Complete functional theory for the fermion density of independent particles subject to harmonic confinement in *d* dimensions for an arbitrary number of closed shells

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(Received 26 June 2002; published 22 November 2002)

In earlier work, expressions have been constructed for the single-particle kinetic-energy functional $T_s[\rho]$ for independent fermions subject to harmonic confinement in low dimensions, with ρ the particle density. Here, the differential equation for ρ is first obtained in d dimensions for an arbitrary number of closed shells. Then, by using the known Euler-Lagrange equation, the functional derivative $\delta T_s/\delta\rho(\mathbf{r})$ is constructed. $T_s[\rho]$ itself is proved to take the form of a linear combination of three pieces: (i) a von Weizsäcker inhomogeneity kinetic energy, but with the original coefficient reduced by a dimensionality factor $1/d$, (ii) a Thomas-Fermi kinetic energy, and (iii) a truly nonlocal contribution that, however, is shown to involve only the density ρ itself and its first derivative. Thus, for this model, which is currently highly relevant to the interpretation of experiments on the evaporative cooling of dilute, and hence almost noninteracting, fermions, a complete density-functional theory now exists.

DOI: 10.1103/PhysRevA.66.054501 PACS number(s): 31.15.Ew, 71.15.Mb

Following earlier experimental studies of the Bose-Einstein condensation in ultracold trapped Bose gases, DeMarco and Jin [1] achieved the evaporative cooling of dilute, and hence almost noninteracting, fermions. Further experimental investigations in Refs. [2–6] add to the motivation for a full theoretical study of many-fermion assemblies that are harmonically confined. The focus in the above experiments was on ultracold vapors of the ^{40}K and ^{6}Li isotopes populating hyperfine states inside magnetic traps. In current experimental approaches, based on axially symmetric magnetic traps, it proves possible to range from a quasi-one-dimensional (1D) trap, through a quasi-2D trap, to a fully spherical 3D trap.

This background, and especially the possibility of exploiting magnetic confinement of many-fermion assemblies having different dimensionality d, has been the prime motivation for the theoretical study to be reported here. The entire focus is on the fermion density ρ, and the theory will be presented for an arbitrary number of closed shells, say $(M+1)$, for general dimensionality of the isotropic harmonic confinement. Thus, $\rho\equiv\rho(r)$, where r is the radial distance from the origin of the confinement in d dimensions. As a starting point, Lawes and March [7] in a very early study gave a third-order linear homogeneous differential equation in 1D, namely

$$-\tfrac{1}{2}\rho(x)V'(x)-(\hbar^2/8m)\,\rho'''=[N\hbar\omega-V(x)]\rho'(x),$$

$$V(x)=m\omega^2x^2/2\,, \tag{1}$$

for N closed shells, where the primes denote spatial derivatives throughout. For uniformity with the notation for dimensionality $d>1$ used below, $N=1$ being the lowest state of Eq. (1), N will be written as $M+1$. This equation (1) was subsequently generalized to 2D by Minguzzi, March, and Tosi [8] to read [their Eq. (11)]

$$(\hbar^2/8m)(\partial/\partial r)\nabla^2\rho(r)+[(M+\tfrac{3}{2})\hbar\omega-V(r)]\rho'(r)+[\partial V(r)/\partial r]\,\rho(r)=0, \tag{2}$$

where the confining potential $V(r)=\frac{1}{2}m\omega^2r^2$. The results (1) and (2) are generalized to d dimensions in the Appendix, where it is argued that

$$(\hbar^2/8m)(\partial/\partial r)\nabla^2\rho(r)+\{[M+(d+1)/2]\hbar\omega-V(r)\}\rho'(r)+(d/2)[\partial V(r)/\partial r]\,\rho(r)=0. \tag{3}$$

To illustrate the basic approach underlying this Brief Report, let us immediately turn to the 2D case of Ref. [8]. There, a result for the (single-particle) kinetic-energy density $t(r)$ was obtained, being expressed in terms of the Thomas-Fermi and von Weizsäcker functionals. Their explicit form was

$$t(r)=\frac{1}{2}t_W(r)+\left[C_2+\frac{\hbar^2}{16m}\int_0^r ds\,\frac{\rho'(s)^2}{\rho(s)^3}\left(\frac{2}{s}+\frac{3\rho'(s)}{\rho(s)}\right)\right]\rho^2(r), \tag{4}$$

with C_2 a constant, where the von Weizsäcker functional is

$$t_W(r)=(\hbar^2/8m)[(\boldsymbol{\nabla}\rho)^2/\rho]\,, \tag{5}$$

while the Thomas-Fermi result is

$$t_{TF}(r)=c_k^{d=2}\rho^2(r),\quad c_k^{d=2}=\pi\hbar^2/m\,. \tag{6}$$

Obviously by integrating Eq. (4) over the whole two-dimensional space, one has $T_s=\int t(r)d^2r$ in terms of $\rho(r)$.

Our first objective therefore is to effect the generalization of this single-particle kinetic-energy expression for $d=2$ to general dimensionality. To do so, we integrate Eq. (3) as a first-order differential equation for the potential energy $V(r)$.

Using an integrating factor, one is led to the result that $V(r)$, within an additive constant, is given in terms of the density $\rho(r)$ for $(M+1)$ closed shells by

$$V(r)=-\frac{\rho^{2/d}}{4d}\int^{r}\frac{1}{\rho^{1+2/d}}\left[\frac{\hbar^2}{m}\frac{\partial}{\partial r}\nabla^2\rho+8\left(M+\frac{d+1}{2}\right)\hbar\omega\frac{\partial\rho}{\partial r}\right]dr, \tag{7}$$

where

$$\nabla^2=(\partial^2/\partial r^2)+[(d-1)/r](\partial/\partial r). \tag{8}$$

In fact Eq. (7) can be directly verified by differentiation to yield Eq. (3). Integration by parts of the final term in Eq. (7) then yields almost immediately

$$V(r)=\left[M+\frac{d+1}{2}\right]\hbar\omega-\frac{\rho^{2/d}}{4d}\frac{\hbar^2}{m}\int^{r}\frac{1}{\rho^{1+2/d}}\frac{\partial}{\partial r}\nabla^2\rho dr. \tag{9}$$

In the Appendix, the differential virial theorem in d dimensions is derived as

$$\partial t/\partial r=-(d/2)\rho(\partial V/\partial r)-(\hbar^2/8m)(\partial/\partial r)\nabla^2\rho. \tag{10}$$

But $\rho^{2/d}\partial\rho/\partial r=(1+2/d)^{-1}\partial\rho^{1+2/d}/\partial r$, and hence one finds for the single-particle kinetic energy $T_s\equiv\int t(r)d^dr$, the result

$$T_s[\rho]=\int_{allspace}\frac{\rho(u)^{1+2/d}}{4(d+2)}\int^{u}\frac{1}{\rho^{1+2/d}}\frac{\partial}{\partial s}\nabla^2\rho\, ds\, du. \tag{11}$$

The constant of integration can be found after some manipulation involving the quotient t'/ρ' (see also the Appendix) in the form

$$t'/\rho'=\{[M+(d+1)/2]\hbar\omega-V(r)\}, \tag{12}$$

and hence one finds

$$t(r)=\frac{d\mu}{d+2}\frac{\rho(r)^{1+2/d}}{\rho(0)^{2/d}}+\frac{\rho(r)^{1+2/d}}{4(d+2)}\int_0^{r}\frac{1}{\rho^{1+2/d}}\frac{\partial}{\partial s}\nabla^2\rho ds-\frac{\hbar^2\nabla^2\rho(r)}{4m(d+2)}, \tag{13}$$

where $\mu=[M+(d+1)/2]\hbar\omega$. As a check of Eq. (13), one can compare with the 1D result of March, Senet, and Van Doren [9], namely

$$t_1(r)=\frac{N\hbar\omega}{3}\frac{\rho^3(r)}{\rho^2(0)}+\frac{\hbar^2\rho^3(r)}{12m}\int_0^{r}\frac{1}{\rho^3(s)}\frac{\partial^3\rho}{\partial s^3}ds-\frac{\hbar^2\rho''}{12m}, \tag{14}$$

which is indeed the special case of Eq. (13) for $d=1$. Obviously from Eq. (13), $T_s[\rho]=\int_{allspace}t(r)d^dr$ through d-dimensional space.

Next one can reduce the order of the derivatives appearing in T_s by repeated integration by parts, and after some considerable manipulation one reaches the desired result for $T_s[\rho]$ in d dimensions:

$$T_s[\rho]=C_d\int\rho(u)^{1+2/d}d^du+\frac{\hbar^2}{8md}\int\frac{\rho'^2(u)}{\rho(u)}d^du+\frac{\hbar^2}{m}\int\rho(u)^{1+2/d}\left[\frac{d-1}{4d}\int_0^{u}\frac{\rho'^2(s)}{s\rho^{2+2/d}}ds+\frac{d+1}{2d(d+2)}\int_0^{u}\frac{\rho'^3(s)}{\rho(s)^{3+2/d}}ds\right]d^du, \tag{15}$$

where

$$C_d=\frac{d}{d+2}\left(M+\frac{d+1}{2}\right)\hbar\omega\frac{1}{\rho^{2/d}(0)}-\frac{\hbar^2}{4m(d+2)}\left[\frac{\nabla^2\rho}{\rho^{1+2/d}}\right]_0-\frac{\hbar^2}{8md}\left[\frac{\rho'^2}{\rho^{2+2/d}}\right]_0, \tag{16}$$

which is the central result of this Brief Report. This is the single-particle kinetic-energy functional $T_s[\rho]$ in d-dimensional harmonic confinement for an arbitrary number $(M+1)$ of closed shells.

The Euler equation of the variational principle for the total energy E given by

$$E=T_s[\rho]+\int\rho Vd^dr, \tag{17}$$

is known to have the form [10]

$$\mu=\delta T_s/\delta\rho(r)+V(r), \tag{18}$$

and we shall next use the known form (3) for the d-dimensional density to extract $\delta T_s/\delta\rho(r)$ from Eq. (18). Obviously, from the Euler equation, we have, again apart from an additive constant,

$$\frac{\delta T_s}{\delta\rho(r)}=\frac{\rho^{2/d}(r)}{4d}\frac{\hbar^2}{m}\int^{r}\frac{1}{\rho^{1+2/d}(s)}\frac{\partial}{\partial s}\nabla^2\rho ds. \tag{19}$$

Repeated integration by parts can be utilized once more to lower the order of the derivatives appearing in Eq. (19). One then finds for the integral appearing in Eq. (19) the equivalent form

$$\int^r \frac{1}{\rho^{1+2/d}(s)}\frac{\partial}{\partial s}\nabla^2\rho ds$$

$$=\frac{\nabla^2\rho(r)}{\rho^{1+2/d}(r)}+(d-1)(1+2/d)\int^r \frac{\rho'^2(s)}{s\rho^{2+2/d}}ds$$

$$+\frac{(1+2/d)}{2}\left[\frac{\rho'^2}{\rho^{2+2/d}}+\int^r \frac{\rho'^3(s)(2+2/d)}{\rho^{3+2/d}(s)}ds\right]. \quad (20)$$

Hence we reach the desired form for $\delta T_s/\delta\rho(r)$, which, we must emphasize, we have extracted using (a) the Euler equation (18), and (b) the known differential equation (3) for the fermion density $\rho(r)$ for harmonic confinement in d dimensions. Evidently, combining Eqs. (19) and (20) yields

$$\frac{\delta T_s}{\delta\rho(r)}=\frac{\hbar^2}{4md}\frac{\nabla^2\rho(r)}{\rho(r)}+\frac{(1+2/d)}{2}\frac{\hbar^2}{m}\frac{\rho'^2}{\rho^2}$$

$$+(d-1)(1+2/d)\rho^{2/d}(r)\frac{\hbar^2}{m}\int^r \frac{\rho'^2(s)}{s\rho^{2+2/d}}ds$$

$$+\frac{\hbar^2(1+2/d)}{2m}\rho^{2/d}(r)\int^r \frac{\rho'^3(s)(2+2/d)}{\rho^{3+2/d}(s)}ds. \quad (21)$$

To confirm the structure of this equation (21) for the functional derivative $\delta T_s/\delta\rho(r)$ in d dimensions, let us write it explicitly for the 1D case. Then we find

$$\frac{\delta T_s}{\delta\rho(x)}=\frac{\hbar^2}{4m}\frac{\rho''(x)}{\rho(x)}+\frac{3\hbar^2}{2m}\frac{\rho'^2}{\rho^2}+6\rho^2(x)\frac{\hbar^2}{m}\int^x \frac{\rho'^3(s)}{\rho^5(s)}ds, \quad (22)$$

which is readily shown by integrating the von Weizsäcker energy density [Eq. (5)]

$$T_W=\frac{\hbar^2}{8m}\int \frac{(\boldsymbol{\nabla}\rho)^2}{\rho}d^dr\equiv\int t_W(r)d^dr \quad (23)$$

to have the form

$$\frac{\delta T_s}{\delta\rho(x)}=\frac{13}{8}\frac{t_W}{\rho}-\frac{\delta T_W}{\delta\rho(x)}+6\rho^2(x)\frac{\hbar^2}{m}\int^x \frac{\rho'^3(s)}{\rho^5(s)}ds, \quad (24)$$

which exhibits clearly the terms having their origin in the von Weizsäcker energy density (23), plus a truly nonlocal part involving, however, only the fermion density $\rho(x)$ and its first derivative.

In summary, the experiment of DeMarco and Jin [1] on harmonically confined fermions has motivated this theoretical study. What has emerged for harmonic confinement is the exact result (15) for the single-particle kinetic energy, which requires only the fermion density $\rho(r)$ for d dimensions with $(M+1)$ closed shells for its evaluation. We have also been able to extract the functional derivative $\delta T_s/\delta\rho(r)$ by invoking the known differential equation for the particle density, in addition to the (constant) chemical potential (Euler) equation (18). Thus, it is fair to claim that the experiments in Refs. [1–6] have motivated a full density-functional theory in d dimensions for harmonically confined independent fermions, for an arbitrary number of closed shells.

APPENDIX

The purpose of this appendix is to confirm the d-dimensional result (3) for the ground-state density $\rho(r)$ for $(M+1)$ closed shells with an isotropic harmonic confinement. We find it instructive to consider the Slater sum $Z(\mathbf{r},\beta)$ defined as

$$Z(\mathbf{r},\beta)=\sum_{all\ i}\psi_i^*(\mathbf{r})\psi_i(\mathbf{r})\exp(-\beta\epsilon_i),\quad \beta=(k_BT)^{-1}, \quad (A1)$$

where the $\psi_i(\mathbf{r})$ are the eigenfunctions, with corresponding eigenvalues ϵ_i, generated by the one-body Hamiltonian $H_{\mathbf{r}}$ defined by

$$H_{\mathbf{r}}=-(\hbar^2/2m)\nabla_{\mathbf{r}}^2+V(\mathbf{r}). \quad (A2)$$

The corresponding Dirac density matrix $\gamma(\mathbf{r},\mathbf{r}_0)$ used below is the off-diagonal generalization

$$\gamma(\mathbf{r},\mathbf{r}_0)=\sum_{i\ occ}\psi^*(\mathbf{r})\psi(\mathbf{r}_0). \quad (A3)$$

From the early work of Sondheimer and Wilson [11], one can then write $Z(r,\beta)$ exactly for d-dimensional harmonic confinement as

$$Z(r,\beta)=(m\omega/2\pi\hbar)^{d/2}[1/\sinh^{d/2}(\beta\hbar\omega)]$$
$$\times\exp[-(m\omega/\hbar)r^2\tanh(\beta\hbar\omega/2)]. \quad (A4)$$

It follows that the differential equation with solution given by Eq. (A4) can be written as

$$\frac{\hbar^2}{8m}\frac{\partial}{\partial r}(\nabla^2 Z)-\left[\frac{\partial}{\partial\beta}+V(r)\right]\frac{\partial Z}{\partial r}-\frac{(d-2)}{2}\frac{\partial V}{\partial r}Z=0, \quad (A5)$$

where here $V(r)=m\omega^2r^2/2$. We next define the "canonical kinetic-energy density" $t_C(\mathbf{r},\beta)$ as

$$t_C(\mathbf{r},\beta)\equiv(-\hbar^2/2m)\nabla_r^2C(\mathbf{r},\mathbf{r}_0,\beta)|_{\mathbf{r}_0=\mathbf{r}}, \quad (A6)$$

with $C(\mathbf{r},\mathbf{r}_0,\beta)$ as the canonical density matrix. But since

$$\nabla_r^2C(\mathbf{r},\mathbf{r}_0,\beta)|_{\mathbf{r}_0=\mathbf{r}}=\beta\int_0^\infty\nabla_r^2\gamma(\mathbf{r},\mathbf{r}_0)\exp(-\beta E)dE$$

$$=-\frac{2m\beta}{\hbar^2}\int_0^\infty t(\mathbf{r},E)\exp(-\beta E)dE, \quad (A7)$$

it follows that

$$t_C(\mathbf{r},\beta)=\beta\int_0^\infty t(\mathbf{r},E)\exp(-\beta E)dE, \quad (A8)$$

and therefore, from the Bloch equation $H_{\mathbf{r}}C(\mathbf{r},\mathbf{r}_0,\beta)=-\partial C/\partial\beta$ and the definition of $H_{\mathbf{r}}$, it follows that

$$t_C(r,\beta)=-(\partial Z/\partial\beta)-V(r)Z(r,\beta), \quad (A9)$$

and thus

$$\partial t_C/\partial r = -VZ' - V'Z - (\partial Z'/\partial \beta) \tag{A10}$$

for an arbitrary dimensionality d. Using Eq. (A5) to eliminate the β derivative in Eq. (A10), we find that

$$\partial t_C/\partial r = -(\hbar^2/8m)(\partial/\partial r)\nabla^2 Z - (d/2)V'Z. \tag{A11}$$

This can immediately, by inverse Laplace transform, be written as a differential virial theorem relating t, ρ, and V:

$$\partial t/\partial r = -(\hbar^2/8m)(\partial/\partial r)\nabla^2\rho - (d/2)V'\rho. \tag{A12}$$

If we define for convenience an ''averaged'' kinetic-energy density $\overline{t} = t + (\hbar^2/8m)\nabla^2\rho$ (the average of the $|\psi'|^2$ and $\psi\nabla^2\psi$ definitions of kinetic-energy density), we can write the above as

$$\partial\overline{t}/\partial r = -(d/2)V'\rho; \tag{A13}$$

then it follows from Eq. (A11) that we can also write correspondingly

$$\partial\overline{t_C}/\partial r = -(d/2)V'Z, \tag{A14}$$

or, dividing by Z',

$$\partial\overline{t_C}/\partial r/Z' = -(d/2)V'(Z/Z'). \tag{A15}$$

But Z'/Z is found from the Sondheimer-Wilson form (A4) for Z to be such that

$$Z'/Z = -2\omega r \tanh(\beta\omega/2), \tag{A16}$$

which is independent of the dimensionality d. Thus, from Eq. (A15), $\overline{t_C{}'}/Z'$ is proportional to d. This is a vital result for establishing the desired ground-state equation for $(M+1)$ closed shells, namely Eq. (12), since it has already been verified for $d=1,2$, and 3 for arbitrary M.

We will establish, in concluding this appendix, the linearity in d for two closed shells using the Dirac density matrices γ in Eq. (A3), calculated by inserting harmonic-oscillator wave functions. These are readily obtained for $d=1-4$ and give

$$\gamma(\xi,\eta) = \gamma\left(\frac{|\mathbf{r}+\mathbf{r}_0|}{2},\frac{|\mathbf{r}-\mathbf{r}_0|}{2}\right) = \left(\frac{m\omega}{\hbar\pi}\right)^{d/2}\exp\left[-\frac{m\omega}{\hbar}(\xi^2+\eta^2)\right]\left[1+2\frac{m\omega}{\hbar}(\xi^2-\eta^2)\right]. \tag{A17}$$

Hence, for instance, the ratio of γ for $d=4$ to the result for $d=1$ is

$$\gamma_4(\xi,\eta)/\gamma_1(\xi,\eta) = \text{const}, \tag{A18}$$

and thus

$$\rho_4/\rho_1 = (m\omega/\hbar\pi)^{3/2}. \tag{A19}$$

The corresponding kinetic-energy density is readily obtained from the differential virial theorem to yield

$$\overline{t_4{}'}/\overline{t_1{}'} = d\rho_4/\rho_1 = d\rho_4'/\rho_1', \tag{A20}$$

with $d=4$. For this example, the linearity in d is established, which is the counterpart of Eq. (A15) for the canonical kinetic-energy density.

To relate Eq. (A20) to Eq. (12) we need, from the line below Eq. (A12), $(\hbar^2/8m)\nabla^2\rho$ to go from $\overline{t}$ to t. This is easily found by putting $\eta=0$ in Eq. (A17) to find $\rho(\xi)$. To prove Eq. (12) in this example, we use

$$\overline{t_4{}'}/\rho_4' = 4\overline{t_1'}/\rho_1' \tag{A21}$$

and insert t_4', t_1', and the associated Laplacian terms to obtain

$$\frac{t_4'}{\rho_4'} - \frac{t_1'}{\rho_1'} = \left[\frac{\overline{t_4{}'}}{\rho_4'} - \frac{\hbar^2}{8m\rho_4'}\frac{\partial}{\partial r}\nabla^2\rho_4\right] - \left[\frac{\overline{t_1{}'}}{\rho_1'} - \frac{\hbar^2}{8m\rho_1'}\frac{\partial}{\partial r}\nabla^2\rho_1\right] = 3\frac{t_1'}{\rho_1'} - \frac{\hbar^2}{8m\rho_4'}\frac{\partial}{\partial r}\nabla^2\rho_4 + \frac{\hbar^2}{2m\rho_1'}\frac{\partial}{\partial r}\nabla^2\rho_1 = \frac{3\omega}{2}, \tag{A22}$$

as predicted by Eq. (12). Thus, for $M=1$, this example reproduces Eq. (12) for $d=1$–4.

N.H.M. acknowledges some financial support from the Francqui Foundation. Thanks are due especially to the Executive Director, Professor L. Eyckmans, for his help and encouragement. I.A.H. wishes to acknowledge support from the Flemish Science Foundation (FWO) under Grant No. G.0347.97, and from the IWT—Flemish region. We also thank the University of Antwerp (RUCA) for its support in the framework of the Visiting Professors Program. This work was also supported by the Concerted Action Program of the University of Antwerp, by the Spanish DGES (Grant No. PB98-0370), and Junta de Castilla y León (Grant No. CO2/199).

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