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Why Matter Occupies so Large a Volume?

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Abstract *The paper represents a rigorous treatment of the underlying quantum theory, not just in words but providing the underlying technical details, as to why matter occupies so large a volume and its intimate connection with the Pauli exclusion principle, as more and more matter is put together, as well as of the contraction or shrinkage of "bosonic matter", upon collapse, for which the Pauli exclusion is abolished. From the derived explicit bounds of integrals of powers of the particle number densities, explicit bounds on probabilities of the occurrences of the events just described are extracted. These probabilities lead one to infer the change of the "size" or extension of such matter, upon expansion or contraction, respectively, as their content is increased.*

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1 Introduction

The fact that matter occupies so large a volume and its connection to the Pauli exclusion principle was emphasized clearly as addressed by Ehrenfest to Pauli in 1931 on the occasion of the Lorentz medal (c.f. [1]) to this effect: "We take a piece of metal, or a stone. When we think about it, we are astonished that this quantity of matter should occupy so large a volume". He went on by stating that the Pauli exclusion principle is the reason: "Answer: only the Pauli Principle, no two electrons in the same state." On the other hand, in regard to "bosonic matter", that is matter for which the exclusion principle is abolished, it is interesting to quote Dyson[2] who states: [Bosonic] matter in bulk would collapse into a condensed high-density phase. The assembly of any two macroscopic objects would release energy comparable to that of an atomic bomb... Matter without the exclusion principle is unstable." In the translated version of the book by Tomonaga on spin,[3] one reads in the Preface: "The existence of spin, and the statistics associated with it, is the most subtle and ingenious design of Nature — without it the whole universe would collapse." The drastic difference between matter, with the exclusion principle, and "bosonic matter", with Coulomb interactions, is that the ground-state energy for the latter, $E_N \sim -N^\alpha$, with $\alpha > 1$, where $(N + N)$ denotes the number of the negatively charged particles plus an equal number of positively charged particles. This behavior for "bosonic matter" is unlike that of matter, with the exclusion principle, for which $\alpha = 1$ (see Refs. [2, 4–13]). A power law behavior with $\alpha > 1$, implies instability, as the formation of a single system consisting of $(2N + 2N)$ particles is favored over two separate systems brought together each consisting of $(N + N)$ particles, and the energy released upon collapse of the two systems into one, being proportional to $[(2N)^\alpha - 2(N)^\alpha]$, will be overwhelmingly large for realistic large N, e.g., $N \sim 10^{23}$. The instability of "bosonic matter" is not a characterstic of the dimensionality of space.[10] We have been particularly interested in recent years on the density limit of matter with[14] and without[15] the exclusion principle, and the size of such matter in bulk as more and more matter is put together from the point of view mentioned above by Ehrenfest, but now also for the "bosonic" counterpart. We provide a rigorous treatment of the underlying quantum theory as to why matter occupies so large a volume and its intimate connection with the exclusion principle. Detailed bounds are derived for the integrals of powers of the particles densities from which explicit bounds on the probabilities of the "extension" of matter for which the exclusion principle is or is not invoked. From these probabilities explicit statements are made on what happens when more and more matter is put together. Our findings are summarized in the concluding section which also pin points the strategy of attack and how the explicit statements of the extension of matter is extracted from the theory. For a pedagogical presentation of problems of stability and instability, in general, c.f. [16]. All the underlying technical details, not just in words, are worked out and are given right here in the bulk of the paper that lead to our explicit conclusions.

In Sec. 2, much emphasis is put on the boundedness of the spectra of the Hamiltonian into consideration is given for the convenience of the reader. Section 3, follows in the derivation of rigorous key bounds on integrals of powers of the particle densities relevant to the investigation of the expansion of matter and the contraction of the "bosonic" one. The investigation of the "size" or extension of matter in both cases is carried out in Sec. 4. The latter section

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is followed by a summary of the strategy of attack of the problem and with our conclusions and are readily interpreted.

2 Boundedness of the Spectrum from Below

The Hamiltonian of consideration in this work is defined by the well known expression

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

where $Z_j|\mathrm{e}|$ denotes the charge of a j-th positively charged particle, $\boldsymbol{x}_i$, $\boldsymbol{R}_j$, correspond, respectively, to positions of negatively and positively charged particles, and m denotes the mass of the negatively charged particles. We also consider neutral matter, that is, $\sum_{j=1}^{k} Z_j = N$.

Let us first consider the situation first without invoking the exclusion principle. To this end, following Ref. [11], let $v(\boldsymbol{x}) > 0$ be an arbitrary real function, such that $v(\boldsymbol{0}) < \infty$, and such that its Fourier transform $\tilde{v}(\boldsymbol{p}) > 0$, as well. Let $\phi(\boldsymbol{x})$ be a real function, and $a_1, \ldots, a_k$ be real and positive numbers, with $k \geq 2$. A Fourier transform allows us to write,

$$\sum_{j=1}^{k} a_j \phi(\boldsymbol{x}_j) = \int \frac{\mathrm{d}^3\boldsymbol{p}}{(2\pi)^3} \frac{\tilde{\phi}(\boldsymbol{p})}{\sqrt{\tilde{v}(\boldsymbol{p})}} \Big(\sum_{j=1}^{k} a_j \mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{x}_j} \sqrt{\tilde{v}(\boldsymbol{p})} \Big). \tag{2}$$

From the Cauchy–Schwartz inequality this gives

$$\Big(\sum_{j=1}^{k} a_j \phi(\boldsymbol{x}_j) \Big)^2 \Big/ \Big(\int \frac{\mathrm{d}^3\boldsymbol{p}}{(2\pi)^3} \frac{|\tilde{\phi}(\boldsymbol{p})|^2}{\tilde{v}(\boldsymbol{p})} \Big) \leq \sum_{i,j=1}^{k} a_i\, a_j v(\boldsymbol{x}_i - \boldsymbol{x}_j). \tag{3}$$

Now for any two real numbers a, b such that $b > 0$, we have $a^2/2b \geq a - b/2$. Hence with

$$a = \sum_{j=1}^{k} a_j \phi(\boldsymbol{x}_j), \quad b = \int \frac{\mathrm{d}^3\boldsymbol{p}}{(2\pi)^3} \frac{|\tilde{\phi}(\boldsymbol{p})|^2}{\tilde{v}(\boldsymbol{p})}, \tag{4}$$

used on the left-hand side of the inequality in Eq. (3), lead to

$$\frac{1}{2} \sum_{i,j=1}^{k} a_i a_j v(\boldsymbol{x}_i - \boldsymbol{x}_j) \geq \sum_{j=1}^{k} a_j \phi(\boldsymbol{x}_j) - \frac{1}{2} \int \frac{\mathrm{d}^3\boldsymbol{p}}{(2\pi)^3} \frac{|\tilde{\phi}(\boldsymbol{p})|^2}{\tilde{v}(\boldsymbol{p})}. \tag{5}$$

Let $V(\boldsymbol{x})$ be a real function such that $V(\boldsymbol{x}) \geq v(\boldsymbol{x})$, and $\rho(\boldsymbol{x})$ be a real function and so far arbitrary. Set

$$\phi(\boldsymbol{x}) = \int \mathrm{d}^3\boldsymbol{x}' \rho(\boldsymbol{x}') V(\boldsymbol{x}' - \boldsymbol{x}). \tag{6}$$

Upon substituting this expression in Eq. (5) gives

$$\sum_{1\leq i<j\leq k} a_i a_j V(\boldsymbol{x}_i - \boldsymbol{x}_j) \geq \sum_{j=1}^{k} a_j \int \mathrm{d}^3\boldsymbol{x} \rho(\boldsymbol{x}) V(\boldsymbol{x} - \boldsymbol{x}_j) - \frac{1}{2} \int \mathrm{d}^3\boldsymbol{x}\mathrm{d}^3\boldsymbol{x}' \rho(\boldsymbol{x}) V(\boldsymbol{x} - \boldsymbol{x}') \rho(\boldsymbol{x}') - \frac{1}{2} v(\boldsymbol{0}) \sum_{j=1}^{k} a_j^2 - \frac{1}{2} \int \frac{\mathrm{d}^3\boldsymbol{p}}{(2\pi)^3} |\tilde{\rho}(\boldsymbol{p})|^2 \Big[\frac{|\tilde{V}(\boldsymbol{p})|^2}{\tilde{v}(\boldsymbol{p})} - \tilde{V}(\boldsymbol{p}) \Big]. \tag{7}$$

In particular with

$$V(\boldsymbol{x}) = \frac{\mathrm{e}^2}{|\boldsymbol{x}|} \geq v(\boldsymbol{x}) = \frac{\mathrm{e}^2(1 - \mathrm{e}^{-\lambda|\boldsymbol{x}|})}{|\boldsymbol{x}|}, \quad \lambda \text{ real and} > 0, \tag{8}$$

we have

$$v(\boldsymbol{0}) = \mathrm{e}^2\lambda, \quad \tilde{V}(\boldsymbol{p}) = \frac{4\pi\mathrm{e}^2}{\boldsymbol{p}^2}, \quad \tilde{v}(\boldsymbol{p}) = \frac{4\pi\mathrm{e}^2\lambda^2}{\boldsymbol{p}^2(\boldsymbol{p}^2 + \lambda^2)}. \tag{9}$$

With $k \geq 2$, Eq. (7) now gives the useful bound

$$\sum_{1\leq i<j\leq k} \frac{\mathrm{e}^2 a_i a_j}{|\boldsymbol{x}_i - \boldsymbol{x}_j|} \geq \sum_{j=1}^{k} \mathrm{e}^2 a_j \int \mathrm{d}^3\boldsymbol{x} \frac{\rho(\boldsymbol{x})}{|\boldsymbol{x} - \boldsymbol{x}_j|} - \frac{2\pi\mathrm{e}^2}{\lambda^2} \int \mathrm{d}^3\boldsymbol{x} \rho^2(\boldsymbol{x}) - \frac{\lambda\mathrm{e}^2}{2} \sum_{j=1}^{k} a_j^2 - \frac{\mathrm{e}^2}{2} \int \mathrm{d}^3\boldsymbol{x}\mathrm{d}^3\boldsymbol{x}' \rho(\boldsymbol{x}) \frac{1}{|\boldsymbol{x} - \boldsymbol{x}'|} \rho(\boldsymbol{x}'). \tag{10}$$

This generalizes a result in Ref. [17]. Now we choose

$$\rho(\boldsymbol{x}) = N \int \mathrm{d}^3\boldsymbol{x}_2 \cdots \mathrm{d}^3\boldsymbol{x}_N |\psi(\boldsymbol{x}, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N)|^2, \tag{11}$$

where ψ is an N boson (spin 0) symmetric normalized wavefunction. We use Eq. (10) twice. Once with $a_j = 1$, $k \to N$, and then again with $a_j = Z_j$, $\boldsymbol{x}_j \to \boldsymbol{R}_j$, for the second and third potentials in Eq. (1), to obtain from Eqs. (10), (11), and (1)

$$\langle\psi|H|\psi\rangle \geq \Big\langle \psi \Big| \sum_{j=1}^{N} \frac{\boldsymbol{p}_j^2}{2m} \Big| \psi \Big\rangle - \frac{4\pi\mathrm{e}^2}{\lambda^2} \int \mathrm{d}^3\boldsymbol{x} \rho^2(\boldsymbol{x}) - \frac{\lambda\mathrm{e}^2}{2} \Big(N + \sum_{j=1}^{k} Z_j^2 \Big), \quad k \geq 2. \tag{12}$$

Optimizing over the parameter λ, this equation gives the bound

$$\langle\psi|H|\psi\rangle \geq \Big\langle \psi \Big| \sum_{j=1}^{N} \frac{\boldsymbol{p}_j^2}{2m} \Big| \psi \Big\rangle - \frac{3\mathrm{e}^2\pi^{1/3}}{2^{2/3}} \Big(\int \mathrm{d}^3\boldsymbol{x} \rho^2(\boldsymbol{x}) \Big)^{1/3} \times \Big(N + \sum_{j=1}^{k} Z_j^2 \Big)^{2/3}. \tag{13}$$

This suggests to derive a lower bound to the kinetic energy term, which is some power of an integral of ρ^2. This is considered next.

Given a real function $f(\boldsymbol{x}) \geq 0$, consider the hypothetical Hamiltonian

$$\tilde{h} = \frac{\boldsymbol{p}^2}{2m} - f(\boldsymbol{x}), \tag{14}$$

in three dimensions. The Schwinger bound,[20–22] details of which are given in Appendix A, for the number of eigenvalues $N(\tilde{h}, -\xi)$ of the Hamiltonian $\tilde{h}$ with energies $\leq -\xi$, for $\xi > 0$, satisfies the inequality

$$N[\tilde{h},-\xi] \leq \Big(\frac{m}{2\pi\hbar^2}\Big)^2 \int \mathrm{d}^3\boldsymbol{x}\mathrm{d}^3\boldsymbol{x}' f(\boldsymbol{x}) \times \frac{\mathrm{e}^{-2|\boldsymbol{x}-\boldsymbol{x}'|\sqrt{2m\xi}/\hbar}}{|\boldsymbol{x}-\boldsymbol{x}'|^2} f(\boldsymbol{x}') \,. \qquad (15)$$

Now we use a particular case of Young's inequality, which for two square integrable real functions $f_1(\boldsymbol{x})$, $f_2(\boldsymbol{x})$, it reads

$$\Big|\int \mathrm{d}^3\boldsymbol{x}\mathrm{d}^3\boldsymbol{x}' f_1(\boldsymbol{x}) G(\boldsymbol{x}-\boldsymbol{x}') f_2(\boldsymbol{x}')\Big| \leq \Big(\int \mathrm{d}^3\boldsymbol{x} f_1^2(\boldsymbol{x})\Big)^{1/2} \Big(\int \mathrm{d}^3\boldsymbol{x}|G(\boldsymbol{x})|\Big) \times \Big(\int \mathrm{d}^3\boldsymbol{x} f_2^2(\boldsymbol{x})\Big)^{1/2}, \qquad (16)$$

which when applied to Eq. (15) gives

$$N[\tilde{h},-\xi] \leq \Big(\frac{m}{2\pi\hbar^2}\Big)^2 \Big(\int \mathrm{d}^3\boldsymbol{x} f^2(\boldsymbol{x})\Big) \times \Big(\int \mathrm{d}^3\boldsymbol{x} \frac{\mathrm{e}^{-2|\boldsymbol{x}|\sqrt{2m\xi}/\hbar}}{|\boldsymbol{x}|^2}\Big) \,. \qquad (17)$$

Using the integral

$$\int \mathrm{d}^3\boldsymbol{x} \frac{\mathrm{e}^{-2|\boldsymbol{x}|\sqrt{2m\xi}/\hbar}}{|\boldsymbol{x}|^2} = \pi\hbar\sqrt{\frac{2}{m\xi}} \,, \qquad (18)$$

we obtain for the Schwinger bound

$$N[\tilde{h},-\xi] \leq \Big(\frac{m}{2\hbar^2}\Big)^{3/2} \frac{1}{\pi\sqrt{\xi}} \int \mathrm{d}^3\boldsymbol{x} f^2(\boldsymbol{x}) \,. \qquad (19)$$

From this equation, one easily obtains a lower bound to the spectrum of the hypothetical Hamiltonian $\tilde{h}$ in Eq. (14). To this end, we may appropriately choose ξ so that $N[\tilde{h},-\xi] = 0$. Indeed, if for any $\epsilon > 0$, we choose

$$-\xi = -\frac{1+\epsilon}{\pi^2}\Big(\frac{m}{2\hbar^2}\Big)^3 \Big(\int \mathrm{d}^3\boldsymbol{x} f^2(\boldsymbol{x})\Big)^2, \qquad (20)$$

then $N[\tilde{h},-\xi] < 1$, that is $N[\tilde{h},-\xi] = 0$, and the spectrum is empty below the value on the right-hand side of Eq. (19). Hence the right-hand side of Eq. (20) gives the following lower bound to the spectrum of $\tilde{h}$

$$\tilde{h} \geq -\frac{1+\epsilon}{\pi^2}\Big(\frac{m}{2\hbar^2}\Big)^3 \Big(\int \mathrm{d}^3\boldsymbol{x} f^2(\boldsymbol{x})\Big)^2, \qquad (21)$$

for any $\epsilon > 0$. Now we choose

$$f(\boldsymbol{x}) = \frac{4}{3}\frac{\rho(\boldsymbol{x})}{\int \mathrm{d}^3\boldsymbol{x}\rho^2(\boldsymbol{x})} T, \quad T = \Big\langle \psi\Big| \sum_{j=1}^{N} \frac{\boldsymbol{p}_j^2}{2m}\Big|\psi\Big\rangle, \qquad (22)$$

where the particle density is given in Eq. (11).

We note that

$$\langle\psi|f|\psi\rangle = \frac{4}{3}T \,. \qquad (23)$$

By noting, in the process, that for bosons, we may put all of the N particles at the bottom of the spectrum of the Hamiltonian $[\sum_{j=1}^{N}(\boldsymbol{p}_j^2/2m - f(\boldsymbol{x}_j))]$, Eq. (20) then gives, the following lower bound to the spectrum of the hypothetical Hamiltonian of N non-interacting bosons but each interacting with a potential energy $f(\boldsymbol{x})$:

$$\langle\psi|\sum_{j=1}^{N}\Big[\frac{\boldsymbol{p}_j^2}{2m} - f(\boldsymbol{x}_j)\Big]|\psi\rangle > -N\frac{1+\epsilon}{\pi^2}\Big(\frac{m}{2\hbar^2}\Big)^3 \Big(\int \mathrm{d}^3\boldsymbol{x} f^2(\boldsymbol{x})\Big)^2 . \qquad (24)$$

From Eqs. (22), (23), this gives

$$-\frac{1}{3}T \geq -N\Big(\frac{4}{3}\Big)^4 T^4 \frac{1+\epsilon}{\pi^2}\Big(\frac{m}{2\hbar^2}\Big)^3 \frac{1}{\big(\int \mathrm{d}^3\boldsymbol{x}\rho^2(\boldsymbol{x})\big)^2} \,, \qquad (25)$$

or

$$T \geq \frac{3\hbar^2}{2mN^{1/3}}\Big(\frac{\pi}{2}\Big)^{2/3} \frac{1}{(1+\epsilon)^{1/3}} \Big(\int \mathrm{d}^3\boldsymbol{x}\rho^2(\boldsymbol{x})\Big)^{2/3} , \qquad (26)$$

for any $\epsilon > 0$.

Upon setting

$$\Big(\int \mathrm{d}^3\boldsymbol{x} f^2(\boldsymbol{x})\Big)^{1/3} = A, \quad \frac{3\hbar^2}{2m(1+\epsilon)^{1/3}}\Big(\frac{\pi}{2}\Big)^{2/3} = B, \qquad (27)$$

Eqs. (13), (26) lead to the following chain of inequalities for $k \geq 2$,

$$\begin{aligned}\langle\psi|H|\psi\rangle &\geq \frac{B}{N^{1/3}}A^2 - \frac{3}{2^{2/3}}\mathrm{e}^2\pi^{1/3}\Big(N + \sum_{j=1}^{k} Z_j^2\Big)^{2/3} A \\ &= \frac{B}{N^{1/3}}\Big[A - \frac{3\mathrm{e}^2\pi^{1/3}N^{1/3}}{2^{5/3}B}\Big(N + \sum_{j=1}^{k} Z_j^2\Big)^{2/3}\Big]^2 \\ &\quad - \frac{9}{8}\frac{\mathrm{e}^4}{2^{1/3}}\frac{\pi^{2/3}}{B}N^{1/3}\Big(N + \sum_{j=1}^{k} Z_j^2\Big)^{4/3} \\ &> -\frac{9}{8}\frac{\mathrm{e}^4}{2^{1/3}}\frac{\pi^{2/3}}{B}N^{1/3}\Big(N + \sum_{j=1}^{k} Z_j^2\Big)^{4/3} \\ &= -1.89\Big(\frac{m\mathrm{e}^4}{2\hbar^2}\Big)N^{1/3}\Big(N + \sum_{j=1}^{k} Z_j^2\Big)^{4/3} ,\end{aligned} \qquad (28)$$

where we have taken ϵ arbitrarily small for N sufficiently large. Upon defining $Z = \max_j Z_j$, we obtain from the above equation the key inequality

$$\langle\psi|H|\psi\rangle > -1.89\Big(\frac{m\mathrm{e}^4}{2\hbar^2}\Big)N^{5/3}(1+Z)^{4/3}, \quad \text{(Bosonic)}, \qquad (29)$$

where we have used the property $\sum_j Z_j = N$. The right-hand side of the inequality in Eq. (29) provides a lower bound to the spectrum.

For the Fermionic case, we follow the traditional approach.[6] To this end, we begin with an inequality that follows from a no-binding theorem originated by Teller.[6,21] This is spelled out in the Appendix. Here, let $\varrho(\boldsymbol{x})$ be an arbitrary positive function, and $\beta > 0$ be an arbitrary dimensionless parameter, then

$$(3\pi^2)^{5/3}\frac{\hbar^2}{10\pi^2 m\beta}\int \mathrm{d}^3\boldsymbol{x}\varrho^{5/3}(\boldsymbol{x}) - \sum_{j=1}^{k} Z_j\mathrm{e}^2 \int \mathrm{d}^3\boldsymbol{x}\frac{\varrho(\boldsymbol{x})}{|\boldsymbol{x}-\boldsymbol{R}_j|}$$

$$+\frac{e^2}{2}\int d^3\boldsymbol{x}d^3\boldsymbol{x}'\varrho(\boldsymbol{x})\frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|}\varrho(\boldsymbol{x}')+\sum_{1\le i<j\le k}\frac{Z_iZ_je^2}{|\boldsymbol{R}_i-\boldsymbol{R}_j|}\ge\beta E_{\rm TF}(1)\sum_{j=1}^{k}Z_j^{7/3}\,, \tag{30}$$

where $E_{\rm TF}(Z)$ is the Thomas-Fermi energy for atoms,

$$E_{\rm TF}(Z)=E_{\rm TF}(1)Z^{7/3}\,,\quad E_{\rm TF}(1)\simeq-1.5375\frac{me^4}{2\hbar^2}\,. \tag{31}$$

From Eq. (30), we may find a lower bound to the (repulsive) potential interaction part between the nuclei to be

$$\sum_{1\le i<j\le k}\frac{Z_iZ_je^2}{|\boldsymbol{R}_i-\boldsymbol{R}_j|}\ge\sum_{j=1}^{k}e^2\int d^3\boldsymbol{x}\frac{\varrho(\boldsymbol{x})}{|\boldsymbol{x}-\boldsymbol{R}_j|}-\frac{e^2}{2}\int d^3\boldsymbol{x}d^3\boldsymbol{x}'\varrho(\boldsymbol{x})\frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|}\varrho(\boldsymbol{x}')$$
$$-(3\pi^2)^{5/3}\frac{\hbar^2}{10\pi^2m\beta}\int d^3\boldsymbol{x}\varrho^{5/3}(\boldsymbol{x})+\beta E_{\rm TF}(1)\sum_{j=1}^{k}Z_j^{7/3}\,. \tag{32}$$

The above inequality, in turn, allows us to find a lower bound to the (repulsive) potential interaction part between the electrons, by making the substitutions: $k\to N$, $Z_j\to1$, $\boldsymbol{R}_j\to\boldsymbol{x}_j$, for $j=1,\ldots,N$:

$$\sum_{1\le i<j\le k}\frac{e^2}{|\boldsymbol{x}_i-\boldsymbol{x}_j|}\ge\sum_{j=1}^{N}e^2\int d^3\boldsymbol{x}\frac{\varrho(\boldsymbol{x})}{|\boldsymbol{x}-\boldsymbol{x}_j|}-\frac{e^2}{2}\int d^3\boldsymbol{x}d^3\boldsymbol{x}'\varrho(\boldsymbol{x})\frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|}\varrho(\boldsymbol{x}')$$
$$-(3\pi^2)^{5/3}\frac{\hbar^2}{10\pi^2m\beta}\int d^3\boldsymbol{x}\varrho^{5/3}(\boldsymbol{x})+\beta E_{\rm TF}(1)N\,. \tag{33}$$

We set

$$\varrho(\boldsymbol{x})=N\sum_{\sigma_1,\ldots,\sigma_N}\int d^3\boldsymbol{x}_2\cdots d^3\boldsymbol{x}_N|\Psi(\boldsymbol{x}\sigma_1,\boldsymbol{x}_2\sigma_2,\ldots,\boldsymbol{x}_N\sigma_N)|^2\,, \tag{34}$$

where $\Psi(\boldsymbol{x}\sigma_1,\boldsymbol{x}_2\sigma_2,\ldots,\boldsymbol{x}_N\sigma_N)$ is a normalized wavefunction, anti-symmetric under the interchange of any pair $(\boldsymbol{x}_i\sigma_i)\leftrightarrow(\boldsymbol{x}_j\sigma_j)$, and the sums are over spins. The total number of particles is obtained by integrating over the number density $\varrho(\boldsymbol{x})$

$$\int d^3\boldsymbol{x}\varrho(\boldsymbol{x})=N\,. \tag{35}$$

Another useful formula for obtaining a lower bound to a Hamiltonian is obtained from Eq. (19) by integrating the latter over ξ. This will give us an upper bound to the sum of negative eigenvalues of a Hamiltonian $\tilde{h}=[\boldsymbol{p}^2/2m-v(\boldsymbol{x})]$ as in Eq. (14). To this end, we use the identity

$$N[h_0-v,-\xi;\xi\ge0]=N\Big[h_0-\Big(v-\frac{\xi}{2}\Big);-\frac{\xi}{2};0\le\xi\le2v(\boldsymbol{x})\Big]\,,\quad h_0=\frac{\boldsymbol{p}^2}{2m}\,. \tag{36}$$

That is,

$$\int_0^\infty d\xi N[h_0-v,-\xi]\le\Big(\frac{m}{2\hbar^2}\Big)^{3/2}\frac{\sqrt{2}}{\pi}\int d^3\boldsymbol{x}\int_0^{2v(\boldsymbol{x})}\frac{d\xi}{\sqrt{\xi}}\Big(v(\boldsymbol{x})-\frac{\xi}{2}\Big)^2\,, \tag{37}$$

which leads to

$$\int_0^\infty d\xi N[h_0-v,-\xi]\le\frac{4}{15\pi}\Big(\frac{2m}{\hbar^2}\Big)^{3/2}\int d^3\boldsymbol{x}(v(\boldsymbol{x}))^{5/2}\,, \tag{38}$$

referred to as a Lieb-Thirring bound,[6] providing an upper bound for the negative of the sum of the negative eigenvalues (if any), counting degeneracy, of a Hamiltonian $\tilde{h}$ such as the one in Eq. (14). Since the ground-state energy cannot be less that than the sum of negative eigenvalues, this equation provides a lower bound for the ground-state energy given by

$$-\frac{4}{15\pi}\Big(\frac{2m}{\hbar^2}\Big)^{3/2}\int d^3\boldsymbol{x}(v(\boldsymbol{x}))^{5/2}\,. \tag{39}$$

An immediate application of this is to derive a lower bound to the average kinetic energy of multi-electron systems. To this end, we consider the hypothetical Hamiltonian $[\sum_{j=1}^N\big(\boldsymbol{p}_j^2/2m-v(\boldsymbol{x}_j)]$, where $v(\boldsymbol{x})$ is taken as

$$v(\boldsymbol{x})=\frac{5}{3}\frac{\varrho^{2/3}(\boldsymbol{x})}{\int d^3\boldsymbol{x}\varrho^{5/3}(\boldsymbol{x})}T,\quad T=\langle\Psi|\sum_{j=1}^{N}\frac{\boldsymbol{p}_j^2}{2m}|\Psi\rangle. \tag{40}$$

It is easily verified that

$$\Big\langle\Psi\Big|\sum_{j=1}^{N}v(\boldsymbol{x}_j)\Big|\Psi\Big\rangle=\frac{5}{3}T\,. \tag{41}$$

Allowing multiplicity and spin degeneracy, we can put the N fermions in the lowest energy levels of the hypothetical Hamiltonian $[\sum_{j=1}^N\big(\boldsymbol{p}_j^2/2m-v(\boldsymbol{x}_j)\big)]$, in conformity with the Pauli exclusion principle, if $N\le$ number of such levels. If N is larger than this number of levels, the remaining free fermions may be chosen to have arbitrary small ($\to0$) kinetic energies, and be infinitely separated, to define the lowest energy of this Hamiltonian. Hence in all cases, this

Hamiltonian is bounded below by 2, for allowing spin orientations, times the sum of the negative energy levels of the Hamiltonian: $\big(\boldsymbol{p}^2/2m - v(\boldsymbol{x})\big)$, allowing in the sum for multiplicity but not for spin degeneracy. Hence we obtain the bound

$$\Big\langle\Psi\Big|\sum_{j=1}^{N}\Big(\frac{\boldsymbol{p}_j^2}{2m}-v(\boldsymbol{x}_j)\Big)\Big|\Psi\Big\rangle \geq -2\frac{4}{15\pi}\Big(\frac{2m}{\hbar^2}\Big)^{3/2}\int \mathrm{d}^3\boldsymbol{x}(v(\boldsymbol{x}))^{5/2}\,. \tag{42}$$

From Eqs. (40), (41),

$$-\frac{2}{3}T \geq -2\frac{4}{15\pi}\Big(\frac{2m}{\hbar^2}\Big)^{3/2}\Big(\frac{5}{3}\Big)^{5/2}T^{5/2}\times\Big(\int \mathrm{d}^3\boldsymbol{x}\varrho^{5/3}(\boldsymbol{x})\Big)^{-3/2}\,, \tag{43}$$

leading to

$$\frac{3}{5}\Big(\frac{3\pi}{4}\Big)^{2/3}\frac{\hbar^2}{2m}\int \mathrm{d}^3\boldsymbol{x}\varrho^{5/3}(\boldsymbol{x}) \leq T\,. \tag{44}$$

Now we have all the ingredients to obtain a lower bound of the Hamiltonian in Eq. (1) for fermionic matter. To this end,

$$\sum_{i=1}^{N}\sum_{j=1}^{k}Z_j\mathrm{e}^2\Big\langle\Psi\Big|\frac{1}{|\boldsymbol{x}_i-\boldsymbol{R}_j|}\Big|\Psi\Big\rangle = \sum_{j=1}^{k}Z_j\mathrm{e}^2\int \mathrm{d}^3\boldsymbol{x}\frac{1}{|\boldsymbol{x}-\boldsymbol{R}_j|}\varrho(\boldsymbol{x})\,. \tag{45}$$

$$\sum_{i=1}^{N}\mathrm{e}^2\int \mathrm{d}^3\boldsymbol{x}\varrho(\boldsymbol{x})\Big\langle\Psi\Big|\frac{1}{|\boldsymbol{x}-\boldsymbol{x}_i|}\Big|\Psi\Big\rangle = \mathrm{e}^2\int \mathrm{d}^3\boldsymbol{x}\mathrm{d}^3\boldsymbol{x}'\varrho(\boldsymbol{x})\frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|}\varrho(\boldsymbol{x}')\,, \tag{46}$$

and hence from Eq. (33)

$$\sum_{1\leq i<j\leq N}\mathrm{e}^2\Big\langle\Psi\Big|\frac{1}{|\boldsymbol{x}_i-\boldsymbol{x}_j|}\Big|\Psi\Big\rangle \geq \frac{\mathrm{e}^2}{2}\int \mathrm{d}^3\boldsymbol{x}\mathrm{d}^3\boldsymbol{x}'\varrho(\boldsymbol{x})\frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|}\varrho(\boldsymbol{x}') -(3\pi^2)^{5/3}\frac{\hbar^2}{10\pi^2 m\beta}\int \mathrm{d}^3\boldsymbol{x}\varrho^{5/3}(\boldsymbol{x})+\beta N E_{\mathrm{TF}}(1)\,. \tag{47}$$

Hence from Eqs. (1), (44)–(47), we have for fermionic matter

$$\begin{aligned}\langle\Psi|H|\Psi\rangle \geq{}& (3\pi^2)^{5/3}\frac{\hbar^2}{10\pi^2 m\beta'}\int \mathrm{d}^3\boldsymbol{x}\varrho^{5/3}(\boldsymbol{x}) - \sum_{j=1}^{k}Z_j\mathrm{e}^2\int \mathrm{d}^3\boldsymbol{x}\frac{1}{|\boldsymbol{x}-\boldsymbol{R}_j|}\varrho(\boldsymbol{x})\\ &+\frac{\mathrm{e}^2}{2}\int \mathrm{d}^3\boldsymbol{x}\mathrm{d}^3\boldsymbol{x}'\varrho(\boldsymbol{x})\frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|}\varrho(\boldsymbol{x}') + \sum_{1\leq i<j\leq k}\frac{Z_iZ_j\mathrm{e}^2}{|\boldsymbol{R}_i-\boldsymbol{R}_j|}+\beta N E_{\mathrm{TF}}(1)\,,\end{aligned} \tag{48}$$

where

$$\frac{1}{\beta'} = \frac{(3/5)(3\pi/4)^{2/3}-[(3\pi^2)^{5/3}/5\pi^2](1/\beta)}{(3\pi^2)^{5/3}/5\pi^2} = \Big(\frac{1}{4\pi}\Big)^{2/3}-\frac{1}{\beta}\,. \tag{49}$$

For a positive β', we must choose $\beta > (4\pi)^{2/3}$.

The sum of the first four terms on the right-hand side of the inequality in Eq. (48) coincide with the expression on the right-hand side of the inequality (30) with β in the latter simply replaced by β'. Hence

$$\langle\Psi|H|\Psi\rangle \geq \beta' E_{\mathrm{TF}}(1)\sum_{j=1}^{k}Z_j^{7/3}+\beta N E_{\mathrm{TF}}(1)\,. \tag{50}$$

Optimizing over β leads to the Lieb-Thirring bound[6]

$$\langle\Psi|H|\Psi\rangle \geq E_{\mathrm{TF}}(1)(4\pi)^{2/3}N\Big[1+\Big(\sum_{j=1}^{k}\frac{Z_j^{7/3}}{N}\Big)^{1/2}\Big]^2\,, \tag{51}$$

where $E_{\mathrm{TF}}(1)$ is given in Eq. (31). Again setting $Z = \max_j Z_j$, we obtain

$$\langle\Psi|H|\Psi\rangle \geq -8.3104\Big(\frac{m\mathrm{e}^4}{2\hbar^2}\Big)N[1+Z^{2/3}]^2\,, \quad \text{(Fermionic)}\,. \tag{52}$$

The numerical value 8.3104 may be further reduced,[22–23] but this will not be important in the subsequent analysis (see also Refs. [24–25]). The right-hand side of the inequality in Eq. (52) provides a lower bound to the spectrum.

3 Integrals of Powers of Particles-Number-Densities

First we note that the negative spectrum of the Hamiltonian in Eq. (1) is not empty for both ordinary matter and the bosonic one. Envisage the situation where we have infinitely separated N clusters: k hydrogenic atoms in their ground states, of nuclear charges $Z_1|\mathrm{e}|,\ldots,Z_k|\mathrm{e}|$, having each one negatively charged particle, and there are also $(N-k)$ free negatively charged particles with vanishingly small kinetic energies. The ground-state of such a system is $-\sum_{i=1}^{k}Z_i^2 m\mathrm{e}^4/2\hbar^2$. Let $|\varphi(m)\rangle$ denote a normalized strictly negative energy state of matter, not necessarily corresponding to the ground-state corresponding either to ordinary matter or to the "bosonic" one. That is,

$$-\varepsilon_{N}[m] \leq \langle\varphi(m)|H|\varphi(m)\rangle < 0\,, \tag{53}$$

where $-\varepsilon_{N}[m] = E_N < 0$ denotes the lower end of the spectrum, and we have emphasized its dependence on the mass m. By definition of the ground-state, the state $|\varphi(m/2)\rangle$ cannot lead for $\langle\varphi(m/2)|H|\varphi(m/2)\rangle$ a numerical value lower than $-\varepsilon_{N}[m]$ for the same Hamiltonian with mass m. That is,

$$-\varepsilon_{N}[m] \leq \langle\varphi(m/2)|H|\varphi(m/2)\rangle\,, \tag{54}$$

where we note that the interaction part V in the Hamiltonian in Eq. (1) is independent of the mass scale m. Accordingly, we may rewrite the above equation in details as

$$-\varepsilon_{N}[m] \leq \langle\varphi(m/2)|\Big[\sum_{i=1}^{N}\frac{\boldsymbol{p}_i^2}{2m}+V\Big]|\varphi(m/2)\rangle\,. \tag{55}$$

This equation, in turn implies that for $m \to 2m$,

$$-\varepsilon_{\scriptscriptstyle N}[2m] \le \big\langle\varphi(m)\big|\Big[\sum_{i=1}^{N}\frac{\boldsymbol{p}_i^2}{4m}+V\Big]\big|\varphi(m)\big\rangle\,. \tag{56}$$

Upon simply writing

$$\sum_{i=1}^{N}\frac{\boldsymbol{p}_i^2}{2m}+V=\Big[\sum_{i=1}^{N}\frac{\boldsymbol{p}_i^2}{4m}+V\Big]+\sum_{i=1}^{N}\frac{\boldsymbol{p}_i^2}{4m}\,, \tag{57}$$

Eq. (56) implies that

$$\big\langle\varphi(m)\big|\sum_{i=1}^{N}\frac{\boldsymbol{p}_i^2}{2m}\big|\varphi(m)\big\rangle \le 2\varepsilon_{\scriptscriptstyle N}[2m]\,, \tag{58}$$

for all states $|\varphi(m)\rangle$ for which Eq. (53) is true.

From the bounds to the spectra in Eqs. (29) and (52), together with the lower bounds of the kinetic energy parts for the respective parts in Eqs. (26) and (44), we then have the following bounds

$$\frac{3\hbar^2}{2mN^{1/3}}\Big(\frac{\pi}{2}\Big)^{2/3}\Big(\int \mathrm{d}^3\boldsymbol{x}\rho^2(\boldsymbol{x})\Big)^{2/3} < \Big\langle\psi\Big|\sum_{i=1}^{N}\frac{\boldsymbol{p}_i^2}{2m}\Big|\psi\Big\rangle < 3.78\Big(\frac{me^4}{\hbar^2}\Big)N^{5/3}\big(1+Z\big)^{4/3}\,, \tag{59}$$

$$\frac{3}{5}\Big(\frac{3\pi}{4}\Big)^{2/3}\frac{\hbar^2}{2m}\int \mathrm{d}^3\boldsymbol{x}\varrho^{5/3}(\boldsymbol{x}) < \Big\langle\Psi\Big|\sum_{i=1}^{N}\frac{\boldsymbol{p}_i^2}{2m}\Big|\Psi\Big\rangle < 16.63\Big(\frac{me^4}{\hbar^2}\Big)N[1+Z^{2/3}]^2\,, \tag{60}$$

for the bosonic and fermionic cases, respectively. These in turn give the following key bounds for integrals of some powers of the particle densities $(\rho(\boldsymbol{x}),\varrho(\boldsymbol{x}))$:

$$\int \mathrm{d}^3\boldsymbol{x}\rho^2(\boldsymbol{x}) < 2.55\frac{m^2e^4}{\hbar^4}N^3[1+Z]^2\,,\quad \text{(Bosonic)}\,, \tag{61}$$

$$\int \mathrm{d}^3\boldsymbol{x}\varrho^{5/3}(\boldsymbol{x}) < 32\frac{m^2e^4}{\hbar^4}N[1+Z^{2/3}]^2\,,\quad \text{(Fermionic)}\,. \tag{62}$$

4 Why Matter Occupies so Large a Volume?

To investigate the question raised above, we proceed as follows. Let $\boldsymbol{x}$ denote the position of an electron relative, for example, to the center of mass of the nuclei, recalling that the Pauli exclusion was invoked in deriving the bound of the power of the electron number-density in Eq. (62). Let

$$\chi_R(\boldsymbol{x})=1\,,\ \text{if}\ \boldsymbol{x}\ \text{lies within a sphere of radius}\ R,\ \text{and}\ =0\,,\ \text{otherwise}\,. \tag{63}$$

Then clearly for the probability to have the electrons within a sphere of radius R, we have

$$\begin{aligned}&\text{Prob}[|\boldsymbol{x}_1|\le R,\ldots,|\boldsymbol{x}_{\scriptscriptstyle N}|\le R]\le \text{Prob}[|\boldsymbol{x}_1|\le R]\\&\quad=\frac{1}{N}\int \mathrm{d}^3\boldsymbol{x}\chi_R(\boldsymbol{x})\varrho(\boldsymbol{x})\\&\quad\le\frac{1}{N}\Big[\int \mathrm{d}^3\boldsymbol{x}\varrho^{5/3}(\boldsymbol{x})\Big]^{3/5}(v_R)^{2/5}\,,\end{aligned} \tag{64}$$

where in the last inequality, we have used Hölder's inequality, the fact that $\chi_R(\boldsymbol{x})^{2/5}=\chi_R(\boldsymbol{x})$, and where $v_R=4\pi R^3/3$.

From Eqs. (62) and (64), we have the fundamental inequality

$$\begin{aligned}&\text{Prob}[|\boldsymbol{x}_1|\le R,\ldots,|\boldsymbol{x}_{\scriptscriptstyle N}|\le R]\Big(\frac{N}{v_R}\Big)^{2/5}\\&\quad<8\Big(\frac{1}{a_0^3}\Big)^{2/5}[1+Z^{2/3}]^{6/5}\,,\quad \text{(Fermionic)}\,,\end{aligned} \tag{65}$$

where $a_0=\hbar^2/me^2$ is the Bohr radius. We may infer from this equation the inescapable fact that necessarily for a non-vanishing probability of having the electrons within a sphere of radius R, the corresponding volume v_R grows not any slower than the first power of N for $N\to\infty$, since otherwise the left-hand side of the inequality would go to infinity and would be in contradiction with the finite upper bound on its right-hand side. That is, necessarily, the radius R grows not any slower than $N^{1/3}$ for $N\to\infty$. No wonder why matter occupies so large a volume! We will see that when the Pauli exclusion is abolished, matter would behave differently in conformity with Ehrenfest's remark above. This is investigated next.

For the bosonic case, the bound on the particle number-density is given in Eq. (61), for which the exclusion principle was not invoked, and a bound on the corresponding probability to the one in Eq. (64) may be written as

$$\text{Prob}[|\boldsymbol{x}_1|\le R,\ldots,|\boldsymbol{x}_{\scriptscriptstyle N}|\le R]\le \text{Prob}[|\boldsymbol{x}_1|\le R]=\frac{1}{N}\int \mathrm{d}^3\boldsymbol{x}\chi_R(\boldsymbol{x})\varrho(\boldsymbol{x})\le\frac{1}{N}\Big[\int \mathrm{d}^3\boldsymbol{x}\varrho^2(\boldsymbol{x})\Big]^{1/2}(v_R)^{1/2}\,, \tag{66}$$

where in the last inequality we have again used Hölder's inequality.

From Eq. (61), we have the fundamental inequality

$$\text{Prob}\big[|\boldsymbol{x}_1|\le R,\ldots,|\boldsymbol{x}_{\scriptscriptstyle N}|\le R\big]\Big(\frac{1}{v_RN}\Big)^{1/2} < 1.61\Big(\frac{1}{a_0^3}\Big)^{1/2}[1+Z]\,,\quad \text{(Bosonic)}\,. \tag{67}$$

From this inequality, we may infer the inescapable fact that if contraction of "bosonic matter" occurs, upon collapse, then for a non-vanishing probability of having the N negatively charged particles within a sphere of radius R, the corresponding volume, necessarily, shrinks not faster than $1/N$ for $N \to \infty$, since otherwise the left-hand side of Eq. (67) would go to infinity and would be in contradiction with the finite upper bound on its right-hand side. That is the radius R shrinks not faster than $1/N^{1/3}$, for $N \to \infty$.

5 Summary and Conclusions

We summarize our conclusions and pin point the strategy of attack of the problem which shows in a definite quantitative manner, not just in words, how the exclusion principle is responsible for matter to occupy such a large volume in conformity with Ehrenfest's remark. To this end, upon defining the electron number density

$$\varrho(\boldsymbol{x}) = N \sum_{\sigma_1,\ldots,\sigma_N} \int \mathrm{d}^3\boldsymbol{x}_2 \cdots \mathrm{d}^3\boldsymbol{x}_N \times |\Psi(\boldsymbol{x}\sigma_1, \boldsymbol{x}_2\sigma_2, \ldots, \boldsymbol{x}_N\sigma_N)|^2 ,$$

where $\Psi(\boldsymbol{x}\sigma_1, \boldsymbol{x}_2\sigma_2, \ldots, \boldsymbol{x}_N\sigma_N)$ is a normalized wavefunction, anti-symmetric under the interchange of any pair $(\boldsymbol{x}_i\sigma_i) \leftrightarrow (\boldsymbol{x}_j\sigma_j)$, the sums are over spins, and the total number of particles is obtained by integrating over the number density $\varrho(\boldsymbol{x})$

$$\int \mathrm{d}^3\boldsymbol{x}\,\varrho(\boldsymbol{x}) = N ,$$

we have seen that

$$\int \mathrm{d}^3\boldsymbol{x}\,\varrho^{5/3}(\boldsymbol{x}) < 32\frac{m^2\mathrm{e}^4}{\hbar^4}N[1+Z^{2/3}]^2 , \quad (\text{Fermionic}) ,$$

where a smaller value than the numerical factor 32 may be obtained, but this is not important for the present investigation. From this bound an explicit upper bound was derived in Eq. (65) which leads to the inescapable conclusion that for a non-vanishing probability of having the electrons within a radius R, the latter necessarily grows not any slower than $N^{1/3}$ for $N \to \infty$, or equivalently the corresponding volume does not grow any slower than the single power of N. No wonder why matter occupies so large a volume. The situation is drastically different when the exclusion principle is abolished, in conformity with Ehrenfest's remark. To this end, definining the negatively charged particle density

$$\rho(\boldsymbol{x}) = N \int \mathrm{d}^3\boldsymbol{x}_2 \cdots \mathrm{d}^3\boldsymbol{x}_N |\psi(\boldsymbol{x}, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N)|^2 ,$$

where ψ is an N boson (spin 0) symmetric normalized wavefunction, we have seen that

$$\int \mathrm{d}^3\boldsymbol{x}\,\rho^2(\boldsymbol{x}) < 2.55\frac{m^2\mathrm{e}^4}{\hbar^4}N^3[1+Z]^2 , \quad (\text{Bosonic}) ,$$

where a smaller numerical value than 2.55 may be obtained, but this is not important for the present investigation. From this bound an explicit upper bound was derived in Eq. (67) which leads to the inescapable conclusion that if contraction of "bosonic matter" occurs, upon collapse, then for a non-vanishing probability of having the negatively charged particles within a radius R, the latter necessarily decreases not faster than $1/N^{1/3}$ for $N \to \infty$, or equivalently the corresponding volume shrinks not any faster than $1/N$.

Appendix A: The Schwinger Bound

Consider the Hamiltonian

$$\tilde{h}(\lambda) = h_0 - \lambda f(\boldsymbol{x}) , \quad h_0 = \frac{\boldsymbol{p}^2}{2m} , \quad f(\boldsymbol{x}) \geq 0 , \tag{A1}$$

in three dimensions, depending on a coupling parameter $\lambda > 0$. Clearly,

$$h_0 - \lambda' f \geq h_0 - \lambda f , \quad \text{for } 0 < \lambda' < \lambda . \tag{A2}$$

Also for the number of eigenvalues $N(h_0 - \lambda f; -\xi) \leq -\xi$, of the Hamiltonian $(h_0 - \lambda f)$, satisfies the inequality

$$N(h_0 - \lambda f; -\xi) \geq N(h_0 - \lambda' f; -\xi) , \quad \text{for } 0 < \lambda' < \lambda , \tag{A3}$$

$$N(h_0 - f; -\xi_2) \geq N(h_0 - \lambda f, -\xi_1) , \quad \text{for } 0 < \xi_2 < \xi_1 . \tag{A4}$$

The number of eigenvalues $N(h_0 - \lambda f; -\xi) \leq -\xi$ of the Hamiltonian $(h_0 - \lambda f)$ satisfies the equality

$$N(h_0 - \lambda f; -\xi) = [\text{Number of } \lambda'\text{s in } 0 < \lambda' \leq \lambda \text{ for which } (h_0 - \lambda' f) \text{ has the eigenvalue } -\xi] . \tag{A5}$$

Accordingly, we are led to consider the eigenvalue problem

$$\Big(\frac{\boldsymbol{p}^2}{2m} - \lambda' f\Big)|\varphi\rangle = -\xi|\varphi\rangle , \quad \|\varphi\| = 1 . \tag{A6}$$

The latter may be rewritten as

$$\Big[\sqrt{f}\frac{1}{(\boldsymbol{p}^2/2m + \xi)}\sqrt{f}\Big]|\phi\rangle = \frac{1}{\lambda'}|\phi\rangle , \tag{A7}$$

$$|\phi\rangle = \sqrt{f}|\varphi\rangle . \tag{A8}$$

Upon setting

$$\Big[\sqrt{f}\frac{1}{(\boldsymbol{p}^2/2m + \xi)}\sqrt{f}\Big] = \Theta , \tag{A9}$$

the positive operator Θ satisfies the inequality

$$\int \mathrm{d}^3\boldsymbol{x}\langle\boldsymbol{x}|\Theta^2|\boldsymbol{x}\rangle \geq \frac{1}{\lambda^2} \times [\text{Number of all } \lambda'\text{s}, \text{ counting degeneracy,as eigenvalues of } \Theta \text{ in (A7), such that } 0 < \lambda' \leq \lambda] . \tag{A10}$$

This leads to

$$N(h_0 - \lambda f; -\xi) \leq \lambda^2 \int \mathrm{d}^3\boldsymbol{x}\langle\boldsymbol{x}|\Theta^2|\boldsymbol{x}\rangle . \tag{A11}$$

In particular

$$N(h_0 - f; -\xi) \leq \int \mathrm{d}^3\boldsymbol{x}\langle\boldsymbol{x}|\Theta^2|\boldsymbol{x}\rangle . \tag{A12}$$

On the other hand,

$$\int \mathrm{d}^3\boldsymbol{x}\langle\boldsymbol{x}|\Theta^2|\boldsymbol{x}\rangle = \int \mathrm{d}^3\boldsymbol{x}\mathrm{d}^3\boldsymbol{x}' f(\boldsymbol{x})\Big|\Big\langle\boldsymbol{x}\Big|\frac{1}{(\boldsymbol{p}^2/2m + \xi)}\Big|\boldsymbol{x}'\Big\rangle\Big|^2 f(\boldsymbol{x}') . \tag{A13}$$

We introduce the Fourier transform

$$\left\langle \boldsymbol{x}\left|\frac{1}{(\boldsymbol{p}^2/2m+\xi)}\right|\boldsymbol{x}'\right\rangle = \int \frac{\mathrm{d}^3\boldsymbol{p}}{(2\pi\hbar)^3}\frac{\mathrm{e}^{\mathrm{i}\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{x}')\hbar}}{(\boldsymbol{p}^2/2m+\xi)}\,. \tag{A14}$$

The angular integration for the latter integral gives

$$\frac{m}{2\pi^2\hbar^2}\frac{1}{\mathrm{i}|\boldsymbol{x}-\boldsymbol{x}'|}\int_{-\infty}^{\infty} p\mathrm{d}p\frac{\mathrm{e}^{\mathrm{i}|\boldsymbol{x}-\boldsymbol{x}'|p/\hbar}}{p^2+2m\xi}\,, \tag{A15}$$

integrating symmetrically over p. In the complex p-plane, the integrand of the above integral has poles at $p=\pm\mathrm{i}\sqrt{2m\xi}$. Closing the contour of integration in the upper plane, we pick up the pole at $p=\mathrm{i}\sqrt{2m\xi}$. The residue theorem then gives from Eqs. (A12)–(A15), the Schwinger bound in Eq. (15).

Appendix B: The No-Binding Theorem

We introduce the functional

$$F[\varrho;Z_1,\ldots,Z_k,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_k] = (3\pi^2)^{5/3}\frac{\hbar^2}{10\pi^2 m\beta}\int \mathrm{d}^3\boldsymbol{x}\varrho^{5/3}(\boldsymbol{x}) - \sum_{j=1}^{k} Z_j\mathrm{e}^2\int \mathrm{d}^3\boldsymbol{x}\frac{\varrho(\boldsymbol{x})}{|\boldsymbol{x}-\boldsymbol{R}_j|}$$
$$+\frac{\mathrm{e}^2}{2}\int \mathrm{d}^3\boldsymbol{x}\mathrm{d}^3\boldsymbol{x}'\varrho(\boldsymbol{x})\frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|}\varrho(\boldsymbol{x}') + \sum_{1\le i<j\le k}\frac{Z_iZ_j\mathrm{e}^2}{|\boldsymbol{R}_i-\boldsymbol{R}_j|}\,, \tag{A16}$$

Here $\varrho(\boldsymbol{x})$ is an arbitrary positive function, and $\beta>0$ is an arbitrary dimensionless parameter. Also $Z_j|\mathrm{e}|$ denotes the charge of a j-th positively charged particle, and the $\boldsymbol{R}_j$, correspond to positions of these positively charged particles — the nuclei. Let ϱ_0 satisfy the equation

$$(3\pi^2)^{2/3}\frac{\hbar^2}{2m\beta}\varrho_0^{2/3}(\boldsymbol{x};k) = \sum_{i=1}^{k}\frac{Z_i\mathrm{e}^2}{|\boldsymbol{x}-\boldsymbol{R}_i|} - \mathrm{e}^2\int \mathrm{d}^3\boldsymbol{x}'\frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|}\varrho_0(\boldsymbol{x}';k)\,. \tag{A17}$$

as obtained by functional differentiation of Eq. (A16) with respect to ϱ, and by setting the result equal to zero as done in Lagrangian mechanics.

Let

$$\varrho(\boldsymbol{x}) = t\varrho_1(\boldsymbol{x}) + (1-t)\varrho_2(\boldsymbol{x}) \quad \equiv t\varrho_1 + (1-t)\varrho_2\,, \tag{A18}$$
$$\varrho(\boldsymbol{x}') = t\varrho_1(\boldsymbol{x}') + (1-t)\varrho_2(\boldsymbol{x}') \equiv t\varrho_1' + (1-t)\varrho_2'\,, \tag{A19}$$

where $0\le t\le 1$, $\varrho_1,\varrho_2\ge 0$. From convexity, we have the elementary inequality

$$(t\varrho_1+(1-t)\varrho_2)^{5/3} \le t(\varrho_1)^{5/3} + (1-t)\varrho_2^{5/3}\,. \tag{A20}$$

We also have

$$(t\varrho_1+(1-t)\varrho_2)(t\varrho_1'+(1-t)\varrho_2') = t\varrho_1\varrho_1' + (1-t)\varrho_2\varrho_2' - t(1-t)(\varrho_1-\varrho_2)(\varrho_1'-\varrho_2')\,. \tag{A21}$$

Hence

$$F[t\varrho_1+(1-t)\varrho_2;Z_1,\ldots,Z_k,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_k] \le tF[\varrho_1;Z_1,\ldots,Z_k,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_k] + (1-t)F[\varrho_2;Z_1,\ldots,Z_k,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_k]\,. \tag{A22}$$

Also

$$\frac{\mathrm{d}}{\mathrm{d}t}F[t\varrho_1+(1-t)\varrho_2;Z_1,\ldots,Z_k,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_k]\Big|_{t=0}$$
$$= \int \mathrm{d}^3\boldsymbol{x}(\varrho_1-\varrho_2)\Big[(3\pi^2)^{2/3}\frac{\hbar^2}{2m\beta}\varrho_2^{2/3}(\boldsymbol{x}) - \sum_{i=1}^{k}\frac{Z_i\mathrm{e}^2}{|\boldsymbol{x}-\boldsymbol{R}_i|} + \mathrm{e}^2\int\frac{\mathrm{d}^3\boldsymbol{x}'}{|\boldsymbol{x}-\boldsymbol{x}'|}\varrho_2'\Big]\,. \tag{A23}$$

Upon choosing $\varrho_2\equiv\varrho_0$, where ϱ_0 satisfies (A17), and $\varrho_1=\sigma$ with the latter arbitrary, we note that the expression within the square brackets in Eq. (A23) vanishes, and we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}F[t\sigma+(1-t)\varrho_0;Z_1,\ldots,Z_k,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_k]\Big|_{t=0} = 0\,. \tag{A24}$$

On the other hand, Eq. (A22) leads to the inequality

$$F[\sigma;Z_1,\ldots,Z_k,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_k] - F[\varrho_0;Z_1,\ldots,Z_k,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_k]$$
$$\ge \frac{1}{t}\Big[F[t\sigma+(1-t)\varrho_0;Z_1,\ldots,Z_k,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_k] - F[\varrho_0;Z_1,\ldots,Z_k,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_k]\Big]\,. \tag{A25}$$

Upon taking the limit $t\to 0$ of the above equation, and using Eq. (A24), we obtain

$$F[\sigma;Z_1,\ldots,Z_k,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_k] \ge F[\varrho_0;Z_1,\ldots,Z_k,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_k]\,. \tag{A26}$$

That is, the solution ϱ_0 of Eq. (A17) provides the smallest value for the functional in Eq. (A16).

From Eq. (A16), we introduce the two functionals

$$F[\varrho;\lambda Z_1,\ldots,\lambda Z_\ell,Z_{\ell+1},\ldots,Z_k,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_k]\,, \tag{A27}$$

$$F[\varrho;\lambda Z_1,\ldots,\lambda Z_\ell,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_\ell]\,, \tag{A28}$$

involving a scaling factor $\lambda > 0$, $\ell < k$.

Let ${}_1\varrho$, ${}_2\varrho$, be the corresponding solutions to Eq. (A17), for the above two functionals, respectively, i.e.,

$$(3\pi^2)^{2/3}\frac{\hbar^2}{2m\beta}{}_1\varrho^{2/3}(\boldsymbol{x}) = \sum_{i=1}^{\ell}\frac{\lambda Z_i \mathrm{e}^2}{|\boldsymbol{x}-\boldsymbol{R}_i|} + \sum_{i=\ell+1}^{k}\frac{Z_i\mathrm{e}^2}{|\boldsymbol{x}-\boldsymbol{R}_i|} - \mathrm{e}^2\int \mathrm{d}^3\boldsymbol{x}'\frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|}{}_1\varrho(\boldsymbol{x}')\,, \tag{A29}$$

$$(3\pi^2)^{2/3}\frac{\hbar^2}{2m\beta}{}_2\varrho^{2/3}(\boldsymbol{x}) = \sum_{i=1}^{\ell}\frac{\lambda Z_i \mathrm{e}^2}{|\boldsymbol{x}-\boldsymbol{R}_i|} - \mathrm{e}^2\int \mathrm{d}^3\boldsymbol{x}'\frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|}{}_2\varrho(\boldsymbol{x}')\,. \tag{A30}$$

For simplicity of the notation, we have suppressed the dependence of ${}_1\varrho$, ${}_2\varrho$ on λ, k, ℓ.

We set

$$(3\pi^2)^{2/3}\frac{\hbar^2}{2m\beta}{}_j\varrho^{2/3}(\boldsymbol{x}) \equiv Q_j(\boldsymbol{x})\,,\quad j=1,2\,, \tag{A31}$$

then

$$Q_1(\boldsymbol{x}) - Q_2(\boldsymbol{x}) = \sum_{i=\ell+1}^{k}\frac{Z_i\mathrm{e}^2}{|\boldsymbol{x}-\boldsymbol{R}_i|} - \frac{1}{3\pi^2}\Big(\frac{2m\beta}{\hbar^2}\Big)^{3/2}\mathrm{e}^2 \times \int \mathrm{d}^3\boldsymbol{x}'\frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|}[Q_1^{3/2}(\boldsymbol{x}') - Q_2^{3/2}(\boldsymbol{x}')]\,. \tag{A32}$$

As in a problem in electrostatics, it is easily shown that

$$Q_1(\boldsymbol{x}) - Q_2(\boldsymbol{x}) \geq 0\,. \tag{A33}$$

In reference to the functional

$$F[\varrho;Z_{\ell+1},\ldots,Z_k,\boldsymbol{R}_{\ell+1},\ldots,\boldsymbol{R}_k]\,, \tag{A34}$$

let ${}_3\varrho(\boldsymbol{x})$ satisfy

$$(3\pi^2)^{2/3}\frac{\hbar^2}{2m\beta}{}_3\varrho^{2/3}(\boldsymbol{x}) = \sum_{i=\ell+1}^{k}\frac{Z_i\mathrm{e}^2}{|\boldsymbol{x}-\boldsymbol{R}_i|} - \mathrm{e}^2\int \mathrm{d}^3\boldsymbol{x}'\frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|}{}_3\varrho(\boldsymbol{x}')\,, \tag{A35}$$

in analogy to Eqs. (A29), (A30).

Now define

$$\begin{aligned} g(\lambda) = {} & F[\varrho;\lambda Z_1,\ldots,\lambda Z_\ell,Z_{\ell+1},\ldots,Z_k,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_k] \\ & - F[\varrho;\lambda Z_1,\ldots,\lambda Z_\ell,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_\ell] \\ & - F[\varrho;Z_{\ell+1},\ldots,Z_k,\boldsymbol{R}_{\ell+1},\ldots,\boldsymbol{R}_k]\,. \end{aligned} \tag{A36}$$

In particular, we note that

$$g(0) = 0\,. \tag{A37}$$

We will show that

$$g(1) \geq 0\,. \tag{A38}$$

From Eq. (A37), we may write

$$g(1) = \int_0^1 \mathrm{d}\lambda\, g'(\lambda)\,. \tag{A39}$$

Thus to show that $g(1) \geq 0$, it is sufficient to show that $g'(\lambda) \geq 0$ for $0 \leq \lambda \leq 1$.

To the above end, we note from Eq. (A16), with $Z_1 \to \lambda Z_1,\ldots,Z_\ell \to \lambda Z_\ell$, $\varrho_1 \to \varrho$, that

$$\begin{aligned} \frac{\partial}{\partial\lambda}F[{}_1\varrho;\lambda Z_1,\ldots,\lambda Z_\ell,Z_{\ell+1},\ldots,Z_k,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_k] = {} & \int \mathrm{d}^3\boldsymbol{x}\Big[(3\pi^2)^{2/3}\frac{\hbar^2}{2m\beta}{}_1\varrho^{2/3}(\boldsymbol{x}) - \sum_{i=1}^{\ell}\frac{\lambda Z_i\mathrm{e}^2}{|\boldsymbol{x}-\boldsymbol{R}_i|} \\ & - \sum_{i=\ell+1}^{k}\frac{Z_i\mathrm{e}^2}{|\boldsymbol{x}-\boldsymbol{R}_i|} + \mathrm{e}^2\int \mathrm{d}^3\boldsymbol{x}'\frac{1}{|\boldsymbol{x}-\boldsymbol{x}'|}{}_1\varrho(\boldsymbol{x}')\Big]\frac{\partial}{\partial\lambda}{}_1\varrho(\boldsymbol{x}) - \sum_{i=1}^{\ell}Z_i\mathrm{e}^2\int \mathrm{d}^3\boldsymbol{x}\frac{1}{|\boldsymbol{x}-\boldsymbol{R}_i|}{}_1\varrho(\boldsymbol{x}) \\ & + \mathrm{e}^2\Big(2\lambda\sum_{i=1}^{\ell-1}\sum_{j=i+1}^{\ell}\frac{Z_iZ_j}{|\boldsymbol{R}_i-\boldsymbol{R}_j|} + \sum_{i=1}^{\ell}\sum_{j=\ell+1}^{k}\frac{Z_j}{|\boldsymbol{R}_i-\boldsymbol{R}_j|}\Big)\,. \end{aligned} \tag{A40}$$

On account of Eq. (A29), the expression within the square brackets in the second/third lines above vanishes. One may easily derive a similar expression for

$$\frac{\partial}{\partial\lambda}F[{}_2\varrho;\lambda Z_1,\ldots,\lambda Z_\ell,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_\ell]\,. \tag{A41}$$

Hence from Eq. (A36), we have

$$\frac{\partial}{\partial\lambda}g(\lambda) = \sum_{i=1}^{\ell}Z_i\Big(\sum_{j=\ell+1}^{k}\frac{Z_j}{|\boldsymbol{R}_i-\boldsymbol{R}_j|} - \mathrm{e}^2\int \mathrm{d}^3\boldsymbol{x}\frac{[{}_1\varrho(\boldsymbol{x}) - {}_2\varrho(\boldsymbol{x})]}{|\boldsymbol{x}-\boldsymbol{R}_i|}\Big) = \sum_{i=1}^{\ell}Z_i[Q_1(R_i) - Q_2(\boldsymbol{R}_i)] \geq 0\,, \tag{A42}$$

where we have used Eqs. (A32), (A33), (A40), thus establishing Eq. (A38). Here we note that the summation over i in the first term on the right-hand side of Eq. (A32) is from $(\ell+1)$ to k, while the one on the extreme right-hand side of Eq. (A42) is over i from 1 to ℓ, and there are no ambiguities in the expression in Eq. (A42).

Accordingly, from Eqs. (A36) and (A38), we obtain

$$F[{}_1\varrho;Z_1,\ldots,Z_k,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_k] \geq F[{}_2\varrho;Z_1,\ldots,Z_\ell,\boldsymbol{R}_1,\ldots,\boldsymbol{R}_\ell] + F[{}_3\varrho;Z_{\ell+1},\ldots,Z_k,\boldsymbol{R}_{\ell+1},\ldots,\boldsymbol{R}_k]\,, \tag{A43}$$

for any $1 \leq \ell < k$, where ${}_1\varrho, {}_2\varrho, {}_3\varrho$ are the densities, which provide the smallest values for the corresponding functionals, respectively.

Since ℓ, k (with $\ell < k$) are arbitrary natural numbers, Eq. (A43) implies that

$$F[\varrho_0; Z_1, \ldots, Z_k, \boldsymbol{R}_1, \ldots, \boldsymbol{R}_k] \geq \sum_{i=1}^{k} F[\varrho_{\mathrm{TF}}^{(i)}; Z_i, \boldsymbol{R}_i] \,, \tag{A44}$$

$$(3\pi^2)^{2/3} \frac{\hbar^2}{2m\beta} \big(\varrho_{\mathrm{TF}}^{(i)}(\boldsymbol{x})\big)^{2/3}(\boldsymbol{x}) = \frac{Z_i}{|\boldsymbol{x} - \boldsymbol{R}_i|} - \mathrm{e}^2 \int \mathrm{d}^3\boldsymbol{x}' \frac{1}{|\boldsymbol{x} - \boldsymbol{x}'|} \varrho_{\mathrm{TF}}^{(i)}(\boldsymbol{x}') \,, \tag{A45}$$

$\varrho_{\mathrm{TF}}^{(i)}$ is the so-called Thomas-Fermi density with $m \to m\beta$, $Z \to Z_i$, and from Eqs. (A26), we have[6,21,26]

$$F[\varrho; Z_1, \ldots, Z_k, \boldsymbol{R}_1, \ldots, \boldsymbol{R}_k] \geq \beta E_{\mathrm{TF}}(1) \sum_{i=1}^{k} Z_i^{7/3} \,, \tag{A46}$$

where

$$E_{\mathrm{TF}}(1) \simeq -1.5375 \frac{m\mathrm{e}^4}{2\hbar^2} \,. \tag{A47}$$

This inequality states that a system identified by the parameters $[Z_1, \ldots, Z_k, \boldsymbol{R}_1, \ldots, \boldsymbol{R}_k]$ cannot have an (optimized) energy functional (A16) less than the sum of (optimized) energy functionals of any two subsystems identified by the parameters $[Z_1, \ldots, Z_\ell, \boldsymbol{R}_1, \ldots, \boldsymbol{R}_\ell]$, $[Z_{\ell+1}, \ldots, Z_k, \boldsymbol{R}_{\ell+1}, \ldots, \boldsymbol{R}_k]$, for $\ell < k$. Because of this, the theorem embodied in the inequality is referred to as a no binding theorem.

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