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Variational Principle for Many-Fermion Systems

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If ψ is a determinantal eigenfunction for the N-fermion Hamiltonian, H, with one- and two-body terms, then $e_0 \leq \langle\psi, H\psi\rangle = E(K)$, where e_0 is the ground-state energy, K is the one-body reduced density matrix of ψ, and $E(K)$ is the well-known expression in terms of direct and exchange energies. If an *arbitrary* one-body K is given, which does not come from a determinantal ψ, then $E \geq e_0$ does not necessarily hold. This Letter proves, however, that if the two-body part of H is positive, then in fact $e_0 \leq e_{\rm HF} \leq E(K)$, where $e_{\rm HF}$ is the Hartree-Fock ground-state energy.

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The variational principle is useful for obtaining accurate upper bounds to the ground-state energy e_0 of an N-particle fermion Hamiltonian, H_N. A normalized wave function ψ_N (or density matrix ρ_N) which *satisfies* the Pauli principle is required; then $e_0 \leq e(\rho_N) \equiv \mathrm{Tr}\rho_N H_N$ (with $\rho_N = |\psi_N\rangle \times \langle\psi_N|$ being a pure state in the wave-function case). In practice, however, it is often possible to make a good guess for ρ_N^1, the reduced single-particle density matrix, but the evaluation of $e(\rho_N)$ is complicated by the reconstruction problem for ρ_N: To evaluate $e(\rho_N)$ we first have to know ρ_N. In the simplest case ρ_N^1 is an N-dimensional projection and ρ_N is a pure state, with ψ_N being a determinantal, or Hartree-Fock (HF) function. Otherwise, ρ_N is a very complicated (and, in general, a nonunique) function of ρ_N^1, and the calculation of $e(\rho_N)$ can be extremely difficult because of the "orthogonality problem." For this reason most variational calculations do not depart very far from a HF calculation.

It is the purpose of this note to show that under a positivity condition on the two-body part of H_N (which, fortunately, holds for one case of major interest—the Coulomb potential) it is possible to obtain an upper bound to e_0 which involves only ρ_N^1; *the reconstruction problem is eliminated.* In the HF case, this bound agrees with $e(\rho_N)$. Moreover, our bound, E, satisfies $E \geq e_{\rm HF}$, where $e_{\rm HF}$ is the *lowest* HF energy. While our bound is thus not superior to the best HF bound, it may be superior in practice because the exact HF orbitals are unknown in general. A possible application might occur in the theory of itinerant ferromagnetism.

Let us make some definitions. Let $z = (x, \sigma)$ denote a single-particle space-spin variable and $\int dz \equiv \sum_\sigma \int dx$. A *single*-particle operator $K(z;z')$ is called *admissible* if it is positive semidefinite and

$$\mathrm{Tr}K = N,\ K \leq I,\ \text{i.e.,}$$

$$\langle\psi, K\psi\rangle \leq \langle\psi,\psi\rangle \text{ for all } \psi. \tag{1}$$

Given ρ_N satisfying the Pauli prinicple,

$$\rho_N^1(z;z') \equiv N\int \rho_N(z, z_2, \ldots, z_N; z', z_2, \ldots, z_N) \times dz_2 \cdots dz_N. \tag{2}$$

Any such ρ_N^1 is admissible. Conversely, given an admissible K there is always at least one ρ_N with $\rho_N^1 = K$. In the HF case $\rho_N = |\psi_N\rangle\langle\psi_N|$ and

$$\psi_N = (N!)^{-1/2} \det[f_i(z_j)],$$
$$\rho_N^1(z;z') = \sum_{j=1}^N f_j(z) f_j^*(z') c_j, \tag{3}$$

with $f_1, \ldots, f_N$ being any N orthonormal functions.

Consider now Hamiltonians of the form

$$H_N = \sum_{j=1}^{N} h_j + \sum_{1\le i<j\le N} v_{ij}, \tag{4}$$

where h and v are self-adjoint operators. v is the two-body part and h is the one-body part [usually $-(h^2/2m)\Delta + U(z)$]. Our method has obvious extensions to higher than two-body interactions, but for brevity only (4) will be considered. Normally v is diagonal [a local potential, such that $v_{ij} = v(z_i, z_j)$], but this is not necessary. *If* ρ_N is of the HF type, then ρ_N^2, defined analogously to (2), satisfies $\rho_N^2 = K_2$, where

$$K_2(z,w;z',w') \equiv K(z;z')K(w;w') - K(z;w')K(w;z'), \tag{5}$$

with $K = \rho_N^1$. In this HF case $e(\rho_N) = E(K)$, where

$$E(K) \equiv \mathrm{Tr}(Kh) + \tfrac{1}{2}\mathrm{Tr}(K_2 v) \tag{6}$$

and

$$\mathrm{Tr}(K_2 v) = \iint v(z,w)K_2(z,w;z,w)dz\,dw \tag{7}$$

in the diagonal case. This formula is well known. For *any* admissible K, (5) and (6) *define* $E(K)$.

The problem addressed here is the following: Given an arbitrary, admissible K, does a ρ_N exist such that $\rho_N^1 = K$ and $e(\rho_N) \le E(K)$? If $v \ge 0$, the answer is yes! Note, however, that $\mathrm{Tr}\rho_N^2 = N(N-1)$ but that $\mathrm{Tr}K_2 = (\mathrm{Tr}K)^2 - \mathrm{Tr}K^2$, and this is $N(N-1)$ if and only if K is an N-dimensional projection as in (3). Otherwise, $\mathrm{Tr}K_2 > N(N-1)$. Therefore the ρ_N which I wish to construct cannot simply satisfy $\rho_N^2 = K_2$. The solution must be more complicated than that.

Our main result is stated as follows:

Theorem.—Let v be positive semidefinite [i.e., in the diagonal case, $v(z,w) \ge 0$ for all z, w], and let K be any admissible single-particle operator. Then (i) there exists a density matrix ρ_N satisfying the Pauli principle such that $\rho_N^1 = K$ and

$$e_0 \le e(\rho_N) \le E(K); \tag{8}$$

(ii) there exists a normalized determinantal function ψ_N such that

$$e_0 \le \langle \psi_N,\, H_N \psi_N\rangle \le e(\rho_N) \le E(K). \tag{9}$$

Note that in (ii) it is not claimed that if $\tilde\rho_N \equiv |\psi_N\rangle\langle\psi_N|$ then $\tilde\rho_N^1 = K$. However, (9) does say that, among all admissible K, an HF-type K [N-dimensional projection (3)] gives the lowest value of $E(K)$. The proof requires the following:

Lemma.—Let $c_1 \ge c_2 \ge \cdots$ be an infinite sequence with $0 \le c_i \le 1$ and $\sum_1^\infty c_i = N$, where N is an integer. Then there exist N orthonormal vectors $V^1, \ldots, V^N$ in L^2 such that $\sum_{i=1}^N |V_j^i|^2 = c_j$.

Proof: Induction on N is used. For $N=1$, choose $V_j^1 = c_j^{1/2}$. Assume that the lemma holds for $N = n-1$; the lemma will first be proved for n under the assumption that $c_j = 0$ for $j \ge 2n$. Define $d_j \equiv 1 - c_j$ $(1 \le j < 2n)$, and $d_j = 0$ $(j \ge 2n)$. The d_j satisfy the hypothesis for $n-1$, so that there exist orthonormal $W^1, \ldots, W^n$ with $\sum_{i=1}^{n-1}|W_j^i|^2 = d_j$. Let $v^1, \ldots, v^n$ be n orthonormal, $(2n-1)$-dimensional vectors which are orthogonal to $W^1, \ldots, W^{n-1}$ [thought of as $(2n-1)$-dimensional vectors]. Then the n vectors $V_j^i = v_j^i$ $(1 \le j < 2n)$ [$V_j^i = 0$ $(j \ge 2n)$] satisfy the lemma. Next, suppose $c_j = 0$ for $j \ge J$. I use induction on J starting with $J = 2n$. Note that $c_{l-1} + c_l \le 1$ when $l \ge 2n$. For $J+1$, apply the lemma (with n and J) to the sequence $b_j = c_j$ $(1 \le j < J-1)$, $b_{J-1} = c_{J-1} + c_J$, and $b_j = 0$ $(j \ge J)$. This sequence may not be decreasing, but that is irrelevant. Let $W^1, \ldots, W^n$ be the orthonormal vectors. The required vectors, V^i, for $J+1$, are given by $V_j^i = W_j^i$ $(1 \le j < J-1)$, $V_{J-1}^i = W_{J-1}^i (c_{J-1}/b_{J-1})^{1/2}$, $V_J^i = W_{J-1}^i (c_J/b_{J-1})^{1/2}$, $V_j^i = 0$ $(j > J)$. Finally, if $c_j > 0$ for all j, choose L so that $b_L \equiv \sum_{j=L}^\infty c_j \le 1$. Then apply the lemma to the finite sequence of length L: $b_j = c_j$ $(1 \le j < L)$, b_L. If $W^1, \ldots, W^n$ are the orthonormal vectors, let $V_j^i = W_j^i$ $(1 \le j < L)$, $V_j^i = W_L^i (c_j/b_L)^{1/2}$ for $j \ge L$. Q.E.D.

Proof of Theorem: Write $K(z;z') = \sum_{j=1}^\infty c_j f_j(z) \times f_j(z')^*$, where the f_j are the orthonormal eigenfunctions of K ("natural orbitals") and the eigenvalues of K, c_j, satisfy the hypothesis of the lemma. Let $V^1, \ldots, V^N$ be the vectors used in the lemma and let $\theta = \{\theta_1, \theta_2, \ldots\}$ be any infinite sequence of reals. The N functions $F_k^\theta(z) = \sum_{j=1}^\infty e^{i\theta_j} V_j^k f_j(z)$ are orthonormal for any θ. Let $\rho_N^\theta = |\psi_N^\theta\rangle\langle\psi_N^\theta|$, where $\psi_N^\theta(z_1, \ldots, z_N) = (N!)^{-1/2}\det[F_k^\theta(z_j)]$. Let $\langle\cdots\rangle_\theta$ denote the average {over $[0, 2\pi) \in Z_+$} with respect to all the θ_j. (Formally, this requires infinitely many integrations $\int_0^{2\pi} d\theta_j/2\pi$, but one can easily make sense of this by taking suitable limits.) It is easy to check, with use of the property of the V^i, that $\rho_N = \langle\rho_N^\theta\rangle_\theta$ satisfies $\rho_N^1 = \langle\rho_N^{\theta,1}\rangle_\theta = K$. Now $\rho_N^2 \ne K_2$, as stated before, but $\rho_N^2 = \langle\rho_N^{\theta,2}\rangle_\theta = K_2 - L_2$, with

$$2L_2(z,w;z',w') = \sum_{a,b=1}^{\infty} W_{ab}[f_a(z)f_b(w) - f_b(z)f_a(w)][f_a^*(z')f_b^*(w') - f_b^*(z')f_a^*(w')]$$

and $W_{ab} = |\sum_{i=1}^{N} V_a{}^i V_b{}^{i*}|^2 \geq 0$. Thus, $e(\rho_N) = E(K) - D$, with $2D = \mathrm{Tr}(L_2 v)$. But clearly L_2 is positive semidefinite, so that $D \geq 0$. This proves (i). To prove (ii), note that $E(K) \geq e(\rho_N) = \langle G^\theta \rangle_\theta$, where $G^\theta = \langle \psi_N{}^\theta, H_N \psi_N{}^\theta \rangle$ is real for each θ. Hence, for some θ, $G^\theta \leq e(\rho_N)$. Q.E.D.

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Note added.—After reading this manuscript, Professor M. B. Ruskai kindly pointed out that the lemma is essentially a consequence of Horn's theorem[1]: Let $y_1 \geq y_2 \geq \cdots \geq y_M$ and $x_1 \geq x_2 \geq \cdots \geq x_M$ be two sets of reals. Then there exists an $M \times M$ hermitean matrix B with eigenvalues $\{x_i\}$ and diagonal elements $B_{ii} = y_i$ if and only if $\sum_{i=1}^{t}(x_i - y_i) \geq 0$ for all $1 \leq t \leq M$, and with equality for $t = M$. The existence of B is equivalent to $y_j = \sum_{i=1}^{M} |U_{ij}|^2 x_i$ for some unitary U. To apply this to the lemma, suppose that $c_j = 0$ for $j > M \geq N$ and take $y_j = c_j$ (for $j \leq M$) and $x_1 = x_2 = \cdots = x_N = 1$, and $x_j = 0$ for $j > N$. The required orthonormal vectors V^i are then $V_j{}^i = U_{ij}$ for $j \leq M$ and $V_j{}^i = 0$ for $j > M$. Finally, if $c_j > 0$ for all j, then an argument such as that given at the end of the proof of the lemma, or something similar, must be used.

[1]A. Horn, Am. J. Math. 76, 620 (1954).

Validity of Scaling to 10^{20} eV and High-Energy Cosmic-Ray Composition

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It is shown that evidence on cosmic-ray showers of energy 3×10^{16} to 10^{20} eV indicates that scaling in the fragmentation region is valid up to the highest energies if (and only if) hadron-air inelastic cross sections continue to rise in the manner observed at lower energies. It is also shown, with use of additional air-shower evidence, that $\langle \ln A \rangle$, the logarithmic mean primary mass number, changes from (4 ± 2) at 1.6×10^{15} eV to $(0^{+0.6}_{-0})$ at and above 3×10^{16} eV.

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Information about some features of nuclear interactions beyond 10^{12} eV can be obtained by the study of high-energy cosmic rays. Beyond 10^{14} eV these studies depend on observations of extensive air showers. Such observations, while not suited for the study of details, are capable of giving information about broad features. In particular, they can be used to test the validity of scaling in the fragmentation region. In this Letter we examine data on the depth of maximum development (X_m) of large air showers as a function of energy (E). The variation of X_m is related to the multiplicity law for the production of high-energy secondaries by the elongation-rate (ER) theorem.[1] By using this relation we show that one of the important predictions of scaling, namely that the multiplicity of high-energy secondaries is asymptotically energy independent,[2] is supported by air-shower evidence up to the highest observed energies, provided that hadron-air interaction cross sections continue to rise in the manner observed at lower energies.

In our analysis we have intentionally disregarded measurements of X_m by Thornton and Clay,[3] as their data have been challenged by Orford and Turver[4] on a number of grounds. We find, however, that the remaining evidence supports their conclusion as to a change in primary composition from heavy to light nuclei between $\sim 10^{15}$ and 3×10^{16} eV.[3] This conclusion is especially interesting astrophysically because it is well established that the cosmic-ray spectrum between 2×10^{15} and 10^{17} eV is significantly steeper than at lower energies,[5] and there is evidence from a variety of experiments that the amplitude of cosmic-ray anisotropy increases rapidly with energy in the same region.[6]

We discuss the data on X_m in terms of D_e, the so-called "elongation rate," equal by definition to $dX_m/d\ln E$. X_m is averaged over fluctuations in shower development, and in case of mixed primary composition over the equal-energy mass spectrum. For numerical results we use "ER per decade," defined similarly in terms of $\log_{10}E$

