Ground state of a low-density aggregate of deuterons in a uniform magnetic field

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Working in second quantization, the ground-state energy and eigenfunction of an interacting aggregate of N spin-1 deuterons confined to a volume Ω in a charge-neutralizing background and immersed in a uniform magnetic field B is estimated. The analysis is appropriate to the low-density limit in which magnetic-field energy is large compared to particle-particle and spin-spin interaction energies. The resulting ground-state energy is given by $E_G \approx N\hbar\omega_c/2 + N(N-1)(e^2 b_c/\Omega^{2/3})\Gamma + N\Phi - \mu_D BN - \gamma f \mu_D^2[N(N-1)/2]$, where ω_c is deuteron cyclotron frequency, b_c is a characteristic magnetic-field length, Φ is background potential, μ_D is the deuteron magnetic moment, Γ represents a nondimensional interaction integral and the constants f,γ model spin-spin correlation and deuteron-deuteron overlap, respectively. The coordinate component of the ground-state wave function is a product of Gaussian forms whereas the spin component is the product of single-particle spin functions corresponding to spins aligned with the imposed magnetic field.

Introduction. The nature of the ground state of an aggregate of deuterons in a steady magnetic field comes into play in the study of hydrogen-rich planets[1–3] and, with respect to the Bose property of deuterons, the possibility of deuteron superfluidity.[4] This study also finds application to a Bose field of spin-aligned hydrogen[5,6] as well as to properties of interstellar pockets of deuterium.[7]

For the most part, many-body studies in the past have addressed spin-zero bosons relevant to superfluidity or spin-$\frac{1}{2}$ fermions relevant to superconductivity as well as Ising modeling of magnetic properties.[8–12] In a number of previous works[13–18] it was shown that a state exists for a collection of spin-zero bosons interacting through a two-body scalar potential which is spatially homogeneous. In the present work this configuration is extended to the case in which particles have spin one and interact with a uniform, constant magnetic field. It is further assumed that the spatial extent of the system is large but finite thereby limiting the magnetic energy to a finite value. The system includes a neutralizing background charge density ensuring overall charge neutrality.

The present study is relevant to a low-density aggregate of deuterons with spin-spin interaction and interparticle interaction energies small compared to magnetic-field energy. Estimates of the ground-state energy and wave function are obtained in this limit.

Starting equations. Our starting Hamiltonian is given by

$$H(\mathbf{r}_i,\ldots,\mathbf{r}_N;\mathbf{S}_1,\ldots,\mathbf{S}_N)=\sum_{i=1}^{N}\frac{1}{2M}\left[\mathbf{p}_i-\left[\frac{e}{c}\right]\mathbf{A}(\mathbf{r}_i)\right]^2+N\Phi+\frac{1}{2}\sum_{i\neq j}V(|\mathbf{r}_i-\mathbf{r}_j|)$$
$$-(\mu_D/\hbar)\sum_{i=1}^{N}\mathbf{S}_i\cdot\mathbf{B}+\tfrac{1}{2}(\mu_D/\hbar)^2\gamma\sum_{i\neq j}f(|\mathbf{r}_i-\mathbf{r}_j|)\mathbf{S}_i\cdot\mathbf{S}_j\;, \tag{1}$$

where $\mathbf{B}=\nabla\times\mathbf{A}$ is the imposed constant magnetic field and $\mathbf{A}$ is its vector potential. The potential of the constant neutralizing background is written Φ, $V(|\mathbf{r}_i-\mathbf{r}_j|)$ is two-body potential, M represents deuteron mass, $f(|\mathbf{r}_i-\mathbf{r}_j|)$ represents a sharply peaked function about $|\mathbf{r}_i-\mathbf{r}_j|=0$, and $e=|e|$ represents deuteron charge. In writing (1) we have assumed that the deuteron magnetic moment, $\mu_D\mathbf{S}/\hbar$, is predominantly in the $\mathbf{S}$ direction,[19] where $\mu_D \simeq 10^{-23}$ erg/G. The constant γ has dimensions $\mathrm{G}^2\,\mathrm{cm}^3$, and together with the short range of the function f, models the deuteron overlap integral. The sign of γ follows from the totally symmetric property of coupled deuteron wave functions appropriate to bosons. In writing (1), we have assumed that the interaction of the neutralizing background with the deuterons is scalar. Furthermore, the preceding Hamiltonian assumes that the interparticle interaction is separable into a scalar potential and a spin-spin interaction.

We rewrite the Hamiltonian (1) in the following form:

$$H=\sum_{i=1}^{N}\frac{1}{2M}\left[\mathbf{p}_i-\left[\frac{e}{c}\right]\mathbf{A}(\mathbf{r}_i)\right]^2+\frac{1}{2}\sum_{i\neq j}V(|\mathbf{r}_i-\mathbf{r}_j|)+N\Phi+H_S+H_{S^2}\;, \tag{2a}$$

where H_{S^2} denotes the spin-spin term in (1) and

$$H_S\equiv-(\mu_D/\hbar)\sum_{i=1}^{N}\mathbf{S}_i\cdot\mathbf{B}\;. \tag{2b}$$

With this form of the Hamiltonian at hand, we turn to the formalism of second quantization.

Second quantization. Expressing the non-spin-dependent terms in the Hamiltonian (2a) in second quantization, one obtains

$$H'=\frac{1}{2M}\int d\mathbf{r}\,\Psi^{\dagger}(\mathbf{r})\left[-i\hbar\nabla-\frac{e}{c}\mathbf{A}(\mathbf{r})\right]^2\Psi(\mathbf{r})+\frac{1}{2}\int\int d\mathbf{r}\,d\mathbf{r}'\Psi^{\dagger}(\mathbf{r}')\Psi^{\dagger}(\mathbf{r})V(|\mathbf{r}-\mathbf{r}'|)\Psi(\mathbf{r})\Psi(\mathbf{r}') \quad (3)$$

$$\equiv\int d\mathbf{r}\Psi^{\dagger}(\mathbf{r})H_K\Psi(\mathbf{r})+\frac{1}{2}\int\int d\mathbf{r}d\mathbf{r}'\Psi^{\dagger}(\mathbf{r}')\Psi^{\dagger}(\mathbf{r})H_V\Psi(\mathbf{r})\Psi(\mathbf{r}')\ , \quad (3a)$$

where the component Hamiltonians H_K and H_V are as implied.

Field operators satisfy the Bose commutation relations

$$[\Psi(\mathbf{r}),\Psi^{\dagger}(\mathbf{r}')]=\delta(\mathbf{r}-\mathbf{r}')\ , \quad (4a)$$

$$[\Psi(\mathbf{r}),\Psi(\mathbf{r}')]=[\Psi^{\dagger}(\mathbf{r}),\Psi^{\dagger}(\mathbf{r}')]=0\ . \quad (4b)$$

When operating on the state function of the system (in Fock space), the field operator, $\Psi^{\dagger}(\mathbf{r})$ creates a particle at $\mathbf{r}$ whereas $\Psi(\mathbf{r})$ annihilates a particle at $\mathbf{r}$ (with occupation number, $N_{\mathbf{r}}$) according to the rules

$$\Psi^{\dagger}(\mathbf{r})|\cdots N_{\mathbf{r}}\cdots\rangle=\sqrt{N_{\mathbf{r}}+1}|\cdots N_{\mathbf{r}}+1\cdots\rangle\ , \quad (4c)$$

$$\Psi(\mathbf{r})|\cdots N_{\mathbf{r}}\cdots\rangle=\sqrt{N_{\mathbf{r}}}|\cdots N_{\mathbf{r}}-1\cdots\rangle\ , \quad (4d)$$

where $N_{\mathbf{r}}$ denotes occupation number at $\mathbf{r}$. These latter relations imply the particle number operators

$$N_{\mathbf{r}}=\Psi^{\dagger}(\mathbf{r})\psi(\mathbf{r}),\quad N=\int d\mathbf{r}\Psi^{\dagger}(\mathbf{r})\Psi(\mathbf{r})\ , \quad (4e)$$

which are seen to commute with H' as given by (3).

Low-density limit. In writing (2) and what follows, the vector potential $\mathbf{A}(\mathbf{r})$ is treated as a c number.[20] We consider the low-deuteron density, high-magnetic-field limit for which H_K is dominant and H_V is viewed as perturbative. Toward these ends we first consider the properties of H_K. Writing the vector potential in the form

$$\mathbf{A}=-\tfrac{1}{2}\mathbf{r}\times\mathbf{B} \quad (5)$$

[where $\mathbf{B}=(0,0,B)$, and B is constant] permits H_K to be written[21]

$$H_K=\frac{\hbar^2}{2M}\nabla^2+\frac{\omega_c}{2}L_z+\frac{\omega_c^2 M}{8}r_\perp^2\ , \quad (6)$$

where

$$r_\perp^2=x^2+y^2\ , \quad (6a)$$

$$L_z=-(\mathbf{r}\times i\hbar\nabla)_z\ , \quad (6b)$$

$$\omega_c\equiv eB/Mc \quad (7)$$

is the deuteron cyclotron frequency.

Working in cylindrical coordinates, eigenstates of H_K are given by

$$H_K\varphi_{nm}=E_{nm}\varphi_{nm}\ , \quad (8a)$$

$$E_{nm}=\hbar\omega_c[n+\tfrac{1}{2}(2m+1)]+\hbar^2k_z^2/2M\ , \quad (8b)$$

where eigenvalues of L_Z are $\hbar m$ and the integers $n,m\geq 0$. The wave functions φ_{nm} are given by

$$\varphi_{nm}(\rho,z,\phi)=\frac{1}{\sqrt{2\pi L}}R_{nm}(\rho)\exp(im\phi)\exp(ik_z z)\ , \quad (9)$$

where R_{nm} are exponentially Gaussian damped Laguerre polynomials[22] and L is the edge length of the volume of confinement.

With the Landau states (9) at hand, the field operators in (3) *et seq.* are expanded as follows:

$$\Psi(\mathbf{r})=\sum_{\nu}a_\nu\varphi_\nu(\mathbf{r})\ . \quad (10)$$

Here we have written $\nu\equiv(n,m)$ so that the summation in (10) is a double sum. In analogy to (4), a_ν operators obey the commutation relations

$$[a_\nu,a_{\nu'}^{\dagger}]=\delta_{\nu,\nu'}\ , \quad (11a)$$

$$[a_\nu^{\dagger},a_{\nu'}^{\dagger}]=[a_\nu,a_{\nu'}]=0\ , \quad (11b)$$

$$N_\nu=a_\nu^{\dagger}a_\nu,\quad \sum_\nu N_\nu=N\ . \quad (11c)$$

In this representation, the expectation-operator $\overline{H}_K$ is given by

$$\overline{H}_K=\int d\mathbf{r}\sum_{\nu}\sum_{\nu'}a_\nu^{\dagger}\varphi_\nu^{\dagger}(\mathbf{r})H_K a_{\nu'}\varphi_{\nu'}(\mathbf{r}) \quad (12)$$

which, with the orthogonality of the basis functions (9) and the relations (11), give

$$\overline{H}_K=\sum_\nu E_\nu a_\nu^{\dagger}a_\nu=\sum_\nu E_\nu N_\nu\ . \quad (13)$$

Evaluating $\overline{H}_K$ in the ground state, with (8b) (corresponding to $n=m=0$), we obtain

$$E_{K,G}=N\hbar\omega_c/2\ . \quad (14)$$

In this relation we interpret N as a c number.

The radial component of the wave function (9) corresponding to the eigenenergy (14) is

$$R_0(\xi)=(1/b_c)e^{-\xi/2}\ , \quad (15)$$

$$\xi\equiv\rho^2/2b_c^2\ , \quad (15a)$$

$$\eta^2\equiv z^2/2b_c^2\ , \quad (15b)$$

$$b_c^2\equiv\hbar/M\omega_c\ , \quad (15c)$$

where (15b) is included for future reference. The limit of large magnetic field as well as large volume of confinement, may be expressed by the condition

$$b_c/L\ll 1\ . \quad (16)$$

With these results at hand we turn next to the spin and potential interaction contribution to the ground state of the system in the said limit.

The expectation operator, $\overline{H}_V$, stems from (3a) and (10) and is given by

$$\overline{H}_V=\int\int d\mathbf{r}'d\mathbf{r}\sum_{\nu}\sum_{\nu'}\sum_{\lambda}\sum_{\lambda'}a_{\nu'}^{\dagger}\varphi_{\nu'}^{\dagger}(\mathbf{r}')a_\nu^{\dagger}\varphi_\nu^{\dagger}(\mathbf{r})H_V a_\lambda\varphi_\lambda(\mathbf{r})a_\lambda(\mathbf{r})a_\lambda{}'\varphi_\lambda{}'(\mathbf{r}')\ . \quad (17)$$

In the present approximation we keep only the leading term corresponding to (9) and (15). With the commutation rules (11) there results

$$\bar{H}_V=\frac{N(N-1)}{2}\iint d\mathbf{r}\,d\mathbf{r}'[\varphi_0(\mathbf{r})]^2[\varphi_0(\mathbf{r}')]^2\frac{e^2}{|r-r'|}\ . \quad (18)$$

Inserting functional forms in the preceding expression gives

$$\bar{H}_V=[N(N-1)e^2b_c/L^2]\Gamma\ , \quad (19)$$

where Γ represents the nondimensional integral

$$\Gamma=\frac{1}{\sqrt{2}\pi^2}\int\frac{d\xi\,d\xi'd\eta\,d\eta'd\phi\,d\phi'}{R(\xi,\eta,\phi;\xi',\eta',\phi')}\ , \quad (20a)$$

$$R^2=\xi+\xi'+\eta^2+\eta'^2-2[\eta\eta'+\sqrt{\xi\xi'}\cos(\phi-\phi')]\ . \quad (20b)$$

The ξ interval of integration is $(0,L^2/2b_c^2)$ whereas the η interval of integration is $(0,L/\sqrt{2}b_c)$. With the condition (16), in the present case both these integration intervals may be replaced by $(0,\infty)$. Expression (19) represents the ground-state contribution from the interaction term in (3a) in the said limit.

The expectation operator $\bar{H}_{S^2}$ in the $\varphi_0(\mathbf{r})$ state is given by

$$\bar{H}_{S^2}=-A\sum_{i\neq j}f_{ij}\mathbf{S}_i\cdot\mathbf{S}_j\ , \quad (21)$$

where

$$f_{ij}\equiv\langle\varphi_0(\mathbf{r}_i)\varphi_0(\mathbf{r}_j)|f(r_{ij})|\varphi_0(\mathbf{r}_i)\varphi_0(\mathbf{r}_j)\rangle\ , \quad (22a)$$

$$A\equiv\tfrac{1}{2}(\mu_D/\hbar)^2\gamma\ . \quad (22b)$$

Further assuming that $f_{ij}=f=$const (see the Appendix) permits (21) to be rewritten

$$\bar{H}_{S^2}=-\frac{Af}{2}\left[S^2-\sum_{i=1}^{N}S_i^2\right]\ , \quad (23)$$

where S^2 is the square of total spin angular momentum. The Hamiltonian, $\bar{H}_{S^2}$, is diagonalized by the eigenstates $|s;m_s;s_1,s_2,\ldots,s_N\rangle$, where

$$s=0,1,\ldots,N,\quad m_s=-s,\ldots,+s,\quad s_i=1\ , \quad (23a)$$

represent quantum numbers of S^2, S_z, S_i^2, respectively. It follows that the ground state of $\bar{H}_{S^2}$ is given by

$$|S^2\rangle_G=|N;m_N;1,\ldots,1\rangle \quad (24a)$$

with corresponding eigenenergy

$$E_{S^2}=Af\hbar^2N(N-1)/2\ . \quad (24b)$$

We turn next to the H_S term in (2b) which may be rewritten [recall statement preceding (6)]

$$H_S=-(\mu_DB/\hbar)\sum_{i=1}^{N}S_{iz}=-(\mu_DB/\hbar)S_z\ . \quad (25)$$

It follows that in the ground state of H_S, all spin projections are $+1$, corresponding to $m_N=N$. Combining this property with the state (24a) gives the overall ground spin state

$$|S^2,S\rangle_G=|N;N;1,\ldots,1\rangle\ , \quad (26)$$

which is noted to diagonalize both H_S and H_{S^2}. In this state,

$$E_S=-\mu_DBN\ . \quad (27)$$

Spin-1 states are represented by three-dimensional column vectors which we label $\alpha_i(1)$, $\beta_i(0)$, $\gamma_i(-1)$, relevant to particle number i. Thus, for example, $S_i^z\alpha_i=\hbar\alpha_i$, etc. A product representation of the spin state (27) is then given by

$$\xi_G(S^N)=\langle\alpha_1\beta_1\gamma_1,\ldots,|N;N;1,\ldots,1\rangle=\alpha_1\alpha_2\cdots\alpha_N\ . \quad (28)$$

Ground-state energy. Collecting terms from (2a), (19), (24b), and (27) gives the ground-state energy

$$E_G\approx\frac{N\hbar\omega_c}{2}+N(N-1)\frac{e^2b_c}{\Omega^{2/3}}\Gamma+N\Phi-\mu_DBN$$
$$-\gamma f\mu_{D^2}[N(N-1)/2]\ , \quad (29)$$

where we have set $\Omega\equiv L^3$.

The ground-state energy (29) is appropriate to the limit where magnetic field energy dominates interaction energy. That is

$$\bar{H}_V\ll\bar{H}_K \quad (30)$$

or, equivalently,

$$N(e^2/L)(b_c/L)\ll\hbar\omega_c \quad (30a)$$

which is obeyed in the high B field, large volume, low-density limit (16). The dependence of the left side of the preceding relation on density $n=N/\Omega$ is obtained by rewriting (30a) in terms of these parameters. There results

$$n\Omega^{2/3}e^2b_c/L\ll\hbar\omega_c \quad (30b)$$

which, with (16), is satisfied in the low-density, high-volume limit providing $n\Omega^{2/3}=$const.

As we are working in an energy representation (10), Fock-space ket vectors are given by $|N_{\nu_1},N_{\nu_2},\ldots,\rangle$ where $N_{\nu_1}=N_{E_G}$ denotes the occupation number of the ground state. In the present limit the ground state is given by the ket vector $|N_{E_G},0,0,\ldots\rangle$. The coordinate component of the ground-state wave function is then given by the inner product[23]

$$\Psi_G(\mathbf{r}^N)=\langle\mathbf{r}_1,\ldots,\mathbf{r}_N|N_{E_G},0,0,\ldots\rangle$$
$$=\varphi_0(\mathbf{r}_1)\cdots\varphi_0(\mathbf{r}_N)\ , \quad (31)$$

where wave functions on the right side of (31) are the ground-state Gaussian forms (9) and (15). Combining this result with the spin function (28) gives the coordinate-spin and ground-state wave function

$$\Psi_G(\mathbf{r}^N,\mathbf{S}^N)=\Psi_G(\mathbf{r}^N)\chi_G(\mathbf{S}^N)\ , \quad (32)$$

which is relevant to the limit (16) and (30) and is seen to be symmetric under particle coordinate and spin exchanges appropriate to a many-body Bose system.

Conclusions. The problem of the quantum states of N deuterons in a steady magnetic field was studied. Working in second quantization, the ground-state energy and related wave function of an aggregate of deuterons in a charge-neutralizing background and immersed in a uniform magnetic field was obtained. This result is relevant to the low-density limit wherein magnetic-field energy is large compared to interaction energy. With minor approximation in the spin-spin term of the Hamiltonian, spin wave functions comprised of products of single-particle spin-1 states were found to diagonalize both spin contributions to the Hamiltonian. An inequality for the validity of these results was obtained which was found to be obeyed in the low-density limit providing $n\Omega^{2/3}=\text{const}$.

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APPENDIX

For a homogeneous equilibrium fluid it may be shown that f_{ij} is constant. First we note that, in general,

$$f_{ij}=\int\int d\mathbf{r}_i d\mathbf{r}_j |\varphi_2(\mathbf{r}_i,\mathbf{r}_j)|^2 f(|\mathbf{r}_i-\mathbf{r}_j|) , \tag{A1}$$

where φ_2 represents the two-particle wave function. Introducing the change of variables: $\mathbf{r}=\mathbf{r}_i-\mathbf{r}_j$ and $2\mathbf{R}=\mathbf{r}_i+\mathbf{r}_j$, gives

$$f_{ij}=\int\int d\mathbf{r}\, d\mathbf{R} |\varphi_2(\mathbf{r},\mathbf{R})|^2 f(\mathbf{r}) . \tag{A2}$$

For a homogeneous equilibrium fluid, the radial distribution function, $g(r)$, is given by

$$d\mathbf{r}\, d\mathbf{R}|\varphi_2(\mathbf{r},\mathbf{R})|^2=\frac{d\mathbf{r}\, d\mathbf{R}}{\Omega^2}g(r) . \tag{A3}$$

Inserting this form into (A3) gives

$$f_{ij}\to f=\int\int \frac{d\mathbf{r}\, d\mathbf{R}}{\Omega^2}g(r)f(r)$$

$$=\frac{4\pi}{\Omega}\int dr\, r^2 g(r)f(r) . \tag{A4}$$

This relation indicates that f_{ij} is constant in the said limit.

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