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碩 士 論 文

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研 究 生：黃晟銘

指導教授：葉立明　教授

中 華 民 國 九 十 五 年 八 月

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學生：黃晟銘　　　　　　　　　　　　　　　指導教授：葉立明

國立交通大學應用數學系（研究所）碩士班

摘　　要

基態能量在量子力學上是代表最低的能量。在研究基態能量時，最主要的困難在於它其中的 exchange correlation energy 不是精確的表示式。有很多關於 exchange correlation energy 的估計。在此篇論文裡，我們用 $\int -\rho^{\frac{4}{3}}(x)+\rho^{\frac{5}{3}}(x)\ln(1+\rho^{-\frac{1}{3}}(x))dx$ 來代表 exchange correlation energy[1]。此篇文章的結果主要參考至[2]。我們把原本的能量 $\varepsilon(\rho)$ 轉換成 $\varepsilon_\alpha(\rho)=\varepsilon(\rho)+\alpha\int\rho dx$ 其中 $\alpha\geq\frac{1}{2}$，而且證明了基態能量的存在性。此外，我們也得到極小值的一些性質。

The ground state energy with new exchange correlation energy

Student: Cheng-Ming Huang **Advisor:** Dr. Li-Ming Yeh

Department of Applied Mathematics
National Chiao Tung University
Hsinchu, Taiwan, R.O.C.

Abstract

The ground state of a quantum mechanical system is its lowest-energy state. The main difficulty of the study of the ground state energy is that the exchange correlation energy is not the exact expression. There are many approximations about the exchange correlation energy. In this paper, we use $\int -\rho^{\frac{4}{3}}(x) + \rho^{\frac{5}{3}}(x)\ln(1+\rho^{-\frac{1}{3}}(x))dx$ to represent the exchange correlation energy(see [1]). The results in this paper primarily refer to [2]. We transform total energy $\mathcal{E}(\rho)$ into $\mathcal{E}_\alpha(\rho) = \mathcal{E}(\rho) + \alpha \int \rho dx$ for $\alpha \geq \frac{1}{2}$ and prove the existence of the ground state energy. Besides, we also get some properties of the minimizer.

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Contents

Notation

Notation	**Definition**
$\rho(x)$	electron density in $\mathbb{R}^3$
$\mathcal{E}(\rho)$	exact ground state energy of any many-electronic system
$T_s[\rho]$	noninteracting kinetic energy
$E_{Coul}[\rho]$	classical Coulomb repulsion energy
$E_{ext}[\rho]$	energy of the electrons due to the external field of the nuclei
$E_{xc}[\rho]$	exchange correlation energy
$E_{xc}^{LDA}[\rho]$	local density approximation to the exchange correlation energy
$E_{x,Dirac}^{LDA}[\rho]$	local density approximation to the exchange energy proposed by Dirac
$E_{xc}^{LSDA}[\rho^a,\rho^b]$	local spin density approximation to the exchange correlation energy
$E_{xc}^{GGA}[\rho^a,\rho^b]$	generalized gradient approximation to the exchange correlation energy
ρ^a	density of spin-up electrons
ρ^b	density of spin-down electrons
$E_{xc}^{WS}[\rho]$	local "Wigner-scaled" exchange correlation energy
α_0	α_0=0.93222
κ	$\kappa = 9.47362 \times 10^{-3}$
$V(x)$	electrostatic potential
z_i	nuclei of charge
R_i	location of nuclei
λ	total electron number
α	α is a any constant larger than $\frac{1}{2}$
$J(\rho)$	$J(\rho) = -\rho^{4/3} + \rho^{5/3}\ln(1+\rho^{-\frac{1}{3}})$
$J_\alpha(\rho)$	$J_\alpha(\rho) = J(\rho) + \alpha\rho$
$\mathcal{E}_\alpha(\rho)$	$\mathcal{E}(\rho) + \alpha\int \rho dx$
G	$G = \{\rho \mid \rho \geq 0, \rho \in L^1 \cap L^3, \nabla\rho^{1/2} \in L^2, D(\rho,\rho) < \infty\}$.

$\tilde{G}$	$\tilde{G} = \{\zeta \mid \zeta \in L^2 \bigcap L^6, \nabla\zeta \in L^2, D(\zeta^2, \zeta^2) < \infty\}$.
$E(\lambda)$	$E(\lambda) = \inf\{\mathcal{E}(\rho) \mid \rho \in G, \int \rho dx = \lambda\}$
$E_\alpha(\lambda)$	$E_\alpha(\lambda) = \inf\{\mathcal{E}_\alpha(\rho) \mid \rho \in G, \int \rho dx = \lambda\}$
$\mathcal{E}_p^{TFW}(\rho)$	energy functional in the Thomas-Fermi-von Weizsäcker theory
$\mathcal{E}_p^{TFDW}(\rho)$	energy functional in the Thomas-Fermi-Dirac-von Weizsäcker theory
U	repulsive electrostatic energy of the nuclei. $U = \sum_{1\le i<j\le k} z_i z_j \lvert R_i - R_j\rvert^{-1}$.
A	$A > 0$ is an adjustable constant. Originally, A was taken to be unity.
h	$h = \hbar/2\pi$
$\hbar$	Planck's constant
C_e	C_e is a positive constant. $C_e = (6/\pi q)^{1/3}$
q	q is a number of spin states (=2 for electrons).
m	electron mass
$B_\delta(R_i)$	ball of radius δ and centered at R_i
ρ_0	minimizer for $\mathcal{E}_\alpha(\rho)$
ψ	$\psi = \rho_0^{1/2}$
$\phi(\rho^{1/2})$	$\phi(\rho^{1/2}) = \mathcal{E}(\rho)$
$\phi_\alpha(\rho^{1/2})$	$\phi_\alpha(\rho^{1/2}) = \mathcal{E}_\alpha(\rho)$

1 Introduction

1.1 Ground State Energy

The fundamental theorem of most modern applications of density functional theory (DFT) is the theorem of Kohn and Sham [3, 4, 5] which states that the exact ground state energy of any many-electronic system is given by

$$\mathcal{E}(\rho) = T_s[\rho] + E_{Coul}[\rho] + E_{ext}[\rho] + E_{xc}[\rho], \tag{1.1}$$

where $T_s[\rho]$ is the noninteracting kinetic energy

$$T_s[\rho] = \int |\nabla \rho^{1/2}(x)|^2 dx,$$

$E_{Coul}[\rho]$ is the classical Coulomb repulsion energy

$$E_{Coul}[\rho] = D(\rho, \rho) \equiv \frac{1}{2} \int\int \rho(x)\rho(y)|x-y|^{-1} dxdy,$$

$E_{ext}[\rho]$ is the energy of the electrons in the external field of the nuclei

$$E_{ext}[\rho] = -\int V(x)\rho(x)dx$$

where

$$V(x) = \sum_{i=1}^{k} z_i |x - R_i|^{-1}$$

and $E_{xc}[\rho]$ is the exchange-correlation (XC) energy. ρ is a non-negative function on three-space, $\mathbb{R}^3$. ρ is called a density and physically is supposed to be the electron density in an atom or molecule. $V(x)$ is the electrostatic potential of k nuclei of charges $z_1, \ldots, z_k > 0$, and located at $R_1, \ldots, R_k \in \mathbb{R}^3$. The R_i are distinct. The wonderful thing about equation (1.1) is that the first three terms on the right hand side of the equation are well-known and readily calculable functionals of the electronic density. The disheartening fact is that the analytic form of the XC functional is not, and probably cannot ever be, known.

1.2 Exchange Correlation Energy

Next, we gives a summary of some of the most important exchange correlation energy functionals and the ideas behind them [6].

1.2.1 Local Density Approximation

The principle of this approximation is to calculate the exchange and correlation energies per particle, $\varepsilon_x(\rho(x))$ and $\varepsilon_c(\rho(x))$, of the homogeneous electron gas as a function of the density. These functions are then used as estimates of the exchange and correlation energies per particle of the relevant inhomogeneous system:

$$E_{xc}^{LDA}[\rho] = \int \rho(x)(\varepsilon_x(\rho(x)) + \varepsilon_c(\rho(x)))dx.$$

One would immediately think that the use of such a functional is only suitable for systems that have slowly varying densities, but the local density approximation yields surprisingly good results for many interesting applications with relatively large density gradients. Already as early as 1930 the first local density approximation to the exchange energy was proposed by Dirac [7]:

$$E_{x,Dirac}^{LDA}[\rho] = -\frac{3}{4} \cdot (\frac{3}{\pi})^{1/3} \cdot \int \rho^{4/3}(x)dx.$$

The functional was used together with the Thomas-Fermi model, in the so called Thomas-Fermi-Dirac model [2], but not lead to any significant improvements, since the inaccuracy of the Thomas-Fermi model primarily is due to the approximation for the kinetic energy functional. The Thomas-Fermi-Dirac-Weizsäcker model [2], which includes gradient corrections to the Thomas-Fermi kinetic energy functional, shows large improvements.

Remark: TFD model and TFDW model are listed below:

$$\mathcal{E}^{TFD}(\rho) = \frac{3}{5}\gamma \int \rho^{5/3}(x) - \frac{3}{4} \cdot (\frac{3}{\pi})^{1/3} \cdot \int \rho^{4/3}(x)dx - \int V(x)\rho(x)dx + D(\rho, \rho).$$

$$\begin{aligned} \mathcal{E}_p^{TFDW}(\rho) &= A \int |\nabla \rho^{1/2}(x)|^2 dx + \frac{\gamma}{p} \int \rho^p(x)dx - \frac{3C_e}{4} \int \rho^{4/3}(x)dx \\ &\quad - \int V(x)\rho(x)dx + D(\rho, \rho) + U \end{aligned}$$

for $p > \frac{4}{3}$. $A > 0$ is an adjustable constant. Originally, A was taken to be unity. $\gamma = (6\pi^2)^{2/3} h^2 (2mq^{2/3})^{-1}$ where $h = \hbar/2\pi$, $\hbar$=Planck's constant, and m is the electron mass. q is the number of spin states (=2 for electrons). $C_e = (6/\pi q)^{1/3}$.

1.2.2 Local Spin Density Approximation

The local density approximation discussed in the previous section leads to the correct results for the spin-compensated homogeneous electron gas, if the correct exchange correlation functional is used. For the descriptions of systems that are subject to an external magnetic field, systems that are polarized or systems where relativistic effects are important, the spin-compensated Kohn-Sham scheme and the local density approximation are not applicable. The spin-polarized Kohn-Sham theory was developed in the early seventies [8, 9], and shortly there-after it was shown that relativistic corrections such as the spin-orbit coupling could be included in this formalism. In the spin-polarized Kohn-Sham scheme with a Local Spin Density Approximation (LSDA) the exchange correlation energy is written as:

$$E_{xc}^{LSDA}[\rho^a, \rho^b] = \int \rho(x)\varepsilon_{xc}(\rho^a(x), \rho^b(x))dx$$

where ρ^a and ρ^b are the densities of spin-up and spin-down electrons respectively.

1.2.3 Generalized Gradient Approximation

In this approximation [10] the gradient is included as the only new variable, and one tries to determine the best scheme that fulfills the relation:

$$E_{xc}^{GGA}[\rho^a, \rho^b] = \int f(\rho^a, \rho^b, \nabla\rho^a, \nabla\rho^b)dx.$$

where ρ^a and ρ^b are the densities of spin-up and spin-down electrons respectively. More details can be found in [11, 12, 13, 14, 15, 16].

1.2.4 Beyond the Generalized Gradient Approximation

The generalized gradient approximation significantly improves upon the results obtained with the local schemes. For the purpose of describing many chemical aspects of molecules, the accuracy of the gradient corrected schemes is still too small. The ultimate goal is to find a density functional which yields so called "chemical accuracy". This essentially means that the method should be able to quantitatively predict chemical properties within the standard deviation offered by the best experimental methods[6].

1.3 Minimization Problem

In this paper, we deal with the exchange-correlation energy functional from Zhao, Q., Parr, R.G.[1] which says that:

> Self-consistent calculations on a number of atoms and ions are carried out with the new local "Wigner-scaled" exchange-correlation functional generated by Zhao, Levy, and Parr:
>
> $$E_{xc}^{WS}[\rho] = -\alpha_0 \int \rho^{4/3}[1 - \kappa\rho^{1/3}\ln(1 + 1/(\kappa\rho^{1/3}))]dx$$
>
> with α_0=0.93222 and $\kappa = 9.47362 \times 10^{-3}$.

For simplicity, we assume

$$E_{xc}[\rho] = -\int \rho^{4/3} + \rho^{5/3}\ln(1 + \rho^{-\frac{1}{3}})dx.$$

This paper is concerned with the energy functional $\mathcal{E}(\rho)$:

$$\mathcal{E}(\rho) = \int |\nabla\rho^{1/2}(x)|^2 dx + \int J(\rho(x))dx - \int V(x)\rho(x)dx + D(\rho, \rho)$$

where

$$J(\rho(x)) = -\rho^{4/3}(x) + \rho^{5/3}(x)\ln\left(1 + \rho^{-\frac{1}{3}}(x)\right).$$

We shall use the function space

$$G = \{\rho | \rho \geq 0, \rho \in L^1 \cap L^3, \nabla\rho^{1/2} \in L^2, D(\rho, \rho) < \infty\}.$$

Define the energy for $\lambda \geq 0$ as

$$E(\lambda) = \inf\{\mathcal{E}(\rho) | \rho \in G, \int \rho dx = \lambda\} \tag{1.2}$$

where λ is the total electron number. A difficulty is that $J(\rho)$ is not positive for $\rho \geq 0$ (see Appendix). This difficulty can be deal with in the following way. Introduce the new function

$$\mathcal{E}_\alpha(\rho) = \mathcal{E}(\rho) + \alpha \int \rho dx$$

with $\alpha \geq \frac{1}{2}$. This amounts to replacing $J(\rho)$ by

$$J_\alpha(\rho) = J(\rho) + \alpha\rho.$$

Note that $J_\alpha(\rho) \geq 0$ and $J'_\alpha(\rho) \geq 0$ for $\rho \geq 0$ (see Appendix). The energy for $\lambda \geq 0$ is

$$E_\alpha(\lambda) = \inf\{\mathcal{E}_\alpha(\rho) | \rho \in G, \int \rho dx = \lambda\}. \tag{1.3}$$

1.4 Related Works

1. In the Thomas-Fermi-von Weizsäcker Theory of Atoms and Molecules [17], they introduce the energy functional

$$\mathcal{E}_p^{TFW}(\rho) = \int |\nabla \rho^{1/2}(x)|^2 dx + \frac{1}{p} \int \rho^p(x) dx - \int V(x)\rho(x) dx + D(\rho, \rho)$$

for $1 < p < \infty$. They are concerned with the following problem

$$\text{Min}\{\mathcal{E}_p^{TFW}(\rho) | \rho \in L^1 \cap L^p, \rho(x) \geq 0, \nabla \rho^{1/2} \in L^2, \int \rho dx = \lambda\}. \tag{1.4}$$

The main result in [17] is the following:

Theorem 1.1 *There is a critical value $0 < \lambda_c < \infty$ depending only on p and V such that*

(a) If $\lambda \leq \lambda_c$, problem (1.4) has a unique solution,

(b) If $\lambda > \lambda_c$, problem (1.4) has no solution,

(c) When $p \geq \frac{4}{3}$, then $\lambda_c \geq Z \equiv \sum_{i=1}^k z_i$,

(d) When $p \geq \frac{5}{3}$ and k=1(atomic case), then $\lambda_c > Z$.

2. In the Thomas-Fermi-Dirac-von Weizsäcker Theory [2], they introduce the energy functional

$$\begin{aligned}\mathcal{E}_p^{TFDW}(\rho) &= A\int|\nabla\rho^{1/2}(x)|^2dx+\frac{\gamma}{p}\int\rho^p(x)dx-\frac{3C_e}{4}\int\rho^{4/3}(x)dx\\ &\quad -\int V(x)\rho(x)dx+D(\rho,\rho)+U\end{aligned}$$

for $p>\frac{4}{3}$. U is the repulsive electrostatic energy of the nuclei,

$$U=\sum_{1\le i<j\le k}z_iz_j|R_i-R_j|^{-1}.$$

$A>0$ is an adjustable constant. Originally, A was taken to be unity. $\gamma=(6\pi^2)^{2/3}h^2(2mq^{2/3})^{-1}$ where $h=\hbar/2\pi$, $\hbar$=Planck's constant, and m is the electron mass. q is the number of spin states (=2 for electrons). C_e is a positive constant. In the original theory (see Dirac, [18]), the value $C_e=(6/\pi q)^{1/3}$ was used for reasons which will be explained in Lieb, E.H.[2].

The function space is

$$G_p=\{\rho|\rho\in L^3\cap L^p,\nabla\rho^{1/2}\in L^2,D(\rho,\rho)<\infty\}.$$

The Thomas-Fermi-Dirac-von Weizsäcker Theory[2] has not been as extensively studied as the above theory. They basically proved the existence of ground state solutions and discuss some properties of the solution by α method. The same technique will be used in our work.

2 Main Results

In this paper, we obtain the following lemmas and theorems. The proof of the lemmas and theorems will be given in the next four sections. First, we prove two lemmas which are useful in the proof of $\min\{\mathcal{E}_\alpha(\rho)|\rho \in G\}$, the existence of ground state solution of (1.3).

Lemma 3.1 For every $\varepsilon > 0$, there is a constant C_ε, depending on V and ε such that

$$\int V(x)\rho(x)dx \leq \varepsilon\|\rho\|_3 + C_\varepsilon D(\rho,\rho)^{1/2}$$

for every $\rho \geq 0$.

Lemma 3.2 There exist positive constants a_0 and C_0 such that

$$\mathcal{E}_\alpha(\rho) \geq a_0(\|\rho\|_3 + \|\nabla\rho^{1/2}\|_2^2 + D(\rho,\rho)) + \int J_\alpha(\rho)dx - C_0.$$

Based on above two lemmas, we prove the existence of $\min\{\mathcal{E}_\alpha(\rho)|\rho \in G\}$.

Theorem 4.1 There exists a minimizer ρ_0 for $\mathcal{E}_\alpha(\rho)$ on G. Every such $\rho_0 \in L^1$, and $\int \rho_0 \leq$ some constant which is independent of ρ_0.

First, the proof of Theorem 4.1 is concerned with a minimizing sequence $\rho_n \in G$. Such minimizing sequence make sense since $\mathcal{E} : G \to \bar{R}$ is well defined where $\bar{R}$ is the range of the mapping $\mathcal{E}_\alpha$.

Next, we derive the Euler equation satisfied by ρ_0. Set $\psi = \rho_0^{1/2}$.

Theorem 4.2 $\rho_0^{1/2}$ satisfies the Euler equation:

$$[-\triangle + W(x)]\psi = 0$$

where

$$W = -\frac{4}{3}\psi^{2/3} - \frac{1}{3}\cdot\frac{\psi^{2/3}}{1+\psi^{-2/3}} + \frac{5}{3}\psi^{4/3}\ln(1+\psi^{-2/3}) + \alpha - V + \mathcal{B}(\psi^2).$$

Now we prove the existence of ground state solution of (1.2). First, we prove one theorem which is useful in the proof of the existence of ground state solution of (1.2).

Theorem 5.1 If $\psi \in \tilde{G}$ satisfies the Euler equation and $\psi(x) \geq 0$ for all x, then ψ is continuous. Moreover, $\psi \in C^{0,\mu}$ for all $\mu < 1$.

Based on the above theorem, we prove the existence of ground state solution of (1.2).

Theorem 5.2 The two functions $E(\lambda)$, $E_\alpha(\lambda)$ are finite and satisfy

$$E(\lambda) = E_\alpha(\lambda) - \alpha\lambda.$$

The solutions of (1.2) and (1.3) are the same. The following theorems discuss the properties of ψ in (1.3). In fact, the minimizer of (1.2) also have the same properties.

Theorem 6.1 If $\psi \in \tilde{G}$ satisfies the Euler equation and $\psi(x) \geq 0$ for all x, either $\psi \equiv 0$ or $\psi > 0$ on $\mathbb{R}^3 \setminus \bigcup_{i=1}^{k}\{R_i\}$.

Define $\phi(g)$ to be

$$\phi(g) = \int |\nabla g|^2 dx - \int g^{8/3} dx + \int g^{10/3}\ln(1+g^{-\frac{2}{3}})dx + D(g^2, g^2).$$

Theorem 6.2 If $V = 0$ in ϕ, there are C^∞ functions of compact support such that $\phi(g) < 0$.

Theorem 6.3 ψ is bounded on $\mathbb{R}^3$ and $\psi(x) \to 0$ as $|x| \to \infty$. Also, $\psi \in H^2$ (i.e., $\psi, \nabla\psi$ and $\triangle\psi \in L^2$).

Theorem 6.4 Let ψ be the positive solution to Euler equation. Then for every $0 < t < \alpha$, there exists a constant M such that

$$\psi(x) \leq M \exp[-t^{1/2}|x|].$$

3 Some Basic Properties of $\mathcal{E}_\alpha$

This section are concerned with some properties of $\mathcal{E}_\alpha$ which are useful in the proof of $\min\{\mathcal{E}_\alpha(\rho)|\rho \in G\}$.

Lemma 3.1 *For every $\varepsilon > 0$, there is a constant C_ε, depending on V and ε such that*

$$\int V(x)\rho(x)dx \leq \varepsilon\|\rho\|_3 + C_\varepsilon D(\rho,\rho)^{1/2} \tag{3.1}$$

for every $\rho \geq 0$.

Proof: Let $\delta > 0$ be a small constant and let $\zeta(x)$ be a smooth function such that $0 \leq \zeta \leq 1$ and

$$\zeta(x) = \begin{cases} 1 & \text{on } \bigcup_{i=1}^k B_\delta(R_i), \\ 0 & \text{outside } \bigcup_{i=1}^k B_{2\delta}(R_i), \end{cases}$$

where $B_\delta(R_i)$ is the ball of radius δ and centered at R_i. δ is chosen such that all these ball $B_{2\delta}$ are disjoint. Let $V = V\zeta + V(1-\zeta) \equiv V_1 + V_2$. It is clear that

$$V_1 \in L^{3/2} \tag{3.2}$$

(since $\int_{B_\delta(0)} |\frac{1}{x}|^{3/2}dx = \int\int_0^\delta |\frac{1}{r}|^{3/2}r^2 dr d\Omega < \infty$). So, by choosing δ small enough we may assume that $\|V_1\|_{3/2} < \varepsilon$. Thus,

$$\int V_1(x)\rho(x)dx \leq \| V_1 \|_{3/2} \| \rho \|_3 \leq \varepsilon \| \rho \|_3 . \tag{3.3}$$

On the other hand define the operator $\mathcal{B}$ to be

$$\mathcal{B}(\rho)(x) = \int \rho(y)|x-y|^{-1}dy.$$

Since $\frac{-1}{4\pi}\mathcal{B}(\rho)(x) = \int \frac{-1}{4\pi}\frac{\rho(y)}{|x-y|}dy$ is the Newtonian potential in $\mathbb{R}^3$(see [19],p18),

$$-\triangle\mathcal{B}(\rho) = 4\pi\rho. \tag{3.4}$$

Thus,

$$\begin{aligned} \int |\nabla\mathcal{B}(\rho)(x)|^2 dx &= -\int \triangle\mathcal{B}(\rho)\cdot\mathcal{B}(\rho)dx \\ &= 4\pi\int \rho(x)\mathcal{B}(\rho)(x)dx \\ &= 4\pi\int\int \frac{\rho(x)\rho(y)}{|x-y|}dxdy \\ &= 8\pi D(\rho,\rho). \end{aligned} \tag{3.5}$$

We deduce from (3.5) and Sobolev's inequality(see [19],p148) that

$$\| \mathcal{B}(\rho)\|_6 \leq CD(\rho,\rho)^{1/2}. \tag{3.6}$$

for some constant C. Consequently, by (3.4) and (3.6),

$$\begin{aligned}
\int V_2(x)\rho(x)dx &= \int V_2(x)\frac{1}{4\pi}(-\triangle\mathcal{B}(\rho)(x))dx \\
&= \frac{1}{4\pi}\int \nabla\mathcal{B}(\rho)(x)\nabla V_2(x)dx \\
&= -\frac{1}{4\pi}\int \triangle V_2(x)\mathcal{B}(\rho)(x)dx \\
&\leq \frac{1}{4\pi}||\triangle V_2||_{6/5}||\mathcal{B}(\rho)||_6 \\
&\leq C_1 \parallel \triangle V_2 \parallel_{6/5} D(\rho,\rho)^{1/2} \qquad (3.7)
\end{aligned}$$

where $C_1 = \frac{1}{4\pi}C$ is a constant. Note that $V(x)$ is the Green's function for the Laplacian, we have

$$\triangle V_2(x) \in C_o^\infty.$$

Combining (3.3) and (3.7), we obtain

$$\int V(x)\rho(x)dx = \int V_1(x)\rho(x)dx + \int V_2(x)\rho(x)dx \leq \varepsilon\|\rho\|_3 + C_\varepsilon D(\rho,\rho)^{1/2}.$$

□

Lemma 3.2 *There exist positive constants a_0 and C_0 such that*

$$\mathcal{E}_\alpha(\rho) \geq a_0(\|\rho\|_3 + \|\nabla\rho^{1/2}\|_2^2 + D(\rho,\rho)) + \int J_\alpha(\rho)dx - C_0. \tag{3.8}$$

Proof: Use (3.1), Young's inequality and Sobolev's inequality,

$$\begin{aligned}
\mathcal{E}_\alpha(\rho) &= \int |\nabla\rho^{1/2}(x)|^2 dx + \int J_\alpha(\rho)dx - \int V(x)\rho(x)dx + D(\rho,\rho) \\
&\geq \int |\nabla\rho^{1/2}(x)|^2 dx + \int J_\alpha(\rho)dx - \varepsilon\|\rho\|_3 - C_\varepsilon D(\rho,\rho)^{1/2} + D(\rho,\rho) \\
&\geq \| \nabla\rho^{1/2}\|_2^2 - \varepsilon C \| \nabla\rho^{1/2}\|_2^2 - C_\varepsilon D(\rho,\rho)^{1/2} + \int J_\alpha(\rho)dx + D(\rho,\rho) \\
&= \frac{1-\varepsilon C}{2} \| \nabla\rho^{1/2}\|_2^2 + \frac{1-\varepsilon C}{2} \| \nabla\rho^{1/2}\|_2^2 - C_\varepsilon D(\rho,\rho)^{1/2} + \int J_\alpha(\rho)dx \\
&\quad + D(\rho,\rho) \\
&\geq \frac{1-\varepsilon C}{2} \| \nabla\rho^{1/2}\|_2^2 + \frac{1-\varepsilon C}{2C} \| \rho \|_3 - C_\varepsilon D(\rho,\rho)^{1/2} + \int J_\alpha(\rho)dx \\
&\quad + D(\rho,\rho) \\
&\geq \frac{1-\varepsilon C}{2} \| \nabla\rho^{1/2}\|_2^2 + \frac{1-\varepsilon C}{2C} \| \rho \|_3 - \left(\frac{C_\varepsilon^2}{2} + \frac{D(\rho,\rho)}{2}\right) + \int J_\alpha(\rho)dx \\
&\quad + D(\rho,\rho) \\
&\geq \frac{1-\varepsilon C}{2} \| \nabla\rho^{1/2}\|_2^2 + \frac{1-\varepsilon C}{2C} \| \rho \|_3 + \frac{1}{2}D(\rho,\rho) + \int J_\alpha(\rho)dx - \frac{C_\varepsilon^2}{2}.
\end{aligned}$$

Since ε can be arbitrary small and C is a fixed number, $\frac{1-\varepsilon C}{2}$ and $\frac{1-\varepsilon C}{2C}$ are positive. Choose

$$a_0 = \min\{\frac{1-\varepsilon C}{2}, \frac{1-\varepsilon C}{2C}, \frac{1}{2}\}.$$

Thus,

$$\mathcal{E}_\alpha(\rho) \geq a_0(\| \rho \|_3 + \| \nabla\rho^{1/2} \|_2^2 + D(\rho,\rho)) + \int J_\alpha(\rho)dx - C_0.$$

□

Since $J_\alpha(\rho) \geq 0$ for $\rho \geq 0$, $\int J_\alpha(\rho)dx \geq 0$ (see Appendix). Hence, $\mathcal{E}_\alpha(\rho)$ has a lower bound.

4 Minimization of $\mathcal{E}_\alpha(\rho)$ with $\rho \in G$ —The Euler Equation

Theorem 4.1 *There exists a minimizer ρ_0 for $\mathcal{E}_\alpha(\rho)$ on G. Every such $\rho_0 \in L^1$, and $\int \rho_0 \leq$ some constant (independent of ρ_0).*

Proof: Let $\rho_n \in G$ be a minimizing sequence. By Lemma 2.2, we have

$$\|\rho_n\|_3 \leq C, \quad \|\nabla \rho_n^{1/2}\|_2 \leq C, \quad D(\rho_n, \rho_n) \leq C.$$

Therefore, we may extract a subsequence, still denoted by ρ_n, such that as $n \to \infty$,

$$\rho_n \to \rho_0 \text{ weakly in } L^3, \tag{4.1}$$

$$\rho_n \to \rho_0 \text{ a.e.,} \tag{4.2}$$

$$\nabla \rho_n^{1/2} \to \nabla \rho_0^{1/2} \text{ weakly in } L^2. \tag{4.3}$$

((4.2)relies on the fact that if Ω is a bounded smooth domain then $H^1(\Omega)$ is relatively compact in $L^2(\Omega)$. (4.1) and (4.3) imply that $\{\rho_n^{1/2}\}$ is bounded in $H^1(\Omega)$. Hence $\{\rho_n^{1/2}\}$ has a subsequence converging in $L^2(\Omega)$ and a.e.). Next, we prove that $\mathcal{E}_\alpha$ is weakly lower semicontinuous at ρ_0. Note that $\nabla \rho_n^{1/2} \to \nabla \rho_0^{1/2}$ weakly in L^2, we have

$$\liminf_{n\to\infty} \int |\nabla \rho_n^{1/2}|^2 dx \geq \int |\nabla \rho_0^{1/2}|^2 dx.$$

Note that $J_\alpha(\rho_n) \geq 0$ and $D(\rho_n, \rho_n) \geq 0$, by Fatou's Lemma, we have

$$\liminf_{n\to\infty} \int J_\alpha(\rho_n) dx \geq \int J_\alpha(\rho_0) dx$$

and

$$\liminf_{n\to\infty} D(\rho_n, \rho_n) \geq D(\rho_0, \rho_0).$$

We now prove that

$$\int V(x)\rho_n(x)dx \to \int V(x)\rho_0(x)dx.$$

We write $V = V_1 + V_2$ as in Lemma 3.1. By (3.2) and (4.1), as $n \to \infty$, we have

$$\int V_1(x)\rho_n(x)dx \to \int V_1(x)\rho_0(x)dx.$$

On the other hand

$$\int V_2(x)\rho_n(x)dx = -\frac{1}{4\pi}\int \triangle V_2\mathcal{B}(\rho_n)dx.$$

It follows from (3.6) that $\mathcal{B}(\rho_n) \to \mathcal{B}(\rho_0)$ weakly in L^6 as $n \to \infty$. Thus, as $n \to \infty$,

$$\begin{aligned}\int V_2(x)\rho_n(x)dx &= -\frac{1}{4\pi}\int \triangle V_2\mathcal{B}(\rho_n)dx \to -\frac{1}{4\pi}\int \triangle V_2\mathcal{B}(\rho_0)dx \\ &= \int V_2(x)\rho_0(x)dx.\end{aligned}$$

Therefore,

$$\mathcal{E}_\alpha(\rho_0) \leq \liminf_{n\to\infty} \mathcal{E}_\alpha(\rho_n).$$

It implies that $\mathcal{E}_\alpha(\rho_0) \leq \inf\{\mathcal{E}_\alpha(\rho)|\rho \in G\}$. Next, It is clear that $\rho_0 \in L^1$. Hence, $\rho_0 \in G$. By the definition, $\inf\{\mathcal{E}_\alpha(\rho)|\rho \in G\} \leq \mathcal{E}_\alpha(\rho_0)$. We get ρ_0 is a minimizer. Therefore, we prove the existence of $\min\{\mathcal{E}_\alpha(\rho)|\rho \in G\}$. It is easy to see from (3.8) that the bound on $\int \rho_0$ is independent of ρ_0.

□

Next, we derive the Euler equation satisfied by $\rho_0^{1/2}$. Set $\psi = \rho_0^{1/2}$.

Theorem 4.2 $\rho_0^{1/2}$ *satisfies the Euler equation:*

$$[-\triangle + W(x)]\psi = 0 \tag{4.4}$$

where

$$W = -\frac{4}{3}\psi^{2/3} - \frac{1}{3}\cdot\frac{\psi^{2/3}}{1+\psi^{-2/3}} + \frac{5}{3}\psi^{4/3}\ln(1+\psi^{-2/3}) + \alpha - V + \mathcal{B}(\psi^2).$$

Proof: Consider the set $\tilde{G} = \{\zeta \in L^2 \cap L^6 | \nabla\zeta \in L^2 \text{ and } D(\zeta^2,\zeta^2) < \infty\}$. (Note that we do not assume $\zeta \geq 0$.) We know $\psi \in \tilde{G}$. If $\zeta \in \tilde{G}$, then $\rho = \zeta^2 \in G$ and

$$\begin{aligned}\mathcal{E}_\alpha(\rho) &= \int |\nabla\zeta|^2dx - \int \zeta^{8/3}dx + \int \zeta^{10/3}\ln(1+\zeta^{-2/3})dx + \alpha\int \zeta^2dx - \int V\zeta^2dx \\ &\quad + D(\zeta^2,\zeta^2) \\ &\equiv \phi_\alpha(\zeta).\end{aligned}$$

Therefore, we find for every $\zeta \in \tilde{G}$

$$\phi_\alpha(\psi) \le \phi_\alpha(\zeta).$$

Let $f \in C_o^\infty$;using the fact that $\frac{d}{dt}\phi_\alpha(\psi + tf)|_{t=0} = 0$.

$$\lim_{t\to 0} \frac{1}{t}\Big(\int |\nabla(\psi + tf)|^2 dx - \int |\nabla\psi|^2 dx \Big)$$

$$\begin{aligned}
&= \lim_{t\to 0} \frac{1}{t} \int |\nabla\psi + t\nabla f|^2 - |\nabla\psi|^2 dx \\
&= \lim_{t\to 0} \frac{1}{t} \int |\nabla\psi|^2 + 2t\nabla\psi\nabla f + t^2|\nabla f|^2 - |\nabla\psi|^2 dx \\
&= \lim_{t\to 0} \int 2\nabla\psi\nabla f + t|\nabla f|^2 dx \\
&= 2\int \nabla\psi\nabla f dx \\
&= -2\int \triangle\psi f dx. \qquad (4.5)
\end{aligned}$$

$$\lim_{t\to 0} \frac{1}{t}\Big[\int (\psi + tf)^{8/3} dx - \int \psi^{8/3} dx \Big]$$

$$\begin{aligned}
&= \lim_{t\to 0} \frac{1}{t} \int \psi^{8/3} + \frac{8}{3}\psi^{5/3} tf + O(t^2) - \psi^{8/3} dx \\
&= \lim_{t\to 0} \int \frac{8}{3}\psi^{5/3} f + O(t) dx \\
&= \frac{8}{3}\int \psi^{5/3} f dx. \qquad (4.6)
\end{aligned}$$

$$\int (\psi + tf)^{10/3} \ln(1 + (\psi + tf)^{-2/3}) dx$$

$$\begin{aligned}
&= \int \Big[\psi^{10/3} + \frac{10}{3}\psi^{7/3} tf + O(t^2)\Big] \cdot \Big[\ln(1+\psi^{-2/3}) - \frac{2}{3}\cdot\frac{\psi^{-5/3}}{1+\psi^{-2/3}} tf + O(t^2)\Big] dx \\
&= \int \psi^{10/3}\Big[\ln(1+\psi^{-2/3}) - \frac{2}{3}\cdot\frac{\psi^{-5/3}}{1+\psi^{-2/3}} tf\Big] + \frac{10}{3}\psi^{7/3} tf \ln(1+\psi^{-2/3}) + O(t^2) dx \\
&= \int \psi^{10/3}\ln(1+\psi^{-2/3}) - \frac{2}{3}\cdot\frac{\psi^{5/3}}{1+\psi^{-2/3}} tf + \frac{10}{3}\psi^{7/3} tf \ln(1+\psi^{-2/3}) + O(t^2) dx.
\end{aligned}$$

So

$$\lim_{t\to 0}\frac{1}{t}\Big[\int(\psi+tf)^{10/3}\ln(1+(\psi+tf)^{-2/3})dx-\int\psi^{10/3}\ln(1+\psi^{-2/3})dx\Big]$$

$$=\int\Big[-\frac{2}{3}\cdot\frac{\psi^{5/3}}{1+\psi^{-2/3}}+\frac{10}{3}\psi^{7/3}\ln(1+\psi^{-2/3})\Big]fdx. \qquad (4.7)$$

$$\lim_{t\to 0}\frac{1}{t}\Big[\int V(\psi+tf)^2dx-\int V\psi^2dx\Big]$$

$$\begin{aligned}
&= \lim_{t\to 0}\frac{1}{t}\int V(\psi^2+2\psi tf+t^2f^2)-V\psi^2dx\\
&= \lim_{t\to 0}\frac{1}{t}\int 2V\psi tf+Vt^2f^2dx\\
&= 2\int V\psi fdx. \qquad (4.8)
\end{aligned}$$

$$\lim_{t\to 0}\frac{1}{t}\Big[\frac{1}{2}\int\int\frac{(\psi+tf)^2(x)(\psi+tf)^2(y)}{|x-y|}dxdy-\frac{1}{2}\int\int\frac{\psi^2(x)\psi^2(y)}{|x-y|}dxdy\Big]$$

$$\begin{aligned}
&= \lim_{t\to 0}\frac{1}{t}\Big[\frac{1}{2}\int\int\frac{(\psi^2+2\psi tf+t^2f^2)(x)\cdot(\psi^2+2\psi tf+t^2f^2)(y)}{|x-y|}dxdy\\
&\quad -\frac{1}{2}\int\int\frac{\psi^2(x)\psi^2(y)}{|x-y|}dxdy\Big]\\
&= \lim_{t\to 0}\frac{1}{t}\Big[\frac{1}{2}\int\int\frac{\psi^2(x)\psi^2(y)+\psi^2(x)2\psi(y)tf(y)+2\psi(x)tf(x)\psi^2(y)+O(t^2)}{|x-y|}dxdy\\
&\quad -\frac{1}{2}\int\int\frac{\psi^2(x)\psi^2(y)}{|x-y|}dxdy\Big]\\
&= \int\int\frac{\psi^2(x)\psi(y)f(y)+\psi(x)f(x)\psi^2(y)}{|x-y|}dxdy\\
&= 2\int\int\frac{\psi^2(y)\psi(x)}{|x-y|}f(x)dxdy\\
&= 2\int\mathcal{B}(\psi^2)\psi fdx. \qquad (4.9)
\end{aligned}$$

$$\lim_{t\to 0}\frac{1}{t}\Big[\alpha\int(\psi+tf)^2dx-\alpha\int\psi^2dx\Big]$$

$$=\lim_{t\to 0}\frac{1}{t}\Big[\alpha\int\psi^2+2\psi tf+t^2f^2-\psi^2dx\Big]=2\alpha\int\psi fdx. \qquad (4.10)$$

By (4.5)(4.6)(4.7)(4.8)(4.9)(4.10), we get ψ satisfies the Euler equation

$$\Big[-\triangle - \frac{4}{3}\psi^{2/3} - \frac{1}{3}\cdot\frac{\psi^{2/3}}{1+\psi^{-2/3}} + \frac{5}{3}\psi^{4/3}\ln(1+\psi^{-2/3}) + \alpha - V + \mathcal{B}(\psi^2)\Big]\psi = 0.$$

□

5 Existence of Ground State Solution

Theorem 5.1 *If $\psi \in \tilde{G}$ satisfies the Euler equation (4.4) and $\psi(x) \geq 0$ for all x, then ψ is continuous. Moreover, $\psi \in C^{0,\mu}$ for all $\mu < 1$.*

Proof: Consider $V(x) = \frac{1}{|x|}$ and $B(0,R) \subset\subset \mathbb{R}^3$. For any $\varepsilon > 0$,

$$\begin{aligned}\int_{B(0,R)} |V|^{3-\varepsilon}dx &= \int_{B(0,R)} \frac{1}{|x|^{3-\varepsilon}}dx = \int\int_0^R \frac{1}{r^{3-\varepsilon}} r^2 dr d\Omega = \int\int_0^R r^{\varepsilon-1} dr d\Omega \\ &= \frac{1}{\varepsilon} r^{\varepsilon}|_0^R \cdot \int d\Omega = \frac{1}{\varepsilon} R^{\varepsilon} \cdot \int d\Omega < \infty.\end{aligned}$$

Hence, $V \in L^{3-\varepsilon}_{loc}$ for any $\varepsilon > 0$. Since $\psi \in L^6$, it follows that $V\psi \in L^{2-\varepsilon}_{loc}$ for any $\varepsilon > 0$ (Since $||V\psi||_{2-\varepsilon} \leq ||V||_{\frac{6(2-\varepsilon)}{4+\varepsilon}} ||\psi||_6$ and $3 - \varepsilon - \frac{6(2-\varepsilon)}{4+\varepsilon} = \frac{-\varepsilon^2+5\varepsilon}{4+\varepsilon} > 0$). It follows from Appendix that for $\psi \geq 0$,

$$-\frac{4}{3}\psi^{2/3} - \frac{1}{3} \cdot \frac{\psi^{2/3}}{1+\psi^{-2/3}} + \frac{5}{3}\psi^{4/3}\ln(1+\psi^{-2/3}) + \alpha \geq 0.$$

By the definition, we also know that $\mathcal{B}(\psi^2) \geq 0$. Therefore, we have

$$-\triangle\psi \leq f$$

where $f = V\psi \in L^{2-\varepsilon}_{loc}$ for any $\varepsilon > 0$ and in particular $f \in L^s_{loc}$ for some $s > \frac{3}{2}$. By Lemma 3.2, $\psi \in H^1$. We may, therefore, apply a result of Stampacchia (see [20], Theorem5.2) to conclude that $\psi \in L^\infty_{loc}$. Going back to (4.4) and using the fact that $\psi \in L^\infty_{loc}$, we now see that $\triangle\psi \in L^{3-\varepsilon}_{loc}$ (since $||V\psi||_{3-\varepsilon} \leq ||V||_{3-\varepsilon}||\psi||_\infty$). By Sobolev imbedding theorem (see Adams, [21], p.98), we have $\psi \in C^{0,\mu}$ for all $\mu < 1$.

□

Theorem 5.2 *The two functions $E(\lambda)$, $E_\alpha(\lambda)$ are finite and satisfy*

$$E(\lambda) = E_\alpha(\lambda) - \alpha\lambda.$$

Proof:

First,

$$\begin{aligned}\mathcal{E}(\rho) &= \int |\nabla\rho^{1/2}|^2 dx - \int \rho^{4/3}dx + \int \rho^{5/3}\ln(1+\rho^{-\frac{1}{3}})dx - \int V(x)\rho(x)dx + D(\rho,\rho) \\ \mathcal{E}_\alpha(\rho) &= \mathcal{E}(\rho) + \alpha\int \rho dx.\end{aligned}$$

It is clear that $\int |\nabla\rho^{1/2}|^2 dx$, $\int \rho^{4/3}dx$, and $D(\rho,\rho)$ are finite (since $\rho \in G$). And

$$\int \rho^{5/3}\ln(1+\rho^{-\frac{1}{3}})dx < \int \rho^{5/3}dx + \int \rho^{4/3}dx < \infty.$$

Let $B_\delta(R_i)$ is the ball of radius δ and centered at R_i for $i = 1, 2, ..., k$. δ is chosen such that all the ball $B_\delta(R_i)$ are disjoint. It is clear that $\int_{B_\delta(R_i)} V(x)\rho(x)dx$ is finite(since ρ is continuous). On the other hand, $\int_{\mathbb{R}^3\setminus B_\delta(R_i)} V(x)\rho(x)dx$ is also finite. Therefore, $\mathcal{E}(\rho)$ and $\mathcal{E}_\alpha(\rho)$ are finite.

Finally, choose any $\rho(x) \in G$ such that $\int \rho(x)dx = \lambda$. We have

$$\mathcal{E}(\rho) \geq E(\lambda).$$

So

$$\mathcal{E}_\alpha(\rho) = \mathcal{E}(\rho) + \alpha\lambda \geq E(\lambda) + \alpha\lambda.$$

Hence,

$$E_\alpha(\lambda) \geq E(\lambda) + \alpha\lambda. \tag{5.1}$$

On the other hand, choose any $\rho(x) \in G$ such that $\int \rho(x)dx = \lambda$. We have

$$E_\alpha(\lambda) \leq \mathcal{E}_\alpha(\rho) = \mathcal{E}(\rho) + \alpha\lambda.$$

So

$$E_\alpha(\lambda) \leq E(\lambda) + \alpha\lambda. \tag{5.2}$$

By (5.1) and (5.2), we have

$$E(\lambda) = E_\alpha(\lambda) - \alpha\lambda.$$

□

6 Properties of the minimizer ψ

Theorem 6.1 *If $\psi \in \tilde{G}$ for $E(\lambda)$ and $E_\alpha(\lambda)$ satisfies the Euler equation (4.4) and $\psi(x) \geq 0$ for all x, either $\psi \equiv 0$ or $\psi > 0$ on $\mathbb{R}^3 \backslash \bigcup_{i=1}^k \{R_i\}$.*

Proof: By Theorem 4.2 and Theorem 5.1, we have $-\triangle\psi = b\psi$ and $b \in L^\infty_{loc}$ on $\mathbb{R}^3 \backslash \bigcup_{i=1}^k \{R_i\}$. The conclusion follows from Harnack's inequality (see Gilbarg, [19]).

□

Define $\phi(g)$ to be

$$\phi(g) = \int |\nabla g|^2 dx - \int g^{8/3} dx + \int g^{10/3} \ln(1 + g^{-\frac{2}{3}}) dx + D(g^2, g^2).$$

Theorem 6.2 *If $V = 0$, there are C^∞ functions of compact support such that $\phi(g) < 0$.*

Proof: Let f be any function in C_o^∞ and let $g(x) = b^2 f(bx)$. Let $\bar{x} = bx$ and $\bar{y} = by$, we have

$$D(g^2, g^2) = b^8 \frac{1}{2} \int\int \frac{f^2(bx) f^2(by)}{|x-y|} dx dy = \frac{1}{2} b^3 \int\int \frac{f^2(\bar{x}) f^2(\bar{y})}{|\bar{x} - \bar{y}|} d\bar{x} d\bar{y}.$$

Let $y = bx$, we have

$$\int |\nabla g|^2 dx = \int |b^2 \nabla f(bx) \cdot b|^2 dx = \int b^6 |\nabla f(bx)|^2 dx = b^3 \int |\nabla f(y)|^2 dy,$$

and

$$\int g^{8/3} dx = b^{16/3} \int f^{8/3}(bx) dx = b^{16/3} \int f^{8/3}(y) b^{-3} dy = b^{7/3} \int f^{8/3}(y) dy,$$

and

$$\int g^{10/3} \ln(1 + g^{-\frac{2}{3}}) dx = \int b^{20/3} f^{10/3}(bx) \ln\left(1 + \frac{1}{b^{4/3} f^{2/3}(bx)}\right) dx$$
$$= b^{11/3} \int f^{10/3}(y) \ln\left(1 + \frac{1}{b^{4/3} f^{2/3}(y)}\right) dy$$

where

$$\ln(1+\frac{1}{b^{4/3}f^{2/3}(y)}) = \ln(1+\frac{1}{f^{2/3}(y)}) - \frac{2}{3}\cdot\frac{f^{-5/3}}{1+f^{-2/3}}(b^{4/3}f^{2/3}-f^{2/3}) + ...$$

We find that the power of b in

$$b^{11/3}\int f^{10/3}(y)\ln\left(1+\frac{1}{b^{4/3}f^{2/3}(y)}\right)dy$$

is lager than $b^{11/3}$. Therefore, the power of b in $\int g^{8/3}dx$ is the smallest one. Hence, for some sufficiently small, but positive b, $\phi(g) < 0$.

□

The next two proofs will use the idea that:

1. If G is the Green's function of an operator L, then the solution for f of the equation $Lf = h$ is given by $f(x) = \int h(s)G(x,s)ds$.

2. (see [22] p.46)
   Let k be a complex number such that Im$k \geq 0$. The function

$$\phi_0(x,y) := \frac{1}{4\pi}\frac{e^{ik|x-y|}}{|x-y|} \quad x,y\in\mathbb{R}^3 \;\; x\neq y$$

   is a solution to the Helmholtz equation

$$\triangle\phi + k^2\phi = 0$$

   with respect to x for any fixed y. Because of polelike singularity at $x \neq y$, the function ϕ_0 is called a fundamental solution to the Helmholtz equation.

Theorem 6.3 *ψ is bounded on $\mathbb{R}^3$ and $\psi(x)\to 0$ as $|x|\to\infty$. Also, $\psi\in H^2$ (i.e., $\psi, \nabla\psi$ and $\triangle\psi\in L^2$).*

Proof: It follows from Appendix that for $\psi \geq 0$,

$$-\frac{4}{3}\psi^{2/3} - \frac{1}{3}\cdot\frac{\psi^{2/3}}{1+\psi^{-2/3}} + \frac{5}{3}\psi^{4/3}\ln(1+\psi^{-2/3}) + \alpha \geq 0.$$

By the definition, we also know that $\mathcal{B}(\psi^2) \geq 0$. Therefore, we have

$$-\triangle\psi \leq V\psi.$$

So

$$(-\triangle + 1)\psi \leq (V + 1)\psi.$$

Since ψ is continuous (Theorem 5.1), it follows that (V+1)$\psi \in L^2$ and thus $\psi \leq (-\triangle + 1)^{-1}[(V + 1)\psi]$(By maximal principle, see [19] Chapter 3). Set $F = (-\triangle + 1)^{-1}[(V + 1)\psi]$. Then

$$(-\triangle + 1)F = (V + 1)\psi \in L^2.$$

So

$$F = \Gamma_0 * (V + 1)\psi$$

where Γ_0 is the Green's function of $-\triangle + 1$. As it is well known, F is bounded and goes to zero as $|x| \to \infty$. Therefore, ψ is bounded and goes to zero as $|x| \to \infty$. Finally, note that

$$\frac{\psi^{5/3}}{1 + \psi^{-2/3}} < \psi^{5/3} \qquad for\ \psi \geq 0$$

and

$$\psi^{7/3}\ln(1 + \psi^{-2/3}) < \psi^{7/3} + \psi^{5/3}.$$

We know that $\psi^{5/3}$ and $\psi^{7/3} \leq d\psi$ for some constant d (since $\psi(x) \to 0$ as $|x| \to \infty$), and $\mathcal{B}(\psi^2)\psi \in L^2$ (since $\psi \in L^3$ and $\mathcal{B}(\psi^2) \in L^6$). So

$$-\frac{4}{3}\psi^{5/3} - \frac{1}{3}\frac{\psi^{5/3}}{1 + \psi^{-2/3}} + \frac{5}{3}\psi^{7/3}\ln(1 + \psi^{-2/3}) + \alpha\psi - V\psi + \mathcal{B}(\psi^2)\psi \in L^2.$$

Therefore, we conclude that $\triangle\psi \in L^2$ and so $\psi \in H^2$.

□

Theorem 6.4 *Let ψ be the positive solution to Euler equation(4.4). Then for every $0 < t < \alpha$, there exists a constant M such that*

$$\psi(x) \leq M \exp[-t^{1/2}|x|].$$

Proof: By (4.4) we have,

$$(-\triangle + W)\psi = 0.$$

So

$$\psi = -(-\triangle + t)^{-1}(W - t)\psi.$$

As $|x| \to \infty$, we know that $V \to 0$ and $\mathcal{B}(\psi^2) \to 0$ (since $\psi(x) \to 0$ as $|x| \to \infty$). From Appendix equation(A.1), as $|x| \to \infty$, we also know that

$$-\frac{4}{3}\psi^{2/3} - \frac{1}{3}\frac{\psi^{2/3}}{1+\psi^{-2/3}} + \frac{5}{3}\psi^{4/3}\ln(1+\psi^{-2/3}) + \alpha \to \alpha.$$

Hence, as $|x| \to \infty$, we have $W \to \alpha$. For $|x| >$ some R, $W - t > 0$ (since $0 < t < \alpha$ and $W \to \alpha > 0$ as $|x| \to \infty$). We know that

$$Y(x-y) := \frac{e^{-\sqrt{t}|x-y|}}{4\pi|x-y|}$$

is the Green's function of $-\triangle + t$ (see [22] p.46). Therefore, since $\psi > 0$,

$$\begin{aligned}
\psi(x) &= -\int Y(x-y)(W(y)-t)\psi(y) \\
&= -\Big(\int_{|y|\le R} Y(x-y)[W(y)-t]\psi(y)dy + \int_{|y|>R} Y(x-y)[W(y)-t]\psi(y)dy\Big) \\
&\le -\int_{|y|\le R} Y(x-y)[W(y)-t]\psi(y)dy \\
&= -\int_{|y|\le R} \frac{e^{-\sqrt{t}|x-y|}}{4\pi|x-y|}[W(y)-t]\psi(y)dy.
\end{aligned}$$

Hence,

$$\psi(x) \le M\exp[-t^{1/2}|x|].$$

□

A Appendix

A.1 Claim that $J(\rho)$ is not positive for $\rho \geq 0$.

Proof:

$$J(\rho) = -\rho^{4/3} + \rho^{5/3}\ln(1+\rho^{-1/3}).$$

So

$$\lim_{\rho\to 0} J(\rho) = \lim_{\rho\to 0}\frac{\ln(1+\rho^{-1/3})}{\rho^{-5/3}} = \lim_{\rho\to 0}\frac{-\frac{1}{3}\rho^{-4/3}}{-\frac{5}{3}\rho^{-8/3}(1+\rho^{-1/3})} = 0.$$

On the other hand,

$$\begin{aligned} J'(\rho) &= -\frac{4}{3}\rho^{1/3} + \frac{5}{3}\rho^{2/3}\ln(1+\rho^{-1/3}) + \rho^{5/3}\frac{-\frac{1}{3}\rho^{-4/3}}{1+\rho^{-1/3}} \\ &= -\frac{4}{3}\rho^{1/3} + \frac{5}{3}\rho^{2/3}\ln(1+\rho^{-1/3}) - \frac{1}{3}\cdot\frac{\rho^{1/3}}{1+\rho^{-1/3}} \\ &= \frac{1}{3}\rho^{1/3}\Big[-4 + 5\rho^{1/3}\ln(1+\rho^{-1/3}) - \frac{\rho^{1/3}}{\rho^{1/3}+1}\Big]. \end{aligned}$$

Let $u = \frac{\rho^{1/3}+1}{\rho^{1/3}} > 1$. Then $\rho^{1/3} = \frac{1}{u-1}$. So

$$-4 + 5\rho^{1/3}\ln(1+\rho^{-1/3}) - \frac{\rho^{1/3}}{\rho^{1/3}+1}$$

$$\begin{aligned} &= -4 + \frac{5}{u-1}\ln(u) - \frac{1}{u} = \frac{-4u-1}{u} + \frac{5}{u-1}\ln(u) \\ &= \frac{1}{u-1}\Big[-\frac{(4u+1)(u-1)}{u} + 5\ln(u)\Big] = \frac{1}{u-1}\Big[-\frac{4u^2-3u-1}{u} + 5\ln(u)\Big]. \end{aligned}$$

Let $y_1 = 5\ln(u)$ and $y_2 = \frac{4u^2-3u-1}{u}$. Then $y_1' = \frac{5}{u}$ and $y_2' = \frac{4u^2+1}{u^2}$. Hence,

$$y_2' - y_1' = \frac{1}{u^2}(4u^2 - 5u + 1) = \frac{(4u-1)(u-1)}{u^2} > 0.$$

Since $y_1(1) = y_2(1) = 0$, we have

$$-4 + 5\rho^{1/3}\ln(1+\rho^{-1/3}) - \frac{\rho^{1/3}}{\rho^{1/3}+1} < 0.$$

Thus, $J'(\rho) < 0$ for $\rho \geq 0$. Combining $\lim_{\rho\to 0} J(\rho) = 0$ and $J'(\rho) < 0$ for $\rho \geq 0$, we get $J(\rho)$ is not positive for $\rho \geq 0$.

A.2 Claim that $J_\alpha(\rho)$ and $J'_\alpha(\rho) \geq 0$ for $\alpha \geq \frac{1}{2}$ is a constant and $\rho \geq 0$.

Proof:

$$J_\alpha(\rho) = -\rho^{4/3} + \rho^{5/3} \ln\left(1 + \frac{1}{\rho^{1/3}}\right) + \alpha\rho.$$

So

$$\begin{aligned} J'_\alpha(\rho) &= -\frac{4}{3}\rho^{1/3} + \frac{5}{3}\rho^{2/3}\ln\left(1+\frac{1}{\rho^{1/3}}\right) + \rho^{5/3}\frac{-\frac{1}{3}\rho^{-4/3}}{1+\frac{1}{\rho^{1/3}}} + \alpha \\ &= -\frac{4}{3}\rho^{1/3} + \frac{5}{3}\rho^{2/3}\ln\left(1+\frac{1}{\rho^{1/3}}\right) - \frac{1}{3}\cdot\frac{\rho^{1/3}}{1+\rho^{-1/3}} + \alpha. \end{aligned}$$

To prove $J'_\alpha(\rho) \geq 0$ for $\rho \geq 0$ it is equivalent to show that $\lim_{\rho\to 0} J'_\alpha(\rho) = \alpha > 0$, $\lim_{\rho\to\infty} J'_\alpha(\rho) \geq 0$, and $J''_\alpha \neq 0$. We find that

$$\begin{aligned} \lim_{\rho\to 0} J'_\alpha(\rho) &= \lim_{\rho\to 0} -\frac{4}{3}\rho^{1/3} + \frac{5}{3}\rho^{2/3}\ln\left(1+\frac{1}{\rho^{1/3}}\right) - \frac{1}{3}\cdot\frac{\rho^{1/3}}{1+\rho^{-1/3}} + \alpha \\ &= \lim_{\rho\to 0} \frac{5}{3}\rho^{2/3}\ln\left(1+\frac{1}{\rho^{1/3}}\right) + \alpha \end{aligned}$$

and

$$\begin{aligned} \lim_{\rho\to 0} \rho^{2/3}\ln\left(1+\frac{1}{\rho^{1/3}}\right) &= \lim_{\rho\to 0}\frac{\ln(1+\frac{1}{\rho^{1/3}})}{\rho^{-2/3}} = \lim_{\rho\to 0}\frac{(-\frac{1}{3}\rho^{-3/4})/(1+\rho^{-1/3})}{-\frac{2}{3}\rho^{-3/5}} \\ &= \lim_{\rho\to 0}\frac{1}{2}\cdot\frac{1}{\rho^{-1/3}(1+\rho^{-1/3})} = 0. \end{aligned}$$

Hence,

$$\lim_{\rho\to 0} J'_\alpha(\rho) = \alpha. \tag{A.1}$$

On the other hand,

$$\begin{aligned} \lim_{\rho\to\infty} J'_\alpha(\rho) &= \lim_{\rho\to\infty} -\frac{4}{3}\rho^{1/3} + \frac{5}{3}\rho^{2/3}\ln\left(1+\frac{1}{\rho^{1/3}}\right) - \frac{1}{3}\cdot\frac{\rho^{1/3}}{1+\rho^{-1/3}} + \alpha \\ &= \lim_{y\to\infty}\frac{1}{3}\left[-4y + 5y^2\ln(1+y^{-1}) - \frac{y}{1+y^{-1}}\right] + \alpha \end{aligned}$$

and

$$\lim_{y\to\infty}\frac{1}{3}\cdot\frac{-4+5y\ln(1+\frac{1}{y}) - \frac{y}{y+1}}{1/y} = \lim_{y\to\infty}\frac{1}{3}\cdot\frac{5\ln(1+\frac{1}{y}) + 5y\frac{y}{y+1}\cdot(-\frac{1}{y^2}) - \frac{1}{(y+1)^2}}{-1/y^2}$$

$$
\begin{aligned}
&= \lim_{y\to\infty} \frac{1}{3} \cdot \frac{5\ln(1+\frac{1}{y}) - \frac{5}{y+1} - \frac{1}{y^2+2y+1}}{-1/y^2} \\
&= \lim_{y\to\infty} \frac{1}{3}\Big[-5y^2 \ln(1+\frac{1}{y}) + 5y^2\frac{1}{y+1} + \frac{y^2}{y^2+2y+1}\Big] \\
&= \frac{1}{3} + \frac{1}{3}\lim_{y\to\infty} 5y^2\Big[-\ln\Big(1+\frac{1}{y}\Big) + \frac{1}{y+1}\Big] = \frac{1}{3} + \frac{1}{3}\lim_{y\to\infty} \frac{-\ln(1+y^{-1}) + \frac{1}{y+1}}{\frac{1}{5}y^{-2}} \\
&= \frac{1}{3} + \frac{1}{3}\lim_{y\to\infty} \frac{-(\frac{y}{y+1})(-\frac{1}{y^2}) - \frac{1}{(y+1)^2}}{\frac{-2}{5}\cdot\frac{1}{y^3}} = \frac{1}{3} + \frac{1}{3}\lim_{y\to\infty} \frac{\frac{1}{y(y+1)^2}}{\frac{-2}{5}\cdot\frac{1}{y^3}} \\
&= \frac{1}{3} + \frac{1}{3}\lim_{y\to\infty} \frac{-5}{2}\frac{y^2}{(y+1)^2} = \frac{1}{3} + \frac{1}{3}\cdot\frac{-5}{2} = \frac{-1}{2}.
\end{aligned}
$$

Hence,

$$
\lim_{\rho\to\infty} J'_\alpha(\rho) \geq 0. \tag{A.2}
$$

We note that

$$
\begin{aligned}
J''_\alpha(\rho) &= -\frac{4}{9}\rho^{-2/3} + \frac{10}{9}\rho^{-1/3}\ln(1+\rho^{-1/3}) + \frac{5}{3}\rho^{2/3}\cdot\frac{-\frac{1}{3}\rho^{-3/4}}{1+\rho^{-1/3}} \\
&\quad -\frac{1}{3}\cdot\frac{\frac{1}{3}\rho^{-2/3}(1+\rho^{-1/3}) - \rho^{1/3}(-\frac{1}{3})\rho^{-4/3}}{(1+\rho^{-1/3})^2} \\
&\neq 0.
\end{aligned} \tag{A.3}
$$

By (A.1)(A.2)(A.3), we have

$$
J'_\alpha(\rho) \geq 0. \tag{A.4}
$$

Note that

$$
\begin{aligned}
\lim_{\rho\to 0} J_\alpha(\rho) &= \lim_{\rho\to 0} -\rho^{4/3} + \rho^{5/3}\ln(1+\rho^{-1/3}) + \alpha\rho \\
&= \lim_{\rho\to 0} \rho^{5/3}\ln(1+\rho^{-1/3}) \\
&= \lim_{\rho\to 0} \frac{\ln(1+\rho^{-1/3})}{\rho^{-5/3}} \\
&= \lim_{\rho\to 0} \frac{(-\frac{1}{3}\rho^{-3/4})/(1+\rho^{-1/3})}{-\frac{5}{3}\rho^{-8/3}} \\
&= \lim_{\rho\to 0} \frac{1}{5\rho^{-4/3}(1+\rho^{-1/3})} \\
&= 0.
\end{aligned} \tag{A.5}
$$

By (A.4) and (A.5), we have $J_\alpha(\rho) \geq 0$ for $\alpha \geq \frac{1}{2}$ and $\rho \geq 0$.

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