รายงานวิจัยฉบับสมบูรณ์

โครงการการวิเคราะห์การพองตัว มิติและพลังงานสูงของสสาร

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มกราคม 2554

สัญญาเลขที่ MRG5080276

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งานวิจัยพิสูจน์ว่าพลังงานที่สถานะพื้นของระบบหลาย(หรือหนึ่ง) อนุภาค ซึ่งมีพลังงานจลน์แบบสัมพัทธภาพสำหรับศักย์กริริยาใดๆ มีขอบเขตบนสอดคล้องกับระบบซึ่งมีปฏิกิริยาพลังงานจลน์แบบไม่สัมพัทธภาพ และงานวิจัยยังพิสูจน์ว่าความเสถียรของสสารที่ไม่เป็นไปตามหลักการกีดกันและมีศักย์แบบลอการิทึมในสองมิติ ขอบเขตล่างของพลังงานสถานะพื้นขึ้นอยู่กับจำนวนอนุภาค N ความสัมพันธ์ระหว่าง N และรัศมี R ของสสารที่ไม่เป็นไปตามหลักการกีดกัน แสดงให้เห็นว่า สสารจะพองตัวเมื่อนำสสารประเภทดังกล่าวมารวมกันเป็นจำนวนมากๆ ภายใต้ศักย์แบบลอการิทึมใน 2 มิติ

Keywords : พลังงานสถานะพื้น ระบบหลายอนุภาค, พลังงานจลน์สัมพัทธภาพ, ปัญหาสเถียรภาพ, ก้อนสสาร, สเถียรภาพของสสารใน 2 มิติ, ศักย์แบบลอการิทึม.

Abstract

Project Code : MRG5080276

Project Title : Inflation, Dimensionality and High-Energy Estimate for Matter

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Project Period : 2 July, 2007 – 1 January, 2011

We prove rigorously that the ground-state energy of many-(or single-) particle systems with relativistic kinetic energies for arbitrary given interaction potentials is bounded above by the corresponding one for systems with non-relativistic kinetic energies and this is true independently of the statistics obeyed by the underlying particles and independently of the dimensionality of space. We also prove rigorously the stability of matter without exclusion principle in two dimensions with logarithmic potential. The lower bound for the ground-state energy of this matter depends on a single power of number of particle, N. The relationship between N and radius R of matter without exclusion principle in this project implies the matter will inflate if we put more and more such matter together .

Keywords : ground-state energy, many-particle systems, relativistic kinetic energies, stability problems, matter in the bulk, stability of matter in 2-dimensions, with logarithmic potentials.

สารบัญ

ความสำคัญและที่มาของปัญหา

การวิเคราะห์เชิงคณิตศาสตร์ที่ชัดเจนโดยใช้หลักการขั้นพื้นฐานของการกีดกันของเพาลีได้พบความมีเสถียรภาพในก้อนสสารที่มีอยู่ช้านานในโลกของเรา โดยได้คำนวณหาขอบเขตล่างและขอบเขตบนหลายวิธีสำหรับพลังงานสถานะพื้นอย่างแม่นตรง

ในปี 1967 Dyson ได้ตีพิมพ์ผลงานซึ่งถือได้ว่าเป็นงานชิ้นแรกที่แสดงให้เห็นถึงความจำเป็นของหลักการกีดกันของเพาลีในการป้องกันการยุบตัวของสสาร โดยเขาใช้คณิตศาสตร์ที่ซับซ้อนและให้ผลการคำนวณอย่างแม่นตรง ซึ่งเขาได้คำตอบคือ สสารที่ละทิ้งหลักการกีดกันของเพาลีจะเป็นสสารที่ไม่เสถียร และถือว่า Dyson ได้บุกเบิกและจุดประกายให้เห็นว่าเสถียรภาพและอเสถียรภาพของสสารสามารถพิสูจน์ได้อย่างแม่นตรงและเป็นแนวทางในการศึกษาวิจัยของนักฟิสิกส์รุ่นต่อๆ มา

ในปี 1991 งานวิจัยของ Prof. E. Leib และ Prof. W. Thirring [1991] ถูกรวบรวมไว้ในหนังสือชื่อ The Stability of Matter From Atoms to Stars โดยมี Prof. W. Thirring [1991] เป็นบรรณาธิการ โดยงานวิจัยที่อยู่ในหนังสือเล่มนนี้ก็มุ่งที่จะอธิบายเสถียรภาพของสสารในธรรมชาติ

ในปี 2004 Manoukian และ Sirininlakul ได้ตีพิมพ์ผลงานในวารสาร physics letter A งานชิ้นนี้ได้ศึกษาขอบเขตล่างที่ชัดเจนของพลังงานสถานะพื้นของสสารทั้งโบซอนและเฟอร์มิออน

ในปี 2005 Manoukian และ Sirininlakul ได้ตีพิมพ์ผลงานในวารสาร Physical Review Letters งานชิ้นนี้ได้ให้คำตอบเกี่ยวกับการเพิ่มของรัศมีของระบบสสารที่มีสปิน 1/2 โดยอิเล็กตรอนในระบบมีความเร็ว v ปฏิกิริยาภายใต้คูลอมบ์ว่า เมื่อเพิ่มจำนวนของอิเล็กตรอนเข้าไปในระบบสสารเรื่อยๆ เงื่อนไขของการที่เราจะพบอิเล็กตรอนในก้อนสสารอันหนึ่งนั้นคือ ความน่าจะเป็นของการพบอิเล็กตรอนในทรงกลมรัศมี R ที่ครอบครองโดยสสารนั้นต้องไม่เท่ากับศูนย์ และเงื่อนไขนี้นำไปสู่พฤติกรรมของรัศมี R ของทรงกลมจำเป็นต้องเพิ่มขึ้นไม่น้อยกว่าลำดับการเพิ่มของ $N^{1/3}$ เมื่อ N มีค่ามากๆ

ในปี 2006 Manoukian และ Sirininlakul ได้ตีพิมพ์ผลงงานวิจัยในวารสาร Reports in Mathematical Physics งานชิ้นนี้ได้ศึกษาเสถียรภาพของสสารเฟอร์มิออนและการขยายตัวของสสารเฟอร์มิออนเมื่อมีการเพิ่มจำนวนของอิเล็กตอนในระบบใน 2 มิติ

แต่จากงานวิจัยต่างๆ ที่กล่าวมาข้างต้น ยังไม่มีงานวิจัยชิ้นไหนที่ได้กล่าวถึง การขยายตัวของระบบที่ประกอบด้วยอิเล็กตอนที่มีความเร็วสูงหรือความเร็วใกล้ความเร็วแสงในระบบและเสถียรภาพของสสารภายใต้เงือนไขที่เพิ่มเติมจากพลังงานจลน์และศักย์คูลอมบ์ ในมิติต่างๆ

งานวิจัยชิ้นนี้จึงมุ่งตอบคำถามดังนี้

1. ถ้าระบบประกอบด้วยอิเล็กตรอนที่มีความเร็วเข้าใกล้แสง ผู้วิจัยจะศึกษาขอบเขตพลังงานจลน์ของระบบในแง่สัมพัทธภาพ เทียบกับระบบในแง่ที่ไม่คิดสัมพัทธภาพ จะยังคงเหมือนเดิมหรือแตกต่างจากเดิมหรือไม่ อย่างไร
2. ของเขตของพลังงานสถานพื้นของระบบภายใต้เงื่อนไขและมิติ มีความสัมพันธ์กันอย่างไรกับเสถียรภาพของสสาร

การตอบปัญหาดังกล่าวจะทำให้เราทราบและเข้าใจลึกซึ้งเกี่ยวกับเสถียรภาพและอเสถียรภาพของสสารมากยิ่งขึ้น นอกจากนี้เราอาจสามารถนำระเบียบวิธีการทางคณิตศาสตร์ (เทคนิค functional ของ J. Schwinger) ที่ใช้คำนวณหาพลังงานสถานะพื้นของระบบไปประยุกต์ใช้กับการหาพลังงานสถานะพื้นของระบบสสารบางอย่างที่มีอยู่จริงในธรรมชาติได้ และองค์ความรู้ที่ได้จากงานวิจัยเป็นองค์ความรู้พื้นฐานทางฟิสิกส์ที่จะคงอยู่ต่อไปตราบนานเท่านาน

วัตถุประสงค์

1. ศึกษาเขตของพลังงานจลน์ของระบบเป็นไปตามทฤษฎีสัมพัทธภาพพิเศษของไอน์สไตน์

2. ศึกษาการเสถียรภาพและขีดจำกัดความหนาแน่นของการพองตัวของสสาร

CHAPTER I

On the ground-state energy of many-particle systems with relativistic kinetic energies

1.1 Introduction

Much progress has been made over the years in deriving rigorous bonds on the ground-state energy of many-particle quantum systems (Dyson (1967), Dyson and Lenard (1968), Lieb and Thirring (1975), Semenoff and Wijewardhana (1987), Lieb (1991), Forte (1992), Geyer (1995), Badhuri, Murthy and Srivastava (1996), Oka (1997) , Manoukian and Sirininlakul (2005)). Particular emphasis was put in these references on the stability problem, or otherwise collapse, of such systems as the number of the underlying particles is made to increase paying special attention, in the process of the investigations, on the statistics obeyed by the underlying particles. The generalization of such analyses to so-call relativistic quantum systems (Dyson (1967)) has been relatively more involved, and an important extension of the earlier studies has been in adopting the relativistic kinetic energies of the underlying particles. The purpose of this communication is to establish rigorously some explicit statements concerning such a generalization

1.2 On the ground-state energy of many-particle systems with relativistic kinetic energies

Consider a Hamiltonian of an N-particle system

$$H_{NR} = \sum_{j=1}^{N} \frac{\mathbf{p_j^2}}{2m_j} + H_I\left(\mathbf{x_1}, \ldots, \mathbf{x_N}\right). \tag{1.1}$$

Where $H_I(\mathbf{x_1, \ldots, x_N})$ is an arbitrary interaction Hamiltonian such that the system admits a ground-state energy which we denote by E_{NR}. For the corresponding Hamiltonian with relativistic kinetic energies of the particles we have

$$H_R = \sum_{j=1}^{N} \left(\sqrt{\mathbf{p_j^2} c^2 + m_j^2 c^4} - m_j c^2 \right) + H_I \left(\mathbf{x_1, \ldots, x_N} \right) \tag{1.2}$$

where c is the speed of light. Let E_R denote the ground-state energy of this Hamiltonian. We then show that

$$E_R \leq E_{NR} \tag{1.3}$$

indenpendently of the statistics obeyed by the particles and *indenpendently* of the dimensionality of space. The demonstration is not difficult but the result is undoubtedly important realizing its generality in applications including for the case $N = 1$. In particular, this established the instability of so-called "*bosonics* matter", obtained by relaxing the Pauli exclusion principle (Dyson and Lenard (1968) Forte (1992), Geyer (1995), Manoukian and Sirininlakul (2005)). with relativistic kinetic energies E_R, i.e., for $-E_R$, with the some power of N as a lower bound obtained for $-E_{NR}$ with non-relativistic kinetic energies for the latter.

Intuitively, so to speak, stability, and the corresponding boundedness of the ground-state energy from below, arises from a balance between the positive kinetic energy terms and the negative part of the interaction Hamiltonian (as well as, of course, of the positive part of the latter). A kinetic energy part has a large (positive) contribution for large values of $|\mathbf{p_j}|$. In the non-relativistic case, a kinetic energy part increases with two power of $|\mathbf{p_j}|$ in contrast to the relativistic case which increases with just a single power. [This argument alone indicates the importance of the generalization to the relativistic case for careful studies involving higher energies.] Accordingly, based on such an intuitive argument, the result stated in (1.3) is expected. The actual technical demonstration of this now follows.

Consider an N-particle wavefunction $\Psi(\mathbf{x_1}\rho_1,\ldots,\mathbf{x}_N\rho_N)$ consistent with the underlying statistics obeyed by the particles, where the denote any additional labels, such as spin, needed to specify the state of a particle. With the Fourier transform defined via

$$\Psi\left(\mathbf{x}_1\rho_1,\ldots,\mathbf{x}_N\rho_N\right)=\int\frac{d^\upsilon\mathbf{p}_1}{\left(2\pi\hbar\right)^\upsilon}\cdots\frac{d^\upsilon\mathbf{p}_N}{\left(2\pi\hbar\right)^\upsilon}\,e^{i\sum\limits_{j=1}^{N}\mathbf{x}_j\cdot\mathbf{p}_j/\hbar}\,\Phi\left(\mathbf{p}_1\rho_1,\ldots,\mathbf{p}_N\rho_N\right)\quad(1.4)$$

where υ denotes the dimensionality of space, we obtain for the expectation value of the relativistic kinetic energy

$$T_R=\sum_{j=1}^{N}\left(\sqrt{-\hbar^2c^2\nabla_j^2+m_j^2c^4}-m_jc^2\right)\quad(1.5)$$

the expression

$$\langle\Psi\,|T_R\rangle\mid\Psi\rangle=\sum_{j=1}^{N}\int\frac{d^\upsilon\mathbf{p}_1}{\left(2\pi\hbar\right)^\upsilon}\cdots\frac{d^\upsilon\mathbf{p}_N}{\left(2\pi\hbar\right)^\upsilon}\left(\sqrt{\mathbf{p}_j^2c^2+m_j^2c^4}-m_jc^2\right)$$

$$\times\left|\Phi\left(\mathbf{p}_1\rho_1,\ldots,\mathbf{p}_N\rho_N\right)\right|^2\quad(1.6)$$

[We note in passing that the square-root operator in (1.5) is a well defined operator.] We use the integral representation

$$\left(\sqrt{\mathbf{p}^2c^2+m^2c^4}-mc^2\right)=\frac{\mathbf{p}^2c^2}{2}\int\limits_0^1dx\frac{1}{\sqrt{\mathbf{p}^2c^2x+m^2c^4}}\quad(1.7)$$

for numericals, to derive the bound

$$\left(\sqrt{\mathbf{p}^2c^2+m^2c^4}-mc^2\right)\leq\frac{\mathbf{p}^2c^2}{2}\int\limits_0^1dx\frac{1}{\sqrt{m^2c^4}}=\frac{\mathbf{p}^2}{2m}\quad(1.8)$$

from which and from (1.6), we obtain the bound

$$\langle\Psi\left|T_R\right|\Psi\rangle \leq \sum_{j=1}^{N}\int\frac{d^v\mathbf{p}_1}{(2\pi\hbar)^v}\cdots\frac{d^v\mathbf{p}_N}{(2\pi\hbar)^v}\frac{\mathbf{p}_j^2}{2m_j}\left|\Phi\left(\mathbf{p}_1\rho_1,\ldots,\mathbf{p}_N\rho_N\right)\right|^2$$

$$= \langle\Psi\left|T_{NR}\right|\Psi\rangle \tag{1.9}$$

with

$$T_{NR} = \sum_{j=1}^{N}\frac{-\hbar^2\nabla_j^2}{2m_j} \tag{1.10}$$

[Needless to say, this inequality, as a rigorous mathematical statement, does not mean that at high energies the kinetic energies are given by the non-relativistic expressions rather than the relativistic ones.]

From (1.1), (1.2) and (1.9), we then obtain the basic inequality

$$\langle\Psi\left|H_R\right|\Psi\rangle \leq \langle\Psi\left|H_{NR}\right|\Psi\rangle\,. \tag{1.11}$$

In particular, for $|\Psi\rangle$ *corresponding to the ground-state energy of* H_{NR}, denoted conveniently by $|\Psi_{NR}\rangle$, i.e., for which $\langle\Psi_{NR}\left|H_{NR}\right|\Psi_{NR}\rangle = E_{NR}, |\Psi_{NR}\rangle$ is not necessarily the ground-state of H_{NR}. That is, $\langle\Psi_{NR}\left|H_R\right|\Psi_{NR}\rangle$ *cannot be any smaller than* E_R . This leads from (1.11) to the inequality

$$E_R \leq \langle\psi_{NR}\left|H_R\right|\psi_{NR}\rangle \leq \langle\psi_{NR}\left|H_{NR}\right|\psi_{NR}\rangle = E_{NR} \tag{1.12}$$

which is the statement in (1.3).

The inequality in (1.3), as stated above, also establishes, as a special case, the instability of so-called "bosonic matter" for which upper bounds for E_{NR} are known as powers of N - the number of underlying particles - leading to

$$E_R \leq -CN^{\gamma} \tag{1.13}$$

where $\gamma > 1$. Here the positive constants C and the exponents γ are estimated from the non-relativistic expressions (Dyson (1967), Dyson and Lenard (1967), Semenoff and Wijewardhana (1987), Forte (1992), Geyer (1995), Badhuri and Murthy (1996), Oka (1997) , Manoukian and Sirininlakul (2005)). We expect that the method of analysis used in this communication will be useful for related developments of relativistic many-particle systems and, in particular, to "fermionic matter". Such investigations will be carried out in a future report.

CHAPTER II

Stability and high density limit of bosonic matter in $2D$

2.1 Introduction

One of the most fundamental problems that quantum mechanics has solved was that of the stability of matter (Lieb and Thirring (1975)). This result is based on two basic properties, one is the boundedness of the ground-state energy from below and the Pauli exclusion principle. For matter, with the exclusion principle and with Coulomb interaction, the ground-state energy $E_N \sim N$, with N denoting the number of electrons in matter, and matter consisting of $(2N + 2N)$ particles, is not favoured over two separate systems brought together, each consisting of $(N+N)$ particles. This is unlike the situation with "matter" without the exclusion principle for which $E_N \sim N^\alpha$ with $\alpha > 1$. It is important to know if such properties are tied down with the dimensionality of space. In particular, there has been interest in recent years in physics in $2D$, e.g. (Kventzel and Katriel (1981), Semenoff and Wijewardhana (1987), Forte (1992), Geyer (1995), Badhuri, Murthy and Srivastava (1996)) and the role of spin and statistics. It is well known that matter is stable (Muthaporn and Manoukian (2004b)) in 2D with $1/r$ potentials with the exclusion principle. On the other hand, it is pertinent to know what the outcome is of one assumes the logarithmic potential in 2D as dictated by the Poisson equation $\nabla^2 \ln r \sim \delta^2(\mathbf{r})$. We prove rigorously that such matter is stable with logarithmic potentials without involving the exclusion principle. To do this, we first review the Thomas-Fermi atom in 2D with logarithmic potentials as well as the No-binding theorem for such a case and finally derive a lower bound for the exact ground-state of matter involving a single power of N. We also establish that such matter would necessarily increase radially not any slower than $N^{1/2}$ with N as it is for ordinary matter in 3D (Manoukian and Sirininlakul (2006)). Unlike the situation with a logarithmic potential, matter with $1/r$ potential is unstable. For reviews of problems of stability of matter see (Lieb (1975),Manoukian and Sirininlakul (2005)).

2.2 The Thomas-Fermi Atom for boson in $2D$

The semi-classical Green function part $G_{\sigma\sigma'}(\mathbf{x}t;\mathbf{x}'0)$ with spin indices σ, σ', with potential $V(\mathbf{x})$ in 2-dimensions is given by (Manoukian, 2006)

$$G_{\sigma\sigma'}(\mathbf{x}\tau;\mathbf{x}'0) = \delta_{\sigma\sigma'} \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \exp \mathrm{i}\left[\frac{\mathbf{p}.(\mathbf{x}-\mathbf{x}')}{\hbar} - \frac{\mathbf{p}^2}{2m}\tau - V(\mathbf{x})\tau\right] \tag{2.1}$$

and for coincident space points $\mathbf{x} = \mathbf{x}'$, we obtain

$$G_{\sigma\sigma'}(\mathbf{x}\tau;\mathbf{x}0) = \delta_{\sigma\sigma'} \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \exp\left[-\mathrm{i}\left(\frac{\mathbf{p}^2}{2m} + V(\mathbf{x})\right)\tau\right]. \tag{2.2}$$

where $\tau = t/\hbar$.

The particle density of (spin 0) bosons $n_{\mathrm{B}}(\mathbf{x})$ may be expressed in terms of the Green function $G_{\sigma\sigma'}(\mathbf{x}\tau;\mathbf{x}0)$ for coincident space points as

$$n_{\mathrm{B}}(\mathbf{x}) = \frac{1}{2\pi\mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon}\, G_{\sigma\sigma}(\mathbf{x}\tau;\mathbf{x}0)\, \mathrm{e}^{\mathrm{i}\xi\tau}\,, \qquad \epsilon \to +0 \tag{2.3}$$

where the spin multiplicity is 1. Substitute (2.2) into (2.3), to obtain

$$n_{\mathrm{B}}(\mathbf{x}) = \frac{1}{2\pi\mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon} \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \exp \mathrm{i}\left[\xi\tau - \frac{\mathbf{p}^2}{2m}\tau - V(\mathbf{x})\tau\right] \tag{2.4}$$

which upon using the integral representation of the step function

$$\Theta(\xi) = \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon}\ \mathrm{e}^{\mathrm{i}\xi\tau} \tag{2.5}$$

and

$$\Theta\left(\xi - V(\mathbf{x}) - \frac{\mathbf{p^2}}{2m}\right) = \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tau}{\tau - \mathrm{i}\varepsilon}\ \exp \mathrm{i}\left(\xi - V(\mathbf{x}) - \frac{\mathbf{p^2}}{2m}\right)\tau \tag{2.6}$$

with

$$\Theta\left(\xi - V(\mathbf{x}) - \frac{\mathbf{p^2}}{2m}\right) = 1 \tag{2.7}$$

for $0 < p < \sqrt{2m(\xi - V(\mathbf{x}))}$, when $p = |\mathbf{p}|$.

By using (2.6) and (2.7), as applied to the right-hand side of (2.4), we obtain

$$\begin{aligned} n_{\mathrm{B}}(\mathbf{x}) &= \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2}\ \Theta\left(\xi - V(\mathbf{x}) - \frac{\mathbf{p^2}}{2m}\right) \\ &= \frac{1}{(2\pi\hbar)^2} \int_0^{\sqrt{2m(\xi - V)}} p\ \mathrm{d}p \int \mathrm{d}\Omega_\nu \\ &= \frac{1}{(2\pi\hbar)^2} \frac{2\pi}{\Gamma(1)} \int_0^{\sqrt{2m(\xi - V(\mathbf{x}))}} p\ \mathrm{d}p \\ &= \frac{1}{(2\pi\hbar)^2} \frac{2\pi}{\Gamma(1)} \frac{\left(\sqrt{2m(\xi - V(\mathbf{x}))}\right)^2}{2} \\ &= \frac{2\pi}{2\ \Gamma(1)} \left(\frac{2m(\xi - V(\mathbf{x}))}{(2\pi\hbar)^2}\right). \end{aligned} \tag{2.8}$$

From (2.8), $V(\mathbf{x}) = 0$ and $n = 0$ at the boundary, we get $\xi = 0$. So that the density of bosons in 2-dimensions is

$$n_{\rm B}(\mathbf{x}) = \frac{2\pi}{2\,\Gamma\,(1)}\left(\frac{-2mV(\mathbf{x})}{(2\pi\hbar)^2}\right). \tag{2.9}$$

The relationship between the particle density $n_{\rm B}(\mathbf{x})$ and the potential $V(\mathbf{x})$ in 2-dimensions, i.e., given by

$$n_{\rm B}(\mathbf{x}) = -\,\frac{m}{2\pi\hbar^2}\;V(\mathbf{x}). \tag{2.10}$$

We may also rewrite (2.10) as

$$V(\mathbf{x}) = -\,\frac{2\pi\hbar^2}{m}\;n_{\rm B}(\mathbf{x}) \tag{2.11}$$

To obtain the sum of the kinetic energies of the bosons in D-dimensions ($T[n_{\rm B}]$), we use the relationship between the kinetic energy and the Green's function :

$$\begin{aligned}
T[n_{\rm B}] =& \sum_{\sigma}\int \mathrm{d}^2\mathbf{x}\;\frac{1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\tau}{\tau-\mathrm{i}\varepsilon}\left[\mathrm{i}\frac{\partial}{\partial\tau}-V(\mathbf{x})\right]G_{\sigma\sigma'}(\mathbf{x}t;\mathbf{x}0)\\
=& \int \mathrm{d}^2\mathbf{x}\;\frac{1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\tau}{\tau-\mathrm{i}\varepsilon}\left[\mathrm{i}\frac{\partial}{\partial\tau}-V(\mathbf{x})\right]G_{\sigma\sigma'}(\mathbf{x}t;\mathbf{x}0)\\
=& \int \mathrm{d}^2\mathbf{x}\,\frac{1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\tau}{\tau-\mathrm{i}\varepsilon}\left[\mathrm{i}\frac{\partial}{\partial\tau}-V(\mathbf{x})\right]\int\frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2}\exp\left[-\mathrm{i}\left(\frac{\mathbf{p}^2}{2m}+V(\mathbf{x})\right)\tau\right]\\
=& \int \mathrm{d}^2\mathbf{x}\;\frac{1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\tau}{\tau-\mathrm{i}\varepsilon}\int\frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2}\,\frac{\mathbf{p}^2}{2m}\;\exp\left[-\mathrm{i}\left(\frac{\mathbf{p}^2}{2m}+V(\mathbf{x})\right)\tau\right].
\end{aligned} \tag{2.12}$$

Upon using the integral representation of the step function

$$\Theta(\xi) = \frac{1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\tau}{\tau-\mathrm{i}\varepsilon}\;\mathrm{e}^{\mathrm{i}\xi\tau} \tag{2.13}$$

we obtain

$$\Theta\left(-\frac{\mathbf{p^2}}{2m}-V(\mathbf{x})\right)=\frac{1}{2\pi\mathrm{i}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\tau}{\tau-\mathrm{i}\varepsilon}\ \exp\mathrm{i}\left(-\frac{\mathbf{p^2}}{2m}-V(\mathbf{x})\right)\tau \tag{2.14}$$

and

$$\Theta\left(-\frac{\mathbf{p^2}}{2m}-V(\mathbf{x})\right)=1 \tag{2.15}$$

for $0<p<\sqrt{-2mV(\mathbf{x})}$.

By using (2.14) and (2.15), as applied to the right-hand side of (2.12), we obtain the relationship between the kinetic energy T and the potential V in 2-dimensions, is then given by

$$\begin{aligned}
T[n_{\mathrm{B}}] &= \int \mathrm{d}^2\mathbf{x}\int\frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2}\,\frac{\mathbf{p}^2}{2m}\ \Theta\left(-\frac{\mathbf{p^2}}{2m}-V(\mathbf{x})\right)\\
&=\frac{1}{(2\pi\hbar)^2}\int\mathrm{d}^2\mathbf{x}\int_0^{\sqrt{-2mV(\mathbf{x})}}\mathrm{d}^2p\ p\ \frac{p^2}{2m}\ \int\mathrm{d}\Omega\\
&=\frac{1}{2m(2\pi\hbar)^2}\frac{2\pi}{\Gamma\left(1\right)}\int\mathrm{d}^2\mathbf{x}\int_0^{\sqrt{-2mV(\mathbf{x})}}\mathrm{d}p\ p^{D+1}\\
&=\frac{1}{2m(2\pi\hbar)^2}\frac{2\pi}{\Gamma\left(1\right)}\int\mathrm{d}^2\mathbf{x}\ \frac{p^4}{4}\bigg|_0^{\sqrt{-2mV(\mathbf{x})}}\\
&=\frac{1}{2m(2\pi\hbar)^2}\frac{2\pi}{\Gamma\left(1\right)}\int\mathrm{d}^2\mathbf{x}\ \frac{(-2mV(\mathbf{x}))^2}{4}\\
&=\frac{1}{8m}\frac{2\pi}{\Gamma\left(1\right)}\int\mathrm{d}^2\mathbf{x}\ (-2mV(\mathbf{x}))\left(\frac{-2mV(\mathbf{x})}{(2\pi\hbar)^2}\right)\\
&=\frac{1}{8m}\frac{2\pi}{\Gamma\left(1\right)}\int\mathrm{d}^2\mathbf{x}\ \left(\frac{4m^2[V(\mathbf{x})]^2}{(2\pi\hbar)^2}\right)\\
&=\frac{m}{4\pi\hbar^2}\int\mathrm{d}^2\mathbf{x}\ [V(\mathbf{x})]^2.
\end{aligned} \tag{2.16}$$

Substitute (2.11) into the right-hand side of (2.16), to obtain

$$\begin{aligned} T[n_{\mathrm{B}}] =& \frac{m}{4\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}\ [V(\mathbf{x})]^2 \\ =& \frac{\pi\hbar^2}{m} \int \mathrm{d}^2\mathbf{x}\ \ [n_{\mathrm{B}}(\mathbf{x})]^2 . \end{aligned} \tag{2.17}$$

The Hamiltonian of a neutral atom consisting of Z bosons and a nucleus of charge $Z|e|$ is taken to be

$$H = \sum_{i=1}^{Z} \left(\frac{\mathbf{p}_i^2}{2m} - Ze^2 V(\mathbf{x}) \right) + \sum_{i<j}^{Z} \ e^2 V(\mathbf{x} - \mathbf{x}') \tag{2.18}$$

where $V(\mathbf{x})$ is the scaled potential satisfying the Poisson's equation given below :

$$\boldsymbol{\nabla}^2 2 \ln \frac{|\mathbf{x}|}{A} = 4\pi\delta^2(\mathbf{x}). \tag{2.19}$$

This is,

$$V(\mathbf{x}) = 2 \ln \frac{|\mathbf{x}|}{A} \tag{2.20}$$

for any dimensional scale factor A.

The expectation value of the Hamiltonian of a neutral atom consisting of Z bosons and a nucleus of charge $Z|e|$ in 2-dimensions is

$$\begin{aligned} \langle\Phi| H |\Phi\rangle = \langle\Phi| \sum_{i=1}^{Z} \frac{\mathbf{p}_i^2}{2m} |\Phi\rangle + 2Ze^2 \langle\Phi| \sum_{i=1}^{Z} \ln \frac{|\mathbf{x}|}{A} |\Phi\rangle \\ - 2e^2 \langle\Phi| \sum_{i<j}^{Z} \ln \frac{|\mathbf{x} - \mathbf{x}'|}{B} |\Phi\rangle \end{aligned} \tag{2.21}$$

where

$$\langle\Phi|\Phi\rangle = \int \mathrm{d}^2\mathbf{x}\ \Phi^*(\mathbf{x})\ \Phi(\mathbf{x})$$

$$= \int \mathrm{d}^2\mathbf{x}\, |\Phi(\mathbf{x})|^2$$

$$=1, \tag{2.22a}$$

$$\int \mathrm{d}^2\mathbf{x}\ n_{\mathrm{B}}(\mathbf{x}) = Z. \tag{2.22b}$$

Here A and B are dimensional scale factors which will be determined below. Form (2.17), we obtain the first term on the right-hand side of (2.21), corresponding to the kinetic energy term $T[n_{\mathrm{B}}] = \frac{\pi\hbar^2}{m} \int \mathrm{d}^2\mathbf{x}\ \left[n_{\mathrm{B}}(\mathbf{x})\right]^2$.

Consider the second term on the right-hand side of (2.21). This is given by

$$2Ze^2\, \langle\Phi| \sum_{i=1}^{Z} \ln \frac{|\mathbf{x}|}{A}\, |\Phi\rangle = 2Ze^2\, \langle\Phi|\, Z \ln \frac{|\mathbf{x}|}{A}\, |\Phi\rangle$$

$$= 2Ze^2\, \langle\Phi| \int \mathrm{d}^2\mathbf{x}\, n_{\mathrm{B}}(\mathbf{x}) \ln \frac{|\mathbf{x}|}{A}\, |\Phi\rangle$$

$$= 2Ze^2 \int \mathrm{d}^2\mathbf{x}\ \ln \frac{|\mathbf{x}|}{A}\ n_{\mathrm{B}}(\mathbf{x}). \tag{2.23}$$

Consider the third term on the right-hand side of (2.22). This is given by

$$2e^2\, \langle\Phi| \sum_{i<j}^{Z} \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\, |\Phi\rangle = 2\frac{e^2}{2} \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^2\mathbf{x}'\ n_{\mathrm{B}}(\mathbf{x})\ n_{\mathrm{B}}(\mathbf{x}') \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\, \langle\Phi|\Phi\rangle$$

$$= e^2 \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^2\mathbf{x}'\ n_{\mathrm{B}}(\mathbf{x})\ n_{\mathrm{B}}(\mathbf{x}') \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}. \tag{2.24}$$

Substitute (2.17), (2.23) and (2.24) into (2.21), to obtain

$$\begin{aligned}\langle\Phi|\, H\, |\Phi\rangle =& \frac{\pi\hbar^2}{m}\int \mathrm{d}^2\mathbf{x}\, [n(\mathbf{x})]^2 + 2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\, n(\mathbf{x}) \\ & - e^2\int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\, n(\mathbf{x}) \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\, n(\mathbf{x}'). \end{aligned} \tag{2.25}$$

Referring to (2.17), (2.23) and (2.24), one may define the interaction of the particle-nucleus system in terms of the boson density, and add to it the kinetic energy term . Let $F[n_{\mathrm{B}}]$ denote the *energy* functional in 2-dimensions as a function of the density $n_{\mathrm{B}}(\mathbf{x})$. From (2.25) we obtain

$$\begin{aligned}F[n_{\mathrm{B}}] =& \frac{\pi\hbar^2}{m}\int \mathrm{d}^2\mathbf{x}\, [n_{\mathrm{B}}(\mathbf{x})]^2 + 2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\, n_{\mathrm{B}}(\mathbf{x}) \\ & - e^2\int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\, n_{\mathrm{B}}(\mathbf{x}) \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\, n_{\mathrm{B}}(\mathbf{x}'). \end{aligned} \tag{2.26}$$

Optimize (2.26) with respect to $n_{\mathrm{B}}(\mathbf{x})$, to obtain

$$\begin{aligned} 0 =& \frac{\delta F[n_{\mathrm{B}}]}{\delta n_{\mathrm{B}}(\mathbf{x})} \\ =& \frac{2\pi\hbar^2}{m}\,[n_{\mathrm{B}}(\mathbf{x})] + 2Ze^2\ln\frac{|\mathbf{x}|}{A} - 2e^2\int \mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\, n_{\mathrm{B}}(\mathbf{x}') \\ -\frac{\pi\hbar^2}{m}\,[n_{\mathrm{B}}(\mathbf{x})] =& Ze^2\ln\frac{|\mathbf{x}|}{A} - e^2\int \mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\, n_{\mathrm{B}}(\mathbf{x}'). \end{aligned} \tag{2.27}$$

The density $n^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x})$ and potential $V^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x})$ may be obtained by functionally differentiating $F[n_{\mathrm{B}}]$ with respect to $n_{\mathrm{B}}(\mathbf{x})$, with solution $n^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x}) = n_{\mathrm{B}}(\mathbf{x})$ satisfying

$$n^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x}) = -\frac{mZe^2}{\pi\hbar^2}\ln\frac{|\mathbf{x}|}{A} + \frac{me^2}{\pi\hbar^2}\int \mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\, n^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x}'). \tag{2.28}$$

From (2.10), we obtain the relationship between $n_{\rm TF}^{\rm B}(\mathbf{x})$ and $V_{\rm TF}^{\rm B}(\mathbf{x})$ as

$$n_{\rm TF}^{\rm B}(\mathbf{x}) = \frac{2\pi}{2\,\Gamma(1)}\left(\frac{-2mV_{\rm TF}^{\rm B}(\mathbf{x})}{(2\pi\hbar)^2}\right)$$

$$= -\frac{m}{2\pi\hbar^2}\,V_{\rm TF}^{\rm B}(\mathbf{x}). \tag{2.29}$$

Substitute (2.28) into (2.29) to obtain

$$V_{\rm TF}^{\rm B}(\mathbf{x}) = Ze^2\left(2\ln\frac{|\mathbf{x}|}{A}\right) - e^2\int \mathrm{d}^2\mathbf{x}'\left(2\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\right)\,n_{\rm TF}^{\rm B}(\mathbf{x}') \tag{2.30}$$

and

$$\nabla^2 V_{\rm TF}^{\rm B}(\mathbf{x}) = Ze^2\nabla^2\left(2\ln\frac{|\mathbf{x}|}{A}\right) - e^2\nabla^2\int \mathrm{d}^2\mathbf{x}'\left(2\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\right)\,n_{\rm TF}^{\rm B}(\mathbf{x}')$$

$$\equiv F_1 - F_2 \tag{2.31}$$

where

$$F_1 = Ze^2\nabla^2\left(2\ln\frac{|\mathbf{x}|}{A}\right)$$

$$= Ze^2 4\pi\delta^2(\mathbf{x}) \tag{2.32}$$

and

$$F_2 = e^2\nabla^2\int \mathrm{d}^2\mathbf{x}'\left(2\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\right)\,n_{\rm TF}^{\rm B}(\mathbf{x}')$$

$$= e^2\int \mathrm{d}^2\mathbf{x}'\,n_{\rm TF}^{\rm B}(\mathbf{x}')\,\nabla^2\left(2\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\right)$$

$$= e^2\int \mathrm{d}^2\mathbf{x}'\,n_{\rm TF}^{\rm B}(\mathbf{x}')\,4\pi\delta^2(\mathbf{x}-\mathbf{x}')$$

$$=4\pi e^2 n_{\rm TF}^{\rm B}(\mathbf{x}). \tag{2.33}$$

Substitute (2.32) and (2.33) into (2.31), to obtain

$$\begin{aligned}\nabla^2 V_{\rm TF}^{\rm B}(\mathbf{x}) =&F_1 - F_2\\ =&4\pi Z e^2 \delta^2(\mathbf{x}) - 4\pi e^2 n_{\rm TF}^{\rm B}(\mathbf{x}).\end{aligned} \tag{2.34}$$

For the integral of the left-hand side of (2.34) over $\mathbf{x}$, we have

$$\int {\rm d}^2\mathbf{x}\ \nabla^2 V_{\rm TF}^{\rm B}(\mathbf{x}) =4\pi Z e^2 \int {\rm d}^2\mathbf{x}\ \delta^2(\mathbf{x}) - 4\pi e^2 \int {\rm d}^2\mathbf{x}\ n_{\rm TF}^{\rm B}(\mathbf{x}). \tag{2.35}$$

The first term on the right-hand side of (2.35) is easily evaluated giving by

$$4\pi Z e^2 \int {\rm d}^2\mathbf{x}\, \delta^2(\mathbf{x}) =4\pi Z e^2. \tag{2.36}$$

For the second-term of the right-hand side of (2.35), we obtain

$$4\pi e^2 \int {\rm d}^2\mathbf{x}\ n_{\rm TF}^{\rm B}(\mathbf{x}) =4\pi Z e^2. \tag{2.37}$$

Substitute (2.36) and (2.37) into (2.35), to obtain

$$\int {\rm d}^2\mathbf{x}\ \nabla^2 V_{\rm TF}^{\rm B}(\mathbf{x}) =4\pi Z e^2 - 4\pi Z e^2 = 0. \tag{2.38}$$

Apply Laplacian operator to the left-hand side of (2.28), to obtain

$$\begin{aligned}\nabla^2 n_{\rm TF}^{\rm B}(\mathbf{x}) =&\nabla^2 \left[-\frac{mZe^2}{\pi\hbar^2} \ln\frac{|\mathbf{x}|}{A} + \frac{me^2}{\pi\hbar^2}\int {\rm d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ n_{\rm TF}^{\rm B}(\mathbf{x}')\right]\\ =&-\frac{mZe^2}{\pi\hbar^2}\nabla^2 \ln\frac{|\mathbf{x}|}{A} + \frac{me^2}{\pi\hbar^2}\int {\rm d}^2\mathbf{x}'\ n_{\rm TF}^{\rm B}(\mathbf{x}')\ \nabla^2 \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\end{aligned}$$

$$= -\frac{mZe^2}{\pi\hbar^2} 2\pi\delta^2(\mathbf{x}) + \frac{me^2}{\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}' \; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}') \; 2\pi\delta^2(\mathbf{x} - \mathbf{x}')$$

$$= -\frac{2mZe^2}{\hbar^2} \delta^2(\mathbf{x}) + \frac{2me^2}{\hbar^2} \int \mathrm{d}^2\mathbf{x}' \; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}') \; \delta^2(\mathbf{x} - \mathbf{x}')$$

$$= -\frac{2mZe^2}{\hbar^2} \delta^2(\mathbf{x}) + \frac{2me^2}{\hbar^2} \; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x})$$

$$\therefore \quad n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}) = Z\delta^2(\mathbf{x}) + \frac{\hbar^2}{2me^2} \nabla^2 n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}). \tag{2.39}$$

Integraling the latter over $\mathbf{x}$ gives

$$\int \mathrm{d}^2\mathbf{x} \; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}) = \int \mathrm{d}^2\mathbf{x} \; Z \; \delta^2(\mathbf{x}) + \frac{\hbar^2}{2me^2} \int \mathrm{d}^2\mathbf{x} \; \nabla^2 n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}). \tag{2.40}$$

From (2.29), we have for the second term

$$\int \mathrm{d}^2\mathbf{x} \; \nabla^2 n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}) = -\frac{m}{2\pi\hbar^2} \int \mathrm{d}^2\mathbf{x} \; \nabla^2 V_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}). \tag{2.41}$$

Substitute (2.41) into the second term on the right-hand side of (2.40), to obtain

$$\int \mathrm{d}^2\mathbf{x} \; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}) = Z \tag{2.42}$$

as expected.

To obtain the exact expressions for the scaling dimensionless constant A and B in the definition of $F[n_{\mathrm{B}}]$ in (2.28), first, apply taking the Laplacian to the left-hand side of (2.28), to obtain

$$\nabla^2 n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}) = \nabla^2 \left[-\frac{mZe^2}{\pi\hbar^2} \ln \frac{|\mathbf{x}|}{A} + \frac{me^2}{\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}' \; \ln \frac{|\mathbf{x} - \mathbf{x}'|}{B} \; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}') \right]$$

$$= -\frac{mZe^2}{\pi\hbar^2} \nabla^2 \ln \frac{|\mathbf{x}|}{A} + \frac{me^2}{\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}' \; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}') \; \nabla^2 \ln \frac{|\mathbf{x} - \mathbf{x}'|}{B} \tag{2.43}$$

Consider the first term on right-hand side of (2.43), to get

$$\begin{aligned}\frac{mZe^2}{\pi\hbar^2}\nabla^2 \ln\frac{|\mathbf{x}|}{A} =& \frac{mZe^2}{\pi\hbar^2}(2\pi\delta^2(\mathbf{x})) \\ =& \frac{2mZe^2}{\hbar^2}\delta^2(\mathbf{x}) \end{aligned} \tag{2.44}$$

Consider the second term on the right-hand side of (2.43), to get

$$\begin{aligned}\frac{me^2}{\pi\hbar^2}\int \mathrm{d}^2\mathbf{x}'\; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}')\;\nabla^2\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B} =& \frac{me^2}{\pi\hbar^2}2\pi\int \mathrm{d}^2\mathbf{x}'\; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}')\;\delta^2(\mathbf{x}-\mathbf{x}') \\ =& \frac{2me^2}{\hbar^2}\; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}). \end{aligned} \tag{2.45}$$

Substitute (2.44) and (2.45) into (2.43), to obtain

$$\nabla^2 n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}) = -\frac{2mZe^2}{\hbar^2}\delta^2(\mathbf{x}) + \frac{2me^2}{\hbar^2}\; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}) \tag{2.46}$$

which upon multiplying (2.46) by r^2, we obtain

$$\begin{aligned} r^2\nabla^2 n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}) =& -\frac{2mZe^2}{\hbar^2}r^2\delta^2(\mathbf{x}) + \frac{2me^2}{\hbar^2}\; r^2\; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}) \\ =& -\frac{2mZe^2}{\hbar^2}r\delta(r)\delta(\theta) + \frac{2me^2}{\hbar^2}\; r^2\; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}) \\ \left(r^2\nabla^2 - \frac{2me^2r^2}{\hbar^2}\right) n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}) =& -\frac{2mZe^2}{\hbar^2}\frac{r\;\delta(r)}{2\pi} \end{aligned} \tag{2.47}$$

where

$$\int_0^\infty r\;\delta(r)\;\mathrm{d}r = 0, \tag{2.48a}$$

$$r\,\delta(r) = 0. \tag{2.48b}$$

We set

$$\frac{r}{r_0} = R. \tag{2.49}$$

The general solution of (2.47) is given by

$$n_{\mathrm{TF}}^{\mathrm{B}}(R) = C_0 K_0(R) + C_1 I_0(R) \tag{2.50}$$

where K_0 and I_0 are modified Bessel functions and

$$r_0 = \left(\frac{\hbar^2}{2me^2}\right)^{1/2}. \tag{2.51}$$

Consider the large R behavior, $I_0(R) \rightarrow \infty$ for $R \rightarrow \infty$ so we have to choose $C_1 = 0$ and the solution of (2.47) becomes

$$n_{\mathrm{TF}}^{\mathrm{B}}(R) = C_0 K_0(R). \tag{2.52}$$

To obtain C_0, substitute (2.52) into (2.42), we get

$$\begin{aligned}
Z =& C_0 \int \mathrm{d}^2\mathbf{x}\ K_0(R) \\
=& C_0 \int_0^\infty \mathrm{d}r \int_0^{2\pi} \mathrm{d}\theta\ r\ K_0(R) \\
=& 2\pi r_0^2\ C_0 \int_0^\infty \mathrm{d}R\ \ R\ K_0(R) \\
=& 2\pi r_0^2\ C_0 \\
=& 2\pi \left(\frac{\hbar^2}{2me^2}\right)\ C_0
\end{aligned}$$

$$C_0 = \left(\frac{mZe^2}{\pi\hbar^2}\right) \tag{2.53}$$

where

$$\int_0^\infty \mathrm{d}R\ R\ K_0(R) = 1. \tag{2.54}$$

Substitute (2.54) into (2.53), to obtain

$$n_{\mathrm{TF}}^{\mathrm{B}}(R) = \left(\frac{mZe^2}{\pi\hbar^2}\right) K_0(R) \quad , \qquad R = \frac{r}{r_0}. \tag{2.55}$$

To obtain A and B, by substitute (2.55) into (2.28) , to obtain

$$\left(\frac{mZe^2}{\pi\hbar^2}\right) K_0\left(\frac{r}{r_0}\right) = -\frac{mZe^2}{\pi\hbar^2} \ln\frac{|\mathbf{x}|}{A} + \frac{me^2}{\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}')$$

$$= Q_1(\mathbf{x}) + Q_2(\mathbf{x}) \tag{2.56}$$

where

$$Q_1(\mathbf{x}) = -\frac{mZe^2}{\pi\hbar^2} \ln\frac{|\mathbf{x}|}{A} \tag{2.57}$$

and

$$Q_2(\mathbf{x}) = \frac{me^2}{\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}'). \tag{2.58}$$

Let $\mathbf{x} = 0$, the left-hand side of (2.55) will become

$$\left(\frac{mZe^2}{\pi\hbar^2}\right) K_0(R) \simeq -\left(\frac{mZe^2}{\pi\hbar^2}\right) \ln R. \tag{2.59}$$

The first term on the right-hand side of (2.56) becomes

$$Q_1(\mathbf{x}) \simeq -\left(\frac{mZe^2}{\pi\hbar^2}\right)\left(\ln\frac{Rr_0}{A}\right). \tag{2.60}$$

The second term on right-hand side of (2.56) becomes

$$
\begin{aligned}
Q_2(0) =& \frac{me^2}{\pi\hbar^2}\left[\int d^2\mathbf{x}' \ \ln\frac{|\mathbf{x}'|}{B} \ n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}')\right] \\
=& \frac{me^2}{\pi\hbar^2}\left[\int d^2\mathbf{x}' \ \ln\frac{|\mathbf{x}'|}{r_0} \ n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}') + \int d^2\mathbf{x}' \ \ln\frac{r_0}{B} \ n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}')\right] \\
=& \frac{me^2}{\pi\hbar^2}\left[\int d^2\mathbf{x}' \ \ln\frac{|\mathbf{x}'|}{r_0} \ n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}') + Z\ln\frac{r_0}{B}\right] \\
=& \frac{me^2}{\pi\hbar^2}(r_0^2)(2\pi)\int dR' \ R' \ \ln R' \ n_{\mathrm{TF}}^{\mathrm{B}}(R') + \frac{me^2}{\pi\hbar^2}Z\ln\frac{r_0}{B} \\
=& \frac{me^2}{\pi\hbar^2}\left(\frac{\hbar^2}{2me^2}\right)(2\pi)\left(\frac{mZe^2}{\pi\hbar^2}\right)\int dR' \ R' \ \ln R' \ K_0(R') \\
&+ \frac{me^2}{\pi\hbar^2}Z\ln\frac{r_0}{B} \\
=& \frac{me^2}{\pi\hbar^2}Z\int dR' \ R' \ \ln R' \ K_0(R') + \frac{me^2}{\pi\hbar^2}Z\ln\frac{r_0}{B} \\
=& \frac{me^2}{\pi\hbar^2}Z[-\gamma + \ln 2] + \frac{me^2}{\pi\hbar^2}Z\ln\frac{r_0}{B}.
\end{aligned} \tag{2.61}
$$

Referring to (2.59)–(2.61), for $R \simeq 0$ we obtain

$$
\begin{aligned}
Q_1(0) + Q_2(0) =& \left(\frac{mZe^2}{\pi\hbar^2}\right)K_0(0) \\
\ln 2 + \ln\frac{r_0}{B} \simeq& -\left(\frac{mZe^2}{\pi\hbar^2}\right)\ln R + \frac{mZe^2}{\pi\hbar^2}\left[\ln\frac{Rr_0}{A} + \gamma\right] \\
-\ln B =& -\ln(2r_0)
\end{aligned} \tag{2.62}
$$

giving

$$
B = 2r_0. \tag{2.63}
$$

To obtain A, substitute (2.63) into (2.56), to obtain

$$\begin{aligned}\left(\frac{mZe^2}{\pi\hbar^2}\right) K_0(R) =& -\frac{mZe^2}{\pi\hbar^2}\ln\frac{|\mathbf{x}|}{A} + \frac{me^2}{\pi\hbar^2}\int \mathrm{d}^2\mathbf{x}' \ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ n^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x}') \\ =& -\frac{mZe^2}{\pi\hbar^2}\ln\frac{|\mathbf{x}|}{2r_0} + \frac{me^2}{\pi\hbar^2}\int \mathrm{d}^2\mathbf{x}' \ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{A}\ n^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x}') \\ =& Q_3(\mathbf{x}) + Q_4(\mathbf{x})\end{aligned} \tag{2.64}$$

where

$$Q_3(\mathbf{x}) = -\frac{mZe^2}{\pi\hbar^2}\ln\frac{|\mathbf{x}|}{2r_0} \tag{2.65}$$

and

$$Q_4(\mathbf{x}) = \frac{me^2}{\pi\hbar^2}\int \mathrm{d}^2\mathbf{x}' \ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{A}\ n^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x}'). \tag{2.66}$$

Let $\mathbf{x}=0$, the left-hand side of (2.64) becomes

$$\left(\frac{mZe^2}{\pi\hbar^2}\right) K_0(R) \simeq -\left(\frac{mZe^2}{\pi\hbar^2}\right)\ln R. \tag{2.67}$$

The first term on right-hand side of (2.64) becomes

$$Q_3(\mathbf{x}) \simeq -\frac{mZe^2}{\pi\hbar^2}\ln\left(\frac{Rr_0}{2r_0}\right). \tag{2.68}$$

For the second term on right-hand side of (2.64) becomes

$$\begin{aligned}Q_4(0) =& \frac{me^2}{\pi\hbar^2}\left[\int \mathrm{d}^2\mathbf{x}' \ \ln\frac{|\mathbf{x}'|}{A}\ n^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x}')\right] \\ =& \frac{me^2}{\pi\hbar^2}\left[\int \mathrm{d}^2\mathbf{x}' \ \ln\frac{|\mathbf{x}'|}{r_0}\ n^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x}') + \int \mathrm{d}^2\mathbf{x}' \ \ln\frac{r_0}{A}\ n^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x}')\right]\end{aligned}$$

$$
\begin{aligned}
&=\frac{me^2}{\pi\hbar^2}\left[\int \mathrm{d}^2\mathbf{x}' \;\ln\frac{|\mathbf{x}'|}{r_0}\; n^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x}') + Z\ln\frac{r_0}{A}\right] \\
&=\frac{me^2}{\pi\hbar^2}(r_0^2)(2\pi)\int \mathrm{d}R'\; R' \;\ln R'\; n^{\mathrm{B}}_{\mathrm{TF}}(R') + \frac{me^2}{\pi\hbar^2}Z\ln\frac{r_0}{A} \\
&=\frac{me^2}{\pi\hbar^2}\left(\frac{\hbar^2}{2me^2}\right)(2\pi)\left(\frac{mZe^2}{\pi\hbar^2}\right)\int \mathrm{d}R'\; R' \;\ln R'\; K_0(R') \\
&\quad + \frac{me^2}{\pi\hbar^2}Z\ln\frac{r_0}{A} \\
&=\frac{me^2}{\pi\hbar^2}Z\int \mathrm{d}R'\; R' \;\ln R'\; K_0(R') + \frac{me^2}{\pi\hbar^2}Z\ln\frac{r_0}{A} \\
&=\frac{me^2}{\pi\hbar^2}Z[-\gamma+\ln 2] + \frac{me^2}{\pi\hbar^2}Z\ln\frac{r_0}{A}. \qquad (2.69)
\end{aligned}
$$

Referring to (2.67)- (2.69), for $R \simeq 0$ we obtain

$$
\begin{aligned}
Q_3(0)+Q_4(0) &= \left(\frac{mZe^2}{\pi\hbar^2}\right)K_0(0) \\
\ln 2 + \ln\frac{r_0}{A} &\simeq -\left(\frac{mZe^2}{\pi\hbar^2}\right)\ln R + \frac{mZe^2}{\pi\hbar^2}\left[\ln\frac{Rr_0}{A}+\gamma\right] \\
-\ln A &= -\ln(2r_0) \qquad (2.70)
\end{aligned}
$$

giving

$$
A = 2r_0. \qquad (2.71)
$$

Substituting the values obtained for B and A in (2.63) and (2.71), into (2.26), we obtain the energy functional $F[n_{\mathrm{B}}]$ as

$$
\begin{aligned}
F[n_{\mathrm{B}}] = \frac{\pi\hbar^2}{m}&\int \mathrm{d}^2\mathbf{x}\,\left[n(\mathbf{x})\right]^2 + 2Ze^2\int \mathrm{d}^2\mathbf{x}\;\ln\left(\frac{|\mathbf{x}|}{2r_0}\right)n_{\mathrm{B}}(\mathbf{x}) \\
&- e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\; n_{\mathrm{B}}(\mathbf{x})\ln\left(\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\right)n_{\mathrm{B}}(\mathbf{x}'). \qquad (2.72)
\end{aligned}
$$

From (2.72), with $n_{\rm B} = n_{\rm TF}^{\rm B}$, we obtain the energy functional $F[n_{\rm TF}^{\rm B}]$:

$$
\begin{aligned}
F[n_{\rm TF}^{\rm B}] =& \frac{\pi\hbar^2}{m} \int \mathrm{d}^2\mathbf{x} \left[n_{\rm TF}^{\rm B}(\mathbf{x})\right]^2 + 2Ze^2 \int \mathrm{d}^2\mathbf{x} \; \ln \frac{|\mathbf{x}|}{2r_0} \, n_{\rm TF}^{\rm B}(\mathbf{x}) \\
& - e^2 \int \mathrm{d}^2\mathbf{x} \, \mathrm{d}^2\mathbf{x}' \, n_{\rm TF}^{\rm B}(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0} \, n_{\rm TF}^{\rm B}(\mathbf{x}'). \qquad (2.73)
\end{aligned}
$$

To obtain the ground-state energy of the TF atom $F[n_{\rm TF}^{\rm B}] \equiv E_{\rm TF}^{\rm B}(Z)$, we refer to (2.28) and (2.73) for the kinetic energy term $T[n_{\rm TF}^{\rm B}]$, given by

$$
T[n_{\rm TF}^{\rm B}] = \frac{\pi\hbar^2}{m} \int \mathrm{d}^2\mathbf{x} \left[n_{\rm TF}^{\rm B}(\mathbf{x})\right]^2. \qquad (2.74)
$$

Substitute (2.55) into (2.74), to obtain

$$
\begin{aligned}
T[n_{\rm TF}^{\rm B}] =& \frac{\pi\hbar^2}{m} \int \mathrm{d}^2\mathbf{x} \left[n_{\rm TF}^{\rm B}(\mathbf{x})\right]^2 \\
=& \frac{\pi\hbar^2}{m} 2\pi \int_0^\infty \mathrm{d}r \; r \; \left[n_{\rm TF}^{\rm B}(r)\right]^2 \\
=& \frac{\pi\hbar^2}{m} 2\pi r_0^2 \int_0^\infty \mathrm{d}R \; R \; \left(\frac{mZe^2}{\pi\hbar^2}\right)^2 \; [K_0(R)]^2 \\
=& \frac{2\pi^2\hbar^2}{m} \left(\frac{\hbar^2}{2me^2}\right) \left(\frac{mZe^2}{\pi\hbar^2}\right)^2 \int_0^\infty \mathrm{d}R \; R \; [K_0(R)]^2 \\
=& \frac{1}{2} Z^2 e^2 \qquad (2.75)
\end{aligned}
$$

where

$$
\int_0^\infty \mathrm{d}R \; R \; [K_0(R)]^2 = \frac{1}{2}. \qquad (2.76)
$$

For the particle-nucleus interaction part, we have

$$\begin{aligned}
E_{e-n}[n_{\rm TF}^{\rm B}] =& 2Ze^2 \int \mathrm{d}^2\mathbf{x} \;\ln\left(\frac{|\mathbf{x}|}{2r_0}\right)\; n_{\rm TF}^{\rm B}(\mathbf{x}) \\
=& 2Ze^2 \int \mathrm{d}^2\mathbf{x} \;\ln\left(\frac{|\mathbf{x}|}{r_0}\right)\; n_{\rm TF}^{\rm B}(\mathbf{x}) - 2Ze^2 \int \mathrm{d}^2\mathbf{x}\; n_{\rm TF}^{\rm B}(\mathbf{x})\; \ln 2 \\
=& 2Ze^2 \int \mathrm{d}^2\mathbf{x} \;\ln\left(\frac{|\mathbf{x}|}{r_0}\right)\; n_{\rm TF}^{\rm B}(\mathbf{x}) - 2Z^2e^2 \ln 2 \\
=& 4\pi Ze^2 \int_0^\infty \mathrm{d}r\; r\; \ln\left(\frac{r}{r_0}\right)\; n_{\rm TF}^{\rm B}(r) - 2Z^2e^2 \ln 2 \\
=& 4\pi Ze^2 r_0^2 \int_0^\infty \mathrm{d}R\; R\; \ln(R)\; \left(\frac{2mZe^2}{2\pi\hbar^2}\right)\; K_0(R) - 2Z^2e^2 \ln 2 \\
=& 4\pi Ze^2 r_0^2 \frac{Z}{2\pi r_0^2} \int_0^\infty \mathrm{d}R\; R\; \ln R\; K_0(R) - 2Z^2e^2 \ln 2 \\
=& 2Z^2e^2 \left[\int_0^\infty \mathrm{d}R\; R\; \ln R\; K_0(R) - \ln 2\right] \\
=& 2Z^2e^2 \left[-\gamma + \ln 2 - \ln 2\right] \\
=& -2\gamma Z^2 e^2
\end{aligned} \tag{2.77}$$

where

$$\int_0^\infty \mathrm{d}R\; R\; K_0(R)\; \ln R = -\gamma + \ln 2, \tag{2.78a}$$

$$\gamma = 0.57722, \tag{2.78b}$$

$$\int_0^\infty \mathrm{d}R\; R\; K_0(R) = 1. \tag{2.78c}$$

The particle-particle interaction part is given by

$$
\begin{aligned}
E_{e-e}[n_{\mathrm{TF}}^{\mathrm{B}}] =& - e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\, n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x})\; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}')\; \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0} \\
=& - e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\, n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x})\; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}')\; \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0} \\
=& + (\ln 2)\, 4\pi^2 e^2 C_0^2 r_0^4 \int \mathrm{d}R\; R\; K_0(\mathbf{R}) \int \mathrm{d}R'\; R'\;\; K_0(\mathbf{R}') \\
& - e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\, n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x})\; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}')\; \ln \frac{|\mathbf{x}-\mathbf{x}'|}{r_0} \\
=& + e^2 Z^2 \ln 2 - e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\, n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x})\; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}')\; \ln \frac{|\mathbf{x}-\mathbf{x}'|}{r_0} \\
=& e^2 Z^2 \ln 2 + I_1
\end{aligned}
\tag{2.79}
$$

where

$$
I_1 = -e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\, n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{r_0}\; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{x}'). \tag{2.80}
$$

By setting $\mathbf{x}/r_0 = \mathbf{R}$, we obtain

$$
\begin{aligned}
\int \mathrm{d}^2\mathbf{x}\,(.) =& \int_0^\infty r\; \mathrm{d}r \int_0^{2\pi} \mathrm{d}\theta\,(.) \\
=& r_0^2 \int_0^\infty R\; \mathrm{d}R \int_0^{2\pi} \mathrm{d}\theta\,(.) \\
=& r_0^2 \int \mathrm{d}^2\mathbf{R}\,(.).
\end{aligned}
\tag{2.81}
$$

Substitute (2.81) into (2.80), to obtain

$$
I_1 = - e^2 r_0^4 \int \mathrm{d}^2\mathbf{R}\, \mathrm{d}^2\mathbf{R}'\; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{R}) \ln |\mathbf{R}-\mathbf{R}'|\; n_{\mathrm{TF}}^{\mathrm{B}}(\mathbf{R}')
$$

$$= -2\pi e^2 \left(\frac{\hbar^2}{2me^2}\right)^2 \left(\frac{mZe^2}{\pi\hbar^2}\right)^2 \Bigg(\int_0^\infty \mathrm{d}R\ R\ K_0(R)\ \int_0^\infty \mathrm{d}R'\ R'\ K_0(R')$$

$$\times \int_0^{2\pi} \mathrm{d}\theta\ \ln(R^2 - 2RR'\cos\theta + R'^2)^{1/2}\Bigg)$$

$$= -\frac{e^2 Z^2}{2\pi} \left[\int_0^\infty \mathrm{d}R\ R\ K_0(R)\ \int_0^\infty \mathrm{d}R'\ R'\ K_0(R')\right.$$

$$\left.\times \int_0^{2\pi} \mathrm{d}\theta\ \ln(R^2 - 2RR'\cos\theta + R'^2)^{1/2}\right]$$

$$= -\frac{e^2 Z^2}{2} \int_0^\infty \mathrm{d}R\ R\ K_0(R)\ \int_0^\infty \mathrm{d}R'\ R'\ K_0(R')\ \ln R_>^2$$

$$= -\frac{e^2 Z^2}{2} \int_0^\infty \mathrm{d}R\ R\ K_0(R)\ f(R) \tag{2.82}$$

where

$$\int_0^{2\pi} \mathrm{d}\theta\ \ln(R^2 - 2RR'\cos\theta + R'^2)^{1/2} = \pi \ln R_>^2 \tag{2.83}$$

and

$$f(R) = \int_0^\infty \mathrm{d}R'\ R'\ K_0(R')\ \ln R_>^2$$

$$= \ln R^2 \int_0^R \mathrm{d}R'\ R'\ K_0(R')\ + \int_R^\infty \mathrm{d}R'\ R'\ K_0(R')\ \ln R'^2$$

$$= \ln R^2 [1 - R\ K_1(R)] + \int_R^\infty \mathrm{d}R'\ R'\ K_0(R')\ \ln R'^2$$

$$= \ln R^2 - R\ K_1(R)\ \ln R^2 + \int_R^\infty \mathrm{d}R'\ R'\ K_0(R')\ \ln R'^2. \tag{2.84}$$

Substitute (2.84) into (2.82), to obtain

$$I_1 = -\frac{e^2 Z^2}{2} \int_0^\infty \mathrm{d}R\ R\ K_0(R)\ \ln R^2$$

$$
\begin{aligned}
&+\frac{e^2Z^2}{2}\int_0^\infty \mathrm{d}R\ R^2\ K_0(R)\ K_1(R)\ \ln R^2 \\
&-\frac{e^2Z^2}{2}\int_0^\infty \mathrm{d}R\ R\ K_0(R)\int_R^\infty \mathrm{d}R'\ R'\ K_0(R')\ \ln R'^2 \\
=&-\frac{e^2Z^2}{2}[-2\gamma+2\ln 2]+\frac{e^2Z^2}{2}[-\frac{1}{2}-\gamma+\ln 2]-(0.615932)\frac{e^2Z^2}{2} \\
=&-e^2Z^2 0.61593 \qquad (2.85)
\end{aligned}
$$

where

$$
\begin{aligned}
&\int_0^\infty \mathrm{d}R\ R\ K_0(R)\int_R^\infty \mathrm{d}R'\ R'\ K_0(R')\ \ln R'^2 \\
&=\int_0^\infty \mathrm{d}R\ R\ K_0(R)\int_0^\infty \mathrm{d}R'\ R'\ K_0(R')\ \ln R'^2 \\
&\quad -\int_0^\infty \mathrm{d}R\ R\ K_0(R)\int_0^R \mathrm{d}R'\ R'\ K_0(R')\ \ln R'^2 \\
&=-2\gamma+2\ln 2-(-0.384068) \\
&=0.615931. \qquad (2.86)
\end{aligned}
$$

Substitute (2.86) into (2.79), to obtain the value for the ground-state energy of the TF atom $E^{\mathrm{B}}_{\mathrm{TF}}\left[n^{\mathrm{B}}_{\mathrm{TF}}\right]$ in 2-dimensions

$$
\begin{aligned}
E^{\mathrm{B}}_{\mathrm{TF}}[n^{\mathrm{B}}_{\mathrm{TF}}] =&T(n^{\mathrm{B}}_{\mathrm{TF}})+E_{en}(n^{\mathrm{B}}_{\mathrm{TF}})+E_{e-e}(n^{\mathrm{B}}_{\mathrm{TF}}) \\
=&\left(\frac{1}{2}Z^2e^2\right)-\left(2\gamma Z^2e^2\right)+\left(Z^2e^2\ln 2-(0.615931)Z^2e^2\right) \\
E^{\mathrm{B}}_{\mathrm{TF}}[n^{\mathrm{B}}_{\mathrm{TF}}] =&-(0.576486)Z^2e^2. \qquad (2.87)
\end{aligned}
$$

For the TF potential energy $V^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x})$ we have from (2.19) and (2.34)

$$\boldsymbol{\nabla}^2 V^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x})(\mathbf{x}) = 4\pi\, Ze^2\, \delta^2(\mathbf{x}) - 4\pi\, e^2 n^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x}) \tag{2.88}$$

with the first term corresponding to the nucleus at the origin, while the second term corresponds to the particle density. Upon integration over $\mathbf{x}$, and using (2.42), we obtain

$$\int \mathrm{d}^2\mathbf{x}\; \boldsymbol{\nabla}^2 V(\mathbf{x}) = 0 \tag{2.89}$$

verifying the neutrality of atom.

It remains to show that $n^{\mathrm{B}}_{\mathrm{TF}}$ provides the smallest possible value for $F[n_{\mathrm{B}}]$ in (2.72), that is

$$F[\sigma] \geqslant F[n^{\mathrm{B}}_{\mathrm{TF}}]. \tag{2.90}$$

To the above end, define a priori a density functional for an arbitrary density $\rho(\mathbf{x}) \geqslant 0$ by

$$\begin{aligned} F[\rho] =& C \int \mathrm{d}^2\mathbf{x}\, [\rho(\mathbf{x})]^2 + 2Ze^2 \int \mathrm{d}^2\mathbf{x}\; \ln \frac{|\mathbf{x}|}{A}\, \rho(\mathbf{x}) \\ & - e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\, \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\, \rho(\mathbf{x}') \end{aligned} \tag{2.91}$$

where

$$C = \frac{\pi\hbar^2}{m}. \tag{2.92}$$

We define the Fourier transform for real function $\rho(\mathbf{x})$

$$\rho(\mathbf{x}) = \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2}\, \tilde{\rho}(\mathbf{p})\, \mathrm{e}^{\mathbf{i}\mathbf{p}\cdot\mathbf{x}/\hbar}, \tag{2.93a}$$

$$\tilde{\rho}^*(\mathbf{p}) = \int \mathrm{d}^2\mathbf{x}\, \rho^*(\mathbf{x})\, \mathrm{e}^{\mathbf{i}\mathbf{p}\cdot\mathbf{x}/\hbar} = \int \mathrm{d}^2\mathbf{x}\, \rho(\mathbf{x})\, \mathrm{e}^{\mathbf{i}\mathbf{p}\cdot\mathbf{x}/\hbar}. \tag{2.93b}$$

We show that the third term on the right-hand side of (2.91) is positive, we start from the solution of the Poisson's equation in (2.19), giving

$$\ln \frac{|\mathbf{x}-\mathbf{x}'|}{B} = 2\pi \left(\boldsymbol{\nabla}^2\right)^{-1} \delta^2(\mathbf{x}-\mathbf{x}'). \tag{2.94}$$

Substitute into the third term on the right-hand side of (2.91), to obtain

$$\begin{aligned} -\int \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}'\rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho(\mathbf{x}') \\ = -2\pi \int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\rho(\mathbf{x}) \left(\boldsymbol{\nabla}^2\right)^{-1} \delta^2(\mathbf{x}-\mathbf{x}')\ \rho(\mathbf{x}'). \end{aligned} \tag{2.95}$$

We use an integral representation of the delta function in 2-dimensions in (2.94) and the Fourier transform of $\tilde{\rho}(\mathbf{p})$ in (2.93), then apply to (2.95), to obtain

$$\begin{aligned} -\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho(\mathbf{x}') \\ = -2\pi \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\rho(\mathbf{x})\ \rho(\mathbf{x}')\ \left(\boldsymbol{\nabla}^2\right)^{-1}\ \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')} \\ = -2\pi \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\rho(\mathbf{x})\ \rho(\mathbf{x}')\ \mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{x}'/\hbar}\ \left(\boldsymbol{\nabla}^2\right)^{-1} \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{x}/\hbar}. \end{aligned} \tag{2.96}$$

The Fourier transform of $\rho(\mathbf{x})$ is

$$\tilde{\rho}(\mathbf{p}) = \int \mathrm{d}^2\mathbf{x}'\ \rho(\mathbf{x}')\ \mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{x}'/\hbar}. \tag{2.97}$$

and

$$\boldsymbol{\nabla}^2 \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{x}/\hbar} = -\left(\frac{\mathbf{p}}{\hbar}\right)^2 \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{x}/\hbar}, \tag{2.98a}$$

$$\left(\boldsymbol{\nabla}^2\right)^{-1} \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{x}/\hbar} = -\left(\frac{\hbar}{\mathbf{p}}\right)^2 \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{x}/\hbar}. \tag{2.98b}$$

Apply (2.97) and (2.98) into (2.96), to get

$$
\begin{aligned}
-\int & \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}'\rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho(\mathbf{x}') \\
&= 2\pi \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \rho(\mathbf{x})\ \rho(\mathbf{x}')\ \mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{x}'/\hbar}\ \left(\frac{\hbar}{\mathbf{p}}\right)^2\ \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{x}/\hbar} \\
&= 2\pi \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi)^2} \int \mathrm{d}^2\mathbf{x}\ \rho(\mathbf{x})\ \tilde{\rho}(\mathbf{p}) \frac{1}{\mathbf{p}^2}\ \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{x}/\hbar}. \qquad (2.99)
\end{aligned}
$$

Since $\rho(\mathbf{x})$ is real function, i.e., $\rho(\mathbf{x}) = \rho^*(\mathbf{x})$, we have

$$
\rho(\mathbf{x}) = \int \frac{\mathrm{d}^2\mathbf{p}'}{(2\pi\hbar)^2}\ \tilde{\rho}^*(\mathbf{p}')\ \mathrm{e}^{-\mathrm{i}\mathbf{p}'\cdot\mathbf{x}}. \qquad (2.100)
$$

Substitute (2.100) into (2.99), to obtain

$$
\begin{aligned}
-\int & \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}'\rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho(\mathbf{x}') \\
&= 2\pi \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \int \frac{\mathrm{d}^2\mathbf{p}'}{(2\pi)^2} \int \mathrm{d}^2\mathbf{x}\ \mathrm{e}^{-\mathrm{i}\mathbf{p}'\cdot\mathbf{x}}\ \tilde{\rho}^*(\mathbf{p}')\ \tilde{\rho}(\mathbf{p}) \frac{1}{\mathbf{p}^2}\ \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{x}/\hbar} \\
&= 2\pi \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi)^2} \int \frac{\mathrm{d}^2\mathbf{p}'}{(2\pi\hbar)^2}\ \tilde{\rho}^*(\mathbf{p}')\ \tilde{\rho}(\mathbf{p}) \frac{1}{\mathbf{p}^2} \int \mathrm{d}^2\mathbf{x}\ \mathrm{e}^{\mathrm{i}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{x}}. \qquad (2.101)
\end{aligned}
$$

By using an integral representation of the delta function in 2-dimensions :

$$
\delta^2(\mathbf{p}-\mathbf{p}') = \int \frac{\mathrm{d}^2\mathbf{x}}{(2\pi\hbar)^2}\ \mathrm{e}^{\mathrm{i}(\mathbf{p}-\mathbf{p}')\cdot\mathbf{x}}, \qquad (2.102a)
$$

$$
F(\mathbf{p}) = \int \mathrm{d}^2\mathbf{p}'\ F(\mathbf{p}')\ \delta^2(\mathbf{p}-\mathbf{p}'). \qquad (2.102b)
$$

Applying into (2.101), to obtain

$$
-\int \mathrm{d}^2\mathbf{x}\mathrm{d}^2\mathbf{x}'\rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho(\mathbf{x}')
$$

$$
\begin{aligned}
&=2\pi \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi)^2}\ \tilde{\rho}(\mathbf{p})\ \frac{1}{\mathbf{p}^2}\ (2\pi\hbar)^2 \int \frac{\mathrm{d}^2\mathbf{p}'}{(2\pi\hbar)^2}\ \tilde{\rho}^*(\mathbf{p}')\ \delta^2(\mathbf{p}-\mathbf{p}') \\
&=2\pi \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi)^2}\ \tilde{\rho}(\mathbf{p})\ \frac{1}{\mathbf{p}^2}\ \tilde{\rho}^*(\mathbf{p}) \\
&=2\pi \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi)^2}\ |\tilde{\rho}(\mathbf{p})|^2\ \frac{1}{\mathbf{p}^2}. \qquad (2.103)
\end{aligned}
$$

So that, from (2.103), we have

$$
-e^2 \int \mathrm{d}^2\mathbf{x}\ \mathrm{d}^2\mathbf{x}' \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho(\mathbf{x}') \geqslant 0 \qquad (2.104)
$$

Let

$$
\begin{aligned}
\rho(\mathbf{x}) &= t\rho_1(\mathbf{x}) + \beta\rho_2(\mathbf{x}) \equiv t\rho_1 + \beta\rho_2\ (=\rho), && (2.105a) \\
\rho(\mathbf{x}') &= t\rho_1(\mathbf{x}') + \beta\rho_2(\mathbf{x}') \equiv t\rho_1' + \beta\rho_2'\ (=\rho'), && (2.105b) \\
1 &= t + \beta, && (2.105c) \\
\beta &= (1-t), && (2.105d)
\end{aligned}
$$

where $0 \leq t \leq 1$ and $\rho_1, \rho_2 \geqslant 0$.

For any real ρ_1, ρ_2, we obtain the inequality

$$
\begin{aligned}
t^2(\rho_1-\rho_2)^2 &\leq t(\rho_1-\rho_2)^2 \\
t^2(\rho_1^2 - 2\rho_1\rho_2 + \rho_2^2) &\leq t(\rho_1^2 - 2\rho_1\rho_2 + \rho_2^2) \\
t^2\rho_1^2 - 2t^2\rho_1\rho_2 + t^2\rho_2^2 &\leq t\rho_1^2 - 2t\rho_1\rho_2 + t\rho_2^2. \qquad (2.106)
\end{aligned}
$$

Subtracting the both-sides of (2.106) by $2t\rho_2^2$, gives

$$t^2\rho_1^2 - 2t^2\rho_1\rho_2 + t^2\rho_2^2 - 2t\rho_2^2 \leq t\rho_1^2 - 2t\rho_1\rho_2 + t\rho_2^2 - 2t\rho_2^2$$

$$t^2\rho_1^2 - 2t^2\rho_1\rho_2 + t^2\rho_2^2 - 2t\rho^2 \leq t\rho_1^2 - 2t\rho_1\rho_2 - t\rho_2^2. \tag{2.107}$$

Add to both-sides of (2.107) the expressions $\rho_2^2 + 2t\rho_1\rho_2$, to obtain

$$t^2\rho_1^2 - 2t^2\rho_1\rho_2 + t^2\rho_2^2 - 2t\rho^2 + \rho_2^2 + 2t\rho_1\rho_2 \leq t\rho_1^2 - t\rho_2^2 + \rho_2^2. \tag{2.108}$$

The left-hand side of (2.108) can be rewritten as

$$\begin{aligned} t^2\rho_1^2 - 2t^2\rho_1\rho_2 + t^2\rho_2^2 - 2t\rho^2 + \rho_2^2 + 2t\rho_1\rho_2 \\ &= t^2\rho_1^2 + (1 + t^2 - 2t)\rho_2^2 + 2t(1-t)\rho_1\rho_2 \\ &= t^2\rho_1^2 + (1-t)^2\rho_2^2 + 2t(1-t)\rho_1\rho_2 \\ &= (t\rho_1 + (1-t)\rho_2)^2. \end{aligned} \tag{2.109}$$

Also the right-hand side of (2.108) is given by

$$t\rho_1^2 - t\rho_2^2 + \rho_2^2 = t\left(\rho_1\right)^2 + (1-t)\left(\rho_2\right)^2. \tag{2.110}$$

Substitute (2.109) and (2.110), to obtain the elementary inequality

$$\left(t\rho_1 + (1-t)\rho_2\right)^2 \leq t\left(\rho_1\right)^2 + (1-t)\left(\rho_2\right)^2. \tag{2.111}$$

Also

$$\left[t\rho_1 + (1-t)\rho_2\right]\left[t\rho_1' + (1-t)\rho_2'\right] = t^2\rho_1\rho_1' + (1-t)^2\rho_2\rho_2' + t(1-t)\rho_1\rho_2'$$

$$
\begin{aligned}
&+t(1-t)\rho_1'\rho_2 \\
=&t^2\rho_1\rho_1' + \rho_2\rho_2' - t^2\rho_2\rho_2' + t\rho_1\rho_2' - t\rho_1'\rho_2 \\
&+t\rho_1'\rho_2 - t^2\rho_1'\rho_2 \\
=&t^2\rho_1\rho_1' + \rho_2\rho_2' - t^2\rho_2\rho_2' + t\rho_1\rho_2' - t\rho_1'\rho_2 \\
&+t\rho_1'\rho_2 - t^2\rho_1'\rho_2 + t\rho_1\rho_1' - t\rho_1\rho_1' \\
=&t\rho_1\rho_1' + (1-t)\rho_2\rho_2' \\
&\quad - t(1-t)(\rho_1-\rho_2)(\rho_1'-\rho_2')
\end{aligned}
$$

$$
\begin{aligned}
\therefore \quad \big[t\rho_1 + (1-t)\rho_2\big]\big[t\rho_1' + (1-t)\rho_2'\big] =&t\rho_1\rho_1' + (1-t)\rho_2\rho_2' \\
&\quad - t(1-t)(\rho_1-\rho_2)(\rho_1'-\rho_2'). \qquad (2.112)
\end{aligned}
$$

From (2.104), replace $\rho(\mathbf{x})$ by $\big[\rho_1(\mathbf{x})-\rho_2(\mathbf{x})\big]$ and replace $\rho(\mathbf{x}')$ by $\big[\rho_1(\mathbf{x}')-\rho_2(\mathbf{x}')\big]$, to obtain

$$
-\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\,\big[\rho_1(\mathbf{x})-\rho_2(\mathbf{x})\big]\ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\big[\rho_1(\mathbf{x}')-\rho_2(\mathbf{x}')\big] \geqslant 0. \qquad (2.113)
$$

From (2.91) and (2.105), replace $\rho(\mathbf{x})$ by $\big[t\rho_1 + (1-t)\rho_2\big]$ and $\rho(\mathbf{x}')$ by $\big[t\rho_1' + (1-t)\rho_2'\big]$, to obtain

$$
\begin{aligned}
F\big[t\rho_1 + (1-t)\rho_2\big] =&A\int \mathrm{d}^2\mathbf{x}\big[t\rho_1 + (1-t)\rho_2\big]^2 \\
&+2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\ \big[t\rho_1 + (1-t)\rho_2\big]
\end{aligned}
$$

$$- e^2 \int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\big[t\rho_1 + (1-t)\rho_2\big] \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \big[t\rho_1' + (1-t)\rho_2'\big]. \tag{2.114}$$

Consider the first term on the right-hand side of (2.114), by using, in the process, the elementary inequality in (2.111) giving

$$A \int \mathrm{d}^2\mathbf{x}\big[t\rho_1 + (1-t)\rho_2\big]^2 \leq A \int \mathrm{d}^2\mathbf{x}\ \left(t\,(\rho_1)^2 + (1-t)\,(\rho_2)^2\right)$$

$$= A \int \mathrm{d}^2\mathbf{x}\ t\,(\rho_1)^2 + A \int \mathrm{d}^2\mathbf{x}\ (1-t)\,(\rho_2)^2$$

$$\therefore\ \ A \int \mathrm{d}^2\mathbf{x}\big[t\rho_1 + (1-t)\rho_2\big]^2 \leq t \left(A \int \mathrm{d}^2\mathbf{x}\ \ (\rho_1)^2\right) + (1-t) \left(A \int \mathrm{d}^2\mathbf{x}\ \ (\rho_2)^2\right). \tag{2.115}$$

Consider the second term on the right-hand side of (2.114) we may write

$$2Ze^2 \int \mathrm{d}^2\mathbf{x}\ \ln \frac{|\mathbf{x}|}{A}\ \big[t\rho_1 + (1-t)\rho_2\big] = 2Ze^2 \int \mathrm{d}^2\mathbf{x}\ \ln \frac{|\mathbf{x}|}{A}\ t\rho_1$$

$$+ 2Ze^2 \int \mathrm{d}^2\mathbf{x}\ \ln \frac{|\mathbf{x}|}{A}\ (1-t)\rho_2$$

$$= t \left(2Ze^2 \int \mathrm{d}^2\mathbf{x}\ \ln \frac{|\mathbf{x}|}{A}\ \rho_1\right)$$

$$+ (1-t) \left(2Ze^2 \int \mathrm{d}^2\mathbf{x}\ \ln \frac{|\mathbf{x}|}{A}\ \rho_2\right). \tag{2.116}$$

Consider the third term on the right-hand side of (2.114), by using (2.112), to obtain

$$-e^2 \int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\big[t\rho_1 + (1-t)\rho_2\big] \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \big[t\rho_1' + (1-t)\rho_2'\big]$$

$$
\begin{aligned}
=&-e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\;\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\;t\rho_1\rho_1' - e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\;\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\;(1-t)\rho_2\rho_2' \\
&+e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\;\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\;\left(t(1-t)(\rho_1-\rho_2)(\rho_1'-\rho_2')\right). \qquad (2.117)
\end{aligned}
$$

From (2.113), the left-hand side of (2.117) is positive, so that (2.117) can be rewritten as

$$
\begin{aligned}
-e^2&\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\big[t\rho_1+(1-t)\rho_2\big]\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\;\big[t\rho_1'+(1-t)\rho_2'\big] \\
&\le -t\left(e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\;\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\;\rho_1\rho_1'\right) \\
&\quad -(1-t)\left(e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\;\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\;\rho_2\rho_2'\right). \qquad (2.118)
\end{aligned}
$$

Substitute (2.115), (2.116) and (2.118) into (2.114), to obtain

$$
\begin{aligned}
F\big[t\rho_1+(1-t)\rho_2\big] \le\;& t\left(A\int \mathrm{d}^2\mathbf{x}\;(\rho_1)^2\right)+(1-t)\left(A\int \mathrm{d}^2\mathbf{x}\;(\rho_2)^2\right) \\
&+t\left(2Ze^2\int \mathrm{d}^2\mathbf{x}\;\ln\frac{|\mathbf{x}|}{A}\;\rho_1\right) \\
&+(1-t)\left(2Ze^2\int \mathrm{d}^2\mathbf{x}\;\ln\frac{|\mathbf{x}|}{A}\;\rho_2\right) \\
&-t\left(e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\;\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\;\rho_1\rho_1'\right) \\
&-(1-t)\left(e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\;\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\;\rho_2\rho_2'\right) \\
=&t\left(A\int \mathrm{d}^2\mathbf{x}\;(\rho_1)^2+2Ze^2\int \mathrm{d}^2\mathbf{x}\;\ln\frac{|\mathbf{x}|}{A}\;\rho_1\right. \\
&\left.-e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\;\ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\;\rho_1\rho_1'\right)
\end{aligned}
$$

$$+ (1-t)\Bigg(A\int \mathrm{d}^2\mathbf{x}\ \left(\rho_2\right)^2 + 2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\ \rho_2$$

$$-e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho_2\rho_2'\Bigg). \tag{2.119}$$

Refer to (2.91), to write

$$F[\rho_1] = A\int \mathrm{d}^2\mathbf{x}\ \left(\rho_1\right)^2 + 2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\ \rho_1$$

$$-e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho_1\,\rho_1' \tag{2.120}$$

and

$$F[\rho_2] = A\int \mathrm{d}^2\mathbf{x}\ \left(\rho_2\right)^2 + 2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{A}\ \rho_2$$

$$-e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho_2\,\rho_2'. \tag{2.121}$$

Substitute (2.119) and (2.121) into the right- hand side of inequality (2.119), to derive the bound :

$$F\big[t\rho_1 + (1-t)\rho_2\big] \le tF[\rho_1] + (1-t)F[\rho_2]. \tag{2.122}$$

Also, from (2.114), we have

$$\frac{\mathrm{d}}{\mathrm{d}t}F\big[t\rho_1 + (1-t)\rho_2\big] = 2A\int \mathrm{d}^2\mathbf{x}\ \big[t\rho_1 + (1-t)\rho_2\big](\rho_1-\rho_2)$$

$$+ 2Ze^2\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}|}{2r_0}\,(\rho_1-\rho_2)$$

$$-2e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ \big[t\rho_1' + (1-t)\rho_2'\big](\rho_1-\rho_2)$$

$$\tag{2.123}$$

and

$$\frac{\mathrm{d}}{\mathrm{d}t} F\big[t\rho_1 + (1-t)\rho_2\big]\bigg|_{t=0}$$

$$= \int \mathrm{d}^2\mathbf{x}\,(\rho_1 - \rho_2)\left[2A\rho_2 + Ze^2 \ln\frac{|\mathbf{x}|}{2r_0} - e^2\int \mathrm{d}^2\mathbf{x}'\,\rho_2'\;\ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\right]. \quad (2.124)$$

By choosing $\rho_2 = n_{\mathrm{TF}}^{\mathrm{B}}$, and $\rho_1 = \sigma \geqslant 0$ arbitrary, we conclude from (2.28) and (2.42) that the expression within the square brackets in (2.116) is zero, thus

$$\frac{\mathrm{d}}{\mathrm{d}t} F\big[t\sigma + (1-t)n_{\mathrm{TF}}^{\mathrm{B}}\big]\bigg|_{t=0} = 0. \quad (2.125)$$

Also (2.106) leads to the bound

$$F\big[\sigma\big] - F\big[n_{\mathrm{TF}}^{\mathrm{B}}\big] \geqslant \frac{F\big[t\sigma + (1-t)n_{\mathrm{TF}}^{\mathrm{B}}\big] - F\big[n_{\mathrm{TF}}^{\mathrm{B}}\big]}{t}. \quad (2.126)$$

Since the left-hand side of (2.126) is independent of t, we may take the limit $t \longrightarrow 0$, leading to

$$F\big[\sigma\big] - F\big[n_{\mathrm{TF}}^{\mathrm{B}}\big] \geqslant \lim_{t\to 0}\left(\frac{F\big[t\sigma + (1-t)n_{\mathrm{TF}}^{\mathrm{B}}\big] - F\big[n_{\mathrm{TF}}^{\mathrm{B}}\big]}{t}\right) \quad (2.127)$$

and use (2.125) to conclude that

$$F\big[\sigma\big] \geqslant F\big[n_{\mathrm{TF}}^{\mathrm{B}}\big] \quad (2.128)$$

with the TF density $n_{\mathrm{TF}}^{\mathrm{B}}$ providing the smallest possible value for the energy functional in (2.91).

2.3 Lower Bound to the Expectation Value of The Exact Kinetic Energy

We first consider the Hamiltonian of a single particle

$$H = H_0 + V \tag{2.129}$$

where H_0 is the free Hamiltonian $\mathbf{p}^2/2m$.

By introducing a variable coupling parameter $g \geqslant 0$, with $g = 1$ corresponding to above the Hamiltonian, we rewrite (2.129) in the form

$$H(g) = H_0 + gV(\mathbf{x}). \tag{2.130}$$

We rewrite the potential, by using in the process the step function

$$\begin{aligned} V(\mathbf{x}) =& V(\mathbf{x})(1) \\ =& V(\mathbf{x}) \left[\Theta(V(\mathbf{x})) + \Theta(-V(\mathbf{x})) \right] \\ =& V(\mathbf{x})\Theta(V(\mathbf{x})) + V(\mathbf{x})\Theta(-V(\mathbf{x})) \\ \geqslant& V(\mathbf{x})\Theta(-V(\mathbf{x})). \end{aligned} \tag{2.131}$$

Since $V(\mathbf{x})\Theta(V(\mathbf{x})) \geqslant 0$, where $\Theta(V(\mathbf{x})) + \Theta(-V(\mathbf{x})) = 1$.

Let $-v = V(\mathbf{x})\Theta(-V(\mathbf{x}))$ where $v(\mathbf{x}) \geqslant 0$, from (2.131) we then obtain

$$V(\mathbf{x}) \geqslant -v(\mathbf{x}). \tag{2.132}$$

Substitute this into (2.130), to obtain

$$H(g) = H_0 + gv(\mathbf{x})$$

$$H(g) \geqslant H_0 - gv(\mathbf{x}). \tag{2.133}$$

Let $N_{-\xi}(H(g))$ denote the number of eigenvalues of $H_g \leq -\xi$, with $\xi > 0$. For future developments, we establish an order relationship between the eigenvalues of two self-adjacent operators $H(g)$ and $H_0 - gv(\mathbf{x})$, whose spectra are bounded from below, such that for all vectors $|\Phi\rangle$ in their domains, we obtain

$$\langle\Phi|H(g)|\Phi\rangle \geqslant \langle\Phi|H_0 - gv(\mathbf{x})|\Phi\rangle \geqslant -\xi. \tag{2.134}$$

Also the number of bound-state of $H_0 - gv(\mathbf{x})$ cannot be less than those of $H(g)$,

$$N_{-\xi}\left(H_0 - gv(\mathbf{x})\right) \geqslant N_{-\xi}\left(H_0 + gv(\mathbf{x})\right). \tag{2.135}$$

Similarly $0 < g' < g$,

$$H_0 - g'v(\mathbf{x}) \geqslant H_0 - gv(\mathbf{x}) \tag{2.136}$$

and

$$N_{-\xi}\left(H_0 - gv(\mathbf{x})\right) \geqslant N_{-\xi}\left(H_0 - g'v(\mathbf{x})\right). \tag{2.137}$$

From (2.131)–(2.137), we have the important relation :

$$N_{-\xi}\left(H_0 - v(\mathbf{x})\right) = [\text{Number of } g'\text{'s in } 0 < g' \leq g \text{ for which}$$
$$H_0 - g'v(\mathbf{x}) \text{ has the eigenvalue} = -\xi] \tag{2.138}$$

so that $H_0 - g'v(\mathbf{x})$ has energy $\equiv -\xi$.

From (2.138), we introduce the new eigenvalue equation :

$$(H_0 - g'v(\mathbf{x}))\,|\Phi\rangle = -\,\xi\,|\Phi\rangle\,, \qquad \langle\Phi|\,\Phi\rangle = 1$$

$$\begin{aligned}
\left(\frac{\mathbf{p}^2}{2m} - g'v(\mathbf{x})\right)\bigg|\,\Phi\bigg\rangle &= -\,\xi\,|\Phi\rangle \\
\left(\frac{\mathbf{p}^2}{2m} + \xi\right)\bigg|\,\Phi\bigg\rangle &= g'v(\mathbf{x})|\Phi\rangle \\
&= g'\sqrt{v(\mathbf{x})}\sqrt{v(\mathbf{x})}\;|\Phi\rangle \\
&= g'\sqrt{v(\mathbf{x})}\;|\Phi\rangle
\end{aligned} \tag{2.139}$$

where $|\Phi\rangle = \sqrt{v(\mathbf{x})}\;|\Phi\rangle$.

Multiply (2.139) by $\sqrt{v(\mathbf{x})}$, to obtain

$$\begin{aligned}
\sqrt{v(\mathbf{x})}\,\left(\frac{\mathbf{p}^2}{2m} + \xi\right)\bigg|\,\Phi\bigg\rangle &= g'\sqrt{v(\mathbf{x})}\;\sqrt{v(\mathbf{x})}|\Phi\rangle \\
\sqrt{v(\mathbf{x})}\,|\Phi\rangle &= g'\sqrt{v(\mathbf{x})}\;\frac{1}{\left(\frac{\mathbf{p}^2}{2m} + \xi\right)}\sqrt{v(\mathbf{x})}|\Phi\rangle \\
|\Phi\rangle &= g'A|\Phi\rangle \\
A|\Phi\rangle &= \frac{1}{g'}|\Phi\rangle
\end{aligned} \tag{2.140}$$

where A is the positive operator

$$A = \sqrt{v(\mathbf{x})}\;\frac{1}{\left(\frac{\mathbf{p}^2}{2m} + \xi\right)}\sqrt{v(\mathbf{x})} \tag{2.141}$$

The eigenvalue of the operator A is $1/g'$ and $0 < g' < g$. Also

$$A^{\rho} = \sum_{j=1}^{\infty} \frac{1}{g_j'^{\rho}} \, |g_j'\rangle\langle g_j'|. \tag{2.142}$$

From earlier equations, (2.129)–(2.141), for $\rho \geqslant 0$, in particular we recall that

$$\begin{aligned}\int \mathrm{d}^{\nu}\mathbf{x} \, \langle \mathbf{x}| \, A^{\rho} \, |\mathbf{x}\rangle \geqslant \frac{1}{g^{\rho}} \times \Big[&\text{Number of all } g'\text{'s as eigenvalues of } A \\ &\text{in } 0 < g' \leq g \text{ for which } H_0 - g' v(\mathbf{x}) \\ &\text{has the eigenvalue } = -\xi\Big] \,.\end{aligned} \tag{2.143}$$

From (2.133) and (2.143), we obtain the so-called Schwinger inequality :

$$N_{-\xi}\left(H_0 - g v(\mathbf{x})\right) \leq g^{\rho} \int \mathrm{d}^{\nu}\mathbf{x} \, \langle \mathbf{x}| \, A^{\rho} \, |\mathbf{x}\rangle \,. \tag{2.144}$$

In two dimensions ($\nu = 2$), we choose $\rho = 2$ on the right-hand side of (2.143). Thus with the definition of A in (2.141), we obtain for the right-hand side of (2.143) with $g = 1$

$$\begin{aligned}\int \mathrm{d}^2\mathbf{x} \, \langle \mathbf{x}| \, A^2 \, |\mathbf{x}\rangle &= \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^2\mathbf{x}' \, \langle \mathbf{x}| \, A \, |\mathbf{x}'\rangle \, \langle \mathbf{x}'| \, A \, |\mathbf{x}\rangle \\ &= \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^2\mathbf{x}' \, \langle \mathbf{x}| \, A \, |\mathbf{x}'\rangle \, \langle \mathbf{x}| \, A \, |\mathbf{x}'\rangle^* \\ &= \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^2\mathbf{x}' \, \left|\langle \mathbf{x}| \, A \, |\mathbf{x}'\rangle\right|^2 \\ &= \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^3\mathbf{x}' \, v(\mathbf{x}) \, v(\mathbf{x}') \left| \left\langle \mathbf{x} \left| \frac{1}{\left[\frac{\mathbf{p}^2}{2m} + \xi\right]} \right| \mathbf{x}' \right\rangle \right|^2 .\end{aligned} \tag{2.145}$$

For $\left\langle \mathbf{x} \left| \left[\frac{\mathbf{p}^2}{2m}+\xi\right]^{-1} \right| \mathbf{x}' \right\rangle$, denote $\left[\frac{\mathbf{p}^2}{2m}+\xi\right]^{-1}$ by $\hat{A}(\mathbf{p})$, to obtain

$$\begin{aligned}
\left\langle \mathbf{x} \left| \frac{1}{\left[\frac{\mathbf{p}^2}{2m}+\xi\right]} \right| \mathbf{x}' \right\rangle &= \left\langle \mathbf{x} \left| \hat{A}(\mathbf{p}) \right| \mathbf{x}' \right\rangle \\
&= \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \int \frac{\mathrm{d}^2\mathbf{p'}}{(2\pi\hbar)^2} \left\langle \mathbf{x} \mid \mathbf{p} \right\rangle \left\langle \mathbf{p} \left| \hat{A}(\mathbf{p}) \right| \mathbf{p'} \right\rangle \left\langle \mathbf{p'} \mid \mathbf{x}' \right\rangle \\
&= \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \int \frac{\mathrm{d}^2\mathbf{p'}}{(2\pi\hbar)^2} \, \mathrm{e}^{\mathrm{i}\frac{\mathbf{p}}{\hbar}\cdot\mathbf{x}} \left\langle \mathbf{p} \left| \hat{A}(\mathbf{p}) \right| \mathbf{p'} \right\rangle \, \mathrm{e}^{-\mathrm{i}\frac{\mathbf{p'}}{\hbar}\cdot\mathbf{x}'} \\
&= \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \int \frac{\mathrm{d}^2\mathbf{p'}}{(2\pi\hbar)^2} \, \mathrm{e}^{\mathrm{i}(\mathbf{p}\cdot\mathbf{x}-\mathbf{p'}\cdot\mathbf{x}')/\hbar} \left\langle \mathbf{p} \left| \hat{A}(\mathbf{p}) \right| \mathbf{p'} \right\rangle \\
&= \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \int \frac{\mathrm{d}^2\mathbf{p'}}{(2\pi\hbar)^2} \, \mathrm{e}^{\mathrm{i}(\mathbf{p}\cdot\mathbf{x}-\mathbf{p'}\cdot\mathbf{x}')/\hbar} \, \hat{A}(\mathbf{p}) \, (2\pi\hbar)^2 \, \delta^2\left(\mathbf{p}-\mathbf{p'}\right) \\
&= \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \, \hat{A}(\mathbf{p}) \, (2\pi\hbar)^2 \int \frac{\mathrm{d}^2\mathbf{p'}}{(2\pi\hbar)^2} \, \mathrm{e}^{\mathrm{i}(\mathbf{p}\cdot\mathbf{x}-\mathbf{p'}\cdot\mathbf{x}')/\hbar} \delta^2\left(\mathbf{p}-\mathbf{p'}\right) \\
&= \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \, \hat{A}(\mathbf{p}) \, \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot(\mathbf{x}-\mathbf{x'})/\hbar} \\
&= \int \frac{\mathrm{d}^2\mathbf{p}}{(2\pi\hbar)^2} \frac{\mathrm{e}^{\mathrm{i}\mathbf{p}\cdot(\mathbf{x}-\mathbf{x'})/\hbar}}{\left[\frac{\mathbf{p}^2}{2m}+\xi\right]}, \qquad \boldsymbol{\eta} = |\mathbf{x}-\mathbf{x'}| \\
&= \frac{1}{(2\pi\hbar)^2} \int_0^\infty \frac{p \, \mathrm{d}p}{\left(\frac{p^2}{2m}+\xi\right)} \int_0^{2\pi} \mathrm{d}\theta \, \mathrm{e}^{\mathrm{i}\eta p\cos\theta/\hbar}.
\end{aligned} \tag{2.146}$$

The angular part is given by

$$\int_0^{2\pi} \mathrm{d}\theta \, \mathrm{e}^{\mathrm{i}\eta p\cos\theta/\hbar} = 2\pi \; J_0\left(\frac{p\eta}{\hbar}\right) \tag{2.147}$$

where $J_0(x)$ is the Bessel function of order zero. On other hand,

$$\int_0^\infty \mathrm{d}x \; \frac{x}{(x^2+a^2)} J_0(x) = K_0(ax) \tag{2.148}$$

where $K_0(ax)$ is the modified Bessel function of order zero.

Apply (2.147) and (2.148) to (2.146), to obtain

$$\left\langle \mathbf{x} \left| \frac{1}{\left[\frac{\mathbf{p}^2}{2m}+\xi\right]} \right| \mathbf{x}' \right\rangle = \frac{1}{(2\pi\hbar)^2} \int_0^\infty \frac{p\ \mathrm{d}p}{\left(\frac{p^2}{2m}+\xi\right)} \int_0^{2\pi} \mathrm{d}\theta\ \mathrm{e}^{\mathrm{i}\eta p\ \cos\theta/\hbar}, \quad \boldsymbol{\eta} = |\mathbf{x}-\mathbf{x'}|$$

$$= \frac{m}{\pi\hbar^2} K_0\left(\frac{|\mathbf{x}-\mathbf{x}'|}{\hbar}\right)\sqrt{2m\xi}. \tag{2.149}$$

Substitute (2.149) into (2.145), to obtain

$$\int \mathrm{d}^2\mathbf{x}\, \langle \mathbf{x}|\, A^2\, |\mathbf{x}\rangle$$

$$= \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^3\mathbf{x'}\ v(\mathbf{x})\ v(\mathbf{x}') \left(\frac{m}{\pi\hbar^2} K_0\left(\frac{|\mathbf{x}-\mathbf{x}'|}{\hbar}\right)\sqrt{2m\xi}\right)^2$$

$$= \left(\frac{m}{\pi\hbar^2}\right)^2 \int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^3\mathbf{x'}\ v(\mathbf{x})\ v(\mathbf{x}') \left(K_0\left(\frac{|\mathbf{x}-\mathbf{x}'|}{\hbar}\right)\sqrt{2m\xi}\right)^2. \tag{2.150}$$

We use Young's inequality

$$\left|\int \mathrm{d}^2\mathbf{x} \int \mathrm{d}^2\mathbf{x}' f(\mathbf{x}) g(\mathbf{x}-\mathbf{x'}) h(\mathbf{x}')\right| \leq \left\{\int \mathrm{d}^2\mathbf{x}\ |f(\mathbf{x})|^p\right\}^{1/p} \left\{\int \mathrm{d}^2\mathbf{x}\ |g(\mathbf{x})|^q\right\}^{1/q}$$

$$\times \left\{\int \mathrm{d}^2\mathbf{x} |h(\mathbf{x})|^s\right\}^{1/s} \tag{2.151}$$

with $p=2,\ s=2,\ q=1$ and

$$f(\mathbf{x}) = v(\mathbf{x}), \tag{2.152}$$

$$g(\mathbf{x}-\mathbf{x'}) = \left(K_0\left(\frac{|\mathbf{x}-\mathbf{x}'|}{\hbar}\right)\sqrt{2m\xi}\right)^2, \tag{2.153}$$

$$h(\mathbf{x}') = v(\mathbf{x}'), \tag{2.154}$$

to obtain

$$\left|\int \mathrm{d}^2\mathbf{x}\int \mathrm{d}^2\mathbf{x'}\ \ v(\mathbf{x})\ \frac{\mathrm{e}^{-2|\mathbf{x}-\mathbf{x'}|\sqrt{2m\xi}/\hbar}}{|\mathbf{x}-\mathbf{x'}|^2}\ v(\mathbf{x}')\right|$$

$$\leq \left(\int \mathrm{d}^2\mathbf{x}\,|v(\mathbf{x})|^2\right)^{1/2}\left(\int \mathrm{d}^2\mathbf{x}\ \left|\left(K_0\left(\frac{|\mathbf{x}-\mathbf{x}'|}{\hbar}\right)\sqrt{2m\xi}\right)^2\right|\right)$$

$$\times\left(\int \mathrm{d}^2\mathbf{x}\,|v(\mathbf{x})|^2\right)^{1/2}$$

$$= \left(\int \mathrm{d}^2\mathbf{x}\ (v(\mathbf{x}))^2\right)^{1/2}\left(\int \mathrm{d}^2\mathbf{x}\ (v(\mathbf{x}))^2\right)^{1/2}$$

$$\times\left(\int \mathrm{d}^2\mathbf{x}\ \left|\left(K_0\left(\frac{|\mathbf{x}-\mathbf{x}'|}{\hbar}\right)\sqrt{2m\xi}\right)^2\right|\right)$$

$$\therefore\ \int \mathrm{d}^2\mathbf{x}\int \mathrm{d}^2\mathbf{x}'\ v(\mathbf{x})\frac{\mathrm{e}^{-2|\mathbf{x}-\mathbf{x'}|\sqrt{2m\xi}/\hbar}}{|\mathbf{x}-\mathbf{x'}|^2}\ v(\mathbf{x}')$$

$$\leq \left(\int \mathrm{d}^2\mathbf{x}\ (v(\mathbf{x}))^2\right)\left(\int \mathrm{d}^2\mathbf{x}\ \left|\left(K_0\left(\frac{|\mathbf{x}-\mathbf{x}'|}{\hbar}\right)\sqrt{2m\xi}\right)^2\right|\right). \qquad (2.155)$$

By using the integral

$$\int \mathrm{d}^2\mathbf{x}\left[K_0\left(\frac{|\mathbf{x}|}{\hbar}\sqrt{2m\xi}\right)\right]^2 = \frac{\pi\hbar^2}{2m\xi} \qquad (2.156)$$

we then have

$$\int \mathrm{d}^2\mathbf{x}\,\langle\mathbf{x}|\,A^2\,|\mathbf{x}\rangle = \frac{m}{2\hbar^2}\frac{1}{\pi\xi}\int \mathrm{d}^2\,\mathbf{x}v^2(\mathbf{x}). \qquad (2.157)$$

From (2.144), this gives

$$N_{-\xi}\left(H_0 - gv(\mathbf{x})\right) \leq \frac{m}{2\hbar^2}\frac{1}{\pi\xi}\int \mathrm{d}^2\mathbf{x}\ v^2(\mathbf{x}). \qquad (2.158)$$

From (2.158) we have $N_{-\xi}\left(H_0 - v(\mathbf{x})\right) < 1$ if we choose

$$\xi = \frac{m}{2\hbar^2}\frac{(1+\delta)}{\pi}\int \mathrm{d}^2\mathbf{x}\; v^2(\mathbf{x}), \quad \delta > 0 \tag{2.159}$$

or

$$-\xi = -\frac{m}{2\hbar^2}\frac{(1+\delta)}{\pi}\int \mathrm{d}^2\mathbf{x}\; v^2(\mathbf{x}). \tag{2.160}$$

On the other hand, $N_{-\xi}(\mathbf{p}^2/2m - v(\mathbf{x})) < 1$, implies that $N_{-\xi}(\mathbf{p}^2/2m - v(\mathbf{x})) = 0$, since $N_{-\xi}$ must be a natural number, and the right-hand side of (2.160) provides a lower bound to the spectrum of $[\mathbf{p}^2/2m - v(\mathbf{x})]$ since its spectrum would then be empty for energies $-\xi$. That is, (2.160) gives the following lower bound for the ground-state energy of the Hamiltonian,

$$-\frac{m}{2\hbar^2}\frac{(1+\delta)}{\pi}\int \mathrm{d}^2\mathbf{x}\; v^2(\mathbf{x}). \tag{2.161}$$

For one particle systems, we first obtain a lower bound for T. First we consider the one particle state with normalization condition $\int \mathrm{d}^2\mathbf{x}\; \rho(\mathbf{x}) = 1$ and define the positive function

$$v(\mathbf{x}) = \gamma \frac{\rho^{\alpha}(\mathbf{x})}{\int \mathrm{d}^2\mathbf{x}\; \rho^{\alpha+1}(\mathbf{x})} T \tag{2.162}$$

where α, γ are to be determined, and $v(\mathbf{x})$ is not the potential energy for any Hamiltonian. It is just introduced in order to be able to obtain a lower bound for T. Substitution (2.162) into $\langle \Phi \left| H_0 - v(\mathbf{x}) \right| \Phi \rangle$, to obtain

$$\left\langle \Phi \left| \frac{\mathbf{p}^2}{2m} - v(\mathbf{x}) \right| \Phi \right\rangle = -(\gamma - 1)\; T \tag{2.163}$$

and in reference to the bound in (2.161), we have

$$\left\langle \Phi \left| \frac{\mathbf{p}^2}{2m} - v(\mathbf{x}) \right| \Phi \right\rangle \geqslant - \frac{m}{2\hbar^2} \frac{(1+\delta)}{\pi} \int \mathrm{d}^2\mathbf{x}\; v^2(\mathbf{x}). \tag{2.164}$$

From (2.163) and (2.164), we may infer that

$$\begin{aligned} -(\gamma - 1)\; T \geqslant & - \frac{m}{2\hbar^2} \frac{(1+\delta)}{\pi} \int \mathrm{d}^2\mathbf{x}\; v^2(\mathbf{x}) \\ = & - \frac{m}{2\hbar^2} \frac{(1+\delta)}{\pi} \int \mathrm{d}^2\mathbf{x} \left(\gamma \frac{\rho^\alpha(\mathbf{x})}{\int \mathrm{d}^2\mathbf{x}\; \rho^{\alpha+1}(\mathbf{x})} T \right)^2 \\ = & - T^2\gamma^2 \frac{m}{2\hbar^2} \frac{(1+\delta)}{\pi} \frac{\int \mathrm{d}^2\mathbf{x}\; \rho^{2\alpha}(\mathbf{x})}{\left(\int \mathrm{d}^2\mathbf{x}\; \rho^{\alpha+1}(\mathbf{x})\right)^2} \end{aligned}$$

$$(\gamma - 1)\; T \leq T^2\gamma^2 \frac{m}{2\hbar^2} \frac{(1+\delta)}{\pi} \frac{\int \mathrm{d}^2\mathbf{x}\; \rho^{2\alpha}(\mathbf{x})}{\left(\int \mathrm{d}^2\mathbf{x}\; \rho^{\alpha+1}(\mathbf{x})\right)^2}. \tag{2.165}$$

This suggests to choose $2\alpha = \alpha + 1$, giving $\alpha = 1$. So the inequality in (2.165) becomes

$$\begin{aligned} (\gamma - 1)\; T \leq & \; T^2\gamma^2 \frac{m}{2\hbar^2} \frac{(1+\delta)}{\pi} \frac{\int \mathrm{d}^2\mathbf{x}\; \rho^2(\mathbf{x})}{\left(\int \mathrm{d}^2\mathbf{x}\; \rho^2(\mathbf{x})\right)^2} \\ = & \; T^2\gamma^2 \frac{m}{2\hbar^2} \frac{(1+\delta)}{\pi} \frac{1}{\int \mathrm{d}^2\mathbf{x}\; \rho^2(\mathbf{x})} \end{aligned}$$

$$T \geqslant \frac{(\gamma - 1)}{\gamma^2} \frac{2\hbar^2\pi}{m(1+\delta)} \int \mathrm{d}^2\mathbf{x}\; \rho^2(\mathbf{x}). \tag{2.166}$$

Optimizing (2.166) over γ

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}\gamma} \frac{\gamma - 1}{\gamma^2} =& 0 \\ \frac{-1}{\gamma^2} + \frac{2}{\gamma^3} =& 0 \end{aligned} \tag{2.167}$$

gives

$$\gamma = 2. \tag{2.168}$$

Substitute γ from (2.168) into (2.166), to obtain the following bound for the expectation value of the kinetic energy T (for one particle systems)

$$T \geqslant \frac{\pi}{(1+\delta)} \frac{\hbar^2}{2m} \int \mathrm{d}^2\mathbf{x}\ \rho^2(\mathbf{x}) \tag{2.169}$$

for arbitrary small $\delta > 0$.

For multi-particle systems, consider N identical bosons, each of mass m and introduce the particle number density in two dimensions :

$$\rho(\mathbf{x}) = N \int \mathrm{d}^2\mathbf{x}_2 ... \mathrm{d}^2\mathbf{x}_N \, |\Phi(\mathbf{x}, \mathbf{x}_2, ..., \mathbf{x}_N)|^2 \quad , \tag{2.170}$$

The total number of particles N is given self consistently from the normalization condition

$$\int \mathrm{d}^2\mathbf{x}\ \rho(\mathbf{x}) = N. \tag{2.171}$$

In reference to (2.162), with $\gamma = 2,\ \alpha = 1$, we obtain the expression for the positive function $v(\mathbf{x})$

$$v(\mathbf{x}) = 2 \frac{\rho(\mathbf{x})}{\int \mathrm{d}^2\mathbf{x}\ \rho^2(\mathbf{x})} T \tag{2.172}$$

where

$$T = \left\langle \Phi \left| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} \right| \Phi \right\rangle. \tag{2.173}$$

It is easily verified that

$$\left\langle \Phi \left| \sum_{i=1}^{N} v(\mathbf{x}_i) \right| \Phi \right\rangle = 2T \tag{2.174}$$

where $\sum_{i=1}^{N} v(\mathbf{x}_i) = v(\mathbf{x})$ and $v(\mathbf{x})$ is not the potential energy for any Hamiltonian. It is just introduced in order to be able to obtain the expectation value of the kinetic energy T (for N identical bosons) in two dimensions.

We consider the operator

$$\sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} - v(\mathbf{x}_i) \right] \tag{2.175}$$

defining a hypothetical Hamiltonian of N non-interacting bosons which, however, interact with the external "potential" $v(\mathbf{x})$.

From (2.173) and (2.174), we have

$$\left\langle \Phi \left| \sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} - v(\mathbf{x}_i) \right] \right| \Phi \right\rangle = -\, T. \tag{2.176}$$

To obtain a lower bound to the spectrum of the "Hamiltonian" (operator) in (2.175), we can put N bosons in the same state without Pauli's exclusion principle (put all of the N bosons at the bottom of the spectrum of $\left[\frac{\mathbf{p}_i^2}{2m} - v(\mathbf{x}_i) \right]$. Hence the Hamiltonian (2.176) is bounded below by N times the ground-state energy in (2.161). This is for N identical bosons we have

$$\left\langle \Phi \left| \sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} - v(\mathbf{x}_i) \right] \right| \Phi \right\rangle \geqslant -\, \frac{mN}{2\hbar^2} \frac{(1+\delta)}{\pi} \int \mathrm{d}^2\mathbf{x}\; v^2(\mathbf{x}). \tag{2.177}$$

Substituting (2.172), (2.176) into (2.177) and using the normalization condition $\int \mathrm{d}^2\mathbf{x}\; \rho(\mathbf{x}) = N$, we obtain for the expectation value of the kinetic energy T (for

N identical bosons)

$$-T \geqslant -\frac{Nm}{2\hbar^2}\frac{(1+\delta)}{\pi}\int \mathrm{d}^2\mathbf{x}\ \left(2\frac{\rho(\mathbf{x})}{\int \mathrm{d}^2\mathbf{x}\ \rho^2(\mathbf{x})}T\right)^2$$

$$= -\ 4NT^2\frac{m}{2\hbar^2}\frac{(1+\delta)}{\pi}\frac{1}{\int \mathrm{d}^2\mathbf{x}\ \rho^2(\mathbf{x})}$$

$$T \geqslant \frac{\pi}{N(1+\delta)}\frac{\hbar^2}{2m}\int \mathrm{d}^2\mathbf{x}\ \rho^2(\mathbf{x}) \tag{2.178}$$

2.4 A Thomas-Fermi Energy Functional and a Lower Bound for The repulsive Interaction

For symmetric normalized functions $\Phi(\mathbf{x}_1,\ldots,\mathbf{x}_N)$ of N particles, we have for the expectation value of the Hamiltonian H

$$\begin{aligned}\langle\Phi|\,H\,|\Phi\rangle =& \sum_{i=1}^{N}\langle\Phi|\,\frac{\mathbf{p}_i^2}{2m}\,|\Phi\rangle + 2\sum_{i=1}^{N}\sum_{j=1}^{k} Z_j e^2\,\langle\Phi|\ln\frac{|\mathbf{x}_i-\mathbf{R}_j|}{2r_0}\,|\Phi\rangle \\ &- 2\sum_{i<j}^{N} e^2\,\langle\Phi|\ln\frac{|\mathbf{x}_i-\mathbf{x}_j|}{2r_0}\,|\Phi\rangle \\ &- 2\sum_{i<j}^{k} Z_i Z_j e^2\,\langle\Phi|\ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0}\,|\Phi\rangle\end{aligned} \tag{2.179}$$

To derive a lower bound to this expectation value, we recall the definition of particle density

$$\rho(\mathbf{x}) = N\int \mathrm{d}^2\mathbf{x}_2\ldots\mathrm{d}^2\mathbf{x}_N\,|\Phi(\mathbf{x},\mathbf{x}_2,\ldots,\mathbf{x}_N)|^2 \tag{2.180}$$

normalized to

$$\int \mathrm{d}^2\mathbf{x}\ \rho(\mathbf{x}) = N \tag{2.181}$$

and

$$
\begin{aligned}
\langle\Phi|\Phi\rangle =& \int \mathrm{d}^2\mathbf{x}, \mathrm{d}^2\mathbf{x}_2 ... \mathrm{d}^2\mathbf{x}_N \ \Phi^*(\mathbf{x}, \mathbf{x}_2, ..., \mathbf{x}_N) \ \Phi(\mathbf{x}, \mathbf{x}_2, ..., \mathbf{x}_N) \\
=& \int \mathrm{d}^2\mathbf{x}, \mathrm{d}^2\mathbf{x}_2 ... \mathrm{d}^2\mathbf{x}_N \, |\Phi(\mathbf{x}, \mathbf{x}_2, ..., \mathbf{x}_N)|^2 \\
=& 1. \qquad (2.182)
\end{aligned}
$$

The lower bound (2.17) to the expectation value of the kinetic energy for particles of mass βm is then given by :

$$
\sum_{i=1}^{N} \langle\Phi| \frac{\mathbf{p}_i^2}{2m\beta} |\Phi\rangle > \frac{\pi\hbar^2}{Nm\beta(1+\delta)} \int \mathrm{d}^2\mathbf{x} \ \ [\rho(\mathbf{x})]^2 \qquad (2.183)
$$

where $\beta > 0$.

In reference to the second term on the right-hand side of (2.179), substitute (2.180) into (2.179), giving

$$
\begin{aligned}
&2 \sum_{i=1}^{N} \sum_{j=1}^{k} Z_j e^2 \, \langle\Phi| \ln \frac{|\mathbf{x}_i - \mathbf{R}_j|}{2r_0} |\Phi\rangle \\
&= 2 \int \mathrm{d}^2\mathbf{x}, \mathrm{d}^2\mathbf{x}_2, \ldots, \mathrm{d}^2\mathbf{x}_N \ \Phi^*(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N) \\
&\quad \times \left(\sum_{i=1}^{N} \sum_{j=1}^{k} e^2 Z_j \ln \frac{|\mathbf{x}_i - \mathbf{R}_j|}{2r_0} \right) \Phi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N) \\
&= 2 \sum_{j=1}^{k} \sum_{i=1}^{N} \int \mathrm{d}^2\mathbf{x}, \mathrm{d}^2\mathbf{x}_2, \ldots, \mathrm{d}^2\mathbf{x}_N \ \Phi^*(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N) \\
&\quad \times \left(\ e^2 Z_j \ln \frac{|\mathbf{x}_i - \mathbf{R}_j|}{2r_0} \right) \Phi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)
\end{aligned}
$$

$$
\begin{aligned}
=&2\sum_{j=1}^{k}\sum_{j=1}^{N}\int \mathrm{d}^2\mathbf{x}\ e^2 Z_j \ln\frac{|\mathbf{x}_i-\mathbf{R}_j|}{2r_0}\\
&\times\sum_{\sigma_1,\dots,\sigma_N}\int \mathrm{d}^2\mathbf{x}_2,\dots,\mathrm{d}^2\mathbf{x}_N\,|\Phi(\mathbf{x},\mathbf{x}_2,\dots,\mathbf{x}_N)|^2\\
=&2\sum_{j=1}^{k}\int \mathrm{d}^2\mathbf{x}\ e^2 Z_j \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}\ \frac{\rho(\mathbf{x})}{N}\\
&+2\sum_{j=1}^{k}\int \mathrm{d}^2\mathbf{x}_2\ e^2 Z_j \ln\frac{|\mathbf{x}_2-\mathbf{R}_j|}{2r_0}\ \frac{\rho(\mathbf{x}_2)}{N}\\
&+\ldots+2\sum_{j=1}^{k}\int \mathrm{d}^2\mathbf{x}_N\ e^2 Z_j \ln\frac{|\mathbf{x}_N-\mathbf{R}_j|}{2r_0}\ \frac{\rho(\mathbf{x}_N)}{N}\\
=&\ldots+2\sum_{j=1}^{k}e^2 Z_j\int \mathrm{d}^2\mathbf{x}\ \rho(\mathbf{x})\ \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}. \qquad (2.184)
\end{aligned}
$$

In reference to the third term on the right-hand side of (2.179), we first note that

$$
-2\sum_{i<j}^{N}e^2\,\langle\Phi|\ln\frac{|\mathbf{x}_i-\mathbf{x}_j|}{2r_0}\,|\Phi\rangle=-e^2\int \mathrm{d}^2\mathbf{x}'\int \mathrm{d}^2\mathbf{x}\ \rho(\mathbf{x})\ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ \rho(\mathbf{x}') \qquad (2.185)
$$

and for the fourth term on the right-hand side of (2.179) , we may write

$$
\begin{aligned}
-2\sum_{i<j}^{k}Z_iZ_je^2\,\langle\Phi|\ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0}\,|\Phi\rangle=&-2\sum_{i<j}^{k}Z_iZ_je^2\ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0}\,\langle\Phi\mid\Phi\rangle\\
=&-2\sum_{i<j}^{k}Z_iZ_je^2\ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0}. \qquad (2.186)
\end{aligned}
$$

From (2.183)–(2.186), we obtain the following lower bound for (2.179)

$$
\langle\Phi|\,H\,|\Phi\rangle>\frac{\pi\hbar^2}{Nm\beta}\int \mathrm{d}^2\mathbf{x}\ \left[\rho(\mathbf{x})\right]^2+2\sum_{j=1}^{k}e^2Z_j\int \mathrm{d}^2\mathbf{x}\ \rho(\mathbf{x})\ \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}
$$

$$- e^2 \int d^2\mathbf{x}\, d^2\mathbf{x}'\, \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ \rho(\mathbf{x}')$$

$$- 2 \sum_{i<j}^{k} Z_i Z_j e^2 \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} \tag{2.187}$$

by closing δ arbitrary small.

We define an *energy* functional $F[\rho]$ in 2-dimensions by

$$\begin{aligned} F[\rho; Z_1, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_j] =& \frac{\pi\hbar^2}{Nm\beta} \int d^2\mathbf{x}\ \ [\rho(\mathbf{x})]^2 \\ &+ 2 \sum_{j=1}^{k} e^2 Z_j \int d^2\mathbf{x}\ \rho(\mathbf{x})\ \ln \frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0} \\ &- e^2 \int d^2\mathbf{x}\, d^2\mathbf{x}'\, \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ \rho(\mathbf{x}') \\ &- 2 \sum_{i<j}^{k} Z_i Z_j e^2 \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} \end{aligned} \tag{2.188}$$

depending on positive parameters $Z_1, \ldots, Z_k$ and $\mathbf{R}_1, \ldots, \mathbf{R}_j$.

Optimize (2.188) over $\rho(\mathbf{x})$, by taking the functional derivative of (2.188), with respect to $\rho(\mathbf{x})$, equal to zero, to obtain

$$\begin{aligned} 0 =& \frac{\delta F[\rho]}{\delta \rho(\mathbf{x})} \\ =& \frac{2\pi\hbar^2}{Nm\beta} \rho(\mathbf{x}) + 2e^2 \sum_{j=1}^{k} Z_j\ \ln \frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0} \\ &- 2e^2 \int d^2\mathbf{x}'\ \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ \rho(\mathbf{x}'). \end{aligned} \tag{2.189}$$

Let $\rho(x) = \rho_0(\mathbf{x}; k)$ satisfy the equation (2.189), this is

$$\frac{2\pi\hbar^2}{Nm\beta}\,[\rho_0(\mathbf{x};k)] = -\,2e^2\sum_{j=1}^{k} Z_j\ \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0} + 2e^2\int \mathrm{d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ \rho(\mathbf{x}'). \tag{2.190}$$

Refer to (2.105)–(2.128), which shows that the TF density actually provides the smallest value, we conclude that $\rho_0(\mathbf{x}; k)$ satisfying (2.190) provides the smallest value for the functional (2.188), with the corresponding solution, $\rho_0(\mathbf{x}; k)$ satisfying the normalization condition

$$\int \mathrm{d}^2\mathbf{x}\ \rho_0(\mathbf{x};k) = \sum_{j=1}^{k} Z_j. \tag{2.191}$$

From (2.128), we then have

$$F[\rho] \geqslant F[\rho_0]$$

$$F[\rho; Z_1,\ldots,Z_k,\mathbf{R}_1,\ldots,\mathbf{R}_k] \geqslant F[\rho_0; Z_1,\ldots,Z_k,\mathbf{R}_1,\ldots,\mathbf{R}_k]. \tag{2.192}$$

We introduce the functionals

$$F[\rho; \lambda Z_1,\ldots,\lambda Z_\ell,\ Z_{\ell+1},\ldots,Z_k,\mathbf{R}_1,\ldots,\mathbf{R}_k] \tag{2.193}$$

and

$$F[\rho; \lambda Z_1,\ldots,\lambda Z_\ell,\mathbf{R}_1,\ldots,\mathbf{R}_\ell] \tag{2.194}$$

where $\ell < k$ and $\lambda > 0$ is arbitrary parameter.

Let $\rho_1(\mathbf{x}), \rho_2(\mathbf{x})$ be the corresponding solutions to (2.189) for the functionals in (2.193), (2.194), respectively. By referring to (2.189), we have

$$\frac{\pi\hbar^2}{Nm\beta}\rho_1(\mathbf{x}) = - e^2\lambda\sum_{j=1}^{\ell} Z_j \ \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0} - e^2 \sum_{j=\ell+1}^{k} Z_j \ \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}$$

$$+ e^2 \int \mathrm{d}^2\mathbf{x}' \ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0} \ \rho_1(\mathbf{x}') \tag{2.195}$$

and

$$\frac{\pi\hbar^2}{Nm\beta}\rho_2(\mathbf{x}) = - e^2\lambda\sum_{j=1}^{\ell} Z_j \ \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0} + e^2 \int \mathrm{d}^2\mathbf{x}' \ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0} \ \rho_2(\mathbf{x}') \tag{2.196}$$

and for the simplicity of the notation only, we have suppressed the dependence of ρ_1, ρ_2 on λ, k, ℓ.

By subtracting (2.195) from (2.196), we obtain

$$Q_1(\mathbf{x}) - Q_2(\mathbf{x}) = - e^2 \sum_{j=\ell+1}^{\ell} Z_j \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0} + e^2 \int \mathrm{d}^2\mathbf{x}' \ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0} \ [\rho_1(\mathbf{x}') - \rho_2(\mathbf{x}')]$$

$$= - e^2 \sum_{j=\ell+1}^{\ell} Z_j \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}$$

$$+ \frac{e^2 Nm\beta}{\pi\hbar^2} \int \mathrm{d}^2\mathbf{x}' \ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0} \ [Q_1(\mathbf{x}') - Q_2(\mathbf{x}')] \tag{2.197}$$

where

$$Q_1(\mathbf{x}) = \frac{\pi\hbar^2\rho_1(\mathbf{x})}{Nm\beta} \tag{2.198}$$

$$Q_2(\mathbf{x}) = \frac{\pi\hbar^2\rho_2(\mathbf{x})}{Nm\beta}. \tag{2.199}$$

Since the sum over j in (2.197) is non-negative, $\big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big]$ cannot be strictly negative for all $\mathbf{x}$ otherwise this will be in contradiction with the equation (2.197) itself.

We introduce the set

$$S = \{\mathbf{x} | Q_1(\mathbf{x}) - Q_2(\mathbf{x}) < 0\} \tag{2.200}$$

which we will show that it is empty, thus concluding that $Q_1(\mathbf{x}) - Q_2(\mathbf{x}) \geqslant 0$.

We assume that S is non-empty and then run into a contradiction. As we move away from the boundary Ω of S, $\big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big]$ changes sign or vanishes, by definition of S, and we then have

$$\hat{\mathbf{n}} \cdot \boldsymbol{\nabla} \big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big] \geqslant 0 \tag{2.201}$$

which $\hat{n}$ is a unit vector perpendicular to the boundary at $\mathbf{x}$, otherwise, we would run into a region beyond S where $\big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big]$ is still strictly negative. [If S is of infinite extension the non-negativity of $\hat{\mathbf{n}} \cdot \boldsymbol{\nabla} \big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big]$ on the boundary still holds.]

The application of the Laplacian to (2.197) gives

$$\begin{aligned}
\nabla^2 \big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big] = & -e^2 \lambda \sum_{j=\ell+1}^{k} Z_j \nabla^2 \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0} \\
& + \frac{e^2 N m \beta}{\pi \hbar^2} \int \mathrm{d}^2\mathbf{x}' \; \nabla^2 \ln \frac{|\mathbf{x} - \mathbf{x}'|}{2r_0} \left[Q_1(\mathbf{x}') - Q_2(\mathbf{x}')\right] \\
= & -4\pi e^2 \sum_{j=l+1}^{k} Z_j \, \delta^2(\mathbf{x} - \mathbf{R_j}) \\
& + \frac{e^2 N m \beta}{\pi \hbar^2} \int \mathrm{d}^2\mathbf{x}' \; \delta^2(\mathbf{x} - \mathbf{x}') \left[Q_1(\mathbf{x}') - Q_2(\mathbf{x}')\right] \\
= & -4\pi e^2 \sum_{j=l+1}^{k} Z_j \, \delta^2(\mathbf{x} - \mathbf{R_j})
\end{aligned}$$

$$+\, 4\pi e^2 \frac{Nm\beta}{\pi\hbar^2} \left[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\right] \tag{2.202}$$

and for $\mathbf{x}$ in the set S, the expression on the right-hand side of this equation is strictly negative since $\Big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\Big] < 0$ for such $\mathbf{x}$ by hypothesis.

Accordingly,

$$0 > \int_S \mathrm{d}^2\mathbf{x}\, \nabla^2 \big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big] = \int_\Omega \mathrm{d}\Omega\, \hat{\mathbf{n}} \cdot \boldsymbol{\nabla} \big[Q_1(\mathbf{x}) - Q_2(\mathbf{x})\big] \tag{2.203}$$

in contradiction with (2.201), hence S is empty and

$$Q_1(\mathbf{x}) - Q_2(\mathbf{x}) \geqslant 0 \tag{2.204}$$

as a function of $\mathbf{x}$.

In reference to the functional

$$F\big[\rho; Z_{l+1}, \ldots, Z_k, \mathbf{R}_{l+1}, \ldots, \mathbf{R}_k\big] \tag{2.205}$$

let $\rho_3(\mathbf{x})$ satisfy

$$\frac{\pi\hbar^2}{Nm\beta}\rho_3(\mathbf{x}) = -e^2 \sum_{j=\ell+1}^{k} Z_j \;\ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0} + e^2 \int \mathrm{d}^2\mathbf{x}' \;\ln \frac{|\mathbf{x} - \mathbf{x}'|}{2r_0}\; \rho_3(\mathbf{x}') \tag{2.206}$$

in analogy to (2.195), (2.196).

We define

$$g(\lambda) = F\big[\rho_1; \lambda Z_1, \ldots, \lambda Z_l, Z_{l+1}, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big]$$

$$-\, F\big[\rho_2; \lambda Z_1, \ldots, \lambda Z_l, \mathbf{R}_1, \ldots, \mathbf{R}_l\big]$$

$$-\, F\big[\rho_3; Z_{l+1}, \ldots, Z_k, \mathbf{R}_{l+1}, \ldots, \mathbf{R}_k\big] \tag{2.207}$$

with $l < k$. Since for $\lambda = 0$, ρ_1 and ρ_3 denote the same density, and ρ_2, in (2.207) is obviously equal to zero for $\lambda = 0$, as the left-hand side of (2.207) is non-negative while the right-hand side is non-positive for $\lambda = 0$, and

$$g(0) = F\big[\rho; Z_{l+1}, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big]$$

$$- F\big[0; \ldots \mathbf{R}_1, \ldots, \mathbf{R}_l\big]$$

$$- F\big[\rho; Z_{l+1}, \ldots, Z_k, \mathbf{R}_{l+1}, \ldots, \mathbf{R}_k\big] \qquad (2.208)$$

we may infer that

$$g(0) = 0. \qquad (2.209)$$

For $\lambda = 1$, gives

$$g(1) = F\big[\rho; Z_1, \ldots, Z_l, Z_{l+1}, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big]$$

$$- F\big[\rho_2; Z_1, \ldots, Z_l, \mathbf{R}_1, \ldots, \mathbf{R}_l\big]$$

$$- F\big[\rho; Z_{l+1}, \ldots, Z_k, \mathbf{R}_{l+1}, \ldots, \mathbf{R}_k\big]. \qquad (2.210)$$

From (2.209) and (2.212), we may write

$$g(1) = \int_0^1 \mathrm{d}\lambda \ g'(\lambda) \qquad (2.211)$$

we infer that $(F[\rho] \geqslant F[\rho_0])$

$$g(1) \geqslant 0 \qquad (2.212)$$

and hence to establish (2.212) it is sufficient to show that $g'(\lambda) \geqslant 0$ for $0 \leq \lambda \leq 1$.

To the above end, we note from (2.188) with $Z_1 \to \lambda Z_1, \ldots, Z_l \to \lambda Z_l$,

$\rho \to \rho_1$, we obtain

$$F\big[\rho_1; \lambda Z_1, \ldots, \lambda Z_l, Z_{l+1}, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big]$$

$$=\frac{\pi\hbar^2}{Nm\beta}\int \mathrm{d}^2\mathbf{x}\ \ [\rho_1(\mathbf{x})]^2$$

$$+\, 2\lambda\sum_{j=1}^{\ell} e^2 Z_j \int \mathrm{d}^2\mathbf{x}\ \rho_1(\mathbf{x})\ \ \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}$$

$$+\, 2\sum_{j=\ell+1}^{k} e^2 Z_j \int \mathrm{d}^2\mathbf{x}\ \rho_1(\mathbf{x})\ \ \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}$$

$$-\, e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \rho_1(\mathbf{x})\ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ \ \rho_1(\mathbf{x}')$$

$$-\, 2\lambda^2\sum_{i=1}^{\ell-1}\sum_{j=\ell+1}^{\ell} Z_i Z_j e^2\ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0}$$

$$-\, 2\sum_{i=1}^{\ell}\lambda Z_i \sum_{j=\ell+1}^{k} Z_j e^2\ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0} \tag{2.213}$$

where

$$2\sum_{i<j}^{k} Z_i Z_j e^2\ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0} = 2\lambda^2\sum_{i=1}^{\ell-1}\sum_{j=\ell+1}^{\ell} Z_i Z_j e^2\ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0}$$

$$+\, 2\sum_{i=1}^{\ell}\lambda Z_i\sum_{j=\ell+1}^{k} Z_j e^2\ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0}. \tag{2.214}$$

By setting the functional partial derivative of (2.213), with respect to λ, we obtain

$$\frac{\partial}{\partial\lambda}F\big[\rho_1; \lambda Z_1, \ldots, \lambda Z_l, Z_{l+1}, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\big]$$

$$=\frac{2\pi\hbar^2}{Nm\beta}\int \mathrm{d}^2\mathbf{x}\ \rho_1(\mathbf{x})\ \frac{\partial}{\partial\lambda}\rho_1(\mathbf{x})$$

$$+ 2\lambda \sum_{j=1}^{\ell} e^2 Z_j \int \mathrm{d}^2\mathbf{x} \ \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0} \frac{\partial}{\partial\lambda} \rho_1(\mathbf{x})$$

$$+ 2 \sum_{j=1}^{\ell} e^2 Z_j \int \mathrm{d}^2\mathbf{x} \ \rho_1(\mathbf{x}) \ \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0}$$

$$+ 2 \sum_{j=\ell+1}^{k} e^2 Z_j \int \mathrm{d}^2\mathbf{x} \ \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0} \ \frac{\partial}{\partial\lambda} \rho_1(\mathbf{x})$$

$$- 2e^2 \int \mathrm{d}^2\mathbf{x} \, \mathrm{d}^2\mathbf{x}' \ln \frac{|\mathbf{x} - \mathbf{x}'|}{2r_0} \ \rho_1(\mathbf{x}') \ \frac{\partial}{\partial\lambda} \rho_1(\mathbf{x})$$

$$- 4\lambda \sum_{i=1}^{\ell-1} \sum_{j=\ell+1}^{\ell} Z_i Z_j e^2 \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0}$$

$$- 2 \sum_{i=1}^{\ell} Z_i \sum_{j=\ell+1}^{k} Z_j e^2 \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0}. \qquad (2.215)$$

Eq.(2.215) can be rewritten as

$$\frac{\partial}{\partial\lambda} F\left[\rho_1; \lambda Z_1, \ldots, \lambda Z_l, Z_{l+1}, \ldots, Z_k, \mathbf{R}_1, \ldots, \mathbf{R}_k\right]$$

$$= \int \mathrm{d}^2\mathbf{x} \left[\frac{2\pi\hbar^2}{Nm\beta} \ \rho_1(\mathbf{x}) + 2\lambda \sum_{j=1}^{\ell} e^2 Z_j \ \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0} \right.$$

$$\left. + 2 \sum_{j=\ell+1}^{k} e^2 Z_j \ \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0} - 2e^2 \int \mathrm{d}^2\mathbf{x}' \ln \frac{|\mathbf{x} - \mathbf{x}'|}{2r_0} \ \rho_1(\mathbf{x}') \right] \ \frac{\partial}{\partial\lambda} \rho_1(\mathbf{x})$$

$$- e^2 \left[4\lambda \sum_{i=1}^{\ell-1} \sum_{j=\ell+1}^{\ell} Z_i Z_j \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} + 2 \sum_{i=1}^{\ell} Z_i \sum_{j=\ell+1}^{k} Z_j \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} \right]$$

$$+ 2 \sum_{j=1}^{\ell} e^2 Z_j \int \mathrm{d}^2\mathbf{x} \ \rho_1(\mathbf{x}) \ \ln \frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0} \qquad (2.216)$$

Refer to (2.195), and note that the expression within the brackets of the **x**-

integral in the first term on the right-hand side of (2.216) is zero. So that (2.216) becomes

$$\frac{\partial}{\partial\lambda}F\big[\rho_1;\lambda Z_1,\ldots,\lambda Z_l,Z_{l+1},\ldots,Z_k,\mathbf{R}_1,\ldots,\mathbf{R}_k\big]$$

$$=-e^2\left[4\lambda\sum_{i=1}^{\ell-1}\sum_{j=\ell+1}^{\ell}Z_iZ_j\ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0}+2\sum_{i=1}^{\ell}Z_i\sum_{j=\ell+1}^{k}Z_j\ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0}\right]$$

$$+2\sum_{j=1}^{\ell}e^2Z_j\int\mathrm{d}^2\mathbf{x}\;\rho_1(\mathbf{x})\;\ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}. \tag{2.217}$$

Refer to (2.216), and in the same way as in (2.217), we obtain

$$\frac{\partial}{\partial\lambda}F\big[\rho_2;\lambda Z_1,\ldots,\lambda Z_l,\mathbf{R}_1,\ldots,\mathbf{R}_l\big]$$

$$=-e^2\left[4\lambda\sum_{i=1}^{\ell-1}\sum_{j=\ell+1}^{\ell}Z_iZ_j\ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0}+2\sum_{i=1}^{\ell}Z_i\sum_{j=\ell+1}^{k}Z_j\ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0}\right]$$

$$+2\sum_{j=1}^{\ell}e^2Z_j\int\mathrm{d}^2\mathbf{x}\;\rho_2(\mathbf{x})\;\ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}. \tag{2.218}$$

Refer to (2.216), and in the same way as in (2.217), we obtain

$$\frac{\partial}{\partial\lambda}F\big[\rho_3;Z_l,\ldots,Z_k\mathbf{R}_{\ell+1},\ldots,\mathbf{R}_k\big]$$

$$=-2e^2\sum_{i=1}^{\ell}Z_i\sum_{j=\ell+1}^{k}Z_j\ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0}. \tag{2.219}$$

Finally refer to (2.210) and (2.217) to (2.219), to obtain

$$\frac{\partial}{\partial\lambda}g(\lambda)=2\sum_{j=1}^{\ell}Z_je^2\int\mathrm{d}^2\mathbf{x}\;\rho_1(\mathbf{x})\;\ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}-2\sum_{j=1}^{\ell}Z_je^2\int\mathrm{d}^2\mathbf{x}\;\rho_2(\mathbf{x})\;\ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}$$

$$
\begin{aligned}
&+2\sum_{i=1}^{\ell} Z_i \sum_{j=\ell+1}^{k} Z_j e^2 \ln \frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0} \\
=&2\sum_{i=1}^{\ell} Z_i \left[\sum_{j=\ell+1}^{k} Z_j e^2 \ln \frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0} + e^2\int \mathrm{d}^2\mathbf{x} \, \ln \frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0} \, [\rho_1(\mathbf{x})-\rho_2(\mathbf{x})]\right] \\
=&2\sum_{i=1}^{\ell} Z_i \,[Q_1(\mathbf{R}_i)-Q_2(\mathbf{R_i})] \\
\geqslant&0
\end{aligned} \tag{2.220}
$$

where we have used (2.204).

Accordingly, from (2.207) and (2.212), we have

$$
\begin{aligned}
F\big[\rho_1; Z_1,\ldots,Z_k,\mathbf{R}_1,\ldots,\mathbf{R}_k\big] \geqslant& F\big[\rho_2; Z_1,\ldots,Z_l,\mathbf{R}_1,\ldots,\mathbf{R}_\ell\big] \\
&+ F\big[\rho_3; Z_{l+1},\ldots,Z_k,\mathbf{R}_{\ell+1},\ldots,\mathbf{R}_k\big]
\end{aligned} \tag{2.221}
$$

for any $1 \leq \ell < k$, where ρ_1, ρ_2, ρ_3 are the densities which provide the smallest values for the corresponding functionals, respectively.

Accordingly, from (2.192) and (2.221), since ℓ, k (with $l < k$) are arbitrary natural numbers,we may conclude that

$$
F\big[\rho_0; Z_1,\ldots,Z_k,\mathbf{R}_1,\ldots,\mathbf{R}_k\big] \geqslant \sum_{i=1}^{k} F\big[\rho^i_{\mathrm{TF}}; Z_i,\mathbf{R}_i\big] \tag{2.222}
$$

where each $F\big[\rho^i_{\mathrm{TF}}; Z_i,\mathbf{R}_i\big]$ is a TF functional.

Consider the solution of the TF functional,(2.27)

$$
-\frac{\pi\hbar^2}{m}\,\big[n^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x})\big] = Ze^2 \ln \frac{|\mathbf{x}|}{2r_0} - e^2 \int \mathrm{d}^2\mathbf{x}' \, \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0} \, n^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x}') \tag{2.223}
$$

where $n^{\mathrm{B}}_{\mathrm{TF}}(\mathbf{x})$ is the TF density.

The ground-state energy $E_{TF}^{B}(Z)$ of the TF atom is given from (2.87) to be

$$E_{TF}^{B}(Z) = -(0.576486)\ e^2 Z^2. \tag{2.224}$$

In TF density $\rho_{\rm TF}^{i}$ with nuclear charge $Z_i|e|$, situated at $\mathbf{R}_i$, and the mass m of each negatively charged particle simply scaled by β, we replace $\mathbf{x}$ by $\mathbf{x}+\mathbf{R}$ and set

$$\rho_{TF}^{i}(\mathbf{x}+\mathbf{R}_i) = n_{\rm TF}^{\rm B}(\mathbf{x})\big|_{m\to m\beta, Z\to Z_i}. \tag{2.225}$$

Substitute this into (2.223),giving

$$-\frac{\pi\hbar^2}{m\beta}\left[\rho_{TF}^{i}(\mathbf{x})\right] = Z_i e^2 \ln\frac{|\mathbf{x}-\mathbf{R}_i|}{2r_0} - e^2\int {\rm d}^2\mathbf{x}'\ \ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ \rho_{TF}^{i}(\mathbf{x}'). \tag{2.226}$$

From (2.192),(2.222) and (2.224), we then have

$$F\big[\rho; Z_1,\ldots,Z_k,\mathbf{R}_1,\ldots,\mathbf{R}_k\big] \geqslant E_{\rm TF}(1)\sum_{i=1}^{k} Z_i^2 \tag{2.227}$$

where $E_{TF}(1) = -(0.576486)e^2$, independent to m.

The basic inequality in (2.221), shows that a system identified by the parameters $\big[Z_1,\ldots,Z_k,\mathbf{R}_1,\ldots,\mathbf{R}_k\big]$ cannot have an (optimized) energy functional (2.188) less than the sum of the (optimized) energy functional of any two subsystems identified by parameters $\big[Z_1,\ldots,Z_l,\mathbf{R}_1,\ldots,\mathbf{R}_l\big]$, $\big[Z_{l+1},\ldots,Z_k,\mathbf{R}_{l+1},\ldots,\mathbf{R}_k\big]$, $l<k$. Because of this last property, the Theorem embodied in the inequalities (2.221), (2.222) is referred to as a "No Binding Theorem".

We now deride a lower bound of the multi-particle repulsive coulomb potential energy. From (2.227) we note that

$$\frac{\pi\hbar^2}{m\beta}\int \mathrm{d}^2\mathbf{x}\,[\rho(\mathbf{x})]^2 + 2\sum_{j=1}^{k} Z_i e^2 \int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}\,\rho(\mathbf{x})$$

$$-e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\,\rho(\mathbf{x})\ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\,\rho(\mathbf{x}') - 2\sum_{i<j}^{k} Z_i Z_j e^2 \ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0}$$

$$\geqslant E_{TF}(1)\sum_{i=1}^{k} Z_i^2. \tag{2.228}$$

The energy density functional, expressed in terms of the density $\rho(\mathbf{x})$ on the left-hand side of (2.228) is in the spirit of the TF energy functional, with the mass m of the particle replaced by $m\beta$, and with the further generalization of including k nuclei, with the last term, involving '$Z_i Z_j\, e^2$', describing their interactions.

The inequality in (2.228) gives rise to a lower bound to the (repulsive) Coulomb potential energy of k particles of charges $Z_1|e|, \ldots, Z_k|e|$, or charges $-Z_1|e|, \ldots, -Z_k|e|$, i.e., for charges of the same signs as follows :

$$-2\sum_{i<j}^{k} Z_i Z_j e^2 \ln\frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0} \geqslant E_{TF}(1)\sum_{i=1}^{k} Z_i^2 - \frac{\pi\hbar^2}{m\beta}\int \mathrm{d}^2\mathbf{x}\,[\rho(\mathbf{x})]^2$$

$$-2\sum_{j=1}^{k} Z_i e^2 \int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}\,\rho(\mathbf{x})$$

$$+e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\,\rho(\mathbf{x})\ln\frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\,\rho(\mathbf{x}'). \tag{2.229}$$

In particular for the interaction of N particles we have, with substitutions $k \to N$, $Z_j \to 1$, $\mathbf{R}_j \to \mathbf{x}_j$ for $j = 1, \ldots, N$:

$$-2\sum_{i<j}^{k} e^2 \ln\frac{|\mathbf{x}_i-\mathbf{x}_j|}{2r_0} \geqslant N E_{TF}(1) - \frac{\pi\hbar^2}{m\beta}\int \mathrm{d}^2\mathbf{x}\,[\rho(\mathbf{x})]^2$$

$$
- 2\sum_{i=1}^{N} e^2 \int d^2\mathbf{x} \ \ln \frac{|\mathbf{x}-\mathbf{x}_j|}{2r_0}\, \rho(\mathbf{x})
$$

$$
+ e^2 \int d^2\mathbf{x}\, d^2\mathbf{x}'\, \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\, \rho(\mathbf{x}') \qquad (2.230)
$$

2.5 Lower Bound for the Exact Ground-state Energy

For symmetric normalized functions $\Phi(\mathbf{x}_1, \ldots, \mathbf{x}_N)$ of N particles, we have for the expectation value of the Hamiltonian H

$$
\langle\Phi| H |\Phi\rangle = \sum_{i=1}^{N} \langle\Phi| \frac{\mathbf{p}_i^2}{2m} |\Phi\rangle + 2\sum_{i=1}^{N}\sum_{j=1}^{k} Z_j e^2 \langle\Phi| \ln \frac{|\mathbf{x}_i-\mathbf{R}_j|}{2r_0} |\Phi\rangle
$$

$$
- 2\sum_{i<j}^{N} e^2 \langle\Phi| \ln \frac{|\mathbf{x}_i-\mathbf{x}_j|}{2r_0} |\Phi\rangle
$$

$$
- 2\sum_{i<j}^{k} Z_i Z_j e^2 \langle\Phi| \ln \frac{|\mathbf{R}_i-\mathbf{R}_j|}{2r_0} |\Phi\rangle \qquad (2.231)
$$

with wavefunction normalization condition.

The lower bound (2.178) to the expectation value of the kinetic energy of bosons :

$$
\sum_{i=1}^{N} \langle\Phi| \frac{\mathbf{p}_i^2}{2m} |\Phi\rangle \geq \frac{\pi}{N} \frac{\hbar^2}{2m} \int d^2\mathbf{x}\ \rho^2(\mathbf{x}) \qquad (2.232)
$$

for δ sufficiently small.

For the second term on the right-hand side of (2.231), substitute (2.180) into (2.231), we obtain

$$
2\sum_{i=1}^{N}\sum_{j=1}^{k} Z_j e^2 \langle\Phi| \ln \frac{|\mathbf{x}_i-\mathbf{R}_j|}{2r_0} |\Phi\rangle
$$

$$
\begin{aligned}
=&2\int \mathrm{d}^2\mathbf{x}, \mathrm{d}^2\mathbf{x}_2, \ldots, \mathrm{d}^2\mathbf{x}_N\ \Phi^*(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)\\
&\times\left(\sum_{i=1}^{N}\sum_{j=1}^{k}\ e^2 Z_j \ln\frac{|\mathbf{x}_i - \mathbf{R}_j|}{2r_0}\right)\Phi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)\\
=&2\sum_{j=1}^{k}\sum_{i=1}^{N}\int \mathrm{d}^2\mathbf{x}, \mathrm{d}^2\mathbf{x}_2, \ldots, \mathrm{d}^2\mathbf{x}_N\ \Phi^*(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)\\
&\times\left(\ e^2 Z_j \ln\frac{|\mathbf{x}_i - \mathbf{R}_j|}{2r_0}\right)\Phi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)\\
=&2\sum_{j=1}^{k}\sum_{j=1}^{N}\int \mathrm{d}^2\mathbf{x}\ e^2 Z_j \ln\frac{|\mathbf{x}_i - \mathbf{R}_j|}{2r_0}\\
&\times\sum_{\sigma_1,\ldots,\sigma_N}\int \mathrm{d}^2\mathbf{x}_2, \ldots, \mathrm{d}^2\mathbf{x}_N\,|\Phi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_N)|^2\\
=&2\sum_{j=1}^{k}\int \mathrm{d}^2\mathbf{x}\ e^2 Z_j \ln\frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0}\ \frac{\rho(\mathbf{x})}{N}\\
&+2\sum_{j=1}^{k}\int \mathrm{d}^2\mathbf{x}_2\ e^2 Z_j \ln\frac{|\mathbf{x}_2 - \mathbf{R}_j|}{2r_0}\ \frac{\rho(\mathbf{x}_2)}{N}\\
&+\ldots+2\sum_{j=1}^{k}\int \mathrm{d}^2\mathbf{x}_N\ e^2 Z_j \ln\frac{|\mathbf{x}_N - \mathbf{R}_j|}{2r_0}\ \frac{\rho(\mathbf{x}_N)}{N}\\
=&2\sum_{j=1}^{k} e^2 Z_j\int \mathrm{d}^2\mathbf{x}\ \rho\ \ln\frac{|\mathbf{x} - \mathbf{R}_j|}{2r_0}.
\end{aligned}
\tag{2.233}
$$

For the third term on the right-hand side of (2.231), we first note that

$$
\begin{aligned}
&-2\sum_{i=1}^{N} e^2\,\langle\Phi|\int \mathrm{d}^2\mathbf{x}\ \ln\frac{|\mathbf{x} - \mathbf{x}_j|}{2r_0}\,\rho(\mathbf{x})\,|\Phi\rangle\\
&\qquad= -2\sum_{j=1}^{N} e^2\int \mathrm{d}^2\mathbf{x}', \mathrm{d}^2\mathbf{x}_2, \ldots, \mathrm{d}^2\mathbf{x}_N\ \Phi^*(\mathbf{x}', \mathbf{x}_2, \ldots, \mathbf{x}_N)
\end{aligned}
$$

$$\times \left(\int \mathrm{d}^2\mathbf{x}\ \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}_j|}{2r_0} \right)\ \Phi(\mathbf{x}', \mathbf{x}_2, \ldots \mathbf{x}_N)$$

$$= -2\sum_{j=1}^{N} e^2 \int \mathrm{d}^2\mathbf{x}' \int \mathrm{d}^2\mathbf{x}\ \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}_j|}{2r_0}$$

$$\times \sum_{\sigma_1,\ldots,\sigma_N} \int \mathrm{d}^2\mathbf{x}_2, \ldots, \mathrm{d}^2\mathbf{x}_N\ \ |\Phi(\mathbf{x}', \mathbf{x}_2, \ldots, \mathbf{x}_N)|^2$$

$$= -2\frac{e^2}{N} \int \mathrm{d}^2\mathbf{x}' \int \mathrm{d}^2\mathbf{x}\ \rho(\mathbf{x})\ \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ \rho(\mathbf{x}')$$

$$+ \frac{e^2}{N} \int \mathrm{d}^2\mathbf{x}_2 \int \mathrm{d}^2\mathbf{x}\ \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}_2|}{2r_0}\ \rho(\mathbf{x}_2)$$

$$+ \ldots + \frac{e^2}{N} \int \mathrm{d}^2\mathbf{x}_N \int \mathrm{d}^2\mathbf{x}\ \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}_N|}{2r_0}\ \rho(\mathbf{x}_N)$$

$$= -2e^2 \int \mathrm{d}^2\mathbf{x}' \int \mathrm{d}^2\mathbf{x}\ \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{2r_0}\ \rho(\mathbf{x}') \tag{2.234}$$

and from (2.230)

$$-2\sum_{i<j}^{k} e^2 \langle\Phi| \ln \frac{|\mathbf{x}_i-\mathbf{x}_j|}{2r_0} |\Phi\rangle \geq N E_{TF}(1) - \frac{\pi\hbar^2}{m\beta} \int \mathrm{d}^2\mathbf{x}\, [\rho(\mathbf{x})]^2$$

$$- e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\ \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho(\mathbf{x}'). \tag{2.235}$$

From (2.232)–(2.235), we obtain the following lower bound for (2.231)

$$\langle\Phi| H |\Phi\rangle \geq \frac{\pi}{N}\frac{\hbar^2}{2m} \int \mathrm{d}^2\mathbf{x}\ \rho^2(\mathbf{x}) + 2\sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^2\mathbf{x}\ \rho\ \ln \frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0}$$

$$+ N E_{TF}(1) - \frac{\pi}{\beta N}\frac{\hbar^2}{2m} \int \mathrm{d}^2\mathbf{x}\, [\rho(\mathbf{x})]^2$$

$$- e^2 \int \mathrm{d}^2\mathbf{x}\, \mathrm{d}^2\mathbf{x}'\ \rho(\mathbf{x}) \ln \frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho(\mathbf{x}')$$

$$- 2\sum_{i<j}^{k} Z_i Z_j e^2 \langle\Phi| \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} |\Phi\rangle \,. \tag{2.236}$$

We set

$$\left(\frac{\pi}{N} - \frac{\pi}{\beta}\right) \times \frac{1}{\pi} = \frac{1}{N} - \frac{1}{\beta} = \frac{1}{\beta'} \tag{2.237}$$

and for positive β' we have to choose $\beta > N$. Apply (2.237) to (2.236), to get

$$\begin{aligned}\langle\Phi| H |\Phi\rangle \geq & \frac{\pi}{\beta'}\frac{\hbar^2}{2m}\int \mathrm{d}^2\mathbf{x}\ \rho^2(\mathbf{x}) + 2\sum_{j=1}^{k} e^2 Z_j \int \mathrm{d}^2\mathbf{x}\ \rho\ \ln\frac{|\mathbf{x}-\mathbf{R}_j|}{2r_0} \\ & - e^2\int \mathrm{d}^2\mathbf{x}\,\mathrm{d}^2\mathbf{x}'\ \rho(\mathbf{x}) \ln\frac{|\mathbf{x}-\mathbf{x}'|}{B}\ \rho(\mathbf{x}') \\ & - 2\sum_{i<j}^{k} Z_i Z_j e^2 \langle\Phi| \ln\frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0} |\Phi\rangle + N E_{TF}(1).\end{aligned} \tag{2.238}$$

Course of E_{TF} is m independent, using (2.228), we can replace β by β' and the sum of the first form on the right-hand side of inequality (2.236) then gives

$$\begin{aligned}\langle\Phi| H |\Phi\rangle \geq & E_{TF}(1)\sum_{j=1}^{k} Z_j^2 + N E_{TF}(1) \\ = & E_{TF}(1)\left(N + \sum_{j=1}^{k}\frac{Z_j^2}{N}\right) \\ \langle\Phi| H |\Phi\rangle \geq & -(0.576486)e^2\left(N + \sum_{j=1}^{k} Z_j Z_{max}\right) \\ = & -(0.576486)e^2\left(N + N Z_{max}\right) \\ = & -(0.576486)e^2 N(1 + Z_{max})\end{aligned}$$

$$\therefore \quad \langle\Phi| H |\Phi\rangle \geq -(0.576486)e^2 N(1 + Z_{max}) \tag{2.239}$$

where

$$Z_j Z_{max} \geq Z_j^2. \tag{2.240}$$

2.6 Inflation of Matter.

Let $|\Phi(m)\rangle$ denote any negative energy-state of matter, not necessarily the ground-state,

$$-\varepsilon_N[m] \leq \langle\Phi(m)| H |\Phi(m)\rangle \tag{2.241}$$

where $-\varepsilon_N[m] = E_N < 0$ is the ground-state energy, and we have emphasized its dependence on the mass m of the particle.

To establish the statement made above, we need upper and lower bounds to the expectation value of the kinetic energy operator

$$T \equiv \left\langle \phi \left| \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} \right| \phi \right\rangle \tag{2.242}$$

To the above end, we rewrite $|\Phi\rangle = |\Phi(m)\rangle$. By definition of the ground-state energy, the state $|\Phi(m/2)\rangle$ cannot lead for $\langle\Phi(m/2)| H |\Phi(m/2)\rangle$ a numerical value lower than $-\varepsilon_N[m]$. That is,

$$-\varepsilon_N[m] \leq \langle\Phi(m/2)| H |\Phi(m/2)\rangle < 0 \tag{2.243}$$

where we note that the interaction part V of the Hamiltonian H in (2.231) is not explicitly dependent on m :

$$V = 2\sum_{i=1}^{N}\sum_{j=1}^{k} Z_j e^2 \ln \frac{|\mathbf{x}_i - \mathbf{R}_j|}{2r_0} - 2\sum_{i<j}^{N} e^2 \ln \frac{|\mathbf{x}_i - \mathbf{x}_j|}{2r_0}$$

$$- 2 \sum_{i<j}^{k} Z_i Z_j e^2 \ln \frac{|\mathbf{R}_i - \mathbf{R}_j|}{2r_0}. \tag{2.244}$$

Accordingly (2.243) implies that

$$-\varepsilon_N[2m] \leq \left\langle \Phi(m) \middle| \left(\frac{T}{2} + V \right) \middle| \Phi(m) \right\rangle . \tag{2.245}$$

Upon writing, trivially,

$$T + V = \frac{T}{2} + \frac{T}{2} + V \tag{2.246}$$

the extreme right-hand of the inequality (2.241) then leads to

$$\left\langle \Phi(m) \middle| \frac{T}{2} \middle| \Phi(m) \right\rangle < - \left\langle \Phi(m) \middle| \left(\frac{T}{2} + V \right) \middle| \Phi(m) \right\rangle \tag{2.247}$$

which upon multiplying by two, (2.245) gives

$$\langle \Phi(m) \left| T \right| \Phi(m) \rangle \leq 2\varepsilon_N \left[2m \right] \tag{2.248}$$

for all states $|\Phi(m)\rangle$ such that (2.241) is true including the ground-state.

Thus from (2.248), (2.240), (2.232), we have the following bounds for the expectation value T of the total kinetic energy of all the particles in such states

$$\frac{\pi}{N} \frac{\hbar^2}{2m} \int \mathrm{d}^2\mathbf{x} \; \rho^2(\mathbf{x}) < T < (2)(0.586476) e^2 N (1 + Z_{max}) \tag{2.249}$$

To investigate the inflation of matter, let $\mathbf{x}$ denote the position of an particle relative, for example, to the center of mass of the nuclei. We define the set function

$$\chi_R(\mathbf{x}) = \begin{cases} 1, & \text{if } \mathbf{x} \text{ lies within a sphere of radius } R \\ 0, & \text{otherwise.} \end{cases} \tag{2.250}$$

We are interested in the expression

$$\text{Prob}\left[|\mathbf{x}_1| \le R, \ldots, |\mathbf{x}_N| \le R\right] = \int \left(\prod_{i=1}^{N} \mathrm{d}^2\mathbf{x}_i \; \chi_R(\mathbf{x}_i) \right) |\Phi(\mathbf{x}_1, \ldots, \mathbf{x}_N)|^2 \quad (2.251)$$

which gives the probability of finding all the particles within a circle of radius R. Clearly,

$$\begin{aligned} \text{Prob}\left[|\mathbf{x}_1| \le R, \ldots, |\mathbf{x}_N| \le R\right] &\le \text{Prob}\left[|\mathbf{x}_1| \le R, \ldots, |\mathbf{x}_j| \le R\right] \\ &\le \ldots \le \text{Prob}\left[|\mathbf{x}_1| \le R\right] \\ &= \frac{1}{N} \int \mathrm{d}^2\mathbf{x} \; \chi_R(\mathbf{x}) \rho(\mathbf{x}) \end{aligned} \quad (2.252)$$

for $j < N$, with $\rho(\mathbf{x})$ given in (2.180).

By Hölder's inequality we have

$$\int \mathrm{d}^2\mathbf{x} \; \chi_R(\mathbf{x}) \rho(\mathbf{x}) \le \left(\int \mathrm{d}^2\mathbf{x} \; \rho^2(\mathbf{x}) \right)^{1/2} \left(\int \mathrm{d}^2\mathbf{x} \; \chi_R^2(\mathbf{x}) \right)^{1/2} \quad (2.253)$$

where $\chi_R^2(\mathbf{x}) = \chi_R(\mathbf{x})$, and

$$\int \mathrm{d}^2\mathbf{x} \; \chi_R(\mathbf{x}) = A_R \quad (2.254)$$

denotes the area in which the particles are confined.

Hence, in particular, (2.252) gives

$$\begin{aligned} \text{Prob}\left[|\mathbf{x}_1| \le R, \ldots, |\mathbf{x}_N| \le R\right] &\le \text{Prob}\left[|\mathbf{x}_1| \le R\right] \\ &\le \frac{(A_R)^{1/2}}{N} \left(\int \mathrm{d}^2\mathbf{x} \; \rho^2(\mathbf{x}) \right)^{1/2} \end{aligned}$$

$$\leq \frac{(A_R)^{1/2}}{N}\left[(2.305944)\frac{me^2N}{\pi\hbar^2}(1+Z_{max})\right]^{1/2} \tag{2.255}$$

where (from (2.249))

$$\left(\int \mathrm{d}^2\mathbf{x}\ \rho^2(\mathbf{x})\right)^{1/2} \leq \left[(2.305944)\frac{me^2N}{\pi\hbar^2}(1+Z_{max})\right]^{1/2} \tag{2.256}$$

finally leads to the simple bound

$$\mathrm{Prob}\left[|\mathbf{x}_1| \leq R, \ldots, |\mathbf{x}_N| \leq R\right]\left(\frac{N}{A_R}\right)^{1/2} < (0.856568)\left[\frac{me^2}{\hbar^2}(1+Z_{\max})\right]^{1/2} \tag{2.257}$$

where $a_0 = \hbar^2/me^2$ is the Bohr radius and $Z_{\max}$ is the maximum of the nuclear charges.

We immediately infer from (2.257) the inescapable fact the *necessarily*, given that there is a non-zero probability of particles to be limit within a circle of radius R, then the corresponding area A_R grows not any slower than the first power of N for $N \to \infty$, since otherwise the left-hand side of (2.257) would go to infinite in this limit while the right-hand side is finite. That is, *necessarily*, the radius R *of spatial extension of matter grows not any slower than* $N^{1/2}$ *for* $N \to \infty$.

We note that N/A_R gives the particle density, and one may infer from (2.257), with a probability non-zero provide that particles are limit within a circle of radius R, the infinite density limit $N/A_R \to \infty$, i.e., of the system collapsing onto itself, does not occur.

2.7 Non-Zero Lower Bound for a Measure of the Extension of Matter

We use define the expectation value

$$\left\langle \sum_{i=1}^{N} \frac{|\mathbf{x}_i|}{N} \right\rangle = \int \mathrm{d}^2\mathbf{x}_1 \ldots \mathrm{d}^2\mathbf{x}_N \left(\sum_{i=1}^{N} \frac{|\mathbf{x}_i|}{N} \right) |\Phi(\mathbf{x}_1, \ldots, \mathbf{x}_N)|^2$$

$$= \frac{1}{N} \int \mathrm{d}^2\mathbf{x}\ |\mathbf{x}| \rho(\mathbf{x}) \tag{2.258}$$

as for a measure of the extension of matter. Using the facts that

$$\frac{1}{N} \int \mathrm{d}^2\mathbf{x}\ |\mathbf{x}| \rho(\mathbf{x}) \geqslant \frac{1}{N} \int_{|\mathbf{x}|>R} \mathrm{d}^2\mathbf{x}\ |\mathbf{x}| \rho(\mathbf{x}) \geqslant \frac{R}{N} \int_{|\mathbf{x}|>R} \mathrm{d}^2\mathbf{x}\ \rho(\mathbf{x})$$

$$= R\ \mathrm{Prob}\left[|\mathbf{x}| > R\right] \tag{2.259}$$

$$\mathrm{Prob}\left[|\mathbf{x}| > R\right] = 1 - \mathrm{Prob}\left[|\mathbf{x}| \leq R\right] \tag{2.260}$$

$A_R = \pi R^2$, and (2.257) we obtain

$$\left\langle \sum_{i=1}^{N} \frac{|\mathbf{x}_i|}{N} \right\rangle \geqslant R \left[1 - \left(\frac{\pi R^2}{N} \right)^{1/2} (1.518534) \left[\frac{me^2}{\hbar^2} (1 + Z_{\mathrm{max}}) \right]^{1/2} \right]. \tag{2.261}$$

Upon optimizing the right-hand side of the above inequality over R, this gives

$$R = (0.329265) \left(\frac{N}{\pi} \frac{\hbar^2}{me^2} \frac{1}{(1 + Z_{\mathrm{max}})} \right)^{1/2}. \tag{2.262}$$

leading for (2.261) to the explicit non-zero lower bound

$$\left\langle \sum_{i=1}^{N} \frac{|\mathbf{x}_i|}{N} \right\rangle \geqslant (0.164632) N^{1/2} \left(\frac{\hbar^2}{\pi me^2} \frac{1}{(1 + Z_{\mathrm{max}})} \right)^{1/2}. \tag{2.263}$$

CONCLUSION

1. We show that

$$E_R \leq E_{NR}$$

indenpendently of the statistics obeyed by the particles and *indenpendently* of the dimensionality of space. The demonstration is not difficult but the result is undoubtedly important realizing its generality in applications including for the case $N = 1$. In particular, this established the instability of so-called "*bosonics* matter", obtained by relaxing the Pauli exclusion principle with relativistic kinetic energies E_R, i.e., for $-E_R$, with the some power of N as a lower bound obtained for $-E_{NR}$ with non-relativistic kinetic energies for the latter. We expect that the method of analysis used in this communication will be useful for related developments of relativistic many-particle systems and, in particular, to "fermionic matter". Such investigations will be carried out in a future report

2. We prove rigorously that such matter is stable with logarithmic potentials with out involving the exclusion principle (bosonic matter). The lower bound for the ground-state energy in 2 dimemsions depends on a single power of N, which is given by

$$\langle\Phi| H |\Phi\rangle \geq -(0.576486)e^2 N(1 + Z_{max}).$$

3. We immediately infer

$$\text{Prob}\left[|\mathbf{x}_1| \leq R, \ldots, |\mathbf{x}_N| \leq R\right] \left(\frac{N}{A_R}\right)^{1/2} \leq (0.856568) \left[\frac{me^2}{\hbar^2}(1 + Z_{\max})\right]^{1/2}$$

the inescapable fact that given that there is a non-zero probability of particles to be limited within a circle of radius R, then the corresponding area A_R grows not any slower than the first power of N for $N \to \infty$, since otherwise the left-hand side of this inequality would go to infinity in this limit while the right-hand side is finite. That is, *necessarily*, the radius R *of spatial extension of matter grows not any slower than* $N^{1/2}$ *for* $N \to \infty$. We note that N/A_R gives the particle density, with a probability non-zero provide that particles are limited within a circle of radius R, the infinite density limit $N/A_R \to \infty$, i.e., of the system collapsing onto itself, does not occur.

4. Non-zero lower bound for a measure of the extension of matter in 2-dimensions is given by

$$\left\langle \sum_{i=1}^{N} \frac{|\mathbf{x}_i|}{N} \right\rangle \geqslant (0.164632) N^{1/2} \left(\frac{\hbar^2}{\pi m e^2} \frac{1}{(1+Z_{\max})} \right)^{1/2}.$$

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OUTPUT

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APPENDIX

Stability of matter without exclusion principle in 2D with logarithmic potentials

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Abstract

We prove rigorously the stability of matter without exclusion principle in 2D with logarithmic potential.

Keywords: matter in the bulk, stability of matter in 2D, with logarithmic potentials.
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One of the most fundamental problems that quantum mechanics has solved was that of the stability of matter [1, 2]. This result is based on two basic properties, one is the boundedness of the ground-state energy from below and the Pauli exclusion principle. For matter, with the exclusion principle and with Coulomb interaction, the ground-state energy $E_N \sim N$, with N denoting the number of electrons in matter, and matter consisting of $(2N + 2N)$ particles is not favoured over two separate systems brought together, each consisting of $(N + N)$ particles. This is unlike the situation with "matter" without the exclusion principle for which $E_N \sim N^{\alpha}$ with $\alpha > 1$. It is important to know if such properties are tied down with the dimensionality of space. In particular, there has been interest in recent years in physics in $2D$, e.g. [3, 4, 5, 6, 7] and the role of spin and statistics. It is well known that matter is stable [8] in 2D with $1/r$ potentials with the exclusion principle. On the other hand it is pertinent to know what the outcome is of one assumes the logarithmic potential in 2D as dictated by the Poisson equation $\nabla^2 \ln r \sim \delta^2(\vec{r})$. We prove rigorously that such matter is stable with logarithmic potentials with out involving the exclusion principle. To do this, we first review the TF atom in 2D with logarithmic potentials as well as the No-binding theorem for such a case and finally derive a lower bound for the exact ground-state of matter involving a single power of N. We also establish that such matter would necessarily increase radially not any slower than $N^{\frac{1}{2}}$ with N as it is for ordinary matter in 3D [9]. Unlike the situation with a logarithmic potential, matter with $1/r$ potential is unstable. For reviews of problems of stability of matter see [2, 10].

We review the TF atom in 2D with logarithmic potentials. We define the TF energy functional

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$F[n_{\rm B}]$ for (spin 0) matter without exclusion principle in 2D:

$$F[n_{\rm B}] = \frac{\pi\hbar^2}{m}\int d^2\vec{x}\,[n_{\rm B}(\vec{x})]^2 + 2Ze^2\int d^2\vec{x}\,\ln\frac{|\vec{x}|}{2r_0}\,n_{\rm B}(\vec{x})$$
$$- e^2\int d^2\vec{x}\,d^2\vec{x}'\,n_{\rm B}(\vec{x})\ln\frac{|\vec{x}-\vec{x}'|}{2r_0}\,n_{\rm B}(\vec{x}') \tag{1}$$

where $r_0 = \left(\hbar^2/2me^2\right)^{1/2}$, and $2r_0$ provides a scale factor [8], and $n_{\rm B}(\vec{x})$ is the particle density. By functional differentiation of $F[n_{\rm B}]$ with respect to $n_{\rm B}(\vec{x})$, we obtain an integral equation satisfied by the TF particle density

$$n^{\rm B}_{\rm TF}(\vec{x}) = -\frac{mZe^2}{\pi\hbar^2}\ln\frac{|\vec{x}|}{2r_0} + \frac{me^2}{\pi\hbar^2}\int d^2\vec{x}'\,\ln\frac{|\vec{x}-\vec{x}'|}{2r_0}\,n^{\rm B}_{\rm TF}(\vec{x}'). \tag{2}$$

The evaluation of the ground-state TF energy is straightforward and is carried out in detail in [8] and is given by

$$E_{\rm TF} = F[n^{\rm B}_{\rm TF}] = -0.576486\,Z^2e^2. \tag{3}$$

Before deriving a lower bound to the exact ground-state of matter, without the exclusion, in 2D, with a logarithmic potential, we also need the following No-Binding Theorem. We define a TF energy-like functional for multi-particle systems with a logarithmic potential :

$$\mathcal{F}[\rho; Z_1,\ldots,Z_k; \vec{R}_1,\ldots,\vec{R}_k] = \frac{\pi\hbar^2}{m\beta}\int d^2\vec{x}\,\rho^2(\vec{x}) + 2\sum_{j=1}^{k} Z_j\,e^2\int d^2\vec{x}\,\rho(\vec{x})\,\ln\left(\frac{|\vec{x}-\vec{R}_j|}{2r_0}\right)$$
$$- 2e^2\sum_{i<j}^{k} Z_i\,Z_j\,\ln\left(\frac{|\vec{R}_i-\vec{R}_j|}{2r_0}\right)$$
$$- e^2\int d^2\vec{x}\,d^2\vec{x}'\,\rho(\vec{x})\,\ln\left(\frac{|\vec{x}-\vec{x}'|}{2r_0}\right)\rho(\vec{x}') \tag{4}$$

where $\beta > 0$ is arbitrary. Here the $\vec{R}_i$ denote the positions of the nuclei.

The No-Binding Theorem now reads [8]

$$\mathcal{F}[\rho; Z_1,\ldots,Z_k; \vec{R}_1,\ldots,\vec{R}_k] \geq -(0.576486)\,e^2\sum_{i=1}^{k} Z_i^2 \tag{5}$$

From (4) and (5), we have the following two useful inequalities

$$-2e^2\sum_{i<j}^{k} Z_i\,Z_j\,\ln\left(\frac{|\vec{R}_i-\vec{R}_j|}{2r_0}\right) \geq -\frac{\pi\hbar^2}{m\beta}\int d^2\vec{x}\,\rho^2(\vec{x}) - 2\sum_{j=1}^{k} Z_j\,e^2\int d^2\vec{x}\,\rho(\vec{x})\,\ln\left(\frac{|\vec{x}-\vec{R}_j|}{2r_0}\right)$$
$$+ e^2\int d^2\vec{x}\,d^2\vec{x}'\,\rho(\vec{x})\,\ln\left(\frac{|\vec{x}-\vec{x}'|}{2r_0}\right)\rho(\vec{x}')$$
$$-(0.576486)\,e^2\sum_{i=1}^{k} Z_i^2. \tag{6}$$

The latter also implies that

$$
\begin{aligned}
-2e^2 \sum_{i<j}^{N} \ln\left(\frac{|\vec{x}_i - \vec{x}_j|}{2r_0}\right) \geq & -\frac{\pi\hbar^2}{m\beta} \int \mathrm{d}^2\vec{x}\, \rho^2(\vec{x}) \\
& - 2\sum_{i=1}^{N} e^2 \int \mathrm{d}^2\vec{x}\, \rho(\vec{x})\, \ln\left(\frac{|\vec{x} - \vec{x}_i|}{2r_0}\right) \\
& + e^2 \int \mathrm{d}^2\vec{x}\, \mathrm{d}^2\vec{x}'\, \rho(\vec{x})\, \ln\left(\frac{|\vec{x} - \vec{x}'|}{2r_0}\right) \rho(\vec{x}') \\
& - (0.576486)\, e^2 N. \qquad (7)
\end{aligned}
$$

To derive a lower bound to the ground-state energy of matter, we need a lower bound to the expectation value of the kinetic energy $\langle\psi| \sum_{i=1}^{N} \vec{p}_i^{\,2}/2m\, |\psi\rangle = T$. To this end, set

$$
f(\vec{x}) = 2\, \frac{\rho(\vec{x})}{\int \mathrm{d}^2\vec{x}\, \rho^2(\vec{x})}\, T \qquad (8)
$$

then

$$
\langle\psi| \sum_{i=1}^{N} \left[\frac{\vec{p}_i^{\,2}}{2m} - f(\vec{x}_i)\right] |\psi\rangle = -T. \qquad (9)
$$

An adaptation of the Schwinger bound [11] for matter without exclusion in 2D, then leads to

$$
T \geq \frac{\pi}{N} \frac{\hbar^2}{2m} \int \mathrm{d}^2\vec{x}\, \rho^2(\vec{x}), \qquad (10)
$$

by using, in the process, that due to the bose character of the N particles, they may all be put in the lowest energy level which accounts for the $1/N$ factor on the right-hand side of the inequality.

We define the total Hamiltonian of the system

$$
\begin{aligned}
H = & \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + 2e^2 \sum_{i=1}^{N} \sum_{j=1}^{k} Z_j\, \ln\left(\frac{|\vec{x}_i - \vec{R}_j|}{2r_0}\right) \\
& - 2e^2 \sum_{i<j}^{N} \ln\left(\frac{|\vec{x}_i - \vec{x}_j|}{2r_0}\right) - 2e^2 \sum_{i<j}^{k} Z_i\, Z_j\, \ln\left(\frac{|\vec{R}_i - \vec{R}_j|}{2r_0}\right). \qquad (11)
\end{aligned}
$$

By using the No-Binding Theorem, from (5), we have the following bound

$$
\begin{aligned}
& \langle\psi| - 2e^2 \sum_{i<j} \ln\left(\frac{|\vec{x}_i - \vec{x}_j|}{2r_0}\right) |\psi\rangle \\
& \quad \geq -\frac{\pi\hbar^2}{m\beta} \int \mathrm{d}^2\vec{x}\, \rho^2(\vec{x}) - e^2 \int \mathrm{d}^2\vec{x}\, \mathrm{d}^2\vec{x}'\, \rho(\vec{x})\, \ln\left(\frac{|\vec{x} - \vec{x}'|}{2r_0}\right) \rho(\vec{x}') \\
& \quad - (0.576486)\, e^2 N \qquad (12)
\end{aligned}
$$

and explicitly

$$
\langle\psi|\, 2e^2 \sum_{i=1}^{N} \sum_{j=1}^{k} Z_j\, \ln\left(\frac{|\vec{x}_i - \vec{R}_j|}{2r_0}\right) |\psi\rangle = 2e^2 \sum_{j=1}^{k} Z_j \int \mathrm{d}^2\vec{x}\, \ln\left(\frac{|\vec{x} - \vec{R}_j|}{2r_0}\right) \rho(\vec{x}). \qquad (13)
$$

From (10)–(13), we obtain

$$\langle\psi|\, H\,|\psi\rangle \geq \frac{2\pi}{\beta'}\frac{\hbar^2}{2m}\int \mathrm{d}^2\vec{x}\,\rho^2(\vec{x}) + 2e^2\sum_{j=1}^{k} Z_j \int \mathrm{d}^2\vec{x}\ \ln\left(\frac{|\vec{x}-\vec{R}_j|}{2r_0}\right)\rho(\vec{x})$$
$$- e^2\int \mathrm{d}^2\vec{x}\,\mathrm{d}^2\vec{x}'\ \rho(\vec{x})\ \ln\left(\frac{|\vec{x}-\vec{x}'|}{2r_0}\right)\rho(\vec{x}')$$
$$- 2e^2\sum_{i<j}^{k} Z_i Z_j\ \ln\left(\frac{|\vec{R}_i-\vec{R}_j|}{2r_0}\right) - (0.576486)\, e^2 N \tag{14}$$

where $(2/\beta') = (1/N) - (2/\beta)$, with $\beta > 2N$, and otherwise arbitrary, chosen for consistency.

With β replaced by β' in (6), the latter in conjunction with (14)-(14) then give

$$\langle\psi|\, H\,|\psi\rangle \geq\ -(0.576486)\, e^2\left[N + \sum_{j=1}^{k} Z_j^2\right]. \tag{15}$$

Finally using the bound

$$\sum_{j=1}^{k} Z_j^2 \leq Z_{\mathrm{MAX}}\sum_{j=1}^{k} Z_j = Z_{\mathrm{MAX}}\, N \tag{16}$$

in equation (16), gives

$$\langle\psi|\, H\,|\psi\rangle \geq\ -(0.576486)\, e^2 N\,[1 + Z_{\mathrm{MAX}}] \tag{17}$$

where Z_{MAX} corresponds to the nucleus with largest charge in units of $|e|$.

It is also important to consider the swelling (inflation) of such matter as the number N is made to increase [9]. To this end the bound (10), (17) lead to the basic inequalities

$$\frac{\pi}{N}\frac{\hbar^2}{2m}\int \mathrm{d}^2\vec{x}\,\rho^2(\vec{x}) \leq T \leq (2)(0.576486)e^2 N(1 + Z_{max}). \tag{18}$$

Now let $\vec{x}$ denote the position of a particle relative, for example, to the center of mass of the nuclei. We define the set function

$$\chi_R(\vec{x}) = \begin{cases} 1, & \text{if } \vec{x} \text{ lies within a sphere of radius } R \\ 0, & \text{otherwise.} \end{cases} \tag{19}$$

We are interested in the expression

$$\mathrm{Prob}\,[|\vec{x}_1| \leq R, \ldots, |\vec{x}_N| \leq R] = \int\left(\prod_{i=1}^{N} \mathrm{d}^2\vec{x}_i\,\chi_R(\vec{x}_i)\right)\left|\Phi(\vec{x}_1, \ldots, \vec{x}_N)\right|^2 \tag{20}$$

which gives the probability of finding all the particles within a circle of radius R. Clearly,

$$\mathrm{Prob}\,[|\vec{x}_1| \leq R, \ldots, |\vec{x}_N| \leq R] \leq \mathrm{Prob}\left[|\vec{x}_1| \leq R, \ldots, |\vec{x}_j| \leq R\right]$$
$$\leq \ldots \leq \mathrm{Prob}\,[|\vec{x}_1| \leq R]$$
$$= \frac{1}{N}\int \mathrm{d}^2\vec{x}\,\chi_R(\vec{x})\rho(\vec{x}) \tag{21}$$

4

for $j < N$, with $\rho(\vec{x})$ is $\rho(\vec{x}) = N \int \mathrm{d}^2\vec{x}_2 \ldots \mathrm{d}^2\vec{x}_N \left|\Phi(\vec{x}, \vec{x}_2, \ldots, \vec{x}_N)\right|^2$.

By Hölder's inequality we have

$$\int \mathrm{d}^2\vec{x}\, \chi_R(\vec{x})\rho(\vec{x}) \leq \left(\int \mathrm{d}^2\vec{x}\, \rho^2(\vec{x})\right)^{1/2} \left(\int \mathrm{d}^2\vec{x}\, \chi_R^2(\vec{x})\right)^{1/2} \tag{22}$$

where $\chi_R^2(\vec{x}) = \chi_R(\vec{x})$, and

$$\int \mathrm{d}^2\vec{x}\, \chi_R(\vec{x}) = A_R \tag{23}$$

denotes the area in which the particles are confined.

Hence, in particular, (21) gives

$$\left(\int \mathrm{d}^2\vec{x}\, \rho^2(\vec{x})\right)^{1/2} \leq \left[(2.305944)\frac{N}{\pi}\frac{me^2}{\hbar^2}(1 + Z_{max})\right]^{1/2} \tag{24}$$

finally leads to the simple bound

$$\mathrm{Prob}\left[|\vec{x}_1| \leq R, \ldots, |\vec{x}_N| \leq R\right]\left(\frac{N}{A_R}\right)^{1/2} \leq (0.856568)\left[\frac{me^2}{\hbar^2}(1 + Z_{\max})\right]^{1/2} \tag{25}$$

where $a_0 = \hbar^2/me^2$ is the Bohr radius and $Z_{\max}$ is the maximum of the nuclear charges.

We immediately infer from (25) the inescapable fact that given that there is a non-zero probability of particles to be limited within a circle of radius R, then the corresponding area A_R grows not any slower than the first power of N for $N \to \infty$, since otherwise the left-hand side of (25) would go to infinity in this limit while the right-hand side is finite. That is, *necessarily*, the radius *R of spatial extension of matter grows not any slower than $N^{1/2}$ for $N \to \infty$.*

We note that N/A_R gives the particle density, and one may infer from (25), with a probability non-zero provide that particles are limited within a circle of radius R, the infinite density limit $N/A_R \to \infty$, i.e., of the system collapsing onto itself, does not occur.

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