v-representability for systems with low degeneracy

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We consider the v-representability of the particle density for a noninteracting system of spinless fermions by introducing the idea of proper order of a set of energy levels. It is shown that if $E_1(\boldsymbol{\lambda})$, $E_2(\boldsymbol{\lambda})$, and $E_3(\boldsymbol{\lambda})$ are three energy levels associated with some local potential $V_{\boldsymbol{\lambda}}(\mathbf{r})$ that is a continuous function of $\boldsymbol{\lambda}=(\lambda_1,\lambda_2,\lambda_3)$ over all possible points $\boldsymbol{\lambda}$, where λ_i is the occupation number of the ith state and $M=\lambda_1+\lambda_2+\lambda_3$ is the total number of particles distributed over the three levels, then there must be at least one $\boldsymbol{\lambda}$ for which the three levels are in so-called proper order, in which the levels below the highest occupied level are filled. This result provides a basis for the proof of ensemble v-representability of some N-particle density for which the ground-state degeneracy of the system is no more than three. As examples, three- and two-dimensional central systems are examined, and an N-particle central density is shown to be ensemble v-representable for small N ($N\le 14$ and $N\le 9$ for three- and two-dimensional cases, respectively). The implications for density-functional theory are discussed.

I. INTRODUCTION

The v-representability [1–5] of a density is an issue in density-functional theory [6]. In addressing the problem of v-representability we ask if, for a given density $n(\mathbf{r})$, there is some local potential $V(\mathbf{r})$ which has the density as its ground-state density. Because of the work of Kohn and Sham [7], who introduced an auxiliary system of noninteracting particles moving in some local effective potential $V_{\text{eff}}(\mathbf{r})$ and having the same density distribution $n(\mathbf{r})$ as the original interacting system, the v-representability of a noninteracting system becomes especially important. In this paper we concern ourselves with the v-representability of densities for noninteracting systems of spinless fermions.

Aryasetiawan and Stott [8,9] gave a systematic approach for deducing $V(\mathbf{r})$ for a noninteracting system based on the reduction of the N one-body Schrödinger equations to a set of $N-1$ nonlinear differential equations

$$-\tfrac{1}{2}\nabla^2\psi_i(\mathbf{r})+V(\mathbf{r})\psi_i(\mathbf{r})=E_i\psi_i(\mathbf{r}),\quad i=1,2,\ldots,N-1 \tag{1}$$

where

$$V(\mathbf{r})=\tfrac{1}{2}\left[n(\mathbf{r})-\sum_{i=1}^{N-1}[\psi_i(\mathbf{r})]^2\right]^{-1/2}\times\nabla^2\left[n(\mathbf{r})-\sum_{i=1}^{N-1}[\psi_i(\mathbf{r})]^2\right]^{1/2}. \tag{2}$$

Their work suggests that any reasonable one-dimensional density is v-representable. This comes about because the energy eigenfunctions of a one-dimensional potential can be ordered with increasing energy according to the number of nodes of the eigenfunctions [10] and there is no degeneracy. The ground-state configuration of N particles must be such that the N single-particle states with the smallest numbers of nodes are occupied, and all other levels are empty. This means there is only one possible ground-state configuration for a one-dimensional system. If a potential $V(x)$ is found such that the given density $n(x)$ can be written in the form

$$n(x)=\sum_{i=0}^{N-1}|\psi_i(x)|^2, \tag{3}$$

where i is the number of nodes of eigenfunction $\psi_i(x)$ for the $V(x)$, then $n(x)$ must be the ground-state density associated with the $V(x)$. It is clear that any reasonable one-dimensional N-particle density is v-representable if the corresponding $N-1$ nonlinear differential equations have such a solution.

The problem is more complicated for three-dimensional systems. For example, for a spherical system, the $2s$ level may be above, below, or equal to the $2p$ level, and possible ground-state configurations for two particles are $1s2s$ ($E_{1s}<E_{2s}<E_{2p}$), $1s2p$ ($E_{1s}<E_{2p}<E_{2s}$), or $1s2s2p$ ($E_{1s}<E_{2s}=E_{2p}$), with the corresponding particle distributions $\boldsymbol{\lambda}=(\lambda_{1s},\lambda_{2s},\lambda_{2p})$: (1,1,0), (1,0,1), and $(1,x,1-x)$, respectively, where x can take any value in the range [0,1]. In contrast to the one-dimensional cases, here there are many configurations which are possible ground states. When the method of Aryasetiawan and Stott [8,9] is applied to deduce the potential $V_{\boldsymbol{\lambda}}(\mathbf{r})$ for a given density, even assuming this can be found, there is no guarantee that the potential has the chosen set of energy levels for its ground state. So it is natural to ask which configuration is the true ground state and whether necessarily there is at least one configuration which is the true ground state. The former question depends obviously on the specific density, but the latter is a basic point which is our main concern in this paper.

As illustrated above, the ground state for a three-dimensional system can be degenerate and in such cases it is useful to introduce the possibility of a density being represented as a linear combination of degenerate ground-state densities corresponding to an ensemble [1,2,11]. In these circumstances we refer to the density as being ensemble v-representable, in contrast to pure-state v-representable. As the latter can be considered as a special case of the former, in what follows we shall not distinguish between the two forms, but refer to both as ensemble v-representable when there is no danger of confusion.

In our recent work [11] we investigated spherical systems with two noninteracting spinless fermions discussed above and showed that any reasonable density which integrates to 2 is either pure-state or ensemble v-representable. In this case v-representability hinges on a simple result concerning two levels which can be degenerate. Using this two-level result and *reductio ad absurdum,* we also proved the ensemble v-representability of spherical densities with $N=3,4,5$. It is clear that results similar to the one above for two levels must be extended to an arbitrary number of levels if the proof of the v-representability is to be carried through for any N. For example, for a spherical system with $N=6$, the possibility of accidental triple degeneracy of 3*s*, 3*p*, and 3*d* levels must first be considered. In this paper we introduce the idea of proper order and use it to define the required extension of the two level result to three energy levels. The proof of proper order for three levels, which is presented in Sec. II, is somewhat less obvious than the two-level result. Not only is this result useful because it allows us to prove ensemble v-representability for a broader class of density functions as we show below, but it is also a step toward a more general treatment of v-representability as it identifies the sort of result that must be proved. In Sec. III we show how the ensemble v-representability of the density for a system whose degeneracy is no more than three can be proved by using the result, and three- and two-dimensional central systems are considered as examples. An N-particle central density is shown to be ensemble v-representable for small N ($N\le 14$ and $N\le 9$ for three- and two-dimensional cases, respectively). Section IV contains the discussion and some concluding remarks.

II. PROPER ORDER OF THREE ENERGY LEVELS

In this section, we want to show the following result: If $E_1(\boldsymbol{\lambda})$, $E_2(\boldsymbol{\lambda})$, and $E_3(\boldsymbol{\lambda})$ are three bound-state energy levels associated with some local potential $V_{\boldsymbol{\lambda}}(\mathbf{r})$, which is a continuous function of $\boldsymbol{\lambda}=(\lambda_1,\lambda_2,\lambda_3)$, where λ_i is the occupation number of the ith state and $\lambda_1+\lambda_2+\lambda_3=M$ is the total number of particles occupying the three levels, then there must be some point $\boldsymbol{\lambda}$ for which there is "proper order," that is the levels below the highest occupied level are filled.

Without loss of generality, we set

$$\lambda_{1_{\max}}\le\lambda_{2_{\max}}\le\lambda_{3_{\max}}\,, \tag{4}$$

where $\lambda_{i_{\max}}$ is the maximum occupation number for level i, and

$$M\le\lambda_{1_{\max}}+\lambda_{2_{\max}}+\lambda_{3_{\max}}\,, \tag{5}$$

so that with $\lambda_i\ge 0$

$$\lambda_1+\lambda_2+\lambda_3=M \tag{6}$$

is a plane in the first octant in λ space subject to the conditions (4) and (5). We also assume that the $E_1(\boldsymbol{\lambda})$, $E_2(\boldsymbol{\lambda})$, and $E_3(\boldsymbol{\lambda})$ are positive, since a constant to $V_{\boldsymbol{\lambda}}(\mathbf{r})$ is trivial, and define a vector $\mathbf{E}$ with $E_0=(E_1^2+E_2^2+E_3^2)^{1/2}$,

$$\mathbf{E}=\left[\frac{E_1}{E_0},\frac{E_2}{E_0},\frac{E_3}{E_0}\right]=(\cos\alpha_1,\cos\alpha_2,\cos\alpha_3) \tag{7}$$

so that all P, the end points of $\mathbf{E}$, are on the surface of a unit sphere in the first octant in E space; see Fig. 1. We call this $\frac{1}{8}$ sphere S. α_i is the angle between vector OP and the axis i. Clearly, if E_1 is smaller than E_2 and E_3, then the angle α_1 is larger than α_2 and α_3, and the point P will be far away from axis 1, and vice versa. There are similar geographic implications for E_2 and E_3. Therefore S can be divided, as shown in Fig. 1, into 3 areas S_1, S_2, and S_3, so that the points inside S_i are points with E_i the smallest of the three. The points on the line L_{ij}, separating S_i and S_j, are points with $E_i=E_j<E_k$, and the point Q has $E_1=E_2=E_3$.

Since $V_{\boldsymbol{\lambda}}(\mathbf{r})$ is assumed to be a continuous function of $\boldsymbol{\lambda}$, $E_1(\boldsymbol{\lambda})$, $E_2(\boldsymbol{\lambda})$, and $E_3(\boldsymbol{\lambda})$ are also continuous through the Feynman-Hellman theorem. Thus we establish a continuous mapping from a plane in λ space to a piece of sphere in E space. This mapping [12] preserves the topological properties of the plane and we see especially that since there are no holes on the λ plane, there are no holes in the region of the image on S.

First we consider the case $1\le M\le\lambda_{1_{\max}}$. The strategy of our proof is to follow in a systematic way possible configurations of proper order and to exclude proper order occurring. We shall show that it is not possible to ac-

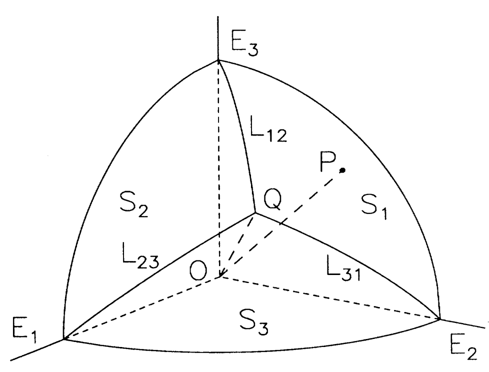

FIG. 1. Energy sphere S defined by Eq. (7). S is divided by L_{12}, L_{23}, and L_{31} into three parts S_1, S_2, and S_3. L_{12} connecting point Q and point (0,0,1) is a line on S with $\alpha_1=\alpha_2$, and similarly for L_{23} and L_{31}. Q is the point with coordinate $(1,1,1)/\sqrt{3}$.

complish this. The possible proper order configurations are (i) no degeneracy with $\lambda_i=M$ and $E_i<\min(E_j,E_k)$; (ii) double degeneracy with $\lambda_i+\lambda_j=M$ and $E_i=E_j<E_k$; and (iii) triple degeneracy with $\lambda_1+\lambda_2+\lambda_3=M$ and $E_1=E_2=E_3$, which is a special case of proper order. We consider these possibilities in turn. The points 1, 2, and 3 in Fig. 2(a) are the vertices of the λ plane at $(M,0,0)$, $(0,M,0)$, and $(0,0,M)$, respectively. If P_1 the image of point 1, is in S_1, then E_1, E_2, and E_3 are in proper order at point 1 because at this point all the M particles occupy E_1, which is lower than E_2 and E_3. We assume this is not the case, so that P_1 must be in S_2 or S_3. Similarly, if points 2 and 3 are not to be proper order points, then their image points P_2 and P_3 must be in S_1 or S_3 and S_1 or S_2, respectively. We now consider the possibility (ii). The lines in Fig. 2(a) connecting P_1, P_2, and P_3 represent the images of lines $\overline{12}$, $\overline{23}$, and $\overline{31}$. If the line P_iP_j crosses boundary L_{ij}, the crossing point would be the image of a proper order point on $\overline{ij}$ of type B as we would have the M particles occupying E_i and E_j with $E_i=E_j<E_k$. We exclude these proper order possibilities by ensuring that the line P_iP_j does not cross L_{ij}. As a consequence of excluding the first two sorts of possible proper order configurations, the lines $P_1P_2P_3P_1$ must encircle the point Q. Because the mapping is continuous, the point Q must be the image of some point on the λ plane, which must be a proper order point. In other words if all else is excluded, there must be some point $\boldsymbol{\lambda}$ at which $E_1=E_2=E_3$, which is a point of proper order.

The case $\lambda_{1_{\max}}<M<\lambda_{2_{\max}}$ is shown in Fig. 2(b). The λ plane has four vertices. The points 2 and 3 are the same as in the case just discussed, and we only need consider points 1′ and 1″ in detail. S_1 is divided into two equal parts $S_{1'}$ and $S_{1''}$ by the extension of L_{23}. If $P_{1'}$ is in $S_{1'}$, where $E_1<E_2<E_3$ with $\boldsymbol{\lambda}_1=(\lambda_{1_{\max}},M-\lambda_{1_{\max}},0)$, then point 1′ will be a proper order point. The point 1″ also is a proper order point if $P_{1''}$ is in $S_{1''}$. Moreover, if $P_{1'}P_{1''}$ crosses the extension line of L_{23}, then the crossing point will be the image of some point $\boldsymbol{\lambda}$ on the line $\overline{1'1''}$ so that the point $\boldsymbol{\lambda}$ is a proper order point with $E_1<E_2=E_3$. If we exclude all possibility that some point is a proper order point due to the positions of $P_{1'}$, $P_{1''}$, P_2, and P_3 and their connections $P_{1'}P_2$, P_2P_3, $P_3P_{1''}$, and $P_{1''}P_{1'}$, then we have Fig. 2(b), which shows that there must be a proper order point with its image at Q.

When different values of M with respect to $\lambda_{1_{\max}}$, $\lambda_{2_{\max}}$, and $\lambda_{3_{\max}}$ are considered, the point 2 may become two points 2′ and 2″ [see Fig. 3(a)], and there are circumstances when the point 2″ coincides with the point 1′ [see Fig. 3(b)], and so on. The proofs for the various cases are easy to carry out if we subdivide S when a point is split into two, or combine regions when points coincide [13]. It is clear that no matter how many vertices the λ plane has (there are at most six vertices), K vertices should be accompanied by the division of S into K pieces, all vertices have similar properties, and the arguments used above can be carried through easily to complete the proof.

If there are restrictions on the relative values of the energies the result that there must be a point of proper order still holds. For example, if the three energy levels under consideration cannot be triply degenerate, then all points P must lie in an area which excludes Q, and because the mapping is continuous, does not surround point Q. Clearly, there must be some point P_i in region S_i or some line P_iP_j crossing L_{ij} which guarantees a point of proper order. As a further example, if $1\le M\le\lambda_{1_{\max}}$ but there are restrictions on the energies so that $E_2>E_3$ with

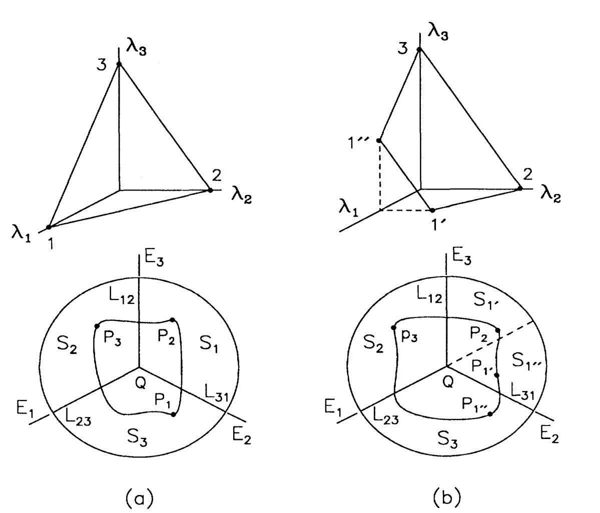

FIG. 2. Schematic mapping relation between λ space and E space for the cases (a) $M\le\lambda_{1_{\max}}$ and (b) $\lambda_{1_{\max}}<M\le\lambda_{2_{\max}}$.

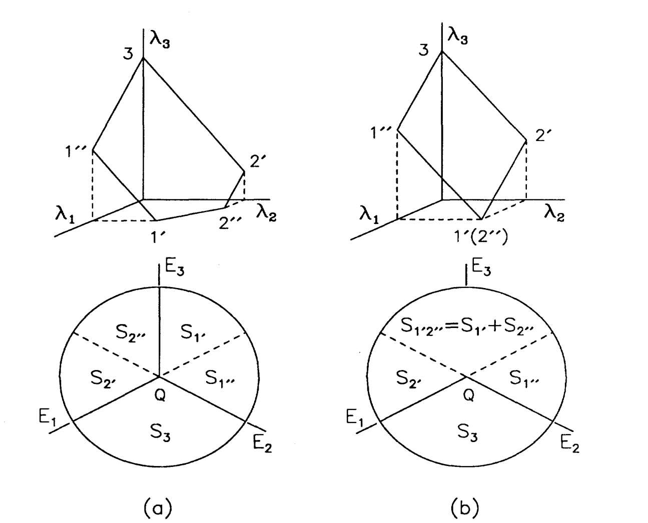

FIG. 3. The forms of λ plane and the divisions of S for two different cases: (a) $\lambda_{2_{\max}}<M<\lambda_{1_{\max}}+\lambda_{2_{\max}}$ $(\le\lambda_{3_{\max}})$; (b) $\lambda_{1_{\max}}+\lambda_{2_{\max}}\le M\le\lambda_{3_{\max}}$.

E_1 taking any value so at most there can be double degeneracy, then points P must lie in the regions S_3 or S_1 of Fig. 2(a), but not on L_{23} or its extension. Furthermore, P_1 and P_3 must be in S_3 and S_1, respectively, if neither is to be a proper order point; consequently P_1P_3 must cross L_{13} with the intersection being a point of proper order. It is straightforward to work through other restricted cases and the result can be applied to any three levels whether or not they can be degenerate.

III. CENTRAL SYSTEMS IN THREE AND TWO DIMENSIONS

A point of proper order of a set of levels is a ground state if all levels above the set are empty and those below filled. Obviously, the results of Sec. II show that the density of a three-level system must be ensemble v-representable. This conclusion by itself is not of much significance because we are not to know, in advance, the number of levels that must be involved in the ground state for an arbitrary density. The three-level result can be applied more usefully to systems where we have some knowledge in advance of the energy-level spectrum. We take systems with central symmetry in three and two dimensions as examples.

For a given spherical density $n(r)$ with

$$\int_0^\infty n(r) 4\pi r^2 dr = N \ , \tag{8}$$

we assume the potential is spherical and hence its energy level E_{nl} is $(2l+1)$-fold degenerate, where n is the principal quantum number and l the orbital angular momentum quantum number. If the $2l+1$ states are equally occupied, then the particle density distribution over these states

$$\rho_{nl}(r) = \frac{4\pi}{2l+1} \sum_{m=-l}^{m=l} |R_{nl}(r) Y_{lm}(\theta,\phi)|^2 r^2 = |U_{nl}(r)|^2 \tag{9}$$

is spherical. The $R_{nl}(r)$ are the usual radial functions and $Y_{lm}(\theta,\phi)$ spherical harmonics. We express $\rho(r)=r^2 n(r)$ in terms of $U_{nl}(r)=rR_{nl}(r)$,

$$\rho(r) = \sum_{n,l} \lambda_{nl} \rho_{nl}(r) = \sum_{n,l} \lambda_{nl} |U_{nl}(r)|^2 \ , \tag{10}$$

with $\sum_{n,l}\lambda_{nl}=N$, where the $2l+1$ states with the same energy E_{nl} are equally occupied each having occupation number $\lambda_{nl}/(2l+1) \le 1$, and the sum runs over all single-particle states from which ground-state configurations can be constructed. For spherical symmetry there are the following restrictions on the energies

$$\begin{aligned} &E_{n'l} > E_{nl}, \quad n' > n \\ &E_{n'l'} > E_{n'-l'+l\, l}, \quad l' > l \ . \end{aligned} \tag{11}$$

The ground-state orbital $U_{1s}(r)$ can be written

$$U_{1s}(r) = \left[\rho(r) - \sum_{n,l \ne 1s} \lambda_{nl} |U_{nl}(r)|^2\right]^{1/2} , \tag{12}$$

and hence the potential can be expressed in terms of $U_{1s}(r)$

$$\begin{aligned} V_\lambda(r) &= \frac{1}{2U_{1s}(r)} \frac{d^2 U_{1s}(r)}{dr^2} + E_{1s} \\ &= \tfrac{1}{2}\left[\rho(r) - \sum_{n,l\ne 1s} \lambda_{nl}|U_{nl}(r)|^2\right]^{-1/2} \\ &\quad \times \frac{d^2}{dr^2}\left[\rho(r) - \sum_{n,l\ne 1s} \lambda_{nl}|U_{nl}(r)|^2\right]^{1/2} + E_{1s} \ , \end{aligned} \tag{13}$$

which explicitly depends on $\rho(r)$ and λ. Substitution of the expression above for $V_\lambda(r)$ into the radial wave equations leads to a set of coupled nonlinear equations for $U_{nl}(r)$.

For a two-particle system all possible ground-state configurations can be constructed from the 1s, 2s, and 2p states. We have shown that for $N=2$ the potential $V_\lambda(r)$ for any λ exists, and the solutions $U_{2s}(r)$ and $U_{2p}(r)$ can be found from the pair of coupled nonlinear equations [11]. However, the order of the energy levels for $V_\lambda(r)$ is such that in general the configuration λ is not a ground state. In the following, for a given N particle spherical density, we assume that a potential $V_\lambda(r)$ can be found for any set of occupation numbers $\lambda=(\lambda_{1s},\lambda_{2s},\ldots)$ and is a continuous function of λ in a λ space prescribed by the density. For the purpose of the proof of v-representability, we can take $\lambda_{1s}=1$ because E_{1s} is always the lowest level.

The ensemble v-representabilities for $N=2,3,4,5$, which were proved earlier [11], can be shown more easily using the three-level result. Let us take $N=4$ as an example. The single-particle states which can be occupied in possible ground-state configurations are 1s, 2s, 3s, 4s, and 2p, and the λ space to be considered is $\lambda=(\lambda_{1s},\lambda_{2s},\lambda_{3s},\lambda_{4s};\lambda_{2p})$ with $\lambda_{1s}=1$. First consider the proper order of E_{2s}, E_{3s}, and E_{2p} with $\lambda_{2s}+\lambda_{3s}+\lambda_{2p}=3$. The only proper order point (p point) that is not guaranteed to be a ground state is $\lambda_1=(1,1,1,0;1)$ with $E_{2p}>E_{3s}$. This is not necessarily a ground-state point (g point) because E_{2p} could be higher than E_{4s}. We then consider the p points of E_{3s}, E_{4s}, and E_{2p} with two particles, and all of these points are g points because all the levels below the occupied E_{4s} or E_{2p} are filled. So any four-particle spherical density is ensemble v-representable.

For $N=6$, the single-particle states to be considered are 1s, 2s, . . . , 6s, 2p, 3p, and 3d. Because one possible ground-state configuration involves accidentally degenerate 3s, 3p, and 3d levels, this case can not be proved using the methods of Ref. [11]. We require the three-level result of Sec. II. We begin by considering the proper order of E_{2s}, E_{2p}, and E_{3d} with $\lambda_{2s}+\lambda_{2p}+\lambda_{3d}=5$. Among the possible p points, the point $\lambda_1=(1,1,0,\ldots,0;3,0;1)$ with $E_{3d}>E_{2s}$ is the only one which is not necessarily a g point because E_{3d} may be higher than E_{3s}. Now we consider the proper order of E_{3s}, E_{3p}, and E_{3d} (the three levels could be degenerate) and there must be a p point among $\lambda=(1,1,\lambda_{3s},\ldots,0;3,\lambda_{3p};\lambda_{3d})$ with $\lambda_{3s}+\lambda_{3p}+\lambda_{3d}=1$. All of the possible p points are assured to be g points except $\lambda_4=(1,1,1,0,0,0;3,0;0)$ with

TABLE I. The main steps for the proofs of ensemble v-representabilities of spherical densities with $N=6$, 10, and 14. The λ spaces are $(\lambda_{1s},\ldots,\lambda_{6s};\lambda_{2p},\lambda_{3p};\lambda_{3d})$, $(\lambda_{1s},\ldots,\lambda_{10s};\lambda_{2p},\ldots,\lambda_{4p};\lambda_{3d};\lambda_{4f})$, and $(\lambda_{1s},\ldots,\lambda_{14s};\lambda_{2p},\ldots,\lambda_{5p};\lambda_{3d},\lambda_{4d};\lambda_{4f})$, respectively. We use an abbreviated symbol for a point in λ space, for example, [4;3;1;0] for (1,1,1,1,0, . . . ,0;3,0, . . . ,0;1,0, . . . ,0;0, . . . ,0).

	$\lambda_1+\lambda_2+\lambda_3=M$				p points that are not	Conditions for the point
N	λ_1	λ_2	λ_3	M	necessarily g points	not to be a g point
6	λ_{2s}	λ_{2p}	λ_{3d}	5	[2;3;1]	$E_{3d}>E_{3s}(E_{3p})$
	λ_{3s}	λ_{3p}	λ_{3d}	1	[3;3;0]	$E_{2p}>E_{4s}$
	λ_{4s}	λ_{5s}	λ_{2p}	3	[5;1;0]	$E_{2p}>E_{6s}$
	λ_{5s}	λ_{6s}	λ_{2p}	2	none	
10	λ_{2s}	λ_{3d}	λ_{4f}	6	[2;3;5;0]	$E_{3d}>E_{3s}(E_{3p})$
	λ_{3s}	λ_{3p}	λ_{3d}	5	[3;6;1;0]	$E_{3d}>E_{4s}(E_{4p})$
	λ_{4s}	λ_{4p}	λ_{3d}	1	[4;6;0;0]	$E_{3p}>E_{5s}$
	λ_{5s}	λ_{3p}	λ_{3d}	3	[5;5;0;0]	$E_{3p}>E_{6s}$
	λ_{6s}	λ_{3p}	λ_{3d}	2	[6;4;0;0]	$E_{3p}>E_{7s}$
	λ_{7s}	λ_{3p}	λ_{3d}	1	[7;3;0;0]	$E_{2p}>E_{8s}$
	λ_{8s}	λ_{9s}	λ_{2p}	3	[9;1;0;0]	$E_{2p}>E_{10s}$
	λ_{9s}	λ_{10s}	λ_{2p}	2	none	
14	λ_{2s}	λ_{3d}	λ_{4f}	10	[2;3;5;4]	$E_{4f}>E_{3s}(E_{3p})$
	λ_{3s}	λ_{3p}	λ_{4f}	4	[3;6;5;0][a]	$E_{3d}>E_{4s}(E_{4p})$ or $E_{3p}>E_{4s}$
	λ_{4s}	λ_{4p}	λ_{3d}	5	[4;9;1;0]	$E_{3d}>E_{5s}(E_{5p})$
	λ_{5s}	λ_{5p}	λ_{3d}	1	[5;9;0;0]	$E_{4p}>E_{6s}$
	λ_{6s}	λ_{4p}	λ_{3d}	3	[6;8;0;0]	$E_{4p}>E_{7s}$
	λ_{7s}	λ_{4p}	λ_{3d}	2	[7;7;0;0]	$E_{4p}>E_{8s}$
	λ_{8s}	λ_{4p}	λ_{3d}	1	[8;6;0;0]	$E_{3p}>E_{9s}$
	λ_{9s}	λ_{3p}	λ_{3d}	3	[9;5;0;0]	$E_{3p}>E_{10s}$
	λ_{10s}	λ_{3p}	λ_{3d}	2	[10;4;0;0]	$E_{3p}>E_{11s}$
	λ_{11s}	λ_{3p}	λ_{3d}	1	[11;3;0;0]	$E_{2p}>E_{12s}$
	λ_{12s}	λ_{13s}	λ_{2p}	3	[13;1;0;0]	$E_{2p}>E_{14s}$
	λ_{13s}	λ_{14s}	λ_{2p}	2	none	

[a]There is more than one such point at this step. It is easy to show that the sequences of steps from those other points will end at the point [3;6;5;0] or some following steps of the sequence listed in the table. For example, [2;6;5;1] with $E_{4f}>E_{4p}$ is such a point, but considering the proper order of E_{3s}, E_{4d}, and E_{4f} with one particle leads back to [3;6;5;0].

TABLE II. The main steps for the proofs of ensemble v-representabilities of two-dimensional central densities with $N=3$ and 9. The λ spaces are $(\lambda_{10},\ldots,\lambda_{30};\lambda_{21})$ and $(\lambda_{10},\ldots,\lambda_{90};\lambda_{21},\ldots,\lambda_{41};\lambda_{32},\lambda_{42};\lambda_{43};\lambda_{54})$, respectively. We use an abbreviated symbol for a point in λ space as we did for spherical densities.

	$\lambda_1+\lambda_2+\lambda_3=M$				p points that are not	Conditions for the point
N	λ_1	λ_2	λ_3	M	necessarily g points	not to be a g point
3	λ_{20}	λ_{30}	λ_{21}	2	none	
9	λ_{20}	λ_{43}	λ_{54}	4	[2;2;2;2;1]	$E_{54}>E_{30}(E_{31})$
	λ_{30}	λ_{31}	λ_{54}	1	$[3-x;2+x;2;2;0]$[a]	$E_{43}>E_{30}(E_{31})$
	λ_{30}	λ_{31}	λ_{43}	3	[3;4;2;0;0][b]	$E_{31}>E_{40}$ or $E_{32}>E_{40}(E_{41})$
	λ_{40}	λ_{41}	λ_{32}	2	[4;5;0;0;0]	$E_{41}>E_{50}$
	λ_{50}	λ_{41}	λ_{32}	1	[5;4;0;0;0]	$E_{31}>E_{60}$
	λ_{60}	λ_{31}	λ_{32}	2	[6;3;0;0;0]	$E_{31}>E_{70}$
	λ_{70}	λ_{31}	λ_{32}	1	[7;2;0;0;0]	$E_{21}>E_{80}$
	λ_{80}	λ_{90}	λ_{21}	2	none	

[a]$0\le x\le 1$.

[b]This step gives more than one such point, and we only list the sequence of steps for the points [3;4;2;0;0].

$E_{3s} < E_{2p} < E_{3d}$ because E_{4s} could be smaller than E_{2p}. So we consider the p point of E_{4s}, E_{5s}, and E_{2p} with three particles and of these only $\lambda_5 = (1,1,1,1,1,0;1,0;0)$ with $E_{5s} < E_{2p}$ is not necessarily a ground state because we may have $E_{6s} < E_{2p}$. But when the proper order of E_{5s}, E_{6s}, and E_{2p} with two particles is considered, all the p points: λ_5 with $E_{5s} < E_{2p} \le E_{6s}$, $\lambda_6 = (1,1,1,1,1,1;0,0;0)$ with $E_{6s} \le E_{2p}$, and $\lambda_7 = (1,1,1,1,1,x;1-x,0;0)(0 \le x \le 1)$ with $E_{6s} = E_{2p}$ are possible g points, and the ensemble v-representability of any six-particle spherical density is proved.

The same general approach can be applied to systems with larger number of particles. The idea is to locate the p points of sets of the possible energy levels and check if they are ground states for the system. We first identify the levels from which possible ground states can be contracted and step through them systematically in sets of three. The points of proper order are considered for each set and conditions are accumulated under which there may not be a ground state. Following this line through we are eventually led to a set of levels whose points of proper order are all inevitably ground states and ensemble v-representability is proved. If larger N is considered, the λ space must be expanded. For $N = 7,8,9$ more s levels must be considered, the number of s levels being equal to N. The $4p$ and $4f$ levels are required for $N = 10,11,12,13$, and $5p$ and $4d$ must be added for $N = 14$. The main steps for proofs of $N = 6$, 10, and 14 are listed in Table I. For $N = 15$, although only one more s level is needed, a possible ground-state configuration involves accidentally degenerate E_{4s}, E_{4p}, E_{4d}, and E_{4f} levels which hold one particle with the other 14 particles filling the levels below the four-fold degenerate one. This case and subsequent ones cannot be covered by the three-level result.

For central systems in two dimensions orbitals are

$$\psi_{n\pm m}(r,\phi) = R_{nm}(r)e^{\pm im\phi} , \tag{14}$$

where $m = 0,1,2,\ldots$ and each energy level E_{nm} can be occupied by two particles for $m \ne 0$.

A similar procedure to that used in the spherical case can be adopted to determine the $V_\lambda(r)$ that yields a given density $n(r)$. If we again assume a $V_\lambda(r)$ can be found, and is continuous in λ, and we observe that similar restrictions to Eq. (11) hold for the energies, then it is straightforward to show the ensemble v-representabilities for $N = 2$ up to 9. The results are summarized in Table II for $N = 3$ and 9. When $N \ge 10$ the fourfold degeneracy of E_{40}, E_{41}, E_{42}, and E_{43} must be considered.

IV. DISCUSSION AND CONCLUSIONS

We proved that for any chosen set of three energy levels, we can find a potential $V_\lambda(\mathbf{r})$ so that the three levels are in proper order. A density is the ensemble ground-state density at this point if levels above the set are empty and those below filled, and hence is ensemble v-representable. This result provides a basis for the proof of ensemble v-representability of some density for which the degeneracy of the ground state of the system is no more than three. By applying the three-level result we have proved that any central density with particle number up to 9 for two dimensions and to 14 for three dimensions is ensemble v-representable.

Symmetry of a density plays an important role in the proof of ensemble v-representability, because the order of energy levels prescribed by the symmetry can be known in advance. For example, Eq. (11) gives general restrictions on the order of energy levels for any central system, and all possible ground-state configurations can be treated systematically. On the other hand, our three-level result does not depend on any special symmetry. If we know the general features of the order of levels for an N-particle density and the degeneracy of the ground state is no more than three, then it is easy to show the ensemble v-representability of the density.

Proper order of a set of energy levels is a key idea in our proofs of ensemble v-representability for various densities. So far we have only considered cases of low accidental degeneracy, and consequently our approach is limited to systems of a few particles. In fact, by using some results from topology we are able to develop the idea for three levels to a set of any number of levels which can be degenerate. From this extension, spherical densities with any N can be shown to be ensemble v-representable, and ensemble v-representabilities of some densities without any special symmetry also can be proved. These generalizations will be presented in a forthcoming paper.

The results given in this paper and our earlier work [11] show that the v-representability of a density is related to the topological properties of the occupation number space and the energy space, and the mapping relationships between the two spaces. These properties and relationships display general features which are independent of specific densities. Thus our results support the general conjecture of Levy and Perdew [2,14,15] that any density is noninteracting ensemble v-representable, and lend formal approval to the Kohn-Sham method [7].

We would like to point out that although we have assumed $V_\lambda(\mathbf{r})$ can be found and is a continuous function of λ, this is only necessary in the region of λ space where there may be ground-state configurations. For example, for a spherical density, we need only consider the subspace

$$\begin{aligned} &\lambda_{n'l} \le \lambda_{nl}, \quad n' > n \\ &\lambda_{n'l'} \le \lambda_{n'-l'+l\,l}, \quad l' > l \end{aligned} \tag{15}$$

and $\lambda_{nl} = \lambda_{nl_{\max}}$ if $\lambda_{n'l} \ne 0$, and $\lambda_{n'-l'+l\,l} = \lambda_{n'-l'+l\,l_{\max}}$ if $\lambda_{n'l'} \ne 0$. In particular we need only consider $\lambda_{1s} = 1$. Furthermore [11], we are able to prove that V_λ exists for the three-level case and an extension to more levels looks straightforward. Numerical examples treated earlier also yield V_λ explicitly. In summary, this assumption does not appear to be a major factor in ensemble v-representability if $n(r)$ is reasonable.

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[13] In Fig. 3(b), the points 1′ coincides with 2″. If $E_3 \geq \max(E_1, E_2)$, then it is a proper order point, which corresponds to its image in $S_{1'2''}$. If $P_{1'(2'')}P_{1''}$ (or $P_{1'(2'')}P_{2'}$) cross the boundary of $S_{1'2''}$ and $S_{1''}$ (or the boundary of $\underline{S_{1'2''}}$ and $\underline{S_{2'}}$), then the image of some point on the line $\overline{1'1''}$ (or $\overline{2'2''}$) will be on the boundary with $E_1 < E_2 = E_3$ (or $E_2 < E_1 = E_3$) so that the point is a proper order point.

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