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LETTER TO THE EDITOR

V-representability in finite-dimensional spaces

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Abstract. In finite dimensions every strictly positive boson density is V-representable.

Let $H(V)=H(0)+V$ be a Hamiltonian with external potential V. Hohenberg and Kohn (1964) proved that for fixed $H(0)$ every one-particle density is the ground-state density of at most one Hamiltonian $H(V)$. (Their restriction to non-degenerate ground states is not necessary, cf Englisch and Englisch (1982).) Their energy functional defined with the help of this uniqueness theorem leads to the problem of whether every density is V-representable, i.e. whether every density describes the ground state of some Hamiltonian $H(V)$. For infinite-dimensional state spaces this question has been answered in the negative by Englisch and Englisch (1982) (and in the special case of pure-state-V-representability by Lieb (1982) and Levy (1982)). Thus the value of the functionals by Levy (1979) and by Lieb (1982) which do not require the V-representability of densities is obvious.

The first application of one of these functionals can be found in Zumbach and Maschke (1983), who present a general method for the calculation of its upper bounds (not, as was asserted in their abstract and in ch IV, a method for its '—in principle—exact calculation').

Epstein and Rosenthal (1978) have shown for systems consisting of one particle with two- and three-dimensional state spaces that every strictly positive density is V-representable. Englisch and Englisch (1983) extended this result to one particle with arbitrary finite-dimensional state spaces. Now the question arises of whether this V-representability is preserved in systems with more than one particle. In the following we show that even for systems of interacting bosons with finite-dimensional state spaces every strictly positive density is V-representable.

Let us consider a system of n bosons where every particle has the state space R^m. The Hamiltonian of this system

$$H(V)=T+U+V \tag{1}$$

acts in the space R^{m^n}. The kinetic part T is given by the sum of discrete Laplacians, one for each particle (i.e. the off-diagonal matrix elements are not positive). We suppose that T has no generalised diagonal form, i.e. there is no subset $A\subset\{1,\ldots,m\}=M$ with $A\neq M$ and $A\neq\varnothing$ for which T maps the subspace $\{\psi|\psi(r_1,\ldots,r_n)=0$ if there is an index i with $r_i\in A\}$ into itself. As usual r_i denotes the (discrete) position of the ith particle. The external potential V and the matrix U describing the interaction between the particles are diagonal matrices. We normalise the external potential by

$$\min_r V(r) = 0. \tag{2}$$

Let the Hamiltonian be symmetric with respect to an interchange of the particles. Then the one-particle density for any symmetric normalised wavefunction ψ is defined by

$$\rho(r) = \sum_{r_2=1}^{m} \dots \sum_{r_n=1}^{m} n\psi^2(r, r_2, \dots, r_n). \tag{3}$$

Let ρ^V denote the density corresponding to the normalised ground state ψ^V (with eigenvalue E^V) of $H(V)$.

The classical results of Stieltjes (1887) and Perron (1907) ensure (cf Englisch and Englisch 1983) that ψ^V is non-degenerate and can be chosen strictly positive. Therefore ρ^V can be identified with a point of the interior of the simplex

$$S_m = \{\rho(1), \dots, \rho(m) | 0 \leq \rho(i) \leq n, \sum \rho(i) = n\}. \tag{4}$$

From the non-degeneracy it follows by theorem 11.8 in Reed and Simon (1978) that ψ^V depends analytically on V. Thus the transformation

$$V \to \rho^V \tag{5}$$

is analytic. Now the uniqueness of the ground state and the Hohenberg–Kohn theorem yield that (5) is a one-to-one map into the interior of S_m. But to prove the V-representability of all strictly positive densities it is necessary to show that (5) maps the potentials *onto* the interior of S_m. For this we need the crucial inequality

$$\psi^V(r_1, \dots, r_n) \leq 2\|H(0)\| \Big/ \sum_{i=1}^{n} V(r_i) \tag{6}$$

where $\|H(0)\|$ is for self-adjoint operators

$$\|H(0)\| = \max_{\|\psi\|=1} |\langle\psi, H(0)\psi\rangle|. \tag{7}$$

For the proof of (6) we assume without loss of generality $V(1) = 0$. We find a function $\bar{\psi}$, namely $\bar{\psi}(r_1, \dots, r_n) = \delta_{1r_1} \dots \delta_{1r_n}$, for which it holds that

$$\langle\bar{\psi}, H(V)\bar{\psi}\rangle = \langle\bar{\psi}, H(0)\bar{\psi}\rangle. \tag{8}$$

Then the Ritz principle, (7) and (8) yield

$$E^V \leq \langle\bar{\psi}, H(V)\bar{\psi}\rangle = \langle\bar{\psi}, H(0)\bar{\psi}\rangle \leq \|H(0)\|. \tag{9}$$

Let us assume that (6) is violated for some ψ^V, i.e. it must have at least one component $\psi^V(s_1, \dots, s_n)$ such that

$$\sum_{i=1}^{n} V(r_i)\psi^V(s_1, \dots, s_n) \geq 2\|H(0)\|. \tag{10}$$

Due to

$$(H(0)\psi)(s_1, \dots, s_n) \geq -\|H(0)\psi\| \geq -\|H(0)\| \tag{11}$$

the eigenvalue equation yields

$$E^V \geq \left(\sum_{i=1}^{n} V(r_i)\psi^V(s_1, \dots, s_n) - \|H(0)\|\right) \Big/ \psi^V(s_1, \dots, s_n). \tag{12}$$

Putting (10) into (12) we get

$$E^V \geq \|H(0)\|/\psi^V(s_1, \ldots, s_n) \geq \|H(0)\|, \tag{13}$$

since $\|\psi^V\| = 1$ implies $\psi^V(s_1, \ldots, s_n) \leq 1$. But (13) contradicts (9), i.e. the inequality (6) must always be valid.

Let us assume that some strictly positive density ρ_0 is not V-representable. We put

$$\min_r \rho_0(r) = c. \tag{14}$$

We denote by $\mathcal{V}^c$ the set of potentials for which there is at least one position r such that

$$V(r) = 2\|H(0)\|(nm^{n-1}/c)^{1/2} \tag{15}$$

and no $V(r)$ is larger than the right-hand side of (15). (The assumption $V(1) = 0$ is no longer made.) Due to (6) the corresponding ρ^V satisfies

$$\rho^V(r) = \sum_{r_2=1}^{m} \ldots \sum_{r_n=1}^{m} n\psi^2(r, r_2, \ldots, r_n) \leq nm^{n-1}(2\|H(0)\|/V(r))^2 = c, \tag{16}$$

i.e. every such ρ^V is less (or equally) far away from the boundary of S_m than ρ_0. A repeated utilisation of the continuity of the map (5) for increasing dimensions of the boundary surfaces of $\mathcal{V}^c$ from 0 to $m-1$ (i.e. for decreasing numbers from $m-1$ to 0 of positions r for which (15) is satisfied) shows that all densities ρ with $\min_r \rho(r) \geq c$ occur in the image of the map $V \to \rho^V$. Therefore the assumption that some strictly positive density is not V-representable must be false.

The analogous conjecture for fermions (with spin degeneracy 2) reads: every strictly positive density ρ with $\rho(r) < 2$, $r = 1, \ldots, m$, is $E - V$-representable, i.e. $\rho = \Sigma\, \lambda_i^2 \rho^{\psi_i}$, where ψ_i are (degenerate) ground states of the same Hamiltonian $H(V)$ and $\Sigma\, \lambda_i^2 = 1$. (ρ^{ψ_i} corresponds to ρ^V as defined below (3).)

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