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A LOWER ENERGY BOUND FOR N-PARTICLES QUANTUM SYSTEMS

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Abstract. It has been shown that the ground state energy E_o of a quantum system of N identical fermi particles satisfies inequality

$$E_o \geqslant \frac{1}{N-n} \sum_{i}^{N-n} \mathcal{E}_i \quad , \tag{1}$$

where n=1,2,...,N-1 and $\mathcal{E}_i$ are the eigenvalues of "n+1 - body Hamiltonian". The summation is performed over the first N-n states.

A generalized lower bound on E_o

The studies of the energy bounds always imply a generele importance. Let us suppose that Hamiltonian of the N-particles homogeneous system reads

$$H = \sum_{n}^{N} p_i^2/2m + \sum_{i<j}^{N} V_{ij}(r_{ij}) \quad , \tag{2}$$

V_{ij} is the pair potential (we do not write spin-coordinates explicitly) and $\vec{r}(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N)$ is a set of coordinates. In "the centre of mass" of kinetic energy ($\sum_i \vec{p}_i = 0$) Hamiltonian becomes

$$H = \sum_{i<j}^{N} (\vec{p}_i - \vec{p}_j)^2/2mN + \sum_{i<j}^{N} V_{ij} \ . \tag{3}$$

Let us now introduce a new set of $\vec{\rho}(\vec{\rho}_1,\vec{\rho}_2,\ldots,\vec{\rho}_N)$ coordinates using the transformation

$$\vec{\rho} = B\,\vec{r} \ . \tag{4}$$

The matrix B is real, nonsingular and enables us to separate the coordinate $\vec{\rho}_1$ of the centre of mass. If $\tilde{B}^{-1}$ is the inverse of the transpose of B, then new momenta are

$$\vec{\pi} = \tilde{B}^{-1}\,\vec{p} \ , \tag{5}$$

where $\vec{\pi}_i = -i\hbar \nabla_{\vec{\rho}_i}$.

For any trial, normalized and antisymmetric (in the particle indices 1,2,...,N) function $\chi(\vec{\rho}_2,\vec{\rho}_3,\ldots,\vec{\rho}_N)$ we have

$$\langle \chi | H | \chi \rangle = \langle \chi | \mathcal{H} | \chi \rangle$$

$$= \langle \chi | \nu^{-1} \sum_{j=2}^{m} \sum_{i=1}^{j-1} H_{ij} | \chi \rangle , \tag{6}$$

where

$$H_{ij} = \frac{1}{4\, m}(\vec{p}_i^{\,2} + \vec{p}_j^{\,2} - 2\vec{p}_i\vec{p}_j) + \frac{1}{2}N(N-1)V_{ij}$$

$$\nu = \frac{m(m-1)}{2} \quad , \qquad m=2,3,\ldots,N \; .$$

Let us suppose that after introducing new coordinates $\vec{\rho}$ and momenta $\vec{\pi}$, Hamiltonian is transformed into

$$\mathcal{H} \longrightarrow \mathcal{H}(\vec{\rho}_2,\ldots,\vec{\rho}_{n+1})$$

with n=1,2,...,N-1, and that we know to solve the eigenvalue problem

$$\mathcal{H}(\vec{\rho}_2,\ldots,\vec{\rho}_{n+1})\,\phi_i(\vec{\rho}_2,\ldots,\vec{\rho}_{n+1}) = \varepsilon_i\,\phi_i(\vec{\rho}_2,\ldots,\vec{\rho}_{n+1}) \tag{7}$$

In order to obtain the lower bound on the energy E_0, let us expand the unknown, ground state function $\psi_0(\vec{\rho}_2,\ldots,\vec{\rho}_N)$ in terms of the normalized eigenstates $\phi_i(\vec{\rho}_2,\ldots,\vec{\rho}_{n+1})$

$$\psi_0(\vec{\rho}_2,\ldots,\vec{\rho}_N) = \sum_i C_i\,\phi_i(\vec{\rho}_2,\ldots,\vec{\rho}_{n+1})\,\psi_i(\vec{\rho}_{n+2},\ldots,\vec{\rho}_N) \; , \tag{8}$$

where C_i are constant coefficientes and ψ_i antisymmetric functions in the individual partisle indices n+2, n+3,...,N, i.e.

$$A(n+2,n+3,\ldots,N)\,\psi_i(\vec{\rho}_{n+2},\ldots,\vec{\rho}_N) = \psi_i(\vec{\rho}_{n+2},\ldots,\vec{\rho}_N) \; ;$$

the operator A is antisymmetrizer. By supposition ψ_0 is antisymmetric and normalized

$$A(1,2,\dots,N)\psi_o = \psi_o$$

$$\langle \psi_o | \psi_o \rangle = \sum_i |C_i|^2 = 1. \tag{9}$$

For the energy of the ground state we have

$$E_o = \langle \psi_o | H | \psi_o \rangle = \langle \psi_o | \mathcal{H} | \psi_o \rangle$$
$$= \sum_i |C_i|^2 \, \mathcal{E}_i \;. \tag{10}$$

An inequality for the coefficients C_i can be obtained using Schwartz inequality, hermiticity, projection property and decomposition of A

$$A(n+1,n+2,\dots,N) = \frac{1}{N-n}\,(1-P_{n+1,n+2}-\dots-P_{n+1,N})A(n+2,\dots,N),$$

where P_{ij} is the exchange operator in the individual particle indices i and j. Namely,

$$|C_i|^2 = |\langle \phi_i \, \psi_i | \psi_o \rangle|^2 = |\langle \phi_i \, \psi_i | A(n+1,\dots N)\, \psi_o \rangle|^2$$
$$= |\langle A(n+1,\dots,N)\phi_i \psi_i \,|\, \psi_o \rangle|^2$$
$$\leq \langle A(n+1,\dots,N)\phi_i \psi_i \,|\, A(n+1,\dots,N)\phi_i \psi_i \rangle$$
$$\leq \frac{1}{N-n} \langle \phi_i \psi_i \,|\, (1 - P_{n+1,n+2} - \dots - P_{n+1,n+2}) *$$
$$* \, \phi_i \psi_i \rangle$$

$$\leq \frac{1}{N-n} \left\{ 1 - \left[N - (n+1) \right] \delta \right\}, \tag{11}$$

where

$$\delta = \int \phi_i^*(\vec{\rho}_2,\ldots,\vec{\rho}_{n+1})\,\psi_i^*(\vec{\rho}_{n+2},\ldots,\vec{\rho}_N)\; P_{n+1,n+2}$$

$$\phi_i(\vec{\rho}_2,\ldots,\vec{\rho}_{n+1})\,\psi_i(\vec{\rho}_{n+2},\ldots,\vec{\rho}_N)\; d\vec{\rho}_2 d\vec{\rho}_3\ldots d\vec{\rho}_N \quad . \tag{12}$$

Let us show that δ is nonnegative for a transformation (4) that satisfies

$$P_{n+1,n+2}\vec{\rho}_{n+1} = \vec{\rho}_{n+2}\,, \quad P_{n+1,n+2}\vec{\rho}_{n+2} = \vec{\rho}_{n+1}$$
$$P_{n+1,n+2}\vec{\rho}_i = \vec{\rho}_i\,, \quad (i \neq n+1,\ n+2)\,. \tag{13}$$

Now for δ we find

$$\delta = \int\cdots\int \left\{\int \phi_i^*(\vec{\rho}_2,\ldots,\vec{\rho}_{n+1})\,\psi_i(\vec{\rho}_{n+1},\vec{\rho}_{n+3},\ldots,\vec{\rho}_N)d\vec{\rho}_{n+1}\right\}\cdot$$
$$\cdot\left\{\int \phi_i(\vec{\rho}_2,\ldots,\vec{\rho}_n,\vec{\rho}_{n+2})\,\psi_i^*(\vec{\rho}_{n+2},\vec{\rho}_{n+3},\ldots,\vec{\rho}_N)d\vec{\rho}_{n+2}\right\} d\vec{\rho}_2\ldots$$
$$d\vec{\rho}_n d\vec{\rho}_{n+3}\ldots d\vec{\rho}_N \quad \geqslant\ 0\,.$$

Hence, from the relation (12) we derive

$$|c_i|^2 \leq \frac{1}{N-n} \quad . \tag{14}$$

Combining this equation with (9) and (10) we have

$$E_o \geqslant \frac{1}{N-n}\sum_{i=1}^{N-n}\mathcal{E}_i \,, \tag{15}$$

where the summation is taken over the first N-n energies of the n+1 - body fictitious Hamiltonian (7).

Let us notice that the relation (15) for n=1 /1/ describes 2-body Jastrow correlations, for n=2 triplet correlations, while with n=N-1 we come back to the original N-body problem as well.

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