

**$v$ -representability of one-body density matrices**

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We consider low-dimensional model systems with a fixed two-body interaction and a variable (nonlocal) one-body potential. It is shown explicitly that an extended domain of allowed ( $N$ -representable) one-body density matrices cannot be generated in this way, the excluded domain depending on the two-body interaction under consideration. This stands in contrast to the behavior of the diagonal part of the density matrix.

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Density-functional theory (DFT) enjoys great success as a practical way of incorporating complex many-body correlations into a manageable computational framework, in particular, for electronic systems [1,2]. Its theoretical foundation as an (in principle) exact description of an interacting system relies on the Hohenberg-Kohn theorems [3], which state that for systems with a fixed two-body interaction and a variable local potential  $v(x)$  the local density  $\rho(x)$  is sufficient to characterize the system completely. As a consequence the ground-state energy is a functional of the local density.

Over the years, there has also been interest in developing density-matrix functional theories (DMFT) [4–8], where instead of the local (diagonal) density  $\rho(x) \equiv \rho(x,x)$  the full one-body density matrix (OBDM) of the ground state  $\Psi_0$ ,

$$\rho(x,x') = \langle \Psi_0 | c^\dagger(x') c(x) | \Psi_0 \rangle, \quad (1)$$

is taken as the central quantity. This would offer significant advantages compared to traditional DFT, because the kinetic energy, as well as the important exchange component of the electronic interaction energy, are completely known functionals of the OBDM. Recently an explicit parameter-free DMFT model was proposed [9] and demonstrated to yield remarkably good results for a test series of small atoms. As shown in [10], however, the functional form proposed in [9] does not obey some rigorous constraints imposed by the properties of a homogeneous electron gas.

In the case of DMFT one has to consider systems with a fixed two-body interaction and a variable one-body potential  $v(x,x')$  that is now, however, allowed to be nonlocal. A given matrix  $\rho(x,x')$  is called  $N$  representable if it corresponds to the OBDM of some properly antisymmetrized  $N$ -fermion wave function. It is called  $v$  representable if, in addition, it corresponds to the OBDM of the ground state of a system interacting with the two-body potential under consideration and subject to some one-body potential  $v(x,x')$ .

Similar definitions are applied to the  $N$  representability and  $v$  representability of the local density, though in general, and apart from a few special cases [1,2], almost any reasonable (normalized, non-negative) local density is both  $N$  representable and  $v$  representable.

In this paper we want to draw attention to the fact that the difference between  $v$  representability and  $N$  representability is much more acute for the OBDM than it is for the local density. The  $N$ -representability conditions for the OBDM are well known [1,2]: the eigenvalues of the OBDM for a fermi-

onic system should be in the interval  $[0,1]$ . We will show with explicit numerical examples that the conditions for  $v$  representability depend in a nontrivial way on the (fixed) two-body interaction under consideration, and that it is impossible to generate every  $N$ -representable OBDM by tuning the one-body potential. This statement is, of course, obvious in the special case when the two-body interaction is absent (because the OBDM is then necessarily idempotent), but it still holds in the presence of a genuine two-body interaction.

In order to prove this we need a model for an interacting fermion system where it is still possible to scan all possible one-body potentials and construct the corresponding OBDM. The simplest such case is for two fermions in a discrete Fock space generated by four single-particle states. Even then it takes 16 independent real parameters to characterize a general Hermitian one-body potential, but this number can be reduced by imposing symmetry requirements.

We impose spherical symmetry and first consider two spin- $\frac{1}{2}$  fermions that can occupy two different  $s$  orbitals. The available single-particle states are created by the operators  $c_{im}^\dagger$ , where  $i=1,2$  distinguishes the orbital and  $m=-\frac{1}{2}, \frac{1}{2}$  is the spin projection. A general (rotationally invariant and Hermitian) one-body potential  $\hat{v}$  can then, apart from an unimportant additive constant, be written in second quantization as

$$\hat{v} = \sum_m [-\epsilon c_{1m}^\dagger c_{1m} + \epsilon c_{2m}^\dagger c_{2m} + \Delta (c_{1m}^\dagger c_{2m} + c_{2m}^\dagger c_{1m})], \quad (2)$$

and requires only two independent real parameters  $\epsilon$ ,  $\Delta$ , which can easily be varied numerically.

The two-fermion subspace with total angular momentum  $J=0$  is spanned by the three orthonormal states  $|\Phi_1\rangle = 1/\sqrt{2}[c_1^\dagger \otimes c_1^\dagger]|0\rangle$ ,  $|\Phi_2\rangle = 1/\sqrt{2}[c_2^\dagger \otimes c_2^\dagger]|0\rangle$ ,  $|\Phi_3\rangle = [c_1^\dagger \otimes c_2^\dagger]|0\rangle$ . The matrix elements of  $\hat{v}$  in this basis are given by  $\langle \Phi_i | \hat{v} | \Phi_j \rangle = -2\epsilon \delta_{ij} (\delta_{i1} - \delta_{i2}) + \sqrt{2}\Delta (1 - \delta_{ij}) (\delta_{i3} + \delta_{j3})$ . A general (rotationally invariant and Hermitian) two-body interaction  $\hat{W}$  is completely determined by its six matrix elements in this basis,  $W_{ij} = \langle \Phi_i | \hat{W} | \Phi_j \rangle$ , with  $i \leq j = 1, 2, 3$ .

For a fixed choice of the  $W_{ij}$  we vary  $\epsilon$  and  $\Delta$  independently over the interval  $[-\infty, +\infty]$ . For each value of  $\epsilon$  and  $\Delta$  the ground state  $|\Psi_0\rangle$  of the total Hamiltonian  $\hat{v} + \hat{W}$  was constructed. The corresponding OBDM is a  $2 \times 2$  matrix,

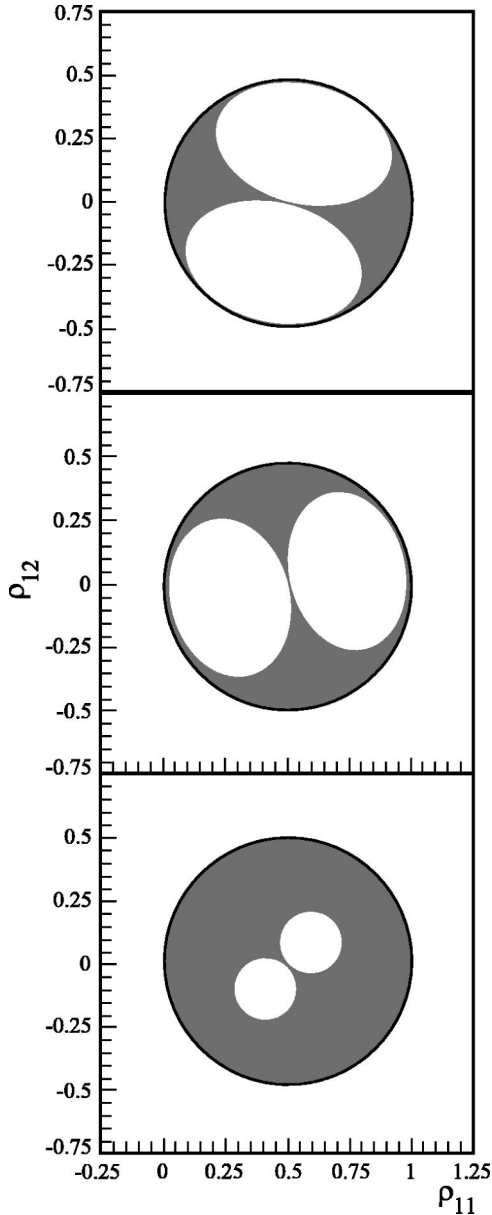


FIG. 1. Domain of  $v$ -representable one-body density matrices, obtained in the model of two fermions in two  $j = \frac{1}{2}$  levels, for a few choices of the two-body interaction  $\hat{W}$ :  $(W_{11}, W_{12}, W_{13}, W_{22}, W_{23}, W_{33}) = (0, 1, 0.5, 0, -0.5, 2)$  (upper panel);  $(0, 0.5, 0.25, 0, -0.25, -2)$  (middle panel);  $(0, 1, 0.05, 0, -0.05, -1)$  (lower panel).

$$\rho_{ij} = \langle \Psi_0 | c_{im}^\dagger c_{jm} | \Psi_0 \rangle, \quad i, j = 1, 2, \quad (3)$$

which can be unambiguously represented by a point in the  $(\rho_{11}, \rho_{12})$  plane, since  $\rho_{12} = \rho_{21}$  and  $\rho_{22} = 1 - \rho_{11}$ . As  $\epsilon$  and  $\Delta$  are varied, these points fill up an area in the  $(\rho_{11}, \rho_{12})$  plane. We have plotted these areas, for a few choices of  $\hat{W}$ , in Fig. 1.

The disk  $(\rho_{11} - \frac{1}{2})^2 + \rho_{12}^2 \leq \frac{1}{4}$  represents the domain of all  $N$ -representable OBDM's, since this condition guarantees that both eigenvalues of  $\rho_{ij}$  lie in the interval  $[0, 1]$ . The edge of the disk corresponds to idempotent matrices, i.e., to the OBDM of a noninteracting system. In our case this can al-

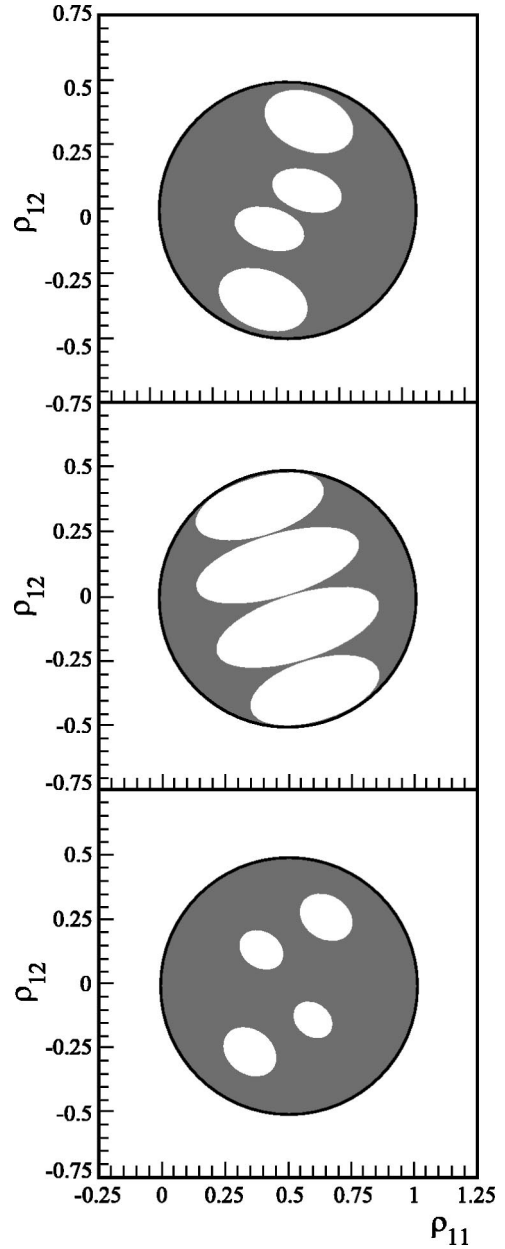


FIG. 2. Domain of  $v$ -representable one-body density matrices, obtained in the model of four fermions in two  $j = \frac{3}{2}$  levels, for a few random choices of the two-body interaction  $\hat{W}$ .

ways be reached in the limit  $\epsilon \rightarrow \infty$  or  $\Delta \rightarrow \infty$ , which is equivalent to having a vanishingly small two-body interaction. More interesting is the presence of two holes in the disk, the position of which depends on  $\hat{W}$ , and which represent regions that cannot be reached by any value of  $\epsilon, \Delta$ . This means that there are subdomains of  $N$ -representable OBDM's that are not  $v$  representable. As expected the diagonal density  $\rho_{11}$  behaves differently in this respect: we checked that by keeping  $\Delta$  fixed and varying  $\epsilon$  the entire allowed interval  $[0, 1]$  was always covered by  $\rho_{11}$ .

In this simple model there is no reduction of the number of degrees of freedom when going from the many-body wave function to the OBDM, since both have essentially two in-

dependent components (taking normalization into account). In order to eliminate the possibility that our result is an artifact of this feature, we have also investigated a (slightly) more involved case of four fermions that can occupy two different levels with angular momentum  $j = \frac{3}{2}$ . The four-fermion subspace with total angular momentum  $J = 0$  is then six dimensional, whereas the general one-body potential and the OBDM both retain the simple two-parameter form of Eqs. (2) and (3). The resulting OBDM's for a few randomly taken choices of  $\hat{W}$  are plotted in Fig. 2, and we observe even more structures in the  $v$  representability domain, with four holes in the  $N$ -representability disk.

We conclude that, in general, the domain of  $v$ -representable OBDM's has complicated boundaries that depend on the underlying two-body interaction, i.e., the structure of some OBDM's is incompatible with a system of particles that interact via this specific two-body interaction. The  $v$ -representable domain is a nontrivial subset of the domain of  $N$ -representable matrices (which has simple boundaries). There is no reason to assume that these features will disappear when going to the continuous Fock space of many-electron systems, where one deals with functionals instead of functions of discrete variables.

This observation does not pose a problem at the conceptual level of DMFT. The exact DMFT functional can be defined, through a constrained-search formalism [5,8], for all  $N$ -representable OBDM's without any reference to  $v$  representability. Nevertheless, if a specific two-body interaction is such that the  $v$  subdomain is considerably different from the  $N$ -representable domain (as in the schematic examples that were treated here), then one may have difficulties in constructing approximate functionals of a simple analytical form, simply because after minimizing over the  $N$ -representable domain the corresponding OBDM may not be  $v$  representable.

We stress that this problem is specific for DMFT and is absent in standard DFT, where the difference between  $v$  rep-

resentability and  $N$  representability is much less acute. The schematic many-body systems in the present paper, can only demonstrate the existence of this problem. Whether it is really serious enough to hinder the development of accurate DMFT functionals for electronic systems, is a question that must be answered by constructing and testing specific model functionals [9,10].

One may argue that if a trial density-matrix functional is a good approximation to the exact functional, then the possible deviation from  $v$  representability for the approximate ground-state OBDM should not be so important. This statement, however, depends on the type of the interparticle interaction. Experience with systems where the interparticle interaction has both medium-range attraction and strong short-range repulsion shows that one has to be careful when declaring a functional to be a good approximation to the exact one. In nuclear physics, e.g., Skyrme-type functionals exist, which can be viewed as density-matrix functionals since they are (quadratic or cubic) functionals of both the nucleon density and kinetic-energy density [11,12]. These functionals are highly successful in predicting ground-state energies and density profiles for nuclei. However, the velocity distributions turn out to be very different from the exact ones (obtained with Green-function Monte Carlo techniques [13]). Due to the short-range repulsion, a significant fraction of the particles move at much higher velocities than predicted by the Skyrme functionals. This can be considered as an example where a successful approximate density-matrix functional yields a density matrix that is not  $v$  representable (it is of the noninteracting type, with occupation numbers zero or one). As a result, the density matrix predicted by the Skyrme functional is excellent on the diagonal, but fails to describe the off-diagonal behavior of the true density matrix.

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