Stability of the high-density ferromagnetic ground state of a chargeless, magnetic-dipolar, quantum Fermi liquid

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We obtain the best upper bound for the ground-state energy of a system of chargeless fermions of mass m, spin $s=1/2$, and magnetic moment $\mu\vec{s}$ as a function of its density in the fully spin-polarized Hartree-Fock determinantal state, specified by a prolate spheroidal plane-wave single-particle occupation function $n_{\uparrow}(\vec{k})$, by minimizing the total energy E at each density with respect to the variational spheroidal deformation parameter $\beta_2, 0 \leqslant \beta_2 \leqslant 1$. We find that at high densities, this spheroidal ferromagnetic state is the most likely ground state of the system, but it is still unstable towards the infinite-density collapse. This optimized ferromagnetic state is shown to be a stable ground state of the dipolar system at high densities, if one has an additional repulsive short-range hardcore interaction of sufficient strength and nonvanishing range.

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The nature of lowest-energy configurations of classical magnetic dipoles fixed on different types of three-dimensional lattices has been studied for a long time [1]. However, the problem of magnetic dipolar quantum Fermi liquid consisting of N particles in volume V_0, of mass m, spin s and magnetic moment $\mu\vec{s}$, with no electric charge, did not attract enough attention in the past. Although, it was expected [2] that even in the quantum Fermi liquid case, having an additional large positive kinetic energy contribution, such a system would be unstable towards an infinite-density collapse, i.e., its total energy per particle $E/N \to -\infty$, as its density $N/V_0 \equiv [3/(4\pi r_0^3)] \to \infty$, we did not come across any detailed study of the nature of its possible high density ground state before the collapse, and how such a system can get stabilized. Recently [3], within the framework of nonrelativistic quantum theory we tried to obtain upper bounds for E/N of such a system as a function of the average interparticle distance r_0, using different forms of variational single-determinant N-particle Hartree-Fock (HF) wave functions. As shown by Lieb [4], unless the particle-particle interaction is repulsive everywhere, which is not the case for the dipole-dipole interaction, one can indeed obtain upper bounds for the ground-state energy if one uses such variational HF functions and not any arbitrary variational positive semidefinite single-particle density matrix [5], which is allowed for variational calculations in the case of the Coulomb interaction between electrons. The problem of ferromagnetism in chargeless magnetic dipolar systems originally attracted our attention in the context of the possibility of ferromagnetism in high density neutrino gas of the early universe, proposed [5] by Yajnik. However, we feel that this is an important problem in many body physics, in itself, and it should be of intrinsic interest to those who study new quantum states of exotic matter or the nature of different interacting fermionic systems, such as quantum dipolar spin liquids and dipolar spin ice systems (see the second paper in Ref. [1]) on a lattice.

For the dipolar system of spin-1/2 particles, using plane waves for the spatial part of single particle states, labeled by the wave vector $\vec{k}$ and spin $\sigma=\uparrow$ or $\downarrow$, we showed [3] that a fully polarized ferromagnetic state with prolate spheroidal occupation function $n_{\uparrow}(\vec{k})=\Theta\{k_{F\uparrow}^2-k^2[1-\beta_2 P_2(\cos\theta_{\hat{k}})]\}$, $P_2(\mu)=(3\mu^2-1)/2$, $0<\beta_2<1$, gives better upper bounds for E/N at high densities compared to other chosen N-particle determinantal HF wave functions, and, as expected, the system was unstable towards the infinite density collapse. Here, $k_{F\uparrow}$ is related to the density N/V_0 and the deformation parameter β_2 due to the fact that the sum over the occupation function must give the total number N of the particles, and $\Theta(x)$ is the usual unit step function. The above analysis was, however, presented only for fixed values of the deformation parameter β_2 in the spheroidal ferromagnetic state, called the JM ferromagnetic state for the purpose of identification, using the small-β_2 approximation. In this paper, we present exact analytical results for the variational ground state energy of the dipolar Fermi liquid in the JM ferromagnetic state at each density for any arbitrary allowed value of the deformation parameter $0 \leqslant \beta_2 \leqslant 1$ and obtain the optimum value $\beta_2^*(r_0)$ of the parameter which gives the lowest upper bound for the energy at that density. Such a variational minimization is crucial to get a correct picture of the nature of the infinite density collapse of E/N in the JM state because in this state the positive kinetic energy contribution $E_{\text{kin}}[\beta_2^*(r_0)]/N$ is found to have a high-density singularity of the type $r_0^{-2}[1-\beta_2^*(r_0)]^{-2/3}$. This leads to the best variational upper bound for the energy in the JM ferromagnetic state as a function of the density parameter r_0, and allows us to determine the actual value of the exponent ν, in the expression $E/E_{\text{kin}}=[1-Cr_0^{-\nu}]$, $C>0$, in the limit $r_0 \to 0$. The exponent ν has to be positive for the infinite density collapse. With this optimum deformation function $\beta_2^*(r_0)$ in the JM ferromagnetic state, we also show how the addition of a suitable short range repulsive hardcore interaction between the particles to

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the dipolar Hamiltonian leads to a stable equilibrium density curve for E/N.

The Hamiltonian for the magnetic dipolar system being considered here is given by [5,3]

$$H=\sum_{i=1}^{N} p_i^2/2m+\sum_{i<j}^{N}\sum^{N} V(\vec{r}_i\vec{s}_i,\vec{r}_j\vec{s}_j), \quad (1)$$

$$V(\vec{r}_1\vec{s}_1,\vec{r}_2\vec{s}_2)=(\mu^2/r^3)[\vec{s}_1\cdot\vec{s}_2-3\vec{s}_1\cdot\hat{r}\vec{s}_2\cdot\hat{r}]$$
$$=(\mu^2/r^3)\sum_{M=-2}^{+2} C_{-M}Y_{2,-M}(\hat{r})N_{12}^{(M)}(\vec{s}_1,\vec{s}_2), \quad (2)$$

$$V_{12}(\vec{q})\equiv\int d^3r e^{-i\vec{q}\cdot\vec{r}}V(\vec{r}_1\vec{s}_1,\vec{r}_2\vec{s}_2)$$
$$=\mu^2\sum_{M=-2}^{+2} h_{-M}N_{12}^{(M)}(\vec{s}_1,\vec{s}_2)Y_{2,-M}(\hat{q})\{1-\delta_{\vec{q},0}\}, \quad (3)$$

where $\vec{r}=\vec{r}_1-\vec{r}_2$, $r=|\vec{r}|$, $\hat{r}=\vec{r}/r$, $\hat{q}=\vec{q}/q$, C_{-M} and h_{-M} are numerical constants, and $N_{12}^{(M)}(\vec{s}_1,\vec{s}_2)$ are two-particle spin operators [5]. While finding the expectation value of the dipole-dipole interaction in a given determinantal HF wave function, only the $M=0$ term contributes, for which $C_0=-(16/\pi)^{1/2}$, $h_0=(4\pi/3)(16/\pi)^{1/2}$, and

$$\bar{N}_{12}^{(0)}(\sigma_1,\sigma_2)\equiv\langle\sigma_2(\vec{s}_1)\sigma_1(\vec{s}_2)|N_{12}^{(0)}|\sigma_1(\vec{s}_1)\sigma_2(\vec{s}_2)\rangle$$
$$=\frac{1}{4}\delta_{\sigma_1,\sigma_2}-\frac{1}{4}(\delta_{\sigma_1,\downarrow}\delta_{\sigma_2,\uparrow}+\delta_{\sigma_1,\uparrow}\delta_{\sigma_2,\downarrow}). \quad (4)$$

We construct any N-particle single determinant HF wave function Ψ_N by choosing N occupied single particle space-spin wave functions $\langle\vec{r}\vec{s}|\vec{k}\rangle=(1/V_0)^{1/2}\exp(i\vec{k}\cdot\vec{r})\chi_\sigma(\vec{s})$. In order to specify a particular Ψ_N, it is enough to know the corresponding values of the occupation function $n_\sigma(\vec{k})$ which is 1 (0) if the single particle state $|\vec{k}\sigma\rangle$ is occupied (unoccupied), with

$$\sum_{\vec{k},\sigma} n(\vec{k})=\sum_\sigma V_0\int(d^3k/8\pi^3)n_\sigma(\vec{k})=N. \quad (5)$$

For any chosen Ψ_N, as described above, the variational energy of the dipolar system is then given by

$$E=\langle\Psi_N|H|\Psi_N\rangle=E_{\rm kin}+E_{\rm exch}, \quad (6)$$

$$E_{\rm kin}=\sum_{\vec{k}\sigma}(\hbar^2k^2/2m)n_\sigma(\vec{k}), \quad (7)$$

$$E_{\rm exch}=-\mu^2\left(\frac{4\pi}{3}\right)\frac{1}{V_0}\sum_{\vec{k}}\sum_{\vec{q}}\sum_{\sigma_1}\sum_{\sigma_2} n_{\sigma_1}(\vec{k}+\vec{q})n_{\sigma_2}(\vec{k})$$
$$\times P_2(\cos\theta_{\hat{q}})\bar{N}_{12}^{(0)}(\sigma_1,\sigma_2). \quad (8)$$

Note that there is no direct interaction term contribution to the energy because $V_{12}(\vec{q})$ vanishes for $\vec{q}=0$, and the exchange term $E_{\rm exch}$ also vanishes if (i) $n_\uparrow(\vec{k})=n_\downarrow(\vec{k})=n(\vec{k})$ or (ii) $n_\sigma(\vec{k})=n_\sigma(|\vec{k}|)$. It is, therefore, necessary to assume $n_\uparrow(\vec{k})\neq n_\downarrow(\vec{k})$ and take $n_\sigma(\vec{k})$ to be nonspherical to obtain any finite negative contribution from the exchange energy, which may be at the expense of increasing the positive kinetic energy contribution. For the particular case of spherical occupation function, only the positive kinetic energy term contributes to the total energy with its minimum value E_0 given by the familiar expression for the paramagnetic state for free spin-half Fermi particles

$$E_0\equiv N(3/5)(\hbar^2/2m)k_{F0}^2\cong N(\hbar^2/2m)\frac{(2.21)}{r_0^2}. \quad (9)$$

As stated earlier, the most likely N-particle determinantal wave function which gives the best upper bound to the ground-state energy at high densities is the fully polarized JM ferromagnetic state with a prolate spheroidal form for the occupation function. This state is specified by the occupation function $n_\sigma(\vec{k})=\delta_{\sigma,\uparrow}n_\uparrow(\vec{k})$, with

$$n_\uparrow(\vec{k})=\Theta\left(1-\frac{(k_x^2+k_y^2)}{k_{Fx}^2}-\frac{k_z^2}{k_{Fz}^2}\right)$$
$$=\Theta(k_{F\uparrow}^2-k^2[1-\beta_2P_2(\cos\theta_{\hat{k}})]), \quad (10)$$

$$k_{Fx}^2=k_{Fy}^2=k_{F\uparrow}^2/(1+\beta_2/2),\quad k_{Fz}^2=k_{F\uparrow}^2/(1-\beta_2),\quad k_{Fz}^2\geqslant k_{Fx}^2, \quad (11)$$

$$k_{F\uparrow}^3=6\pi^2[(1+\beta_2/2)(1-\beta_2)^{1/2}]N/V_0,\quad 0\leqslant\beta_2\leqslant 1. \quad (12)$$

In the JM state, for any β_2 we are able to obtain here the following exact analytic expressions for the kinetic energy as well as exchange energy contributions

$$E_{\rm kin}=E_0[(2)^{2/3}(1-\beta_2/2)(1+\beta_2/2)^{-1/3}(1-\beta_2)^{-2/3}], \quad (13)$$

$$E_{\rm exch}=-E_0\Bigg[\frac{1}{4\times(2.21)}\frac{r_m}{r_0}\frac{1}{\beta_2}\times\Bigg\{1-(1+\beta_2/2)(1-\beta_2)^{1/2}(2/(3\beta_2))^{1/2}\times\sin^{-1}\left(\frac{3\beta_2}{(2+\beta_2)}\right)^{1/2}\Bigg\}\Bigg], \quad (14)$$

where the magnetic length $r_m\equiv(2m/\hbar^2)\mu^2$. The optimum value of the variational deformation parameter β_2 is obtained by minimizing $E=E_{\rm kin}+E_{\rm exch}$ with respect to β_2, at each density, i.e., for each density parameter $r_{0m}\equiv r_0/r_m$. This leads to the required optimum value of the deformation parameter, to be called $\beta_2^*(r_{0m})$, as a function of the density parameter r_{0m}. This function is plotted in Fig. 1. We see that at low densities $\beta_2^*(r_{0m})$ is very small compared to 1, whereas at high densities $\beta_2^*(r_{0m})$ is close to 1, i.e., $t^*(r_{0m})\equiv 1-\beta_2^*(r_{0m})$ is small compared to 1. In fact, in these two limiting cases expressions in Eqs. (13) and (14) get greatly simplified. We find (i) $\beta_2\ll 1$:

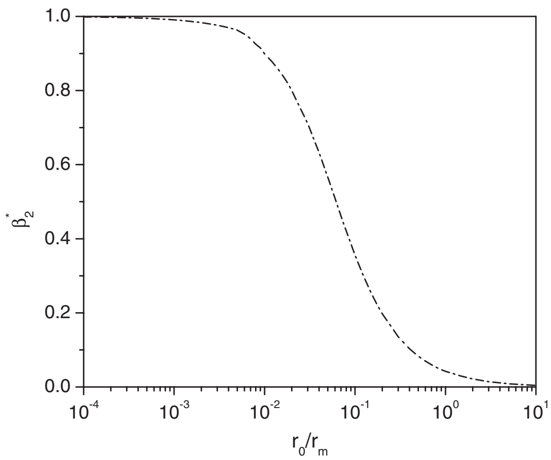

FIG. 1. Plot of the optimum variational deformation parameter β_2^* as a function of the density parameter r_0/r_m, in the spheroidal JM ferromagnetic state of the magnetic dipolar system.

$$E/E_0 \to 2^{2/3}(1+\beta_2^2/4) - \frac{3}{40\times(2.21)}\frac{1}{r_{0m}}(\beta_2+5\beta_2^2/14), \tag{15}$$

$$\beta_2^*(r_{0m}) \to 0.04275[r_{0m}-5/7\times(0.04275)]^{-1}, \quad \text{valid for } r_{0m} \gg 0.1, \tag{16}$$

(ii) $t=1-\beta_2 \ll 1$:

$$E/E_0 \to \frac{1}{(3)^{1/3}t^{2/3}} - \frac{1}{4\times(2.21)}\frac{1}{r_{0m}}[1-(3/2)^{1/2}(\pi/2)t^{1/2}+2t], \tag{17}$$

$$t^*(r_{0m}) = 1-\beta_2^*(r_{0m}) \to 3.4552(r_{0m})^{6/7}, \quad \text{valid for } r_{0m} \ll 0.1. \tag{18}$$

Thus, at high densities as we approach the infinite density collapse, in the JM ferromagnetic state we find that E_{kin}/N varies as $(+)r_0^{(-2-4/7)}$ and E_{exch}/N varies as $(-)r_0^{-3}$. Explicitly, as $r_0 \to 0$, we get

$$E/E_{\text{kin}} = [1-C(r_0)^{-\nu}], \quad \text{with } \nu=3/7 \quad \text{and } C=0.373(r_m)^{\nu}. \tag{19}$$

Since $\nu > 0$, the infinite density collapse of the dipolar liquid remains real. The large spheroidal deformation of the fully spin polarized Fermi sphere makes the divergence of the positive kinetic energy stronger, but not strong enough to dominate the diverging dipolar exchange energy. Note that the high-density variation of the kinetic energy does not violate the bound for fermionic kinetic energy derived by Lieb and Thirring [6]. The curve in Fig. 2, labeled by $\Gamma_{cm}=0$, gives the plot of E/E_0 in the JM ferromagnetic state as a function of the density parameter $r_{0m}=r_0/r_m$, with the optimum deformation parameter $\beta_2^*(r_{0m})$ at each density. This, of course, gives much lower upper bound at each density for the energy of the dipolar system compared to earlier results [3] obtained for fixed values of β_2.

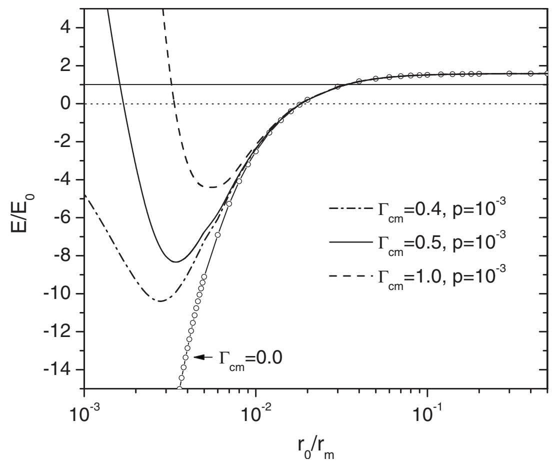

FIG. 2. Plots for the total ground-state energy E in the spheroidal JM ferromagnetic state for the magnetic dipolar system in the units of the paramagnetic free fermion energy E_0, as a function of the density parameter r_0/r_m, with the hardcore range parameter $p \equiv a/r_m = 10^{-3}$; $r_m \equiv (2m\mu^2/\hbar^2)$. The curves are for different values of the ratio of the hardcore and dipolar coupling constants $\Gamma_{cm} \equiv U_0 a^3/\mu^2$, including the case in which $\Gamma_{cm}=0$.

To stop the infinite density collapse of the dipolar system, one has to add a repulsive hardcore interaction between the particles at very short distances, which may originate from some higher-level theories valid at very short distances involving appropriate relativistic quantum field theory depending upon the nature of the particles. Here, we add it to the dipolar Hamiltonian given by Eqs. (1)–(3), as a phenomenological interaction, working still within the framework of the nonrelativistic quantum mechanics. We have considered different forms for the central hard core repulsive interaction $V_C(r)$ to obtain a stable JM ferromagnetic state, which include the usual three-dimensional repulsive square-barrier [3,7] of strength U_0 and range a. If we adjust the numerical constants such that for each form of the hardcore interaction, its Fourier transform at $\vec{q}=0$, $V_C(\vec{q}=0)$, is equal to $(4\pi/3)U_0 a^3$, all those forms lead to similar results for the stability of the dipolar system as long as the ratio of the hardcore and dipolar coupling constants $\Gamma_{cm} \equiv U_0 a^3/\mu^2$ is not very small compared to 1 and the range a in the units of r_m does not vanish. For the case of vanishing range of the hardcore potential, in the fully polarized JM ferromagnetic case the direct and the exchange terms arising from the hardcore will cancel each other, as is the case for the conventional fully polarized ferromagnetic state with a delta-function interaction. For definiteness, we present here our results only for the square barrier potential, for which

$$V_C(r) = U_0, \quad r \le a; V_C(r) = 0, \quad r > a;$$

$$V_C(\vec{q}) = (4\pi U_0 a^3/3)[(3\sin qa - 3qa\cos qa)/q^3a^3]. \tag{20}$$

For this case, using the optimized JM ferromagnetic state with the deformation function $\beta_2^*(r_{0m})$ obtained earlier for the purely dipolar case, we find the following form for additional contribution to the energy

$$E_C/E_0 = \frac{\Gamma_{cm}}{r_{0m}}[19.2/(27\pi)][W_{C,\text{direct}} - W_{C,\text{exch}}(p/r_{0m},\beta_2^*)],$$

$$p \equiv a/r_m, \quad \Gamma_{cm} \equiv \frac{U_0 a^3}{\mu^2}, \tag{21}$$

$$W_{C,\text{direct}} = (1+\beta_2^*/2)(1-\beta_2^*)^{1/2}\int_0^1 \frac{d\mu}{[1-\beta_2^*(3\mu^2-1)/2]^{3/2}} = 1. \tag{22}$$

The direct positive contribution from the hardcore interaction is independent of the deformation parameter $\beta_2^*(r_{0m})$ and the range a, as displayed in Eq. (22). We also have the exact form for the negative hardcore exchange contribution, but here it is enough to state that its magnitude is always less than the direct contribution if the range a of the interaction is finite.

In Fig. 2, we plot the ratio of total energy E and E_0, including the kinetic energy part, the dipolar exchange part and the total of the direct and exchange parts from the hardcore interaction, as a function of the density parameter $r_{0m} = r_0/r_m$. Plots are for different values of the ratio of the coupling constants Γ, including its value 0 representing the energy of the dipolar system in the absence of the hardcore interaction, with the range parameter of the hardcore interaction $p = a/r_m$ taken to be 10^{-3}, as an example. There is no longer any infinite density collapse of the quantum dipolar Fermi liquid in the presence of the repulsive short-range hardcore interaction of sufficient strength and nonvanishing range.

In summary, we have obtained the best variational bound on the energy of a dipolar quantum fluid using a single determinant spheroidal ferromagnetic HF state with or without a hardcore repulsion. In the absence of the hardcore repulsion, the system collapses (energy/particle $\to -\infty$) to an infinite density state due to the dominance of the negative dipolar energy over the positive kinetic energy. However as the system collapses it tends to polarize the particles in the momentum space, i.e., the particles tend to move in the z direction resulting from the limiting form of the spheroidal deformation $[\beta_2^*(r_0) \to 1$, as $r_0 \to 0]$ of the occupied fully spin polarized Fermi sphere. The effect of this optimum deformation at very high densities is to change the nature of the singularity of the kinetic energy, from $1/r_0^2$ to $1/r_0^{(2+4/7)}$ as $r_0 \to 0$, without affecting (in the leading order) the negative dipolar exchange energy, which still varies as $1/r_0^3$ in this limit. The inclusion of hardcore repulsion of sufficient strength arrests the high-density collapse. However one needs a finite repulsive length scale (range a) for this to be true. As it is clear from the curve for $\Gamma_{cm}=0$ in Fig. 2, the fully polarized JM ferromagnetic state is not the correct ground state for the purely dipolar system in the low density limit ($r_{0m} > 2 \times 10^{-2}$). At sufficiently low densities, even the paramagnetic state corresponding to free fermions, with energy E_0, gives a better upper bound than the energy in the JM ferromagnetic case. In the low density limit, the lowest upper bound for the ground-state energy may correspond to particles in the system localized on a suitable three-dimensional lattice with spin configurations which may be similar to the classical results of Luttinger and Tisza [1], but we must reanalyze and correct those results by adding positive contributions from the corresponding zero point energy associated with spin fluctuations. Note that in our units, for proper comparison their [1] μ has to be changed to $\mu/2$. We plan to investigate this interesting case of the possible cross over, in the future.

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