Energy of many-particle quantum states

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We derive a functional form for the energy of interacting many-particle systems from first principles. Our main contribution is that we define the effective zero-point energy of an interacting system in terms of fluctuations of momentum and the Coulomb electric field. An uncertainty equation can be derived, relating the interaction energy in terms of the kinetic energy and local charge density. The Lieb-Thirring bound is then applied to constrain the kinetic energy which takes particle (anti-)symmetry into account, and the resulting functional form applies to fermionic as well as bosonic systems; in the uniform density case, the functional form agrees with the entire range of avail-
able Quantum Monte Carlo (QMC) data of many-particle systems, to within chemical accuracy. Furthermore, the functional form shows promising agreement with QMC phase transition data found in the literature, and in the high density case, where QMC data is not as readily available for a BCC Wigner state, predicts the stability of a BCC Wigner crystal agreeing qualitatively with Unrestricted Hartree-Fock. Seen in this way, many-particle wavefunctions are minimum uncertainty states in coherence with the electromagnetic bath, where the coupling is a self-generated scalar potential.
We consider the many-body Schrödinger equation,
\[
\left( -\sum_\alpha \frac{\nabla^2 \alpha}{2} + \sum_{\alpha \neq \beta} \frac{1}{2 |x_\alpha - x_\beta|} + \hat{V}_{\text{ext}} \right) \Psi = E \Psi
\]  
(1)

where \( \hat{T} = -\sum_\alpha \frac{\nabla^2 \alpha}{2} \) and \( \hat{V}_{ee} = \frac{1}{|x_\alpha - x_\beta|} \) denote kinetic and electron-electron interaction energies respectively, with \( \Psi \) (anti)symmetric under permutation of coordinate labels. Within density functional theory (DFT) (1–5), the ground state total energy is determined by,
\[
E[n] = \langle \Psi_n^{\text{min}} | \hat{T} + \hat{V}_{ee} | \Psi_n^{\text{min}} \rangle + \int V_{\text{ext}}(r)n(r)
\]  
(2)

where \( V_{\text{ext}}(r) \) denotes the external potential, and \( n(r) \) is the charge density. By convention, one starts with the Kohn-Sham ansatz, considering antisymmetry first – one assumes a single-determinant solution by introducing an effective single-particle Hamiltonian as a function of charge density, that when diagonalized, results in eigenstates that are occupied or unoccupied. For a given charge density, existing bounds on \( \langle V_{ee} \rangle \) and \( \langle T \rangle \) (4, 6–10) can be used to inform a hierarchy of functional forms of exchange correlation energy (11–15). Uncontrolled approximations can arise in this context because the relationship between kinetic and potential energy of many-particle quantum systems has not been proposed so far; here we provide a physical constraint that relates kinetic and electron-electron interaction energies to one another.

Let us start by setting the total momentum, \( \langle \hat{p} \rangle = 0 \), i.e. the many-electron system is not undergoing translation – this is not essential but simplifies our derivation. Particle indistinguishability then implies (9, see p. 320) \( \langle \hat{p}_{1,i} \rangle = \langle \hat{p}_{2,i} \rangle = \ldots = \langle \hat{p}_{N,i} \rangle = 0 \), and the kinetic
energy is the sum of fluctuations of momentum,
\[
\langle \hat{T} \rangle = \sum_{\alpha=1}^{N} \sum_{i=1}^{3} \frac{\Delta p_{\alpha,i}^2}{2}
\]
(3)

where \( \alpha \) denotes particle labels and \( i \) denotes \( xyz \)-directions.

The scalar potential at \( r \) is given by \( \hat{V}(r) = \sum_{\alpha=1}^{N} \frac{1}{|r-x_\alpha|} \Psi(x_1, \ldots, x_N) \), and its gradient, \( \hat{E}(r) = -\nabla_r V(r) \). Using what we know from classical electrostatics, i.e. the square of the Coulomb electric field denotes the energy density of interaction between charged particles, let us expand the quantum product

\[
\int_r \langle \Psi | \hat{E}(r) \cdot \hat{E}(r) | \Psi \rangle = \sum_{\alpha,\beta} \int_r \langle \Psi | \frac{1}{|r-x_\alpha|} \cdot \frac{1}{|r-x_\beta|} | \Psi \rangle \]

(4)

integrating by parts in \( r \), setting the surface term to zero, and using the identity, \( \nabla^2_r \frac{1}{|r-x|} = -4\pi \delta(r-x) \) in 3 dimensions results in

\[
\int_r \langle \Psi | \hat{E}(r) \cdot \hat{E}(r) | \Psi \rangle = 8\pi \langle \Psi | \hat{V}_{ee} | \Psi \rangle + 4\pi N \int_r \frac{\delta(r-x_1)}{|r-x_1|} \langle \Psi \rangle \]

(5)

with the last term simplifying to a constant, \( \frac{4\pi N}{(\sqrt{2\pi})} \int_k \frac{1}{|k|^2} \). A similar analysis for a classical product of operators shows

\[
\int_r \langle \Psi | \hat{E}(r) | \Psi \rangle \cdot \langle \Psi | \hat{E}(r) | \Psi \rangle = 8\pi \int_{r,r'} \frac{n(r)n(r')}{2 |r-r'|} \]

(6)

Taking the difference between Eqs 5 and 6, the left-hand-side denotes fluctuations of the
Coulomb field, $\int r \sum_{j=1}^{3} \Delta E_j^2(r)$, and rearrangement leads to

$$\langle \hat{V}_{ee} \rangle = \int_{r,r'} \frac{1}{2} \frac{n(r)n(r')}{|r - r'|} + \frac{1}{8\pi} \int_{r} \sum_{j} \Delta E_j^2(r) - \frac{N}{2 (\sqrt{2\pi})^3} \int \frac{1}{|k|^2} d^3k$$

(7)

Thus, $E[n] = E_{\text{classical}} + E_{\text{quantum}}$ where

$$E_{\text{classical}} = \int V_{\text{ext}}(r)n(r) + \frac{1}{2} \int_{r,r'} \frac{n(r)n(r')}{|r - r'|} - \frac{N}{2 (\sqrt{2\pi})^3} \int \frac{1}{|k|^2}$$

(8)

$$E_{\text{quantum}} = \sum_{\alpha,j} \Delta p_{\alpha,j}^2 + \frac{1}{8\pi} \int_{r} \sum_{j} \Delta E_j^2(r)$$

(9)

Next, we focus on $E_{\text{quantum}}$ by inspecting the relationship between the momentum and electric field operators via commutation

$$[\hat{p}_{j,\alpha}, \hat{E}_j(r)]\Psi = \frac{\hbar}{i} \frac{\partial E_j(r)}{\partial x_{j,\alpha}} \Psi = -\frac{\hbar}{i} \left( -\partial^2_{r_j} \frac{1}{|r - x_{\alpha}|} \right) \Psi$$

(10)

where applying the Cauchy-Schwartz inequality following Robertson (16), results in a relationship between fluctuations of the kind, $\Delta p_{j,\alpha} \Delta E_j(r) \geq \frac{\hbar}{2} \langle \Psi | -\partial^2_{r_j} \frac{1}{|r - x_{\alpha}|} |\Psi \rangle$. Using $|g(x)| \geq g(x)$, summing over three dimensions, and using $\nabla^2 \frac{1}{|r - x|} = -4\pi \delta(r - x)$, eventually leads to the relation $\sum_{j=1}^{3} \Delta p_{j,\alpha} \Delta E_j(r) \geq 2\pi \langle \hat{n}_\alpha(r) \rangle$. Summation over particle labels, assuming isotropy of fluctuations, and using particle indistinguishability we get

$$3N \Delta p \Delta E(r) \geq 2\pi n(r)$$

(11)

which has not been derived before, to constrain total energy of many particle systems. We
combine this constraint with the well-known Lieb-Thirring bound on kinetic energy (10),

\[
\langle T \rangle = 3N\Delta p^2/2 \geq C_{ke} \int n^{5/3}(r)
\]

(12)

which also takes the effect of (anti)symmetry under coordinate exchange into account to obtain

\[ E[n] = E_{quantum}[n] + E_{classical}[n] \]

as follows:

\[ E[n] = C_{ke} \int n^{5/3}(r) + \frac{\pi}{2C_{ke}N} \int n^2 + \int V_{ext}(r)n(r) + \frac{1}{2} \int \frac{n(r)n(r')}{|r - r'|} - \frac{N}{2(\sqrt{2\pi})^3} \int k \frac{1}{|k|^2} \]

(13)

where the first term is due to the constraint on kinetic energy, and the second term arises from the constraint on the local electric field. The remaining terms are from \( E_{classical}[n] \). In the

\[ ^{1} \text{Alternatively, one can also develop meta functionals in the Jacob’s ladder of functional complexity, for example, by computing the kinetic energy, } \propto \Delta p^2, \text{ from Kohn-Sham wavefunctions.} \]
uniform density limit, one can simplify:

\[
E[n] = C_{ke} \int \frac{n^{5/3}(r)}{r^2} \, dr + \frac{\pi}{2 C_{ke} N} \int \frac{n^2}{n^{5/3}} \, dr + \int V_{ext}(r)n(r) + \frac{1}{2} \int \frac{n(r)n(r')}{|r - r'|} - \frac{N}{2} \left( \frac{\sqrt{2\pi}}{3} \right)^3 \int \frac{1}{|k|^2} \sim_{\text{const.}}
\]

where we have used the fact that a uniform positively charged background provides the external potential, \( V_{ext}(r) = -\int r' \frac{n(r')}{|r - r'|} \), and the Wigner-Seitz radius, \( r_s \), is defined by \( \frac{4\pi}{3} r_s^3 = \frac{1}{n} \).

The functional form thus presented in Equation 14 holds true for bosonic and fermionic wavefunctions, and are fitted (with different \( \{c_1, \ldots, c_4\} \)) to Quantum Monte Carlo data from (17). Figure 2 shows the efficacy of the functional form derived in this work for the known four macroscopic quantum states. Discrete points show Quantum Monte Carlo data from (17) while continuous plots represent parametric fits to the functional form, and fitting to QMC data using various schemes (least-squares, setting \( c_1 \) to be constant, setting \( c_1 \) and \( c_4 \) to constant) all lead to deviations within \( \pm 1.5 \) mHa. The agreement is remarkable given that, usually, exchange and correlation energies are parameterized separately by combining energy of the bosonic fluid and Dirac exchange respectively. Furthermore, the functional form in the uniform limit is obtained for free from the generalized description of Equation 14.

One set of fitting parameters is presented in Table 1 where all parameters were allowed to vary freely. Note that the sign of \( c_2 \), coefficient of the term which accounts for the quantum fluctuation of the Coulomb electric field, is negative – the scalar potential, \( A_0(r) \rightarrow V(r) \), relativistically would require the Minkowski metric. Given that the QMC data fits neatly to the functional form within \( \pm 1.5 \) mHa even with a least-squares fit (see Supplementary information), we investigated whether the functional form can say more about quantum phase tran-
Figure 2: Total energy of quantum many-body systems in the uniform density limit for four different quantum states. Discrete points in each plot denote Quantum Monte Carlo (QMC) data from (17) while the continuous lines represent parametric fits to the functional form in Equation 14. Each discrete point also has an associated error bar that denotes deviation from the QMC values, which are within chemical accuracy (see Figure 3b).

sitions, and therefore fit our parameters to minimize not just deviation from the QMC data, but also relative deviation of different states, for example, $|\text{error}(BF) - \text{error}(PMF)|$, for a given $r_s$. The results are very promising: Figure 3b shows the corresponding error for all four quantum states: not only are they all within 1.5 mHa, deviations from the reference values are systematic, both in sign as well as in the magnitude of error – previously not possible with density functionals – indicating that the functional form encapsulates physics common to the four coherent macroscopic states.
Table 1: Parametric fits of the functional form obtained in 14 for the ground state energy of many-body quantum states to Quantum Monte Carlo simulations (17).

| Quantum state description            | $c_1$  | $c_2$  | $c_3$  | $c_4$  |
|-------------------------------------|--------|--------|--------|--------|
| Boson fluid (BF)                    | -0.0042| -1.2300| 0.7783 | -1.8025|
| Paramagnetic Fermion (PMF)          | -0.0039| -1.2630| 2.5674 | -0.1264|
| Ferromagnetic Fermion (FMF)         | -0.0038| -1.2890| 3.4322 | 2.7008 |
| Wigner Crystal (BCC)                | -0.0043| -1.2252| 2.0053 | 837.9585|

Figure 3: Errors estimating energies of different systems can be minimized in-tandem. Not only are deviations from QMC data less than 1.5 mHa, they can be minimized in-tandem.

The systematic behavior of errors allows one to investigate phase transitions, that are determined by smaller differences in energy, in the meV-range, which are presented in Figure 4. In particular, Figure 4a presents the energy of different fermionic states – FMF, PMF and Wigner BCC crystal – in comparison to the uniform boson fluid (BF). The BCC-BF transition is correctly predicted near $r_s = 160$, consistent with results in (17). Figure 4b presents transitions between different fermionic states, and shows that the ferromagnetic fluid is energetically favorable compared to the paramagnetic between $32 < r_s < 51$, agreeing with (18) and (19), which predict ferromagnetic stability in the regions $26 < r_s < 67$ and $20 \pm 5 < r_s < 40 \pm 5$ respec-
Figure 4: (A) Energy of different fermionic states – FMF, PMF and Wigner BCC crystal – in comparison to the uniform boson fluid (BF). The BCC-BF transition occurs near $r_s = 160$, consistent with results in (17). (B) Phase transitions between fermions: the ferromagnetic fluid is energetically favorable compared to the paramagnetic between $32 < r_s < 51$, agreeing with (18, 19), but not with (17). At higher $r_s$, the BCC Wigner crystal is favored over the ferromagnetic state above $r_s > 75$, denoting rearrangement of excited states, while the paramagnetic fluid remains the ground state, until $r_s > 128$, when Wigner crystal is the ground state, agreeing with (18, 19) but again not with (17, 20), which predict Wigner crystallization at $r_s = 106 \pm 1$. In both cases, imposing an ordering-constraint between the paramagnetic and ferromagnetic states at $r_s = 50$, and $r_s = 100$ leads to agreement with (17, 20), without significant change in total error – (see Supplementary Materials) – suggesting that an additional spin-fluctuation related constraint orders polarization. Finally, in the small $r_s$ region where QMC data for the Wigner crystal state do not exist, the functional form predicts Wigner crystallization at about $r_s < 20$, in agreement with Unrestricted Hartree-Fock theory (21, 22).

Other calculations, for example (17), predict ferromagnetic stability between $50 < r_s < 100$. The functional form can be fit to result in ferromagnetic stability at $50 < r_s < 100$ instead but it requires an additional constraint of preserving the ordering of the polarized and unpolarized macroscopic states during the fitting process, at $r_s = 50$ and $r_s = 100$, with no change in the accuracy of energy prediction, but with a different order. This constraint likely arises due to spin, and will be investigated in the future in the context of uncertainty relations of the electromagnetic field due to fermions. Going further to the low density regime, the functional form...
predicts the favorability of BCC Wigner crystal over the ferromagnetic state above $r_s > 75$, denoting rearrangement of excited states. However, the paramagnetic fluid remains the ground state, until $r_s > 128$, at which point the paramagnetic to Wigner crystal transition occurs. For comparison to QMC simulations, (18) predict lower and upper bounds for Wigner crystallization – one at $r_s = 67 \pm 5$ and another due to extrapolation from the exact boson solution at $r_s = 90 \pm 20$, while (19) predict a ferromagnetic-to-Wigner crystal transition at $r_s = 65 \pm 10$. Other calculations (17, 20) put the onset of Wigner crystallization at $r_s = 106 \pm 1$. Again, imposing an ordering-constraint for the paramagnetic and ferromagnetic states at $r_s = 50$, and $r_s = 100$ leads to agreement with (17, 20), vs. predictions in (18, 19).

So far, the functional form has predicted known results from Quantum Monte Carlo simulations; next we note that Figure 4b also shows Wigner crystallization in the high density limit, $r_s < 20$ where QMC data does not exist, and has not been used in parameter-fitting. Instead, the BCC Wigner crystal is the ground state solution, supposedly incorrect, of the Unrestricted Hartree-Fock theory (21, 22). The high-density limit of BCC Wigner crystals at zero-temperature is underexplored: Unrestricted Hartree-Fock (UHF) simulations of (22) were motivated in part to obtain trial wavefunctions for QMC simulations, and they report an antiferromagnetic BCC Wigner crystal at $r_s = 7$ for a simulation with 54 electrons, although at $r_s = 4$, there is no bcc structure (fcc). On the other hand, QMC simulations of (20) were motivated by the necessity of understanding the deviation of UHF-predictions from QMC-predictions after UHF predicted bcc Wigner crystallization in the high density, low $r_s$ region (21).

In the low density limit, Wigner crystal formation is driven by competition between $1/r_s$ – scaling interaction and $1/r_s^2$ – scaling kinetic energy. The derivations in this work suggest that in the high density limit, $1/r_s$ scaling arises from quantum-mechanical fluctuations of the interaction field, while the classical interaction energy scales as $1/r_s^6$. Scaling of kinetic energy remains $1/r_s^2$. The functional form presented in this work is consistent with predictions of QMC.
where QMC data are found, but they also suggest the validity of some kind of UHF-like ground state for low $r_s$. More work is necessary – particularly, incorporating spin degrees of freedom, generalizations to current density functionals, and the effect of anisotropy of fluctuations.

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Supplementary Materials: Energy of many-particle quantum states

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I. INTRODUCTION

Let $x_\alpha = \{x_1, \ldots, x_N\}$ denote particle coordinates, and $r$ denote generic spatial coordinates. The charge density operator, $\hat{n}(r, \{x_\alpha\})$, and the Coulomb electric field operator, $\hat{E}(r, \{x_\alpha\})$, act on the many-body wavefunction $\Psi(x_1, \ldots, x_N)$, and result in observables defined on $r$. Within density functional theory [1–5], for a given charge density, $n(r)$, one is interested in obtaining the energy functional:

$$F[n(r)] = \min_{\Psi \rightarrow n(r)} \langle \Psi | \hat{T} + \hat{V}_{ee} | \Psi \rangle$$

where $\langle \hat{T} \rangle$ denotes the kinetic energy operator, $\langle \hat{V}_{ee} \rangle$ denotes the electron-electron interaction, and the minimization is over all antisymmetric wavefunctions $\Psi$ that also result in the charge density $n(r)$. The energy functional is generally written as the sum of three terms:

$$F[n] = T_s[n] + U[n] + E_{xc}[n]$$

where $T_s[n]$ denotes the minimum kinetic energy $\langle \Phi_n | \hat{T} | \Phi_n \rangle$, where $\Phi_n$ is the antisymmetric wavefunction that minimizes $\langle \hat{T} \rangle$ for fixed $n(r)$. $U[n]$ denotes the classical Coulomb interaction for a given charge density distribution $\frac{1}{2} \int_{r,r'} \frac{n(r)n(r')}{|r-r'|}$, and $E_{xc}[n]$ denotes the exchange correlation functional. Using coupling-constant integration[6–8] and Hellmann-Feynmann theorem, it is possible to write $E_{xc}[n]$ as[9, Chapter 1]:

$$E_{xc}[n] = \langle \Psi_{n}^{\text{min},\lambda} | \hat{T} + \lambda \hat{V}_{ee} | \Psi_{n}^{\text{min},\lambda} \rangle \bigg|_{\lambda=1} - \langle \Psi_{n}^{\text{min},\lambda} | \hat{T} + \lambda \hat{V}_{ee} | \Psi_{n}^{\text{min},\lambda} \rangle \bigg|_{\lambda=0} - U[n]$$

$$E_{xc}[n] = \int_{0}^{1} d\lambda \langle \Psi_{n}^{\text{min},\lambda} | \hat{V}_{ee} | \Psi_{n}^{\text{min},\lambda} \rangle - U[n]$$

where $\Psi_{n}^{\text{min},\lambda}$ denotes the many body wavefunction results in $n(r)$ and minimizes $\langle \hat{T} + \lambda \hat{V}_{ee} \rangle$. However, the integral never directly evaluated, as it requires obtaining $\Psi_{n}^{\text{min},\lambda}$ for every coupling strength $\lambda$. Instead, coordinate scaling[10], exact exchange [11], and lower bounds on the correlation energy[12], provide important constraints on the exchange-correlation energy. Using these constraints and limiting norms (for eg. homogenous electron gas, single electron, $N \rightarrow \infty$), a hierarchy of exchange correlation functionals can be constructed[13]. The Strongly Constrained and Appropriately Normed(SCAN)[14] exchange-correlation func-
tional, for instance, uses 7 constraints for exchange, and 10 constraints for correlation, in addition to 5 norms.

II. KINETIC ENERGY

Let the expectation value of momentum of an electron in a finite bound, many-electron system equal zero. Else, $\langle p_{\alpha} \rangle \neq 0 \implies \dot{x} \neq 0$ [15], resulting in net translation.

$$\langle \hat{p}_{\text{total},i} \rangle = \langle \hat{p}_{1,i} \rangle + \ldots \langle \hat{p}_{N,i} \rangle = 0$$

Particle indistinguishability[16, see p. 320] implies $\langle \hat{p}_{1,i} \rangle = \langle \hat{p}_{2,i} \rangle = \ldots = \langle \hat{p}_{N,i} \rangle$. As a result, kinetic energy is the sum of variances of single-particle momenta, $\Delta p_{\alpha,i}^2$

$$\langle \hat{T} \rangle = \sum_{\alpha,i} \frac{\langle \hat{p}_{\alpha,i}^2 \rangle}{2} = \sum_{\alpha,i} \frac{\langle \hat{p}_{\alpha,i} \rangle^2 + \Delta p_{\alpha,i}^2}{2} = \sum_{\alpha,i} \frac{\Delta p_{\alpha,i}^2}{2} \quad (5)$$

Thus,

$$E_{\text{total}} = \sum_{\alpha,i} \Delta p_{\alpha,i}^2 + \langle \Psi | \hat{V}_{ee} | \Psi \rangle + \int V_{\text{ext}}(r) n(r)$$

Lieb and Thirring have shown that there is a lower bound on the kinetic energy of particles[16, 17],

$$\langle \hat{T} \rangle \geq C_{ke} \int n^{5/3}(r) \quad (6)$$

where the constant $C_{ke}$ differs for bosons and fermions by a factor of $N^{-2/3}$. Therefore,

$$\frac{3N\Delta p_{j,\alpha}^2}{2} \geq C_{ke} \int n^{5/3}(r) \quad (7)$$

III. ELECTRON-ELECTRON INTERACTION

Let the electrostatic potential at $r$ due to wavefunction $\Psi(\{x_{\alpha}\})$ be

$$\hat{V}(r) = \sum_{\alpha} \frac{1}{|r - x_{\alpha}|}$$

$$\langle \Psi | \hat{V}(r) | \Psi \rangle = \langle \Psi | \sum_{\alpha} \frac{1}{|r - x_{\alpha}|} | \Psi \rangle \quad (8)$$
And the corresponding electric field (longitudinal in Coulomb gauge) is the gradient of the scalar potential,

$$\langle \Psi | \hat{E} (r) | \Psi \rangle = \langle \Psi | - \nabla_r \hat{V}(r) | \Psi \rangle$$

$$\hat{E}(r) = - \nabla_r \sum_\alpha \frac{1}{|r-x_\alpha|}$$  \hspace{1cm} (9)

We show that the electron-electron interaction $\hat{V}_{ee}$ can be written as the spatial integral of the square of the Coulomb electric field $\int_r \langle \psi | \hat{E}(r) \cdot \hat{E}(r) | \psi \rangle$.

This is a well-known property in classical electrostatics as well as in non-relativistic molecular quantum electrodynamics\cite{18–20} where Coulomb interactions (and interactions with electromagnetic fields) are defined in terms of the polarizability vector, which differs from the electric field by a dielectric constant.

We are interested in integral:

$$\int_r \langle \psi | \hat{E}(r) \cdot \hat{E}(r) | \psi \rangle = \sum_{\alpha,\beta} \int_r \langle \psi | \frac{1}{4\pi\varepsilon_0} \frac{\nabla^2}{|r-x_\alpha|} \frac{1}{4\pi\varepsilon_0} \frac{1}{|r-x_\beta|} | \psi \rangle$$  \hspace{1cm} (10)

Using integration by parts, and setting the surface terms to zero:

$$= - \sum_{\alpha,\beta} \int_r \langle \psi | \frac{1}{4\pi\varepsilon_0} \frac{\nabla^2}{|r-x_\alpha|} \frac{1}{4\pi\varepsilon_0} \frac{1}{|r-x_\beta|} | \psi \rangle$$  \hspace{1cm} (11a)

$$= \sum_{\alpha,\beta} \frac{1}{4\pi\varepsilon_0^2} \int_r \langle \psi | \frac{\delta(r-x_\beta)}{|r-x_\alpha|} | \psi \rangle$$  \hspace{1cm} (11b)

$$= \frac{1}{4\pi\varepsilon_0^2} \sum_{\alpha \neq \beta} \langle \psi | \frac{1}{|x_\alpha-x_\beta|} | \psi \rangle + \frac{1}{4\pi\varepsilon_0^2} \sum_{\alpha = \beta} \langle \psi | \int_r \frac{\delta(r-x_\alpha)}{|r-x_\alpha|} | \psi \rangle$$  \hspace{1cm} (11c)

The second integral results in a related expression. Again, by using integration by parts and $\nabla^2 \frac{1}{|r-x|} = 4\pi \delta(r-x)$ in a similar way, it can be shown that

$$\int_r \langle \Psi | \hat{E}(r) | \Psi \rangle \cdot \langle \Psi | \hat{E}(r) | \Psi \rangle = 8\pi \int \frac{1}{|r-r'|} \frac{n(r)n(r')}{2}$$  \hspace{1cm} (12)
The variance of the electric field,
\[ \int_r \Delta E_x^2(r) + \Delta E_y^2(r) + \Delta E_z^2(r) = \int_r \left( \langle E_x^2 \rangle - \langle E_x \rangle^2 \right) + \left( \langle E_y^2 \rangle - \langle E_y \rangle^2 \right) + \left( \langle E_z^2 \rangle - \langle E_z \rangle^2 \right) \] (13a)

\[ = \int_r \langle \Psi|E(r) \cdot E(r)|\Psi \rangle - \langle \Psi|E(r)|\Psi \rangle \cdot \langle \Psi|E(r)|\Psi \rangle \] (13b)

\[ = 8\pi \langle \hat{V}_{ee} \rangle + 4\pi N \int_{\mathbf{k}} \frac{1}{|\mathbf{k}|^2} d^3k - 8\pi \int_{r,r'} \frac{1}{2} n(r) n(r') \] (13c)

OR,
\[ \langle \hat{V}_{ee} \rangle = \int_{r,r'} \frac{1}{2} n(r) n(r') + \frac{1}{8\pi} \int_r \sum_j \Delta E_j^2(r) - \frac{N}{2} \int \frac{1}{|\mathbf{k}|^2} d^3k \] (13d)

So that the total energy is,
\[ E_{total} = \sum_{\alpha,j} \frac{\Delta p_{\alpha,j}^2}{2} + \frac{1}{8\pi} \int_r \sum_j \Delta E_j^2(r) + \int_r V_{ext}(r) n(r) + \frac{1}{2} \int_{r,r'} \frac{n(r) n(r')}{|r-r'|} - \frac{N}{2} \int \frac{1}{|\mathbf{k}|^2} \] (14)

\[ E_{quantum}[n] = \sum_{\alpha=1}^{N} \sum_{j=1}^{3} \frac{\Delta p_{\alpha,j}^2}{2} + \frac{1}{8\pi} \int_r \sum_{j=1}^{3} \Delta E_j^2(r) \] (15)

IV. UNCERTAINTY RELATIONS

A. Derivation of the uncertainty relation

The uncertainty relation can be derived by using the Schwarzian inequality[21, 22] for inner products [23]. Let \( \hat{A} \) and \( \hat{B} \) be hermitian operators, we follow [24] to show:

\[ [\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = \frac{\hbar}{i} C \implies \Delta A \Delta B \geq \frac{\hbar |C_0|}{2} \]

\[ \tilde{f}_1(x) = (\hat{A} - A_0)\Psi(x) = f_2(x) \] (16)

\[ \tilde{g}_1(x) = (\hat{B} - B_0)\Psi(x) = -g_2(x) \] (17)

Define the inner product
\[ \langle f, g \rangle = \int f_1(x) \tilde{g}_1(x) + f_2(x) \tilde{g}_2(x) dx = \int f_1(x) \tilde{g}_1(x) + \tilde{g}_2(x) f_2(x) \] (18)
\[
\int \left[ \left( \hat{A} - A_0 \right) \Psi(x) \right]^\dagger \left( \hat{B} - B_0 \right) \Psi(x) - \left[ \left( \hat{B} - B_0 \right) \Psi(x) \right]^\dagger \left( \hat{A} - A_0 \right) \Psi(x) \tag{19}
\]

Using hermiticity of the operators, \( \hat{A}^\dagger = \hat{A} \) and \( \hat{B}^\dagger = \hat{B} \)

\[
= \langle \Psi | (\hat{A} - A_0)(\hat{B} - B_0) - (\hat{B} - B_0)(\hat{A} - A_0) | \Psi \rangle \tag{20}
\]

\[
= \langle \Psi | \hat{A} \hat{B} - \hat{B} \hat{A} | \Psi \rangle = \langle \Psi | [\hat{A}, \hat{B}] | \Psi \rangle \tag{21}
\]

Using the Cauchy-Schwartz inequality for inner products: \( |\langle f, g \rangle|^2 \leq \langle f, f \rangle \cdot \langle g, g \rangle \) The RHS can be substituted and expanded as follows:

\[
| \langle f, f \rangle | = \left| \int f_1(x) \bar{f}_1(x) + f_2(x) \bar{f}_2(x) \right| \tag{22}
\]

, where

\[
\int f_1(x) \bar{f}_1(x) dx = \int \Psi^*(x)(\hat{A} - A_0)^2 \Psi(x) \tag{23}
\]

\[
= \langle \Psi | \hat{A}^2 - \hat{A} A_0 - A_0 \hat{A} + A_0^2 | \Psi \rangle = \Delta A^2 \tag{24}
\]

Similarly, we can expand, \( RHS = (2\Delta A^2)(2\Delta B^2) \), and combining LHS and RHS

\[
| \langle [\hat{A}, \hat{B}] \rangle |^2 \leq 4\Delta A^2 \Delta B^2 \tag{25}
\]

If \( [\hat{A}, \hat{B}] = \hat{C} \implies 4\Delta A^2 \Delta B^2 \geq | \langle \hat{C} \rangle |^2 \). Taking the square root on both sides, we obtain,

\[
\Delta A \Delta B \geq \frac{\langle \hat{C} \rangle}{2} \tag{26}
\]

**B. Canonical uncertainty relation**

In the canonical case, let \( A = \hat{p} = \hbar \frac{\partial}{\partial x} \), and \( \hat{B} = \hat{x} \), the commutation between the two is given by:

\[
[\hat{p}, \hat{x}] \Psi = \hbar i \frac{\partial}{\partial x} (x \Psi) - \frac{\hbar}{i} \frac{\partial}{\partial x} x \Psi \tag{27}
\]

\[
= \hbar \frac{\partial}{\partial x} \Psi + x \hbar \frac{\partial}{\partial x} (\Psi) - x \frac{\hbar}{i} \frac{\partial}{\partial x} \Psi \tag{28}
\]

\[
= \frac{\hbar}{i} \Psi \tag{29}
\]
Thus,
\[ \Delta p \Delta x \geq \frac{\hbar}{2} \]  

(30)

**C. Uncertainty relation between variances**

We now obtain a relation between variances of the electric field and momentum, \( \Delta E_j(r) \) and \( \Delta p_{\alpha,j} \). Our derivation relies on a specific case of a general relation [24]

\[ [\hat{p}, \hat{F}(x, r)] \psi(x) = \frac{\hbar}{i} \frac{\partial}{\partial x}(\hat{F}(x, r)\psi) - \hat{F}(x, r)i \frac{\partial}{\partial x}\psi = \frac{\hbar}{i} \frac{\partial F(x, r)}{\partial x}\psi(x) \]  

(31)

Replacing \( F(\ldots) \) by the electric field along \( j \) direction at \( r \), \( \hat{E}_j(r) \), the commutation between momentum and electric field operators,

\[ [\hat{p}_{j,\alpha}, \hat{E}_j(r)] \psi = \frac{\hbar}{i} \frac{\partial E_j(r)}{\partial x_{j,\alpha}} \psi \]  

(32)

Since \( \hat{E}_j(r) = -\partial_{r_j} V(r) = -\partial_{r_j} \sum_{\beta} \frac{1}{|r-x_{\beta}|} \),

\[ [\hat{p}_{j,\alpha}, \hat{E}_j(r)] \psi = \left( -\frac{\hbar}{i} \partial_{x_{j,\alpha}} \partial_{r_j} \sum_{\beta} \frac{1}{|r-x_{\beta}|} \right) \psi \]  

(33)

\[ [\hat{p}_{j,\alpha}, \hat{E}_j(r)] \psi = -\frac{\hbar}{i} \left( -\partial_{r_j} \frac{1}{|r-x_{\alpha}|} \right) \psi \]  

(34)

The commutation relation implies

\[ \Delta p_{j,\alpha} \Delta E_j(r) \geq \frac{\hbar}{2} \left| \langle \psi | -\partial_{r_j}^2 \frac{1}{|r-x_{\alpha}|} |\psi \rangle \right| \]  

(35a)

Using \( |g(x)| \geq g(x) \),

\[ \Delta p_{j,\alpha} \Delta E_j(r) \geq \frac{\hbar}{2} \langle \psi | -\partial_{r_j}^2 \frac{1}{|r-x_{\alpha}|} |\psi \rangle \]  

(35b)

\[ \frac{\hbar}{2} \left| \langle \psi | \left( -\partial_{r_j}^2 \frac{1}{|r-x_{\alpha}|} \right) |\psi \rangle \right| \geq \frac{\hbar}{2} \langle \psi | -\partial_{r_j}^2 \frac{1}{|r-x_{\alpha}|} |\psi \rangle \]  

(35c)

Summation over three directions results in

\[ \sum_{j=x,y,z} \Delta p_{j,\alpha} \Delta E_j(r) \geq \frac{\hbar}{2} \langle \psi | -\nabla_r^2 \frac{1}{|r-x_{\alpha}|} |\psi \rangle \]  

(35d)
\[ \Delta p_{x,\alpha} \Delta E_x(r) + \Delta p_{y,\alpha} \Delta E_y(r) + \Delta p_{z,\alpha} \Delta E_z(r) \geq \frac{\hbar}{2} \langle \hat{n}_\alpha(r) \rangle \quad (35e) \]

\( \hat{n}_\alpha(r) = \delta(r-x_\alpha) \), is the charge density due to particle \( \alpha \). Summation of Equation 35 over \( \alpha \), results in an expression that relates variances of momentum and electric field directly to the total charge density as follows:

\[ \sum_\alpha \Delta p_{x,\alpha} \Delta E_x(r) + \sum_\alpha \Delta p_{y,\alpha} \Delta E_y(r) + \sum_\alpha \Delta p_{z,\alpha} \Delta E_z(r) \geq \frac{\hbar n(r)}{2} \quad (36) \]

Under the assumption of isotropic variances, i.e., \( \Delta E_x(r) = \Delta E_y(r) = \Delta E_z(r) \), \( \Delta E_x(r) \) can be factored out, resulting in:

\[ \Delta E_x(r) \left( \sum_\alpha \Delta p_{x,\alpha} + \Delta p_{y,\alpha} + \Delta p_{z,\alpha} \right) \geq \frac{\hbar n(r)}{2} \quad (37) \]

\[ \Delta E_x(r) \left( \sum_{\beta,j=x,y,z} \Delta p_{j,\beta} \right) \geq \frac{\hbar n(r)}{2\epsilon_0} \quad (38) \]

Therefore, assuming isotropy of local fluctuations, Equation 36 simplifies to

\[ \Delta E_z(r) = \Delta E_y(r) = \Delta E_x(r) \geq \frac{\hbar n(r)}{2} \frac{1}{\sum_{j,\alpha} \Delta p_{j,\alpha}} \quad (39) \]

Using particle indistinguishability and assuming isotropy of momentum fluctuations, we get:

\[ \sum_{\beta=1}^{N} \sum_{j=1}^{3} \Delta p_{j,\beta} \Delta E_j(r) \geq \frac{\hbar n(r)}{2\epsilon_0} \quad (40) \]
V. MINIMIZATION WITH UNCERTAINTY RELATION BUT WITHOUT PARTICLE (ANTI-)SYMMETRY

Let us minimize $E_{\text{quant}}[n]$ under only one constraint – the uncertainty constraint defined above in Equation 40

$$E_{\text{quant}}[n] = \min_{\Psi \rightarrow n(r)} \left[ \sum_{\alpha,x,y,z} \frac{(\Delta p_{\alpha})^2}{2m} + \frac{\epsilon_0}{2} \int_{r} \sum_{j=x,y,z} (\Delta E_j(r))^2 \right]$$  \hspace{1cm} (41)

Substituting for $\Delta E_x(r), \Delta E_y(r), \Delta E_z(r)$, we get:

$$E_{\text{quant}}[n] = \sum_{\alpha=1}^{N} \sum_{i=1}^{3} \frac{(\Delta \hat{p}_{i,\alpha})^2}{2m} + \frac{3\epsilon_0}{2} \int_{r} \left( \frac{\hbar n(r)}{2\epsilon_0} \right)^2 \left( \sum_{\beta=1}^{N} \sum_{j=1}^{3} \Delta p_{j,\beta} \right)^2 \hspace{1cm} (42)$$

Let $\frac{3\epsilon_0}{2} \int_{r} \left( \frac{\hbar n(r)}{2\epsilon_0} \right)^2 = \mathcal{G}[n(r)]$ is a density-dependent constant for fixed charge density, $n(r)$, and where $\frac{1}{2m} = b$. Then,

$$E_{\text{quant}}[n] \geq b \sum_{\alpha,j=x,y,z} \Delta p_{\alpha,j}^2 + \frac{\mathcal{G}[n(r)]}{(\sum_{\alpha,j=x,y,z} \Delta p_{\alpha,j})^2} \hspace{1cm} (43)$$

and the minimization problem is a simple one. Next, we minimize $E_{\text{quant}}$, w.r.t fluctuations of momentum, $\Delta p$. The first and second derivatives are $\frac{\partial E_{\text{quant}}[n]}{\partial \Delta p_{\alpha,j}} = 2b\Delta p_{\alpha,j} - 2 \frac{\mathcal{G}[n]}{(\sum_{\alpha,j} \Delta p_{\alpha,j})^3}$ and $\frac{\partial^2 E_{\text{quant}}[n]}{\partial \Delta p_{\alpha,j} \partial \Delta p_{\alpha',j'}} = 2b \delta_{\alpha,\alpha'} \delta_{j,j'} + 6 \frac{\mathcal{G}[n]}{(\sum_{\alpha,j} \Delta p_{\alpha,j})^4} \geq 0$, respectively.

Setting the first derivative to zero (the second derivatives are $\geq 0$) results in $\Delta p_{\alpha,j} = \left( \frac{1}{b \mathcal{G}[n]} \right)^{1/4}$, for all $\alpha, j$, reflecting indistinguishability of particles and isotropy of fluctuations. Thus, the minimum value for $E_{\text{quant}}[25]$ is given by:

$$E_{\text{quant}}[n] = b \cdot 3N \left[ \left( \frac{1}{b \mathcal{G}[n]} \right)^{1/4} \right]^2 + \frac{\mathcal{G}[n(r)]}{3N \cdot \left( \frac{1}{b \mathcal{G}[n]} \right)^{1/4}} \hspace{1cm} (44)$$

$$E_{\text{quant}}[n] = \frac{\hbar}{2\sqrt{m\epsilon_0}} \sqrt{\int_{r} n^2(r) \frac{1}{N}} \hspace{1cm} (45)$$
\[ E_{\text{total}}[n(r)] = \int_r V_{\text{ext}}(r)n(r) + \frac{1}{2} \int_{r,r'} \frac{n(r)n(r')}{|r - r'|} - \frac{N}{2} \int_k \frac{1}{|k|^2} + \sqrt{\pi} \int_r n^2(r) \frac{1}{N} \]  

(46)

Where atomic units, \(\hbar = 1, m_e = 1, 4\pi\varepsilon_0 = 1\) are used. For the case of uniform density, \(n = \frac{N}{V}\), where \(N\) is the number of particles and \(V\), the system volume, is independent of position, and using the Wigner-Seitz radius, \(\frac{4\pi}{3}r_s^3 = \frac{1}{n}\), we obtain:

\[ \text{Energy}[r_s] = c_1 + c_2 \frac{1}{r_s^{3/2}} + c_3 \frac{1}{r_s^6} \]  

(47)

Here we note that there is no way to include antisymmetry of particles, and one needs a Dirac exchange term in addition to the energy predicted by the uncertainty relation. This is one way to make an incorrect, uncontrolled approximation.

FIG. 1. Total energies for the uniform electron and boson gas densities, fitted to the functional form obtained due to the uncertainty relation between variances of momentum and electric field. Just one constraint is insufficient, as the constraint on \(\Delta p\Delta E\) does not take particle symmetry into account, and Dirac exchange was added to the paramagnetic fermion case.
VI. USING BOTH CONSTRAINTS ON UNCERTAINTY AND PARTICLE (ANTI-)SYMMETRY

To summarize our derivation so far, the total energy can be written in terms of the charge density, and variances of the electric field and momentum operators.

\[
E_{\text{total}} = \sum_{\alpha,j} \frac{\Delta p_{\alpha,j}^2}{2} + \int r V_{\text{ext}}(r)n(r) + \frac{1}{2} \int_{r,r'} \frac{n(r)n(r')}{|r - r'|} + \frac{1}{8\pi} \int r \sum_j \Delta E_j^2(r) - \frac{N}{2} \int_k \frac{1}{|k|^2} \quad (48)
\]

Since variances of the electric field can be constrained by variances of the momentum (as derived from the uncertainty relation in the previous section), the total energy is:

\[
E_{\text{total}} \geq \sum_{\alpha,j} \frac{\Delta p_{\alpha,j}^2}{2} + \int r V_{\text{ext}}(r)n(r) + \frac{1}{2} \int_{r,r'} \frac{n(r)n(r')}{|r - r'|} + \frac{3}{8\pi} \int r \left( \frac{\hbar n(r)}{2} \sum_{j,\alpha} \frac{1}{\Delta p_{j,\alpha}} \right)^2 - \frac{N}{2} \int_k \frac{1}{|k|^2} \quad (49)
\]

For fixed \(n(r)\), \(E_{\text{total}}\) is constrained only by variances of the momentum as follows:

\[
E_{\text{total}} \geq \sum_{\alpha,j} \frac{\Delta p_{\alpha,j}^2}{2} + \frac{3}{8\pi} \int r \left( \frac{\hbar n(r)}{2} \sum_{j,\alpha} \frac{1}{\Delta p_{j,\alpha}} \right)^2 + A[n] - C \quad (50)
\]

Furthermore, the Lieb-Thirring bound on kinetic energy constrains variances of the momentum as follows.

\[
3N \Delta p_{i,\alpha}^2 \geq C_{ke} \int n^{5/3}(r) \quad (51)
\]

Figure 2 presents a schematic description of energy minimization for a given charge density, \(n(r)\), where the horizontal axis denotes the variance of momentum, and the vertical axis denotes total energy. The solid blue line in Figure 2 represents the constraint on total energy, from Equation 50, and the vertical, dashed, red line denotes the Lieb-Thirring bound on kinetic energy, Equation 51. The shaded region represents the feasible region of energy that satisfies Equations 50 and 51. Assuming that both constraints are active, the minimum total energy of the system is as follows:

\[
= C_{ke} \int n^{5/3}(r) + \int V_{\text{ext}}(r)n(r) + \frac{1}{2} \int \frac{n(r)n(r')}{|r - r'|} + \frac{\hbar^2}{64\pi C_{ke} N} \int n^2 - \frac{N}{2} \int_k \frac{1}{|k|^2} \quad (52)
\]
A. Uniform charge density

In the limit of uniform charge density, a uniform positive charge density was used to obtain $V_{\text{ext}}$. Therefore, $V_{\text{ext}}(\mathbf{r}) = -\int \frac{n(r')}{|\mathbf{r} - \mathbf{r}'|}$, and $n(\mathbf{r}) = n(\mathbf{r}) = n$, where $n$ is a constant. Then, the energy expression becomes:

$$E = C_{ke}n^{2/3}V - \frac{1}{2} \int \frac{n^2}{|\mathbf{r} - \mathbf{r}'|} + \frac{\hbar^2}{64\pi C_{ke}N n^{1/3}} - \frac{N}{2} \int_k \frac{1}{|k|^2}$$  \hspace{1cm} (53)

where $V$ denotes the volume. Using $V = N/n$, removes explicit dependence on volume, so that:

$$E_{\text{total}} = N C_{ke}n^{2/3} - \frac{n^2}{2} \int \frac{1}{|\mathbf{r} - \mathbf{r}'|} + \frac{\hbar^2 n^{1/3}}{64\pi NC_{ke}} - \frac{N}{2} \int_k \frac{1}{|k|^2}$$  \hspace{1cm} (54)

For purposes of comparison with numerical data, we use $\frac{4\pi}{3} r_s^3 = \frac{1}{n}$, where $r_s$ denotes the Wigner radius. Furthermore, the last term due to self-interaction, is a renormalizable constant $[\text{constant}]$, and is treated as constant $c_1$. In terms of the Wigner radius, the total energy is obtained as follows.

$$E_{\text{total}} = c_1 + c_2 \frac{1}{r_s} + c_3 \frac{1}{r_s^2} + c_4 \frac{1}{r_s^3}$$  \hspace{1cm} (55)

Thus, after using $\frac{4\pi}{3} r_s^3 = \frac{1}{n}$ to substitute $n$ by $r_s$, and adding the effect of the external potential $\int V_{\text{ext}} n(\mathbf{r}) = \int \frac{n^2}{|\mathbf{r} - \mathbf{r}'|}$, as the uniform gas is held in place by a fixed uniform charge distribution of opposite charge in the background, the functional form of the total energy is
FIG. 3. QMC results (discrete values), parametric fit (continuous curve), and resulting absolute errors from fitting to the functional form denoted by Equation 55, for the uniform (A) electron and (B) bosons gases. We note that the same functional form is capable of reproducing the total energy behavior of both bosons and fermions within a wide range of particle densities, $1 \leq r_s \leq 100$ for fermions and $2 \leq r_s \leq 200$ for bosons, within quantum chemical accuracy, $err \leq 1.5 \text{ mHa}$.

| $c_1$   | $c_2$   | $c_3$   | $c_4$   |
|---------|---------|---------|---------|
| -0.0052 | -1.2486 | -0.1147 | 2.5425  |

TABLE I. Parameters for paramagnetic fermion fluid obtained via least sum-of-squares minimization of the functional form given in Equation 55 against Quantum Monte Carlo data[26].

as follows:

$$E_{\text{total}} = F[n] + \int V_{\text{ext}} n(r) = c_1 + c_2 \frac{1}{r_s} + c_3 \frac{1}{r_s^6} + c_4 \frac{1}{r_s^2}$$  \hspace{1cm} (56)

A single functional form, Equation 56, describes the total energy of bosons as well as fermions. Above, $c_1, \ldots, c_4$ are not fitting coefficients but constants that arise from the expression in Equation 55, and depend on the number of particles, and the effect of periodic boundary conditions. In particular, both the functional form of Equation 55, as well as Quantum Monte Carlo simulations in [26], pertain to simulations of finite systems – in [26], simulations of 38 to 246 particles were empirically extrapolated to the infinite case. Thus,
we obtain the coefficients, \( \{c_1, \ldots, c_4\} \), semi-empirically against the reference values in [26].

VII. PROPERTIES OF THE WAVEFUNCTION

A. Indistinguishability

Let a two-electron wavefunction be constructed from plane waves:

\[
\Psi(x_1, x_2) = \frac{1}{\sqrt{2}} \left( e^{i k_1 \cdot x_1} e^{i k_2 \cdot x_2} \pm e^{i k_1 \cdot x_2} e^{i k_2 \cdot x_1} \right)
\] (57)

The single particle momentum is then,

\[
\hat{p}_1 = \frac{\hbar}{i} \frac{1}{\sqrt{2}} \left( i k_1 e^{i k_1 \cdot x_1} e^{i k_2 \cdot x_2} \pm i k_2 e^{i k_1 \cdot x_2} e^{i k_2 \cdot x_1} \right)
\]

\[
\hat{p}_2 = \frac{\hbar}{i} \frac{1}{\sqrt{2}} \left( i k_2 e^{i k_1 \cdot x_1} e^{i k_2 \cdot x_2} \pm i k_1 e^{i k_1 \cdot x_2} e^{i k_2 \cdot x_1} \right)
\]

B. Effect of antisymmetry

Let \( \psi_c(x_1, \ldots, x_N) \) be the solution to the coupled many-body problem,

\[
\hat{H} \psi_c(x_1, \ldots, x_N) = E \psi_c(x_1, \ldots, x_N)
\]

, with distinguishable particle labels. The corresponding symmetric wavefunction can be constructed as a symmetric sum over all permutations of coordinate labels[12], \( \Psi_S = \frac{1}{\sqrt{N!}} \sum_{\mathcal{P}(x_1, \ldots, x_N)} \psi_c(\mathcal{P}(x_1, \ldots, x_N)) \), where \( \mathcal{P}(x_1, \ldots, x_n) \) denotes permutation of coordinate labels. The antisymmetric wavefunction, \( \Psi_A \), is related to the symmetric wavefunction \( \Psi_A(x_1, \ldots, x_N) = \Psi_S(x_1, \ldots, x_N) \theta(x_1, \ldots, x_N) \), where \( \theta(x_1, \ldots, x_N) \) equals \( \pm 1 \) everywhere except over a set whose measure is zero[12]. Inclusion of the sign-function, and the associated discontinuities at regions where \( x_\alpha = x_\beta \), does not affect \( \hat{n}(r) \), or \( \hat{V}_{ee} \), as \( \theta^2 = 1 \), everywhere except a set of points that contribute zero to the integral[12]. The effect of the sign-function on momentum and momentum-squared, is non-trivial: the differential operator acts on \( \Psi_A \) as:

\[
\langle \Psi_A | \nabla_\alpha | \Psi_A \rangle = \int \Psi_S^\dagger \nabla_\alpha \Psi_S + \int |\Psi_S|^2 \theta \nabla_\alpha \theta
\] (58a)
Similarly, the laplacian, \( \langle \Psi_A | \nabla^2_\alpha | \Psi_A \rangle \), is:

\[
\begin{align*}
\langle \Psi_A | \nabla^2_\alpha | \Psi_A \rangle &= \int \Psi^\dagger_S \nabla^2_\alpha \Psi_S + \int \Psi^\dagger_S \nabla_\alpha \Psi_S \cdot \theta \nabla_\alpha \theta + \int |\Psi_S|^2 \theta \nabla^2_\alpha \theta^0 \\
&= \int \Psi^\dagger_S \nabla^2_\alpha \Psi_S + \int \Psi^\dagger_S \nabla_\alpha \Psi_S \cdot \theta \nabla_\alpha \theta + \int |\Psi_S|^2 \theta \nabla^2_\alpha \theta^0 
\end{align*}
\]  

(58b)

where \( \nabla_\alpha \theta \) is non-zero only at \( x_\alpha = x_\beta \), along the direction of the \( \pm 1 \) jump, while the second derivative, \( \partial^2_\alpha \theta = 0 \). Thus, the difference between symmetric and antisymmetric wavefunctions that are related by a multi-dimensional sign-function appears in the variance of momentum. Interestingly, in 1D, antisymmetry introduces a product of generalized functions, as \( \theta \nabla \theta = \theta \delta(x) \) that anticommutes[27][28], with additional implications in higher dimensions [29, 30].

We note that the bound on the total energy remains unchanged in terms of the charge density for bosonic and fermionic systems. In particular, let us assume that a function, \( \psi_c(x_1, \ldots, x_N) \), satisfies the coupled many-body problem, \( \hat{H} \psi_c = E \psi_c(x_1, \ldots, x_N) \). Following Lieb[12, between Eqs. 8 and 9], the corresponding bosonic solution, \( \Psi_S \) – symmetric wrt particle-label exchange, can be constructed by taking sums over all permutations of \( x_1, \ldots, x_N \). The antisymmetric solution can be constructed formally as :

\[
\Psi_A = \Psi_S \theta(x_1, \ldots, x_N)
\]  

(59)

where \( \theta(x_1, \ldots, x_N) \) equals \( \pm 1 \) everywhere except over a set whose measure is zero. Thus, bounds on \( \langle \Psi_A | \hat{H} | \Psi_A \rangle \) as a function of charge density hold for symmetric or antisymmetric wavefunctions, with the caveat that the constructed symmetric and antisymmetric \( \Psi \) from the same classical function, will result in different charge densities.

C. Wavefunction eigenstates

So far, the uncertainty relations have been used to obtain the energy functional of the many-body Hamiltonian; the inequality between inner-products becomes an exact equality when two vectors (or functions) under consideration are linearly dependent, i.e.

\[
(\hat{\rho}_\beta - \langle \hat{\rho}_\beta \rangle) \Psi \equiv A(r) \left( \hat{\mathbf{E}}(r) - \langle \hat{\mathbf{E}}(r) \rangle \right) \Psi
\]  

(60)
where the proportionality constant can be a function of \( r \). Ignoring constants, \( \Psi \) satisfies

\[
\hat{p}_1 \Psi(x_1, \ldots, x_N) \equiv A(r) \hat{E}(r) \Psi(x_1, \ldots, x_N)
\]  

(61)

Using \( \hat{E}(r) = -\nabla_r \sum_{\alpha} \frac{1}{4\pi^{3/2}|r-x_\alpha|^3} \), and taking its Fourier transform with respect to \( r \to k \) from [19, page 12, Table II],

\[
\hat{p}_1 \Psi(x_1, \ldots, x_N) \equiv A(r) \sum_{\alpha} \frac{(r-x_\alpha)}{|r-x_\alpha|^3} \Psi(x_1, \ldots, x_N) \hat{p}_1 \Psi \equiv A(r) \sum_{\alpha} \int_k \frac{e^{ik(r-x_\alpha)} - i\kappa}{4\pi k^2} \Psi
\]  

(62)

Let \( \Psi(x_1, \ldots, x_N) \) be written as the sum of many-particle basis functions (here Slater determinants) \( \Phi_S \) defined by the set of any \( N \) non-repeating plane waves, \( S = (q_1, \ldots, q_N) \):

\[
\Phi_S = \frac{1}{\sqrt{N!}} \sum_{\mathcal{P}} (-1)^{\mathcal{P}} e^{i\mathcal{P} \cdot x_1} e^{i\mathcal{P} \cdot x_2} \cdots e^{i\mathcal{P} \cdot x_N}
\]  

(63)

where \( \mathcal{P} \) denotes the permutation of coordinate labels necessary to obtain the many-body wavefunction of indistinguishable particles. Expanding \( \Psi = \sum_S c_S \Phi_S \), multiplying by \( (\Phi_S')^\dagger \) on the left, and taking the inner product (with each index \( S \) and \( S' \) denoting \( N \) three dimensional momenta, \( \{q_1, \ldots, q_N\} \)), we obtain a generalized matrix eigenproblem:

\[
\langle \Phi_{S'}|\hat{p}_1|\Psi \rangle = A(r) \int_k e^{ikr} \langle \Phi_{S'}|\sum_{\alpha} \frac{e^{-ik \cdot x_\alpha}}{4\pi \kappa^2} |\Psi \rangle
\]  

(64a)

\[
\langle \Phi_S|\hat{p}_1|\Phi_S \rangle c_S = A(r) \int_k e^{ikr} \langle \Phi_S|\sum_{\alpha} \frac{e^{-ik \cdot x_\alpha}}{4\pi \kappa^2} |\Phi_S \rangle c_S
\]  

(64b)

where repetition of index \( S \) denotes summation. The LHS results in:

\[
LHS = \sum_S \sum_{\mathcal{P}(S)} \sum_{\mathcal{P}'(S')} (-1)^{\mathcal{P} + \mathcal{P}'} \int_x e^{-i\mathcal{P}' \cdot x_1} \cdots e^{-i\mathcal{P}' \cdot x_N} (\hbar \mathcal{P}') e^{i\mathcal{P} \cdot x_1} \cdots e^{i\mathcal{P} \cdot x_N} c_S
\]  

(64c)

\[
= \sum_{S, \mathcal{P}(S), \mathcal{P}'(S')} (-1)^{\mathcal{P} + \mathcal{P}'} (\hbar \mathcal{P}') \prod_{\alpha=1}^N \delta(q_{\mathcal{P}'_\alpha} - q_{\mathcal{P}_\alpha}) c_S
\]  

(64d)

\[
= P_{S'S} c_S
\]  

(64e)
The RHS results in (removing factor of $A(r)$ for now):

\[
= A(r) \sum_{S,P,P'} (-1)^{P+P'} \int_{X,k} \frac{k}{4\pi k^2} e^{i k \cdot r} \sum_{\alpha} e^{-i k \cdot x_\alpha} e^{-i q_{\varphi'_1} \cdot x_1} \ldots e^{-i q_{\varphi''_N} \cdot x_N} e^{i q_{\varphi_1} \cdot x_1} \ldots e^{i q_{\varphi'_N} \cdot x_N} c_S
\]

\[
= A(r) \sum_{S,P,P'} (-1)^{P+P'} \int_{X,k} \frac{k}{4\pi k^2} e^{i k \cdot r} \sum_{\alpha} \delta(q_{\varphi'_1} - q_{\varphi_1}) \ldots \delta(q_{\varphi''_N} - q_{\varphi'_N}) \ldots \delta(q_{\varphi'_N} - q_{\varphi'_N}) c_S
\]  

\[
= \sum_{S,P,P'} (-1)^{P+P'} \sum_{\alpha} \frac{(q_{\varphi'_N} - q_{\varphi_1})}{4\pi (q_{\varphi'_1} - q_{\varphi_1})^2} e^{-i (q_{\varphi'_1} - q_{\varphi_1}) \cdot r} c_S
\]

\[
= \Lambda(r) E_{SS'} c_S
\]

We note that each index $S$ represents $N$ three-dimensional plane waves, and the determination of the matrix elements involves, in particular, sums over all permutations denoted by $P$ and $P'$. In addition, two cutoffs have to be introduced – for the maximum value of $q$, and a resolution for discreteness between two vectors $q$ and $q + \delta q$. These factors determine the size of the problem, and solution of this generalized eigenvalue problem then results in vectors $c_S$, which satisfy the uncertainty relations obtained from commutation between $\hat{p}$ and $\hat{E}(r)$ exactly. Each eigenvector, however, may correspond to a different charge density. Furthermore, linear combinations of these eigenvectors can be used to construct other states that also satisfy this Schwarzian equality. The charge densities from generated by these states, thus provide one way to determine the domain of $v-$representable charge densities[3, 31, 32], as well as candidate charge density distributions $n(r)$ for any external potential $V_{ext}(r)$.

\[\text{VIII. MINIMIZATION CODE AND PRODUCED FEATURES/TABLES}\]

Here, we present several minimization schemes to show the robustness of the derived functional form for the uniform density case, as well as the changes due to additional constraints during parameter-fitting.
A. Minimization 1a

Least-squares fit (matrix-inversion) of QMC data, while constraining $c_1$ and $c_4$ to be the same across all phases. By inverting the relationship:

$$E_{BF} = c_1 + c_4 \frac{1}{r_s^6} + c_{BF} \frac{1}{r_s} + c_{BF}^2 \frac{1}{r_s^2}$$

$$E_{PMF} = c_1 + c_4 \frac{1}{r_s^6} + c_{PMF}^1 \frac{1}{r_s} + c_{PMF}^2 \frac{1}{r_s^2}$$

$$E_{FMF} = c_1 + c_4 \frac{1}{r_s^6} + c_{FMF}^1 \frac{1}{r_s} + c_{FMF}^2 \frac{1}{r_s^2}$$

$$E_{BCC} = c_1 + c_4 \frac{1}{r_s^6} + c_{BCC}^1 \frac{1}{r_s} + c_{BCC}^2 \frac{1}{r_s^2}$$

or

$$E(r_s) = \tilde{A}(r_s)c$$

where in total 25 datapoints from QMC simulations [26] were fitted for 10 coefficients: $c_1, c_4$ fixed for all phases, and $c_2, c_3$ allowed to be different for each phase of matter. The row null-space of $\tilde{A}$ is non-empty: i.e. there exist more than one solution to reasonably fit the data, and is specific to the algorithm used. Fitting parameters using the left-division in MATLAB[33], we obtain the set of parameters:
FIG. 4. Energies predicted from coefficient inversion. Note slightly higher errors for BF and BCC cases.

B. Minimization 1b

One can instead seek to sample different possible values in the neighborhood of \( c \). The Nelder-Mead simplex starts with an \( N \)-dimensional simplex (where \( N \) is the number of coefficients), which expands, contracts, and reflects based on the values of the objective function, increasing the chances of finding a local minimum. Minimization of deviation from QMC data, while holding \( c_1 \) and \( c_4 \) constant, using the Nelder-Mead simplex results in:
FIG. 5. Energies predicted Nelder-Mead simplex minimization of deviation from QMC data. Note slightly higher errors for BF and BCC cases.

C. Minimization 2a

To predict phase diagrams, it is insufficient to predict energies to within $\pm 1.5 \text{ mHa}$. The difference between energies of different phases should also be consistent. In turn, this also reduces error in energy. In particular, we allow all coefficients, $c_1, c_2, c_3, c_4$, for every phase of matter (16 coefficients in total) to change.
Let:

\[ dE_{QMC}(BF - PMF) = E_{QMC}(BF) - E_{QMC}(PMF) \] (67)

\[ dE_{\text{functional}}(BF - PMF) = E_{\text{functional}}(BF) - E_{\text{functional}}(PMF) \] (68)

\[ \Delta E(BF, PMF) = dE_{QMC}(BF - PMF) - dE_{\text{functional}}(BF - PMF) \] (69)

for different pairs of matter. Then, we minimize:

\[ \|E_{QMC} - E_{\text{functional}}\|_2 + \|\Delta E(BF, PMF)\|_2 + \|\Delta E(BF, FMF)\|_2 + \|\Delta E(BF, BCC)\|_2 + \ldots \] (70)

The results of this minimization scheme is presented in the paper.
D. Minimization 2b

We minimize the same objective function and variables as Minimization 2a, but with the added constraint that at $r_s = 50$ and $r_s = 100$, the polarization order of PMF-v-FMF phases agree with the QMC data. This results in:

\[
\begin{array}{cccc}
\text{BF} & -0.0042 & -1.2301 & 0.7784 & -1.8037 \\
\text{PMF} & -0.0039 & -1.2630 & 2.5674 & -0.1264 \\
\text{FMF} & -0.0038 & -1.2890 & 3.4322 & 2.7008 \\
\text{BCC} & -0.0043 & -1.2252 & 2.0066 & 0 \\
\end{array}
\]

TABLE III.
FIG. 6. Energies predicted Nelder-Mead simplex minimization of deviation from QMC data. Note slightly higher errors for BF and BCC cases.

E. Minimization 2c

Finally, we minimize the same objective function, and constraint as Minimization 2b but with a multistart global optimization with 1000 starting points.
TABLE IV. Coefficients obtained via minimization using the Multistart method within MATLAB’s global optimization toolbox[33]. We note that the search for global optimization was ended due to maximum number of iterations, and not because a global optimum was reached.

|   | BF  | PMF  | FMF      | BCC       |
|---|-----|------|----------|-----------|
| BF | -0.0042 | -1.2301 | 0.7784 | -1.8036 |
| PMF| -0.0039 | -1.2630 | 2.5674 | -0.1264 |
| FMF| -0.0038 | -1.2890 | 3.4321 | 2.7011 |
| BCC | -0.0043 | -1.2252 | 2.0065 | 830.4583 |

FIG. 7. Energies predicted using the Multistart fmincon global minimization scheme in MATLAB with 1000 starting points. See code in Supplementary materials.
IX. CONCLUSION

A variety of optimization methods, constraints, and coefficient-degrees of freedom are used to understand and test the robustness of the functional form provided in this work against available data.

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