v-representability for systems of a few fermions

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The v-representability of the particle density for a system of noninteracting fermions is considered. It is shown that any reasonable spherical density for two spinless fermions is either the nondegenerate ground-state density or a linear combination of degenerate ground-state densities for some effective local potential, and is therefore ensemble v-representable. The results of model calculations are given that illustrate various possible situations for two-particle systems. An extension of this result for systems of more particles is made and the implications for density-functional theory are discussed.

I. INTRODUCTION

Density-functional theory addresses the behavior of systems of interacting particles such as the electrons in an atom or molecule. An objective is to describe properties of the system, particularly the ground-state energy, in terms of the particle density distribution, which is likely to be a much simpler quantity than the many-particle wave function, Green's functions, or similar devices. There could be considerable merit in such a description for a system with a large number of particles such as a solid because the density distribution remains a function of a single variable, whereas other quantities such as the wave function become inordinately complicated for an interacting many-particle system. Although approximate schemes such as the Thomas-Fermi method were in common use, the theoretical framework of the density-functional approach was laid in 1964 by Hohenberg and Kohn [1]. They showed that for a system with a nondegenerate ground state there is a one-to-one relationship between the ground-state density distribution $n_0(\mathbf{r})$ and the external field $V_{\text{ext}}(\mathbf{r})$ in which the particles move, consequently the system may be equally well characterized by $n_0(\mathbf{r})$ or $V_{\text{ext}}(\mathbf{r})$. The result of Hohenberg and Kohn was also extended to cover a system with a degenerate ground state [2–4].

Hohenberg and Kohn [1] went on to introduce the ground-state energy functional of the density $E[n]$, which is subject to the variational principle $E[n] \geq E_0$, where E_0 is the true ground-state energy and the equality is obtained upon substitution of the corresponding ground-state density. As originally presented, the functional $E[n]$ is defined only for densities which are ground-state densities for some external field—the so called interacting v-representable densities. However, the formulation by Levy [2] in terms of the constrained-search functional overcomes this restriction and the v-representability of a density is no longer an issue for an interacting system.

Although the physical systems of interest consist of many interacting particles, companion systems of noninteracting particles are useful in density-functional theory because of the work of Kohn and Sham [5]. They introduced an auxiliary system of noninteracting particles moving in some local effective potential $V_{\text{eff}}(\mathbf{r})$ and having the same density as the original interacting system. Given a prescription for the effective field, the noninteracting problem can be treated by solving self-consistently the set of single-particle Schrödinger equations. The ground-state energy and density of the interacting system then follow. In practice, it is necessary to approximate the effective field, but the local-density approximation for the electron exchange and correlation contribution to the energy and the effective potential is simple to apply and has proved very successful in treatments of the ground-state energy and density and related quantities for atoms, molecules, and condensed matter. This Kohn-Sham scheme assumes that the density of the interacting system under consideration is also the ground-state density of the auxiliary noninteracting system for some $V_{\text{eff}}(\mathbf{r})$, in other words $n_0(\mathbf{r})$ is assumed to be noninteracting v-representable. This assumption merits examination because there are many examples of "reasonable" densities for which there is no corresponding noninteracting ground-state wave function for any local effective potential, for example, those suggested by Levy [3] and Lieb [6]. Furthermore, Levy [3] has shown that any density that can be represented as a linear combination of degenerate ground-state densities is not pure-state v-representable, by which we mean it cannot be the density corresponding to a nondegenerate ground state for a local potential.

In this paper we shall investigate the relationship between the electron density and the potential for a noninteracting system of particles and focus on the potential that has a given density as its ground state. This inverse problem to determine $V_{\text{ext}}[n]$ has been studied for a small number of particles by a number of authors and of particular relevance to this paper is the work of Aryasetiawan and Stott [7,8], Nagy and March [9–11], and Li and Krieger [12]. The former authors gave a systematic approach for deducing V based on the reduction of the N one-body Schrödinger equations to a set of $N-1$ nonlinear differential equations. The approach was used to obtain Kohn-Sham effective potentials for Be and Ne atoms and further applications were made to a number of one-dimensional and spherical three-dimensional model systems. A number of densities for one-dimensional systems with two and three spinless fermions were considered and all the examples treated were found to be pure-state v-representable. It was shown that any density for two spinless fermions is pure-state v-representable and it seemed likely that the same is true for any number of particles in one dimension. In contrast, densities for spherical, three-dimensional systems with two particles were given which did not correspond to a nondegenerate ground state for any local potential, e.g., $n(r)=ce^{-ar}$. The way in which this can come about is interesting.

If we consider initially a $1s2s$ configuration for the two spinless fermions, then a potential can be found for which $n(r)=R_{1s}^2+R_{2s}^2$, where R_{nl} is a radial wave function and this is always possible. This could be the ground-state configuration for the potential, but not necessarily so. For example [8], in the case of the exponential density it was found on examination that the $2p$ (and the $3d$) levels lay below the $2s$, the $1s2s$ configuration is not the ground state, and the density is not pure-state v-representable. To investigate the possibility of this density being a linear combination of degenerate ground-state densities of some other effective potential, that is, a Levy-Lieb density, a configuration was considered with one particle in the $1s$ state, and with each of the three $2p$ levels $\frac{1}{3}$ occupied so that the density would have the form $n(r)=R_{1s}^2+R_{2p}^2$. Again, the effective potential can be deduced and this time the $2p$ level is found to be below the $2s$, the $1s2p$ configuration is the triply degenerate ground state, and the density is representable as a linear combination of degenerate ground-state densities.

In this paper we shall show that for specific cases of a small number of spinless fermions any reasonable spherically symmetric density is the nondegenerate ground-state density, or a linear combination of degenerate ground-state densities for some local potential. In what follows we shall refer to these alternatives as pure-state and ensemble v-representability, respectively, and we note that the former can, of course, be considered as a special case of the latter. We refer to both as ensemble v-representability when there are no special implications. The v-representability of any reasonable density even in these restricted circumstances of a small number of particles and spherical symmetry is nontrivial and lends support for the more general conjecture of Levy and Perdew [3,13,14] that such v-representability is extremely likely for any number of particles.

The proof of ensemble v-representability for any spherical density for two spinless fermions is given in Sec. II. Section III presents the results of calculations which illustrate the salient points of Sec. II. Section IV describes the extension of the results to larger N, and Sec. V contains the discussion and some concluding remarks.

II. TWO-PARTICLE SYSTEMS

We consider a density distribution $n(r)$ corresponding to two particles, and which is spherically symmetric, so that

$$\int_0^\infty n(r)4\pi r^2 dr = N \ , \tag{1}$$

with $N=2$, and ask if $n(r)$ can be the nondegenerate ground-state density or a linear combination of degenerate ground-state densities for a system of two noninteracting, spinless fermions moving in some local, effective potential. This system could be the auxiliary noninteracting Kohn-Sham system. We choose the potential to be itself spherically symmetric; this choice will be justified later. The two particles must occupy the two lowest states for this potential. The lowest bound state must be the $1s$, but the next level can be either the $2s$ or the $2p$ or a mixture of the $2s$ and $2p$ if they prove to be degenerate.

To investigate the various possibilities we look for a potential $V_\lambda(r)$ such that the three lowest states given by

$$\begin{aligned} &\left[-\frac{1}{2}\frac{d^2}{dr^2}+V_\lambda(r)\right]U_{1s}(r)=E_{1s}U_{1s}(r) \ , \\ &\left[-\frac{1}{2}\frac{d^2}{dr^2}+V_\lambda(r)\right]U_{2s}(r)=E_{2s}U_{2s}(r) \ , \\ &\left[-\frac{1}{2}\frac{d^2}{dr^2}+V_\lambda(r)+\frac{1}{r^2}\right]U_{2p}(r)=E_{2p}U_{2p}(r) \end{aligned} \tag{2}$$

yield the given density $\rho(r)=r^2 n(r)$ through

$$\rho(r)=U_{1s}^2+\lambda U_{2s}^2+(1-\lambda)U_{2p}^2 \ , \tag{3}$$

where $U_{nl}=rR_{nl}$ are normalized radial functions and with $0\le\lambda\le1$, where λ can be viewed as the occupation number of the $2s$ state. The contribution to the density of the $2p$ states is spherically symmetric and comes about from equal occupation of the $m=0$ and ±1 states.

We assume for the moment that a solution of Eqs. (2) and (3) can always be found for any value of λ in the allowed range and for any reasonable $n(r)$ and that the energies are continuous functions of λ. The remaining issue is the order of the lowest energy levels of $V_\lambda(r)$. Consider the various possibilities. If for $\lambda=1$ the resulting potential has the $2s$ state below the $2p$ then the density is $1s2s$ pure state v-representable and all is well. Let us assume this is not the case and the order of the levels is $1s, 2p, \ldots, 2s, \ldots$. Now turn to the solution for $\lambda=0$. If the $2p$ level is below the $2s$, then the density is ensemble v-representable with the three $2p$ states each $\frac{1}{3}$ occupied and the other particle in the $1s$. But if the $2s$ proves to be the lower level, then we have a density that is not v-representable for $\lambda=0$ or 1 and for which the $2s$ is lower than the $2p$ at $\lambda=0$ and vice versa at $\lambda=1$. If we track the $2s$ and $2p$ energies as functions of λ they must cross for some λ_0 between 0 and 1. At this crossing point the $2s$ and $2p$ levels are degenerate and the density is an ensemble ground-state density with occupation numbers λ_0 and $1-\lambda_0$ for the $2s$ and $2p$ levels, respectively. This covers all possibilities and we must conclude that the density $n(r)$ is always pure-state or ensemble v-representable.

All possibilities are illustrated schematically in Fig. 1. It might appear that there can be some duplication. If, for instance, the chosen density gives a level diagram such as Fig. 1(c), then we would conclude that the density is pure-state v-representable because $E_{2s}<E_{2p}$ at $\lambda=1$, but at $\lambda=0$, $E_{2p}<E_{2s}$ and the density is ensemble v-representable for some different potential. Furthermore,

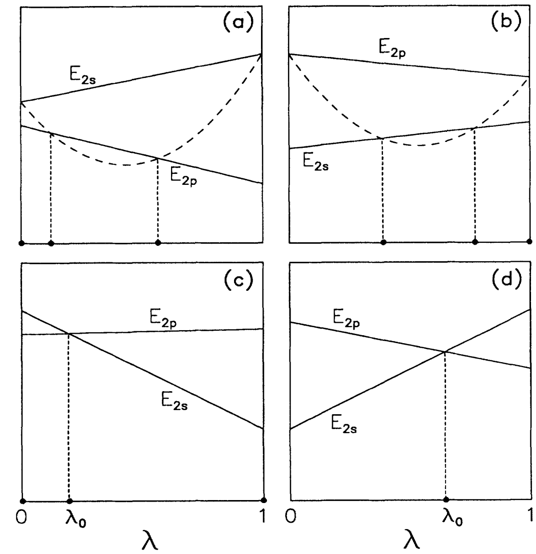

FIG. 1. Illustration of the four types of possible behavior of the energy levels as functions of occupation number λ for a two-particle density.

the crossing point at λ_0 implies that there must be yet another potential for which $n(r)$ is the ensemble ground-state density with the $1s$ and the degenerate $2s$ and $2p$ levels occupied. However, the level diagram illustrated in Fig. 1(c) is excluded because Levy [3] has shown that a density which can be represented as a convex sum of degenerate ground-state densities for some potential and is therefore ensemble v-representable cannot simultaneously be the pure ground-state density for some other potential. Levy's result also leads us to exclude the possibility of the dashed line in Fig. 1(b) occurring where the $2p$ state dips below the $2s$ for some intermediate range of λ as this would imply that the density is a pure ground-state density at $\lambda=1$ and simultaneously an ensemble ground-state density at the two crossing points.

Englisch and Englisch [4] have extended Levy's argument and shown that a given density cannot be an ensemble ground-state density for two different potentials, and since for a given potential different ensembles must give different densities [15], we are led to exclude the possibilities of the dashed line in Fig. 1(a) and multiple crossing points in Fig. 1(d). The only physical possibilities are covered by the solid lines of Fig. 1(a), 1(b), or 1(d) representing, respectively, ensemble v-representability with $\lambda=0$, pure-state v-representability with $\lambda=1$, or ensemble v-representability at λ_0; but there can be only a single crossing point.

We now attend to some details. It was assumed that Eqs. (2) and (3) could be solved and a potential V_λ could be found for any λ between 0 and 1. This is shown to be so in the Appendix by simple extensions of the arguments of Aryasetiawan and Stott [8]. Also addressed in the Appendix is our assumption that the energy levels are continuous functions of λ.

We have studied the case of a spherically symmetric density and assumed that the potential $V_\lambda(r)$ is central. However, we have seen that any reasonable $n(r)$ is ensemble v-representable with a central $V_\lambda(r)$. But from Levy's result [3] or its generalization [4] this $n(r)$ cannot be simultaneously ensemble v-representable with another, noncentral potential, and it was sufficient to consider just central $V_\lambda(r)$. Finally, we regard a density which is positive, twice differentiable and which integrates to N to be a reasonable one.

III. CALCULATIONS

Calculations have been performed for a number of model densities for two spinless fermions to illustrate points made in Sec. II. Rather than a direct numerical evaluation on Eqs. (2) we have found it convenient to use the transformation introduced by Dawson and March [16], namely

$$\begin{aligned} U_{1s}(R) &= [\rho(r)]^{1/2}\sin\theta(r)\cos\phi(r)\ , \\ U_{2s}(r) &= \left[\frac{\rho(r)}{\lambda}\right]^{1/2}\sin\theta(r)\sin\phi(r)\ , \\ U_{2p}(r) &= \left[\frac{\rho(r)}{1-\lambda}\right]^{1/2}\cos\theta(r)\ . \end{aligned} \tag{4}$$

Equation (3) is satisfied automatically and Eqs. (2) become

$$\begin{aligned} &\ddot{\phi}+\left[\frac{\dot{\rho}}{\rho}+2\dot{\theta}\cot\theta\right]\dot{\phi}=-\varepsilon_{2s}\sin 2\phi\ , \\ &\ddot{\theta}+\frac{\dot{\rho}}{\rho}\dot{\theta}=\sin 2\theta\left[\frac{1}{2}\dot{\phi}^2+\varepsilon_{2p}-\frac{1}{r^2}-\varepsilon_{2s}\sin^2\phi\right]\ , \end{aligned} \tag{5}$$

where $\varepsilon_{2s}=E_{2s}-E_{1s}$ and $\varepsilon_{2p}=E_{2p}-E_{1s}$, and the effective potential is given by

$$\begin{aligned} V_\lambda(r) = &-\frac{1}{8}\left[\frac{\dot{\rho}}{\rho}\right]^2+\frac{1}{4}\frac{\ddot{\rho}}{\rho}-\frac{1}{2}\dot{\theta}^2-\frac{1}{2}\sin^2\theta\dot{\phi}^2 \\ &+\cos^2\theta\left[\varepsilon_{2p}-\frac{1}{r^2}\right]+\varepsilon_{2s}\sin^2\phi\sin^2\theta+E_{1s}\ . \end{aligned} \tag{6}$$

The boundary conditions on θ and ϕ follow from the required nodal behavior of the orbitals and we find ϕ is a monotonically decreasing function with one node and $0\le\phi(0)\le\pi/2$ with $\phi(\infty)=-\pi/2$. The function θ is restricted to $0\le\theta\le\pi/2$ with $\theta(0)=\pi/2$, while $\theta(\infty)$ takes the values $\pi/2$ or 0, depending on which of the $2p$ or $2s$ has the higher energy [$\theta(\infty)$ has an intermediate value if the $2p$ and $2s$ are degenerate]. Normalization requires

$$\begin{aligned} &\int_0^\infty \rho(r)\sin^2\theta\cos^2\phi\, dr=1\ , \\ &\int_0^\infty \rho(r)\sin^2\theta\sin^2\phi\, dr=\lambda\ , \end{aligned} \tag{7}$$

which give the occupation number of the $2s$ state once θ and ϕ have been found.

We first consider densities of a type introduced by Levy [3] and Lieb [6] and given by

$$\rho(r)=[R_{1s}^2+\alpha R_{2s}^2+(1-\alpha)R_{2p}^2]r^2\ , \tag{8}$$

where R_{nl} is the radial wave function for a free hydrogenic system with $Z=2$, and $0 \le \alpha \le 1$. Our chosen density is therefore by construction a linear combination of degenerate ground-state densities. We have treated the cases $\alpha=0$, 0.5, and 1.

The other two-particle density we have examined is

$$\rho(r)=a^3 r^2 e^{-ar} , \tag{9}$$

for which the scaling $r'=ar$, $\varepsilon'=\varepsilon/a^2$ in Eqs. (5) and (9) eliminates the exponent from the calculations. Aryasetiawan and Stott [8] considered this density and tried to represent it by a two-level system at the end points $\lambda=0$ and 1. We have examined the representation of the exponential density and those given by Eq. (8) as a function of $2s$ occupation number λ. The four densities considered are illustrated in Fig. 2. The procedure was to solve Eqs. (5) with the appropriate boundary conditions using a fourth-order Runge-Kutta formula to obtain θ and ϕ, and ε_{2p} and ε_{2s}. The corresponding effective potential was found from Eq. (6) and E_{1s} was adjusted so that $V_\lambda(r\rightarrow\infty)=0$. The value of λ was obtained from Eqs. (7).

The energies of the $1s$, $2s$, and $2p$ levels as functions of λ for different two-particle densities are shown in Fig. 3. The energies go smoothly to the values at the end points of $\lambda=0$ and 1. The limiting values agree with results obtained by considering the appropriate two-level system, $1s2p$ in the case of $\lambda=0$, and $1s2s$ for $\lambda=1$. The curves demonstrate the v-representability of the densities. The Coulombic density with $\alpha=1$ is pure-state v-representable because the point $\lambda=1$ is a ground state. It is also unique because the $2s$ levels are below the $2p$ for other values of λ. For $\alpha=0$, the density is ensemble v-representable because the $2s$ and $2p$ levels are degenerate at $\lambda=0$ with the $2p$ below the $2s$ level for $\lambda\neq0$. The case with $\alpha=0.5$ shows the $2s$ and $2p$ levels crossing at $\lambda_0=0.5$ at which point the system is in its ground state and the density is therefore ensemble v-representable. The potential for which the densities are ground-state densities is Coulomb for the three cases considered in accordance with the construction of the densities, and the degeneracy of the $2s$ and $2p$ levels at the values of λ giving a ground state is accidental Coulomb degeneracy. The potentials $V_\lambda(r)$ for other values of λ are non-Coulomb as illustrated for $\alpha=0.5$ in Fig. 4.

The dependence of the energy levels on λ for the ex-

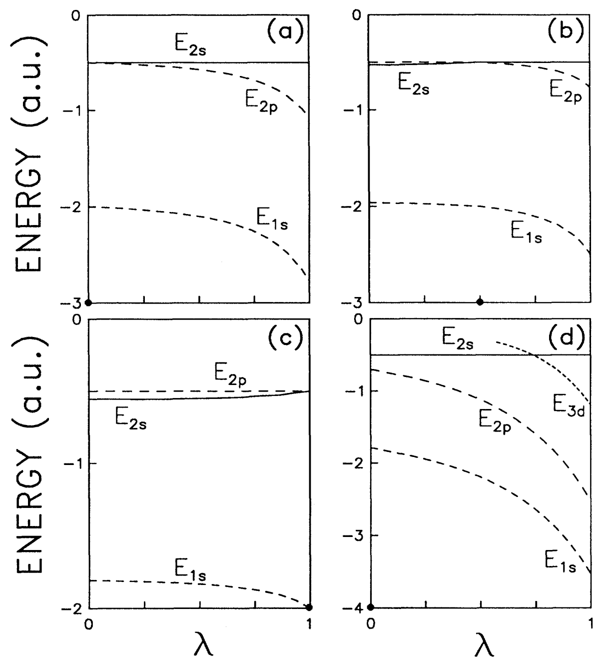

FIG. 3. Energy levels as functions of λ for the four densities shown in Fig. 2. The dots denote values of λ which correspond to the ground-state configurations.

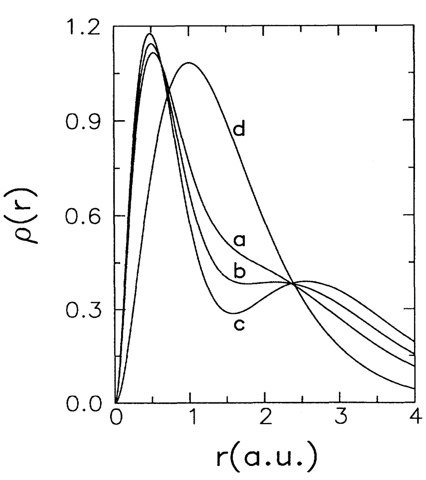

FIG. 2. Radial densities $\rho(r)=r^2 n(r)$ for the Coulomb potential from Eq. (8) with curve a, $\alpha=0$; curve b, $\alpha=0.5$; and curve c, $\alpha=1$. Curve d shows the exponential density given by Eq. (9) with $a=2$.

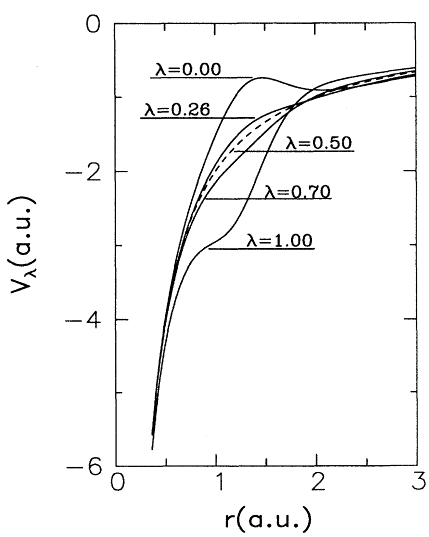

FIG. 4. Representative potentials $V_\lambda(r)$, which give the Coulomb density Eq. (8) with $\alpha=0.5$. Only the potential for $\lambda=0.5$ has $\rho(r)$ for its ground-state density.

ponential density shows the $2p$ levels below the $2s$ for all λ, and the density is therefore ensemble v-representable because the point $\lambda=0$ is a ground state. In all the cases considered the energy of the highest of the three levels shown is independent of λ, this is because the asymptotic form of the density is governed by the tail of the highest occupied orbital which in turn is determined by the orbital energy [17].

In compliance with our result that the potential for which ρ is the ground-state density, either for a pure state or an ensemble, is unique, we see at most one crossing point for the $2s$ and $2p$ energies as a function of λ. Furthermore, the energies vary smoothly with λ.

IV. EXTENSION TO MORE PARTICLES

It is straightforward to extend the proof of ensemble v-representability to spherical densities with greater numbers of particles than 2. We give the proof for $N=3$ and show how the same approach can be used for up to $N=5$. A new significant feature is involved for the six-particle systems.

We consider the single-particle states which can be occupied in possible ground states. For $N=3$ this amounts to the $1s$, $2s$, $3s$, and $2p$ states where we continue to use the atomic notation to designate the single-particle states. We wish to show that the given density is a ground-state density for some local potential and therefore has the form

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

where the sum extends over the $1s$, $2s$, $3s$, and $2p$ states and the U_{nl} are normalized radial functions for the spherical local potential. The occupation numbers satisfy $0\le\lambda_{nl}\le 2l+1$ and $\sum_{n,l}\lambda_{nl}=3$.

We assume that a potential V_λ can be found for any set of occupation numbers $\boldsymbol{\lambda}=(\lambda_{1s},\lambda_{2s},\lambda_{3s},\lambda_{2p})$. We also assume that the single-particle energies for V_λ are continuous functions of $\boldsymbol{\lambda}$. As we have seen for the two-particle case, merely finding the potential for a given $\boldsymbol{\lambda}$ is not a problem. The difficulty is that in general the order of the energy levels for V_λ will be such that $\rho(r)$ will not be a ground-state density of V_λ, but will correspond to some excited state. We shall show that there is always one choice for $\boldsymbol{\lambda}$ giving a V_λ which has $\rho(r)$ as its ground state.

The strategy of the proof is to select those configurations or $\boldsymbol{\lambda}$ which can correspond to a ground state and then progress through them in a prescribed fashion. We can then show, using general conditions on the order of the energy levels, that there must be a $\boldsymbol{\lambda}$ with a corresponding V_λ for which the order of energy levels is such that $\boldsymbol{\lambda}$ gives the ground-state configuration. General conditions on the levels are

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

so that for any ground state $\lambda_{1s}=1$ and $\lambda_{3d}=0$, and only the distribution of the other two particles among the $2s$, $3s$, and $2p$ levels remains to be considered, which of course, depends on the position of the $2p$ level with respect to the $2s$ and $3s$ levels.

We begin by considering $\boldsymbol{\lambda}_1=(1,0,0,2)$. This would be the ground state if $E_{2s}\ge E_{2p}$, but there can be no assurance that V_{λ_1} gives this order. Let us assume that this is not the ground state so that $E_{2p}>E_{2s}$ at $\boldsymbol{\lambda}_1$. Now consider the $\boldsymbol{\lambda}$ along the line $(1,x,0,2-x)$, with $0\le x\le 1$, from $\boldsymbol{\lambda}_1$ to $\boldsymbol{\lambda}_2=(1,1,0,1)$ and track the $2s$, $3s$, and $2p$ energy levels as functions of x. If for some $x=x_0$ the $2s$ and $2p$ levels cross in a point of accidental degeneracy, then $\boldsymbol{\lambda}_0=(1,x_0,0,2-x_0)$ is the ground state. But if there has been no crossing when $\boldsymbol{\lambda}_2$ has been reached, then at $\boldsymbol{\lambda}_2$, $E_{2p}>E_{2s}$. The point $\boldsymbol{\lambda}_2$ would be the ground state if in addition $E_{3s}\ge E_{2p}$, but let us continue along this line of argument and assume that $\boldsymbol{\lambda}_2$ is not a ground state so that $E_{2p}>E_{3s}>E_{2s}$. The final step is to proceed from $\boldsymbol{\lambda}_2$ to $\boldsymbol{\lambda}_3=(1,1,1,0)$ along the line $(1,1,x,1-x)$, with $0\le x\le 1$. If the $2p$ and $3s$ levels do not cross on the way to $\boldsymbol{\lambda}_3$, so that a ground state has not been encountered in passing from $\boldsymbol{\lambda}_1$ to $\boldsymbol{\lambda}_3$ via $\boldsymbol{\lambda}_2$, then at $\boldsymbol{\lambda}_3$ we must have $E_{2p}>E_{3s}$ and $\boldsymbol{\lambda}_3$ must be the ground state wherever the $2p$ level lies in the region above E_{3s}. In other words, if all else fails the ground state must be $1s,2s,3s$. Any spherical density for three particles is therefore ensemble v-representable.

The proof of ensemble v-representability with $N=4$ and 5 follow along similar lines. For $N=4$ the $4s$ must be added to the set of levels and with $\boldsymbol{\lambda}=(\lambda_{1s},\lambda_{2s},\lambda_{3s},\lambda_{4s},\lambda_{2p})$. The progression through the possible ground states is (1,0,0,0,3), (1,1,0,0,2), (1,1,1,0,1), and finally to (1,1,1,1,0). The $3d$ is involved for $N=5$ (the $3p$ level is not involved in a ground state because it must lie above the $2s$ level), and with $\boldsymbol{\lambda}=(\lambda_{1s},\lambda_{2s},\lambda_{3s},\lambda_{4s},\lambda_{5s},\lambda_{2p},\lambda_{3d})$, and ensemble v-representability of a $\rho(r)$ can be proved easily by following the path (1,0,0,0,0,3,1), (1,1,0,0,0,3,0), (1,1,1,0,0,2,0), (1,1,1,1,0,1,0), (1,1,1,1,1,0,0,).

For $N\le 5$ it was only necessary to consider double degeneracy and possible ground states could be sampled by following a line in $\boldsymbol{\lambda}$ space. The possibility of accidental triple degeneracy of the $3s$, $3p$, and $3d$ levels must be considered for $N=6$, and possible ground states spread over a plane in $\boldsymbol{\lambda}$ space. Triple and higher degeneracies are key features for larger numbers of particles. We have been able to account for the triple degeneracy and carry through the proof of ensemble v-representability for $N=6$ up to 14. These results we shall present in a separate paper. The proof can be extended to larger numbers of particles, but it becomes increasingly laborious for larger N as higher-order degeneracies enter at $N=15$, but it seems likely that a spherical density is ensemble v-representable for any N.

V. DISCUSSION AND CONCLUSIONS

We have shown that any spherical density for $N=2$, 3, 4, or 5 noninteracting spinless fermions is pure state or ensemble v-representable. This means that any reasonable function $\rho(r)$, which is positive definite and integrates to the required N, is the nondegenerate ground-state density or a linear combination of degenerate ground-state densities for some local potential $V(\mathbf{r})$, which itself is spherical. Furthermore, to within an additive constant $V(\mathbf{r})$ is unique. This result supports the general conjecture of Levy and Perdew [3,13,14] that any density is noninteracting ensemble v-representable.

Li and Krieger [12] have also considered the representation of a spherical density for $N=2$ by the ground state of a two-level system, and Nagy and March [11] have discussed representation by two- and three-level systems. These authors suggest that if a potential can be obtained for a given density through solution of the appropriate set of single-particle equations, e.g., Eqs. (2) and (3), then the Kohn-Sham potential for the density has been found. Arasetiawan and Stott [8] explained that this was the case for one-dimensional systems, but not in general for the spherical systems addressed by these authors. The mistake comes about because there is no guarantee that the potential has the chosen set of energy levels for its ground state. However, our results above show that it is always possible to find a set of levels and occupation numbers that yield a potential that has the density for its ensemble ground state.

Degeneracy plays an important role in the proof of ensemble v-representability as we have presented it for systems of two spinless fermions and for the extensions to larger numbers of particles. Two sorts of degeneracy enter. For the spherical densities considered here most of the cases of degeneracy are a direct consequence of the spherical symmetry. The equal occupation of the three degenerate $2p$ levels in the case we have considered is one example. We should expect this degeneracy to be less prevalent for nonspherical densities and absent when there is no special symmetry. The possibility of accidental degeneracy is also important as seen in the case of the Coulomb potential, but it is not restricted to that situation. For nonspherical densities where the degeneracy resulting from symmetry is lifted we should anticipate that the class of functions which are pure-state v-representable is increased and only in the relatively infrequent cases of accidental degeneracy will the density be ensemble ground-state v-representable.

We are encouraged to suggest that the class of functions which are candidates for the ensemble ground-state density of a system of noninteracting fermions is broad and the exceptions are easily excluded on physical grounds.

ACKNOWLEDGMENT

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APPENDIX

Some properties of the solutions of the set of single particle equations for a given density are presented.

Equations (5) can be obtained from a variational principal. Minimization of the kinetic-energy functional

$$T[\theta,\phi]=\int_0^\infty t[\theta,\phi]dr$$
$$=2\pi\int_0^\infty \rho\left[\dot\theta^2+\sin^2\theta\dot\phi^2+\cos^2\theta\frac{2}{r^2}\right]dr \qquad \text{(A1)}$$

with respect to $\theta(r)$ and $\phi(r)$, subject to the constraints

$$\int_0^\infty \rho(r)\sin^2\theta\cos^2\phi\,dr=1\ , \qquad \text{(A2)}$$

$$\int_0^\infty \rho(r)\sin^2\theta\sin^2\phi\,dr=\lambda\ , \qquad \text{(A3)}$$

gives Eqs. (5). That solutions that minimize T exist can be shown by replacing the space by a lattice and applying Weierstrass theorem [18] in the manner used by Aryasetiawan and Stott [8].

In order to show that a density is ensemble v-representable, not only did we assume that a solution to the set of single particle Eqs. (2) could be found for a given λ, but we also assumed that the resulting single-particle energies obtained from V_λ were continuous functions of λ. An interesting result related to this latter assumption follows by applying the Feynman-Hellman theorem to the single-particle energies E_{1s}, E_{2s}, and E_{2p} regarded as functions of λ

$$\frac{dE_{1s}}{d\lambda}+\lambda\frac{dE_{2s}}{d\lambda}+(1-\lambda)\frac{dE_{2p}}{d\lambda}=\frac{d}{d\lambda}\int_0^\infty V_\lambda\rho\,dr\ . \qquad \text{(A4)}$$

Substitution of V_λ in (A4) in terms of ρ, θ, and ϕ using Eq. (6) yields

$$\varepsilon_{2s}+\varepsilon_{2p}=-\frac{dT_m}{d\lambda}\ , \qquad \text{(A5)}$$

where $T_m=T[\theta_m,\phi_m]$ is the value of $T[\theta,\phi]$ at the minimum for a given λ. The result (A5) suggests that T_m is a continuous function of λ because the minimization of Eq. (A1) exists and therefore the energy differences ε_{2s} and ε_{2p} are bounded. If for a given ρ we are able to take the derivative under the integral in Eq. (A5), i.e.,

$$\frac{d}{d\lambda}\int_0^\infty t[\theta_m,\phi_m]dr=\int_0^\infty \frac{d}{d\lambda}t[\theta_m,\phi_m]dr\ , \qquad \text{(A6)}$$

then the solutions of Eqs. (5) will be expected to be continuous functions of λ over range $r=[0,\infty)$ and therefore E_{1s}, E_{2s}, and E_{2p} should be continuous.

The numerical solutions for the specific densities chosen as examples gave us no cause to suspect that the set of equations (5) is not well behaved. The V_λ and the corresponding energies were found without great difficulty and they proved to be smooth functions of λ.

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