{B} \right] \Pi_>, \\ &\ge \frac{1}{2}\Pi_>[(\mathbf{p} + \mathbf{A})^2 + B]\Pi_>. \end{aligned}$$

In the last inequality, we used $B \ge \pm\sigma \cdot \mathbf{B}$.

For the second way, we decompose $\tilde{H}^\alpha$:

$$\tag{2.14} \begin{aligned} \tilde{H}^\alpha = \sum_{l=1}^{K} [\, \frac{\tilde{T}^\alpha}{K} - (1+\varepsilon^{-1}) Z_l \sum_{i \notin \alpha} |x^i - R_l|^{-1} \\ - \frac{3\varepsilon^{-1}}{K} \sum_{i \notin \alpha} (\sum_{j \in \alpha} |x^i - x^j|^{-1}) - \frac{3\varepsilon^{-1}}{K} \sum_{\substack{i<j \\ i,j \notin \alpha}} |x^i - x^j|^{-1} \,] \\ =: \sum_{l=1}^{K} \tilde{H}_l^\alpha. \end{aligned}$$

We treat each $\tilde{H}_l^\alpha$ and use (2.5) again. By translation, we can let $R_j = 0$ in each term. Note that $\tilde{H}^\alpha$ contains no differentiation with respect to $x^i (i \in \alpha)$ so that $x^i (i \in \alpha)$ in $\tilde{H}_l^\alpha$ can be treated as fixed points whose values are adjusted to give the lowest possible energy of $\Pi^\alpha \tilde{H}_l^\alpha \Pi^\alpha$. Now consider that any antisymmetric function $\Psi(x^1, \cdots, x^n)$(of $n := N - n_\alpha$variables) and its corresponding density $\rho_\Psi(x)(x \in \mathbf{R}^3)$. We can always translate Ψ by letting $x \mapsto x + y$ such that the maximum of $z \mapsto \int \rho_\Psi(x+z)|x|^{-1}dx$ occurs at $z = 0$. After this translation, the maximum of $x^j \mapsto \int \rho_\Psi |x - x^j|^{-1} dx$ occurs at $x^j = 0$ that means $\inf_{x^j, j \in \alpha} \int \cdots \int \Pi^\alpha \Psi \tilde{H}_l^\alpha \Pi^\alpha \Psi \overbrace{dx^{i_1} \cdots dx^{i_n}}^{i \notin \alpha}$ occurs if $x^j = 0 (j \in \alpha)$.

Due to the two arguments above, we conclude that $\inf spec(\Pi^\alpha \tilde{H}^\alpha \Pi^\alpha) \geq \inf spec(\Pi^\alpha \bar{H}^\alpha \Pi^\alpha)$, where $\bar{H}^\alpha = \sum_{l=1}^K \bar{H}_l^\alpha$ and

$$\bar{H}_l^\alpha := \frac{nB}{2K} + \frac{1}{2} \sum_{i=1}^n \frac{(\mathbf{p}^i + \mathbf{A})^2}{K} - \left\{ (1 + \varepsilon^{-1}) Z_l + \frac{3\varepsilon^{-1}}{K} \right\} \sum_{i=1}^n |x^i|^{-1} - \frac{3\varepsilon^{-1}}{K} \sum_{1 \leq i < j \leq n} |x^i - x^j|^{-1}. \tag{2.15}$$

We decompose further using $\sum_{i=1}^n = \frac{1}{n-1} \sum_{i=1}^n \sum_{\substack{j=1 \\ j \neq i}}^n$:

$$\begin{aligned} \bar{H}_l^\alpha = \frac{nB}{2K} + \frac{1}{n-1} \sum_{i=1}^n \Bigg\{ \sum_{\substack{k=1 \\ k \neq i}}^n \Bigg[& \frac{1}{2K} (\mathbf{p}^k + \mathbf{A}(x^k))^2 \\ & - \left((1 + \varepsilon^{-1}) Z_l + \frac{3\varepsilon^{-1}}{K} \right) |x^k|^{-1} \\ & - \frac{3(n-1)\varepsilon^{-1}}{2K} |x^k - x^i|^{-1} \Bigg] \Bigg\}, \\ =: \frac{nB}{2K} + \frac{1}{n-1} \sum_{i=1}^n H_l^{(i)}. & \end{aligned} \tag{2.16}$$

We bound each operator $H_l^{(i)}$ by letting $x^i = 0$ due to the same argument as above. Therefore we reached the no-interacting Hamiltonian and we shall estimate it using Lieb-Thirring inequality that says the sum of the absolute value of negative eigenvalues of $\sum\{\frac{1}{2}(\mathbf{p}+\mathbf{A})^2 - V\}$ is bounded above by $(const.)\int V^{5/2}(x)dx$. To apply this, we cut off the Coulomb potential. For $R>0$, define $v(x) = |x|^{-1} - R^{-1}$ for $|x|<R$ and $v=0$ if $|x|>R$ so that $-|x|^{-1} \geq -v(x) - R^{-1}$. We estimate $H_l^{(i)}$

$$H_l^{(i)} \geq \frac{1}{K}\left\{\frac{1}{2}(\mathbf{p}^k + \mathbf{A}(x^k))^2 - \varepsilon^{-1}[2KZ_l + 3N]|x^k|^{-1}\right\}. \tag{2.17}$$

We use $-|x^k|^{-1} \geq -v(x^k) - R^{-1}$ and apply Lieb-Thirring inequality to v which concludes

$$\begin{aligned} H_l^{(i)} \geq -\frac{1}{K}\{&(const.)R^{1/2}\varepsilon^{-5/2}(2KZ_l+3N)^{2/5} \\ &- \varepsilon^{-1}(2KZ_l+3N)\frac{n}{R}\}. \end{aligned} \tag{2.18}$$

By maximizing the RHS of (2.18) with respect to R, we obtain

$$H_l^{(i)} \geq -\frac{1}{K}\{(const.)\varepsilon^{-2}(N-n_\alpha)^{1/3}(2KZ_l+3N)^2\}. \tag{2.19}$$

Thus, we arrived at the position of estimating $\bar{H}^\alpha$.

$$\begin{aligned} \bar{H}^\alpha &= \sum_{l=1}^{K} \bar{H}_l^\alpha = \sum_{l=1}^{K}\left(\frac{nB}{2K} + \frac{1}{n-1}\sum_{i=1}^{n} H_l^{(i)}\right), \\ &\geq \frac{N-n_\alpha}{2}B - (const.)\varepsilon^{-2}(N-n_\alpha)^{1/3}(K^2Z^2\sum k_j^2 + KN^2). \end{aligned} \tag{2.20}$$

Let K^α be the number such that

$$K^\alpha = \text{RHS of (2.11)} + \text{RHS of (2.20)}, \tag{2.21}$$

so that Step 2 and Step 3 yields

$$\Pi^\alpha H^\alpha \Pi^\alpha \geq \Pi^\alpha K^\alpha. \tag{2.22}$$

Step 4.

It suffices to show that ε (>0) which first appeared in Step1 can be taken to depend on $\lambda^{2/3}\beta = Z^{-2}N^{2/3}B$ and Λ such that

$$K^{\alpha} \geq E^{Q}_{conf}(N, \{Z_j\}, B, \{R_j\}) + \delta(\lambda^{2/3}\beta, \Lambda)E^{Q}(N, \{Z_j\}, B, \{R_j\}), \tag{2.23}$$

for every α, and $\delta \to 0$ and as $\lambda^{2/3}\beta \to \infty$ for each fixed Λ. We can easily derive theorem 1.1 from (2.23) since

$$(\Psi, H_N\Psi) \geq \sum_{\alpha} K^{\alpha}(\Psi, \Pi^{\alpha}\Psi) \text{ and } (\Psi, \Psi) = \sum_{\alpha}(\Psi, \Pi^{\alpha}\Psi). \tag{2.24}$$

In proving (2.23), we first note that we can replace n_{α} by N in (2.11) since $E^{Q}_{conf}(n_{\alpha}, \{Z_j\}, B, \{R_j\}) \geq E^{Q}_{conf}(N, \{Z_j\}, B, \{R_j\})$ (it holds because we can always make particles throw away to infinity[LS1]). (2.11) already satisfies the conditions of (2.23) if we can let $\varepsilon > 0$ arbitrary small when $\lambda^{2/3}\beta \to \infty$. For the contribution of (2.22), we needs to consider two cases, namely $B \ll Z^3$ and $B \gg Z^3$. When $B \ll Z^3$, the contribution of (2.21) can be bounded below by omitting the B term. The rest is bounded below by

$$\begin{aligned} &-(const.)(K^2 \sum k_j^2 + K\Lambda)\varepsilon^{-2}(\lambda^{2/3}\beta)^{-2/5} Z^{6/5} N^{3/5} B^{2/5} \\ &\geq (const.)(K^2 \sum k_j^2 + K\Lambda)\varepsilon^{-2}(\lambda^{2/3}\beta)^{-2/5} \\ &\quad \times E^{Q}(N, \{Z_j\}, B, \{R_j\}). \end{aligned} \tag{2.25}$$

This inequality comes from the upper bound of E^Q(it can be obtained by mimicking the proof of theorem 5.3 of [LSY1]). When $B \gg Z^3$, (2.21) is easily seen to be positive as $\lambda^{2/3}\beta \to \infty$ provided that Z is bounded below which follows easily from $N/Z \leq \Lambda$. Hence we can let $\varepsilon \to 0$ as $\lambda^{2/3}\beta \to \infty$ with satisfying (2.21) is positive.

3. The Density Matrix Functional

In this section, we see the various properties of $\mathcal{E}^{DM}$ such as the existence and uniqueness of the minimizer. These proofs are essentially the same as in section 4 of [LSY1], so we will give only the sketch.

At first we need the bound for the energy of one-dimensional Coulomb potential which is the lemma 2.1 of [LSY1].

Lemma 3.1. *Let us consider the one-dimensional Schrödinger operator on* $L^2(\mathbf{R})$

$$\hat{h}_{\{Z_j\},\{R_j\}\{a_j\}} := -\frac{d^2}{dx^2} - \sum_{j=1}^{K} \frac{Z_j}{\sqrt{(x-R_j)^2 + a_j^2}},$$

where $\{Z_j\}$ *denotes the set* $\{Z_1, \cdots, Z_K\}$,*etc. Let* $-\mu_n(\hat{h}_{\{Z_j\},\{R_j\}\{a_j\}})$ *be the n-th eigenvalues of* $\hat{h}_{\{Z_j\},\{R_j\}\{a_j\}}$ *counting multiplicity. Then they satisfy the following estimates*

$$-\mu_1(\hat{h}_{\{Z_j\},\{R_j\}\{a_j\}}) \geq -K \sum_{j=1}^{K} Z_j^2 \left\{1 + \left[\sinh^{-1}\left(\frac{1}{K a_j Z_j}\right)\right]^2\right\},$$

$$-\mu_{2n}, -\mu_{2n+1}(\hat{h}_{\{Z_j\},\{R_j\}\{a_j\}}) \geq -\frac{1}{4n^2} \sum_{j=1}^{K} Z_j^2. \tag{3.1}$$

Proof. We decompose the Hamiltonian

$$\hat{h}_{\{Z_j\},\{R_j\}\{a_j\}} = \sum_{j=1}^{K} \left(-\frac{1}{K}\frac{d^2}{dx^2} - \frac{Z_j}{\sqrt{(x-R_j)^2 + a_j^2}}\right) =: \sum_{j=1}^{K} \hat{h}_j.$$

We use

$$-\mu_n(\hat{h}_{\{Z_j\},\{R_j\}\{a_j\}}) \geq -\sum_{j=1}^{K} \mu_n(\hat{h}_j). \tag{3.2}$$

In lemma 2.1 of [LSY1], $\mu_n(\hat{h}_j)$ is estimated

$$-\mu_1(\hat{h}_j) \geq -K Z_j^2 \left(1 + \left[\sinh^{-1}\left(\frac{1}{K Z_j a_j}\right)\right]^2\right),$$

$$-\mu_{2n}, -\mu_{2n+1}(\hat{h}_j) \geq -\frac{KZ_j^2}{4n^2}. \tag{3.3}$$

Putting this into (3.2), the lemma 3.1 is proved. □

REMARK. If we adopt the method used in lemma 2.1 of [LSY1] directly, we obtain slightly different bound

$$-\mu_1 \geq -\left[\left\{\sum_{j=1}^{K} Z_j \sinh^{-1}(a_j^{-1})\right\}^2 + \sum_{j=1}^{K} Z_j\right],$$

$$-\mu_{2n,2n+1} \geq -\frac{1}{4n^2}\sum_{j=1}^{K} Z_j^2. \tag{3.4}$$

In the following, we see the estimates related to $\Gamma \in \mathcal{G}_B^{DM}$ which can be proved essentially in the same way as in [LSY1].

PROPOSITION 3.2. *If $\Gamma \in \mathcal{G}_B^{DM}$, it holds that*

(1)

$$\int \rho_\Gamma dx = \int_{\mathbf{R}^2} Tr_{L^2(\mathbf{R})}[\Gamma_{x_\perp}]dx_\perp, \tag{3.5}$$

(2)

$$\int_{\mathbf{R}} \left(\frac{\partial\sqrt{\rho_\Gamma}}{\partial x_3}\right)^2 dx_3 \leq Tr_{L^2(\mathbf{R})}\left[-\frac{\partial^2}{\partial x_3^2}\Gamma_{x_\perp}\right], \text{ for a.e. } x_\perp \in \mathbf{R}^2, \tag{3.6}$$

(3)

$$\int \rho_\Gamma^3 dx \leq \left(\frac{3B^2}{\pi^2}\right) Tr_{L^2(\mathbf{R})}\left[-\frac{\partial^2}{\partial x_3^2}\Gamma_{x_\perp}\right], \tag{3.7}$$

(4) *If $\int \rho_\Gamma dx \leq N$ and*

$$\hat{h}_{\{Z_j\},\{R_j\},x_\perp} := -\frac{d^2}{dx_3^2} - \sum_{j=1}^{K} Z_j|x - R_j|^{-1}, \tag{3.8}$$

which is an one-dimensional Schrödinger operator on $L^2(\mathbf{R})$. Then,

$$\int_{R^2} Tr_{L^2(\mathbf{R})}[\hat{h}_{\{Z_j\},\{R_j\},x_\perp}\Gamma_{x_\perp}]dx_\perp \geq -(const.)K^{1/5}N^{3/5}\sum_{j=1}^{K} Z_j^{6/5}B^{2/5}, \tag{3.9}$$

and

$$\int_{R^2} Tr_{L^2(\mathbf{R})}[\hat{h}_{\{Z_j\},\{R_j\},x_\perp}\Gamma_{x_\perp}]dx_\perp \geq -(const.)NK\sum_{j=1}^{K} Z_j^2\left\{1+\left(ln\frac{B}{K^2NZ_j^2}\right)^2\right\}. \tag{3.10}$$

Using these inequalities, we can prove the existence and uniqueness of minimizer of $\mathcal{E}^{DM}$. Theorem 4.3 of [LSY1] applies to this with no change.

THEOREM 3.3. *$\mathcal{E}^{DM}$ has an unique minimizer Γ^{DM}. $E^{DM}(N,\{Z_j\}, B,\{R_j\})$ is a monotonically non-increasing, convex function of N and non-increasing function of B.*

Next, we set the linearized functional of $\mathcal{E}^{DM}$. It is defined as

$$\mathcal{E}_{lin}^{DM}[\Gamma] := \int_{R^2} Tr_{L^2(\mathbf{R}^2)}[h_{x_\perp}^{DM}\Gamma_{x_\perp}]dx_\perp \tag{3.11}$$

where $h_{x_\perp}^{DM}$ is the one-dimensional Schrödinger operator

$$h_{x_\perp}^{DM} := -\frac{d^2}{dx_3^2} - \phi_{x_\perp}^{DM}(x_3), \tag{3.12}$$

where

$$\phi_{x_\perp}^{DM}(x_3) = \sum_{j=1}^{K} Z_j|x-R_j|^{-1} - |x|^{-1} * \rho^{DM}, \tag{3.13}$$

which is the effective potential. We set the minimizing problem similarly as (1.9)

$$E_{lin}^{DM} = \inf\{\mathcal{E}_{lin}^{DM}[\Gamma] : \Gamma \in \mathcal{G}_B^{DM}, \int Tr_{L^2(\mathbf{R}^2)}[\Gamma_{x_\perp}]dx_\perp \leq N\}. \tag{3.14}$$

The following theorem is proved in [LSY1,theorem 4.4].

THEOREM 3.4. *Γ^{DM} is also the minimizer of E_{lin}^{DM}.*

This is used to prove the uniqueness of Γ^{DM}(the uniqueness of ρ^{DM} is proved without the aid of $\mathcal{E}_{lin}^{DM}$, so that $\mathcal{E}_{lin}^{DM}$ is well- defined) and also used to prove the lower bound to E^Q in terms of E^{DM} (in section 4).

The virial inequality has the following form

LEMMA 3.5. *If we write as $E^{DM} = K^{DM} - A^{DM} + R^{DM}$, they satisfy the following estimates.*

$$R^{DM} \leq A^{DM} - 2K^{DM} + X, \quad K^{DM} \leq A^{DM} - 2R^{DM} + X, \tag{3.15}$$

$$\begin{aligned} &A^{DM} \leq 3|E^{DM}| + X, \quad K^{DM} \leq |E^{DM}| + X, \\ &R^{DM} \leq |E^{DM}| + X, \end{aligned} \tag{3.16}$$

where

$$X = \sum_{j=1}^{K} \int \frac{Z_j}{|x - R_j|} \sum_{i=1}^{3} \left(\frac{\partial \rho^{DM}}{\partial x_i} \right) dx. \tag{3.17}$$

REMARK.

$$|X| \leq \sum_{j=1}^{K} Z_j \int 3R_j \rho^{DM}(x)dx \leq (const.)N \sum_{j=1}^{K} Z_j R_j, \tag{3.18}$$

and it is lower order than E^Q when $B \gg Z^{4/3}$(by mimicking theorem 5.3 of [LSY1]).

Finally, this is the estimate of ρ^{DM} which can be proved by mimicking proposition 4.9 in [LSY1].

PROPOSITION 3.6.

$$\int_{\mathbf{R}} \left(\frac{\partial \sqrt{\rho^{DM}}}{\partial x_3} \right)^2 dx_3 \leq (const.) KB \sum_{j=1}^{K} Z_j^2 \left\{ \left[\sinh^{-1} \left(\frac{1}{KZ_j |x_\perp - R_j^\perp|} \right) \right]^2 + 1 \right\}. \tag{3.19}$$

The above estimates will be used to bound the E^Q in terms of E^{DM}.

4. Proof of Theorem 1.2

This is the section we prove the main theorem. We derive the upper and lower bound of E^Q and estimate the error.

THEOREM 4.1. *E^Q, E^Q_{conf} satisfy the following estimates.*

$$\begin{aligned} E^Q(N, \{Z_j\}, B, \{R_j\}) &\leq E^Q_{conf}(N, \{Z_j\}, B, \{R_j\}), \\ &\leq E^{DM}(N, \{Z_j\}, B, \{R_j\}) + R_U. \end{aligned} \tag{4.1}$$

R_U is estimated :

$$R_U \leq (const.) K (\sum_{j=1}^{K} Z_j)^{4/3} N^{1/3} B^{1/3}, \quad \textit{and}$$

$$(const.) K^{1/3} (\sum_{j=1}^{K} Z_j)^2 N^{2/3} \left\{ 1 + \left[ln \left(\frac{B}{K^2 N (\sum_j Z_j)^2} \right) \right]^2 \right\}^{5/6}. \tag{4.2}$$

It is proved by the same way as theorem 5.1 of [LSY1] except the $\sum_j Z_j$ treatment and the virial inequality. Proposition 3.2, lemma 3.5 and proposition 3.6 are used to do this.

To lower E^Q, it is sufficient to use theorem 7.1 of [LSY1] which is the estimate of the Coulomb repulsion.

THEOREM 4.2. *When $N = \lambda Z$, $Z_j = k_j Z$,*

$$H_N \geq \sum_{i=1}^{N} \Big((1 - Z^{-1/3}) H_A^i - \phi^{DM}(x^i) \Big) - D(\rho^{DM}, \rho^{DM}) - C_{\lambda, k_j} (1 + \lambda^5)(1 + Z^{8/3})(1 + [ln(B/Z^3)]^2), \tag{4.3}$$

where $\phi^{DM}(x) = \sum_{j=1}^{K} Z_j |x - R_j|^{-1} - |x|^{-1} * \rho^{DM}$.

Using the above theorems, propositions and lemmas together lead to the theorem 1.2. In more detail, we can refer to the section 8 of [LSY1] so that we omit the proof.

5. The proof of theorem 1.3

The proof of the convergence of ρ^Q is the same as [LSY1] which is omitted here. Next, we prove the convergence of each term of the energy. We will only see the attraction energy only here since the other is essentially the same. We use the method of [LS1]. At first we define the modified Hamiltonian for $\alpha > 0$:

$$H_N^\alpha := \sum_{i=1}^{N} \{ (\mathbf{p}^i + \mathbf{A}(x^i)^2 + \sigma^i \cdot \mathbf{B} \} - \alpha \sum_{i=1}^{N} V(x^i) + \sum_{i<j} |x^i - x^j|^{-1}. \tag{5.1}$$

Let E_α^Q denotes the ground state energy of H_N^α defined similarly as (1.2). Moreover, we define $\mathcal{E}_\alpha^{DM}[\Gamma]$ whose Coulomb attractions are all multiplied by α. E_α^{DM} denotes its infimum. Let Γ_α^{DM} be the minimizer of E_α^{DM}. It is easy to show $\Gamma_\alpha^{DM} \to \Gamma_1^{DM}$ in $L^3 \cap L^{6/5}$ as $\alpha \to 1$(To see this, note that when α moves near 1, $\int \left(\frac{\partial \sqrt{\rho_\alpha^{DM}}}{\partial x_3} \right)^2 dx$ is uniformly bounded. Hence we can use the argument used in the proof of theorem 2.2 in [LSY1]). Then it follows that

$$\begin{aligned} \alpha^{-1}[E_\alpha^{DM} - E_1^{DM}] &\leq \alpha^{-1} \left(\mathcal{E}_\alpha^{DM}[\Gamma_1^{DM}] - \mathcal{E}_1^{DM}[\Gamma_1^{DM}] \right), \\ &= A_1^{DM}, \\ &\geq \alpha^{-1} \left(\mathcal{E}_\alpha^{DM}[\Gamma_\alpha^{DM}] - \mathcal{E}_1^{DM}[\Gamma_\alpha^{DM}] \right), \end{aligned} \tag{5.2}$$

$$= A_\alpha^{DM}.$$

Since $|x|^{-1} \in L^{3/2} + L^6$, we see $A_\alpha^{DM} \to A_1^{DM}$ as $\alpha \to 1$. Hence

$$\frac{\partial E_\alpha^{DM}}{\partial \alpha}\Big|_{\alpha=1} = A_1^{DM}. \tag{5.3}$$

Due to the same argument, we can show

$$\frac{\partial E_\alpha^{Q}}{\partial \alpha}\Big|_{\alpha=1} = A_1^{Q}. \tag{5.4}$$

We can apply the proof of theorem 1.2 and conclude that

$$\frac{E_\alpha^Q(N, \{k_j Z\}, B, \{Z^{-1}\tilde{R}_j\})}{E_\alpha^{DM}(N, \{k_j Z\}, B, \{Z^{-1}\tilde{R}_j\})} \to 1 \ \ as \ \ Z \to \infty, \ B \gg Z^{4/3}. \tag{5.5}$$

If $\{k_j\}, \{\tilde{R}_j\}, \eta$ fixed, we can use the scaling property and derive

$$\begin{aligned} Z^{-3} E_\alpha^Q&(N, \{k_j Z\}, B, \{Z^{-1}\tilde{R}_j\}) \\ &\to E_\alpha^{DM}(\lambda, \{k_j\}, 2\pi\eta, \{\tilde{R}_j\}) \ \ as \ Z \to \infty. \end{aligned} \tag{5.6}$$

Because E_α^Q and E_α^{DM} are concave with respect to α, we can derive the convergence of the derivative(since when a function is concave or convex, its derivative is monotone)

$$Z^{-3}\frac{\partial}{\partial\alpha} E_\alpha^Q(N, \{k_j Z\}, B, \{Z^{-1}\tilde{R}_j\}) \to \frac{\partial}{\partial\alpha} E_\alpha^{DM}(\lambda, \{k_j\}, 2\pi\eta, \{\tilde{R}_j\}). \tag{5.7}$$

Putting $\alpha = 1$, we reach the conclusion.

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