Spin-polarized ^{3}He in a density-functional frame

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The properties of spin-polarized liquid helium are analyzed in a density-functional framework. It is shown that the BHN functional [M. Barranco *et al.*, Phys. Rev. B **54**, 7394 (1996)] designed to describe the thermodynamics and the response of the unpolarized liquid also reproduces reasonably well recent experimental results at low magnetization. In particular, the present description reproduces the magnetic field data for the weakly polarized liquid, and is also consistent with the existence of a near-metamagnetic transition at a polarization close to 0.2. We indicate the various difficulties associated with the extension of the current scenario to highly and fully magnetized systems. [S0163-1829(98)09541-1]

I. INTRODUCTION

The theoretical description of spin polarized liquid ^{3}He (Refs. 1 and 2) has attracted the interest of various research groups for almost 20 years. The properties of the liquid in the vicinity of solid-liquid coexistence after fusion of the polarized solid have been thoroughfully explored,[3,4] following an early proposal by Castaing and Nozières.[2] Another suggestion advanced by Lhuillier and Laloë,[1] namely, to employ optical pumping techniques in order to polarize either the gas or the liquid, has been also exploited to study the influence of nuclear orientation upon liquid-gas coexistence.[5] Theoretical approaches have also encountered a prosperous field; the simplification introduced by the symmetry of the wave function of the helium atoms of the totally polarized liquid in spin space made room for microscopical descriptions[6–9] that provide indications of the expected range of energies and densities at saturation, of the size of the effective mass of the spin-up particles, and of the possible trend of energy and effective mass as functions of the density. Moreover, phenomenological descriptions based on Landau's theory of Fermi liquids[10–12] have also shed light on various aspects of the fully[10] and partially polarized[11,12] liquid. In particular, near-metamagnetic behavior at high pressures has been predicted[12] in fair agreement with early experimental data close to melting pressure[3] and opposite to the predictions of both the paramagnon[13] and the Gutzwiller model.[14] However, a decrease of the magnetic susceptibility with growing polarization is to be expected in the frame of the paramagnon model; experimental data on viscosity of the magnetized liquid[15,16] may also favor this behavior. More recent experimental results for the induced magnetic field at a pressure close to 26 bars (Refs. 17 and 18) might exclude a near-metamagnetic state, since the slope of the curve of magnetization vs field appears to decrease monotonically. This apparently contradicting evidence[3,17,18] poses an interesting challenge to be sorted by more conclusive data and makes room for further theoretical speculation, due to the fact that the metamagnetic behavior reported in Ref. 3 strongly relies on an interpretation of the dynamics of the melting process, while the magnetic field results[17,18] are derived on thermodynamic grounds and are thus model independent.

Density-functional theory has been also applied to magnetized liquid helium.[19,20] Stringari[19] has shown that a density functional devised to describe the bulk properties of ^{3}He can account for various features of the liquid at low polarization, and that an extension of the above model via the incorporation of higher powers of the magnetization is also able to treat several aspects of the fully polarized system. In a similar spirit, the study of the liquid-gas phase transition in spin-polarized systems has been performed, showing the appearance of both density and magnetization instability regimes in some regions of parameter space.[20]

More recently, a density functional for liquid ^{3}He has been proposed[21] which, in addition to describing the equation of state of the unpolarized liquid up to the monopole and dipole Landau parameters in both the density and spin channels, is capable of providing a reasonable description of the dynamical response in these channels, in good agreement with available experimental data. It is then interesting to examine the extent to which the density functional of Ref. 21 [hereafter referred to as Barranco, Hernández, and Navarro (BHN)] accounts for the most important features of polarized liquid helium. For this sake, we investigate which experimentally determined properties of the weakly polarized system can be pictured by the BHN functional, and discuss different scenarios according to particular choices of the still-undetermined force parameters. The major outcome of this analysis is the fact that the BHN functional is adequate to describe the magnetic behavior of the liquid at polarizations below 0.3, in addition to the various thermodynamic quantities. We also indicate that in order to account for observed and/or expected properties of the highly polarized system in a continuous fashion, it may be necessary to incorporate energy terms that depend upon noninteger powers of the magnetization. However, the appearance of two species with different densities associated with the spin-up and spin-down particles provokes increasing complexity of the effective force strengths, which in turn demands a large number of new parameters.

This paper is organized as follows. In Sec. II we revise the foundations of the BHN density functional and derive the equation of state of arbitrarily polarized helium. Section III is devoted to exploring the properties of the weakly magnetized liquid and the different scenarios, while in Sec. IV we discuss the limitations and perspectives of the above functional as applied to the highly polarized system, and summarize the present results.

II. BHN DENSITY FUNCTIONAL

The BHN density functional[21] is derived from an effective particle-particle (pp) interaction of the form

$$V(1,2)=\mathcal{V}_0\delta(\mathbf{r}_1-\mathbf{r}_2)+\frac{1}{2}[\mathbf{k}'^2\mathcal{V}_1\delta(\mathbf{r}_1-\mathbf{r}_2)+\delta(\mathbf{r}_1-\mathbf{r}_2)\mathcal{V}_1\mathbf{k}^2]+\mathbf{k}'\cdot\mathcal{V}_2\delta(\mathbf{r}_1-\mathbf{r}_2)\mathbf{k}, \quad (2.1)$$

with Kronecker's delta function $\delta(\mathbf{r})$ and with the relative momentum operators $\mathbf{k},\mathbf{k}'$ respectively acting on the right and on the left, $\mathcal{V}_n$ being

$$\mathcal{V}_0=t_0+t_0'\rho^{\gamma}+u_0\rho^{\beta}\mathbf{S}\cdot\mathbf{S}+v_0(\mathbf{J}\cdot\mathbf{J}-\mathbf{S}\cdot\mathbf{T}) \quad (2.2)$$

and

$$\mathcal{V}_n=t_n+t_n'\rho+u_n\mathbf{S}\cdot\mathbf{S}+v_n(\mathbf{J}\cdot\mathbf{J}-\mathbf{S}\cdot\mathbf{T}) \quad (2.3)$$

for $n=1,2$. The various densities appearing in this expression as well as in the total energy are the particle, particle kinetic energy, and particle current density and the corresponding spin ones, respectively:

$$\{\rho(\mathbf{r}),\tau(\mathbf{r}),\mathbf{j}(\mathbf{r}),\mathbf{S}(\mathbf{r}),\mathbf{T}(\mathbf{r}),\mathbf{J}(\mathbf{r})\}=\sum_{ij}\phi_i\phi_j^*\rho_{ij}\left\{\delta_{\sigma_i\sigma_j},\mathbf{k}_i\cdot\mathbf{k}_j\delta_{\sigma_i\sigma_j},\frac{\mathbf{k}_i+\mathbf{k}_j}{2}\delta_{\sigma_i\sigma_j},\langle\sigma_j|\vec{\sigma}|\sigma_i\rangle,\mathbf{k}_i\cdot\mathbf{k}_j\langle\sigma_j|\vec{\sigma}|\sigma_i\rangle,\frac{\mathbf{k}_i+\mathbf{k}_j}{2}\langle\sigma_j|\vec{\sigma}|\sigma_i\rangle\right\}, \quad (2.4)$$

where ρ_{ij} is the occupation number matrix, and the single-particle wave functions ϕ_i are plane waves normalized to unity in the volume Ω. Let us recall that the combination $\mathbf{J}\cdot\mathbf{J}-\mathbf{S}\cdot\mathbf{T}$ entering $\mathcal{V}_n$ is required to guarantee Galilean invariance.[21]

Since in thermal equilibrium $\rho_{ij}=\delta_{ij}n_i$, one has

$$\rho=\sum_i\frac{n_i}{\Omega}=\rho_++\rho_-=\frac{k_F^3}{3\pi^2}, \quad (2.5)$$

$$\tau=\sum_i\frac{n_i}{\Omega}k_i^2=\tau_++\tau_-, \quad (2.6)$$

whereas for species $\sigma(=\pm)$ one has $k_{F_\sigma}=(6\pi^2\rho_\sigma)^{1/3}$ and $\tau_\sigma=3/5\rho_\sigma k_{F_\sigma}^2$. Furthermore, both currents $\mathbf{j}$ and $\mathbf{J}$ vanish in a homogeneous system while, along the polarization axis $\hat{z}$, $S_z=\rho_+-\rho_-$ and $T_z=\tau_+-\tau_-$. In the case of a finite polarization $\Delta=S_z/\rho$, these quantities read

$$\rho_\sigma=\frac{\rho}{2}(1+\sigma\Delta), \quad (2.7)$$

$$k_{F_\sigma}=k_F(1+\sigma\Delta)^{1/3}, \quad (2.8)$$

$$\tau_\sigma=\frac{3}{10}\rho k_F^2(1+\sigma\Delta)^{5/3}, \quad (2.9)$$

$$T_z=\frac{3}{10}\rho k_F^2[(1+\Delta)^{5/3}-(1-\Delta)^{5/3}]. \quad (2.10)$$

Let us now consider the total energy

$$E=\sum_{ij}\frac{\hbar^2}{2m}\langle j|-\nabla^2|i\rangle\rho_{ij}+\frac{1}{2}\sum_{ijlm}\langle jm|V|il\rangle_A\rho_{ij}\rho_{lm}, \quad (2.11)$$

where

$$\langle jm|V|il\rangle_A=\frac{1}{\Omega}\left\{\left[\mathcal{V}_0+\frac{1}{8}\mathcal{V}_1[(\mathbf{k}_i-\mathbf{k}_l)^2+(\mathbf{k}_j-\mathbf{k}_m)^2]\right]\times(\delta_{\sigma_i\sigma_j}\delta_{\sigma_l\sigma_m}-\delta_{\sigma_i\sigma_m}\delta_{\sigma_j\sigma_l})+\frac{1}{4}\mathcal{V}_2(\mathbf{k}_i-\mathbf{k}_l)\cdot(\mathbf{k}_j-\mathbf{k}_m)(\delta_{\sigma_i\sigma_j}\delta_{\sigma_l\sigma_m}+\delta_{\sigma_i\sigma_m}\delta_{\sigma_j\sigma_l})\right\}. \quad (2.12)$$

After carrying the various summations, the total energy density can be written as

$$\frac{E(\rho,\Delta)}{\Omega}=\frac{\hbar^2}{2m}(\tau_++\tau_-)+\frac{1}{2}\mathcal{V}_0(\rho^2-\rho_+^2-\rho_-^2)+\frac{\mathcal{V}_1+3\mathcal{V}_2}{4}(\rho\tau-\rho_+\tau_+-\rho_-\tau_-)+\frac{\mathcal{V}_2}{2}(\rho_+-\rho_-)(\tau_+-\tau_-), \quad (2.13)$$

The form $\mathcal{V}_1+3\mathcal{V}_2$ simply corresponds to the contribution of the singlet and triplet spin pairs in the unpolarized system; expression (2.13) brings into evidence the pair-breaking effect of the polarizing field, which in addition to separating the partial densities $\rho_\pm$, $\tau_\pm$ in the singlet-plus-triplet energy introduces an extra term, proportional to $\mathcal{V}_2$, which represents an alignment energy of the ''equal spin pairs.'' It is then clear that this term vanishes for $\Delta=0$, whereas in such a case, the spin singlet-plus-triplet interaction energy adopts the form already obtained for the unpolarized system.[21] Moreover, only the extra term appears in the fully polarized case. For practical use of the density functional in the $\Delta \neq 0$ case one requires the values of the coefficients t_n, t_n', u_n, and v_n for $n=1,2$. We recall that in the case of the BHN functional the values of $t_{1,2}$ and $t'_{1,2}$ have been determined so as to reproduce the experimental surface tension of the unpolarized liquid.[22] To analyze the polarized case we need some criterium to decouple the coefficients $u_{1,2}$ and $v_{1,2}$. This subject is further discussed in Sec. III.

The first and second derivatives of the total energy with respect to the density ρ respectively yield the pressure P and the inverse compressibility modulus $1/\kappa\rho = mc^2$ related to the sound velocity c, whereas the corresponding derivatives with respect to the magnetization give the induced magnetic field B and the inverse magnetic susceptibility C/χ at zero temperature, C being the Curie constant. The first and second functional variations of the total energy with respect to the occupation numbers respectively give the mean single-particle field and the effective particle-hole (ph) interaction. We leave out the corresponding expressions, as they are rather cumbersome, and give instead a hint on the calculation of the functional variations. The general expression for the mean field is

$$U_i = \frac{\delta E}{\delta \rho_{ii}} = \frac{\hbar^2}{2m} k_i^2 + \sum_{lm} \langle im|V|il\rangle_A \rho_{lm} + \frac{1}{2} \sum_{lmnp} \left\langle nm \left| \frac{\delta V}{\delta \rho_{ii}} \right| pl \right\rangle_A \rho_{lm}\rho_{pn}. \tag{2.14}$$

In view of Eqs. (2.1)–(2.4), the explicit derivative of the pp interaction can be calculated using

$$\frac{\delta}{\delta \rho_{ij}} = \phi_i \phi_j^* \left\{ \delta_{\sigma_i \sigma_j} \left[\frac{\partial}{\partial \rho} + \mathbf{k}_i \cdot \mathbf{k}_j \frac{\partial}{\partial \tau} + (\mathbf{k}_i + \mathbf{k}_j)_\alpha \frac{\partial}{\partial j_\alpha} \right] + \langle \sigma_i | \sigma_\alpha | \sigma_j \rangle \left[\frac{\partial}{\partial s_\alpha} + \mathbf{k}_i \cdot \mathbf{k}_j \frac{\partial}{\partial T_\alpha} + \frac{(\mathbf{k}_i + \mathbf{k}_j)_\beta}{2} \frac{\partial}{\partial J_{\alpha\beta}} \right] \right\}. \tag{2.15}$$

Once this explicit operation is performed as well as the summations entering Eq. (2.14), one gets the final expression for the mean field. The coefficient of k_i^2 gives the effective mass for species σ, which turns out to be

$$\frac{\hbar^2}{m_\sigma^*} = \frac{\hbar^2}{m} + \frac{\mathcal{V}_1 + 3\mathcal{V}_2}{2} \rho_{-\sigma} + \mathcal{V}_2(\rho_\sigma - \rho_{-\sigma}) - \sigma(\rho_+ - \rho_-) \times \left[\frac{v_0}{2} \rho^2 (1-\Delta^2) + \frac{v_1 + 3v_2}{2} (\rho_+ \tau_- + \rho_- \tau_+) + 2v_2 (\rho_+ - \rho_-)(\tau_+ - \tau_-) \right]. \tag{2.16}$$

This expression reflects the scheme intrinsic to the energy and mean field, where an ''equal spin'' contribution adds up to the spin singlet-plus-triplet one. However, the double-functional variation that gives rise to the effective interaction does not preserve this scheme, which is nevertheless reencountered in the Landau parameters at $\Delta=0$. Since these coefficients only depend on the combination $\mathcal{V}_1 + 3\mathcal{V}_2$, they do not provide any condition to determine the separate values of the parameters $u_{1,2}$ and $v_{1,2}$.

III. WEAKLY POLARIZED LIQUID

In order to shed light on the structure of the equation of state of the polarized liquid within the BHN frame, it is convenient to examine the expression of the energy (2.13) in terms of the polarization Δ. For this sake, we first note that the equal spin contribution carries the factor

$$(\rho_+ - \rho_-)(\tau_+ - \tau_-) = \frac{3}{10} \rho^2 k_F^2 \Delta^2 [1 + f(\Delta)], \tag{3.1}$$

with $f(\Delta)$ an even analytical function vanishing at the origin. On the other hand, the force strength functions (2.2) are even functions of the polarization and, consequently, the energy density of the ''equal spin pairs'' depends at least quadratically on Δ, i.e.,

$$\mathcal{V}_2(\rho_+ - \rho_-)(\tau_+ - \tau_-) = A(\rho; t_2, t_2')\Delta^2 + C(\rho; u_2, v_2)\Delta^4 + \mathcal{O}(\Delta^6). \tag{3.2}$$

It becomes then clear that the energy and its derivatives of any order with respect to density and up to third order with respect to polarization, evaluated at $\Delta=0$, are independent of the separate coefficients u_2 and v_2. Among these quantities, the parameter β, giving the strength of the finite-temperature correction to the magnetic susceptibility,

$$\chi(T) = \chi(0)[1 - \beta \chi(0)^2 T^2], \tag{3.3}$$

with χ in units of the Curie constant, has been employed in Ref. 19 as a criterium for a relationship among unknown force coefficients of the density functional proposed there. To test the BHN density functional, we extract an explicit expression for β, performing a Sommerfeld expansion of the energy per particle $\epsilon = E/N$ as

$$\epsilon(\Delta, T) = \epsilon_0(\Delta) + \epsilon_2(\Delta) T^2 = \epsilon_0(\Delta) + [\epsilon_{20} + \epsilon_{22}\Delta^2 + \mathcal{O}(\Delta^4)] T^2, \tag{3.4}$$

from which we get the magnetic susceptibility at constant temperature (in units of the Curie constant) as

$$\chi(T) = \chi(0) \left[1 + 2 \frac{\epsilon_{22} \chi(0)}{C} T^2 \right], \tag{3.5}$$

with $C/\chi(0) = \partial^2 \epsilon_0 / \partial \Delta^2$; i.e., we have $\beta = -2\epsilon_{22}/[C\chi(0)]$.

As discussed above, the coefficient β is a linear function of all force coefficients appearing in $\mathcal{V}_1 + 3\mathcal{V}_2$, in addition to t_2 and t_2'. The BHN density functional predicts β values ranging between 0.66 and 0.79 for densities between the saturation one ρ_0 and $1.4\rho_0$, which are not inconsistent with the available experimental data[23] giving β around 0.5–0.55 in that interval.

TABLE I. Slopes of the relative variation of the sound velocity at constant pressure in the BHN frame vs experimental figures taken from Ref. 4.

P (bar)	BHN	Experimental values
12	0.019	0.020
15.6	0.015	0.016
26.2	0.006	0.005
28.5	0.007	0.010

On the other hand, the relative variation of the sound velocity $\delta c/c$ at constant pressure has been shown to depend linearly upon Δ^2;[4] since the expression for these variations depends only on derivatives of the total energy at zero polarization,[19] this quantity is a basis for a further test. We have verified that the BHN density functionals provide very close fits to these variations. This is shown in Table I where the present results are compared to the experimental slopes of $\delta c/c$ vs Δ^2 in Ref. 4.

We now investigate to what extent other properties of the weakly polarized liquid allow us a determination of the unknown force parameters u_2 and v_2. For this sake, we explore the scenario that takes place in the (ρ,Δ) plane for $\rho_0 \leqslant \rho \leqslant 1.5\rho_0$ and low magnetizations, according to three viewpoints.

(1) BHN0 parametrization: adjusting the experimental susceptibility data[3] at the lowest polarizations (on the left hand side of the metamagnetic peak) we set the values $u_2\rho_0^2 = -9261.08$ K Å^5 and $v_2\rho_0^2 = -11\,726.8$ K Å^7. In this case, the susceptibility is a decreasing function of Δ at the origin, as predicted by the paramagnon model,[13] and presents a pole slightly above $\Delta = 0.2$. Examination of the total energy density indicates that the liquid remains bound in the above polarization interval and in a wide range of densities. Moreover, the system remains stable against density fluctuations. However, although the slope of the induced magnetic field in terms of the polarization at the origin reproduces the data at $P = 26$ bars, the field remains too low as compared to experimental evidence.[18]

(2) BHN1 parametrization: we demand that the susceptibility at melting pressure adopt values compatible with the experimental data[3] at two different magnetizations. We set $u_2\rho_0^2 = 3017.66$ K Å^5 and $v_2\rho_0^2 = 4030.68$ K Å^7. This procedure gives rise to near-metamagnetic behavior of the susceptibility for $0 \leqslant \Delta \leqslant 0.4$ with a peak localized at $\Delta = 0.2$, in agreement with results from Fermi liquid[12] and density functional theories.[19] The liquid is bound and stable against density fluctuations; the induced magnetic field is compatible with experimental data up to $\Delta \approx 0.1$, but it increases very rapidly for larger polarizations.

(3) BHN2 parametrization: we adjust the induced magnetic field at a pressure $P = 26$ bars (Ref. 18) for the lowest magnetizations, with the values $u_2\rho_0^2 = 1953.25$ K Å^5 and $v_2\rho_0^2 = 2748.49$ K Å^7. We find that the susceptibility exhibits a weak near-metamagnetic peak at $\Delta \approx 0.2$. The system is bound and stable against density fluctuations; however, magnetic instabilities show up, in particular at the highest densities where the pattern resembles the BHN0 one.

A possible question concerns the capability of the BHN density functional to deal with highly polarized liquids. Extension of the above scenarios to polarizations above 0.4 rapidly lead to an unbound system, and in particular, the fully magnetized liquid lies at positive energies. An exploration of the evolution of the scenario in parameter space shows that negative values of u_2 are needed in order to obtain a bound liquid in the limit $\Delta = 1$, with a binding energy close to that of the unpolarized system. However, in such a situation, there always exist broad domains of the (ρ,Δ) space where the system is unstable, either with respect to density or to spin fluctuations (i.e., the BHN0 and BHN2 choices), or to both of them. In addition, the BHN1 parametrization predicts localization[14] in some regions where the effective mass diverges. One can verify that the size of those instability domains enlarges as one decreases u_2. This analysis leads us to conclude that the BHN density functional, which has been devised to describe the unpolarized liquid, can provide a reference for the weakly polarized system up to a rough 30%; this is illustrated in Fig. 1, where we show the induced magnetic field calculated with the parametrization BHN2 as a function of magnetization up to $\Delta = 0.4$, together with the experimental data from Ref. 17.

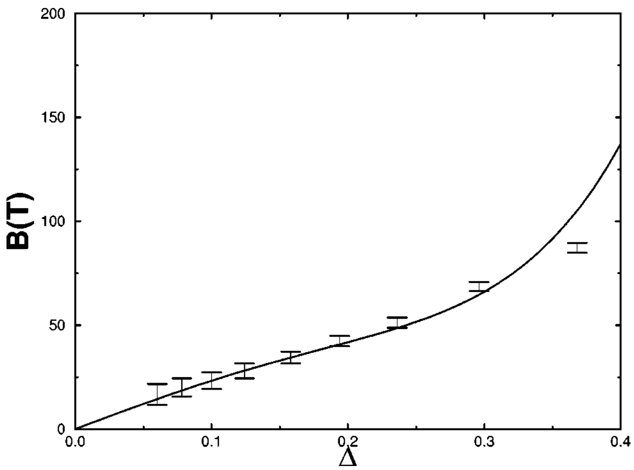

FIG. 1. The induced magnetic field calculated with the BHN2 parametrization at zero pressure as a function of polarization. The experimental points are those of Ref. 17.

In previous works by some of us[21,24–27] it has been shown that the random phase approximation (RPA) response of quantum liquids, either polarized or unpolarized, can be carried out almost exactly in the current density-functional frame, both at zero and at finite temperatures. An important feature of these calculations, which on the other hand demand a clear understanding of the properties of the effective ph interaction in polarized matter,[27] is the possibility of investigating the behavior of zero sound and the paramagnon resonance with increasing polarization, as well as the exploration of the existence of collective magnetic states. Although the effective ph interaction for finite transferred momentum enters the dynamical response in a rather complicated fashion,[26,27] the Landau parameters $F_l^{s,a}$ may indicate possible changes in the structure pattern. These parameters are displayed in Fig. 2 for $l = 0$ and 1 as functions of the magnetization, computed at saturation density of the unpolarized system with the parametrization BHN2. We notice that the Landau parameters in the antisymmetric spin channel change sign at polarizations near 0.1 and 0.2 (F_0^s and

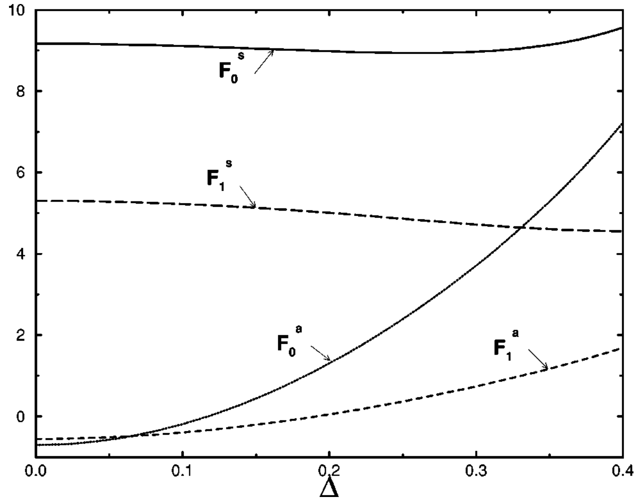

FIG. 2. The Landau parameters $F_{0,1}^{s,a}=N(0)f_{0,1}^{s,a}$, calculated with the BHN2 parametrization at zero pressure as function of polarization, where $N(0)$ is the density of states of the unpolarized liquid.

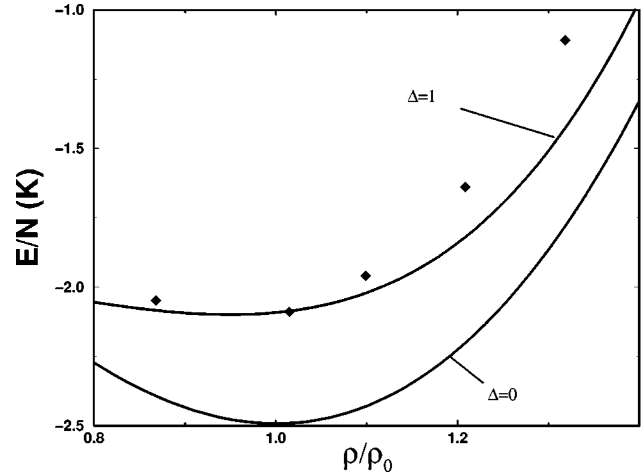

FIG. 3. Energy per particle as a function of density for polarizations zero and unity, computed according to the GHN Ansatz described in the text. The points are the results of Ref. 7 for the fully polarized liquid. ρ_0 is the equilibrium density of the unpolarized liquid at zero pressure.

F_0^a, respectively); in other words, the magnetic strength becomes repulsive, making room for the appearance of collective spin modes. A detailed analysis of these effects, correlating the evolution of the structure pattern to the behavior of the effective interactions in the low-magnetization limit, has been performed recently.[28]

IV. DISCUSSION AND PERSPECTIVES

As we compare the BHN functional with the one introduced by Stringari in Ref. 19, we find that the general appearance of these two functionals is rather similar, the most noticeable difference lying in the fact that in the BHN picture, the effective mass arises from the exchange term of the pp interaction. Moreover, the BHN functional has been adjusted to reproduce the monopole and dipole Landau parameters, in addition to the equation of state of the bulk liquid. This gives rise to dipole Landau fields $f_1^{\sigma\sigma'}$ that depend upon transferred momenta above the Landau limit, an important fact for future dynamical susceptibility calculations. In the low-polarization limit, the BHN functional yields an accurate description of the variations of the sound velocity at constant pressure, overestimated in Ref. 19. By contrast, the BHN predictions of the susceptibility coefficient β are 15–30% higher than the data, whereas in Ref. 19 these data have been employed to extract unknown parameters of the density functional. We have shown in this work that various choices of the criterium to determine the free force coefficients lead to scenarios which cannot be extended to describe the fully polarized liquid.

Up to the present day, experimental data for fully polarized liquid helium are not available. Various microscopic Ansätze[6–9] nevertheless indicate that such a system is bound at both density and binding energy slightly below those of the unpolarized system, with the effective mass of the spin-up particles at saturation being close to the bare one. One might then intend to generalize the BHN density functional so as to include higher dependences of the effective force strengths on spin density, spin kinetic energy density, and spin current density. We have verified that a series expansion in powers of the magnetization, with BHN being the second-order approximation, is not appropriate to continuously describe the full range of polarizations and liquid densities. Although one might have naively expected that most properties of spin-polarized matter would be associated with the spin-triplet pp interaction (i.e., $i=2$), this happens to be not true; we have encountered that a significant increase in the number of parameters of the functional is needed. This apparent drawback reflects the fact that spin densities are associated with a degree of freedom that was not present in the original construction of the BHN functional, whose existence introduces complexities comparable to those associated with the mass density itself.

As an Ansatz, to be hereafter indicated as Gatica, Hernández, and Navarro (GHN), one may look for modifications of the force strengths $\mathcal{V}_n$ of the form $u_i'\rho^{\alpha_1}\mathbf{S}^{2\alpha_2}+v_i'\rho^{\beta_1}\mathbf{S}^{2\beta_2}(\mathbf{J}^2-\mathbf{S}\cdot\mathbf{T})$, in order to parallel the dependence upon the density of the form ρ^{γ}, already proved convenient

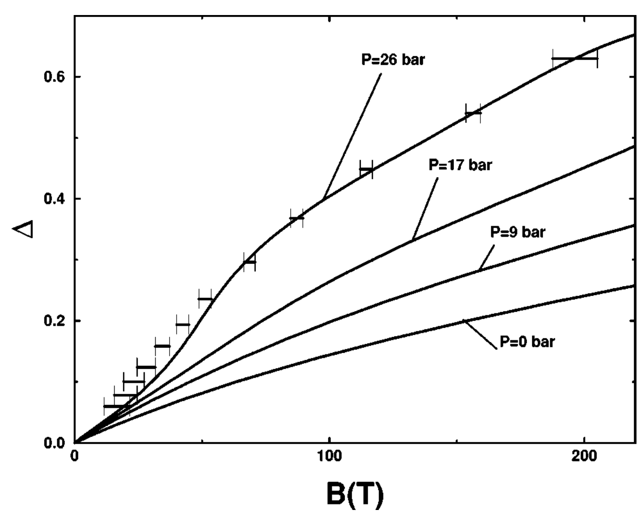

FIG. 4. Magnetization as a function of the induced magnetic field at various pressures for the GHN Ansatz. The experimental points are those of Ref. 17.

to reproduce the Landau parameters of the liquid in the density channel. The noninteger exponents thus control the curvature of the energy surface as a function of density and polarization. We have determined the above force parameters looking for the closest fit to the measured magnetic field as a function of polarization up to $\Delta=0.7$,[17] setting the energy of the fully polarized liquid equal to -2.1 K at a density equal to $0.95\rho_0$, the effective mass of the spin up species equal to unity at that density, and choosing three experimental points for the magnetic field. We have also minimized the dispersion of the microscopically calculated points of the energy of the fully polarized liquid[7] as well as the dispersion of the remaining magnetic field data. These choices are not unique; in fact, the exponents can vary within some moderate ranges, giving very similar patterns for any calculated magnitude. As an illustration we select one set of the extra parameters and depict in Fig. 3 the energy per particle of the fully polarized liquid as a function of the density, together with the microscopic results from Ref. 7, and the energy curve for the unpolarized system. We appreciate that while the trend of the microscopic prediction is well reproduced, the present results slightly underestimate the inverse compressibility. The magnetization as a function of the induced magnetic field is pictured in Fig. 4 for various densities, together with the experimental results of Ref. 17. We observe that in spite of the good fit to the high-field data, the adjustment of the low-polarization region is poorer that that provided by the BHN2 parametrization (cf. Fig. 1). No clear monotonic tendency in the slope of the field vs magnetization is evident and in particular, at the density $0.95\rho_0$, the susceptibility presents a singularity at $\Delta\approx0.65$. This is consistent with the metamagnetic behavior reported by Bonfait *et al.*[3] and theoretically described by previous authors,[12,19] since for a pressure of about 30 bars we predict a metamagnetic peak, however twice as large as the experimental value.[3] We also note that at the lowest polarizations the magnetic susceptibility predicted by these calculations is a decreasing function of Δ as indicated by the paramagnon model[13] and in agreement with viscosity measurements.[17,18] In view of the scarcity of experimental evidence, more data are requested in order to discern whether near-metamagnetic behavior should be ruled out as claimed by the authors in Refs. 17 and 18, especially, measurements of the induced field and the susceptibility as a function of the polarization at various pressures.

It should be also kept in mind that the present study describes a liquid at zero temperature; however, no substantial departures from the qualitative patterns should be expected in the degenerate Fermi liquid regime. A simple Sommerfeld expansion of the total energy predicts temperature corrections in the induced field of the type $B(T,\Delta)=B(0,\Delta)(1+\alpha T^2)$. This correction is not significant for the present discussion, since the largest deviation is below 10%. We also wish to stress that the results presented in Figs. 3 and 4 are only exploratory in the spirit of the BHN density functional. Nevertheless, a feature of these results, as well as of those arising from the BHN parametrizations, is the fact that they do not rule out metamagnetic behavior. In this sense, the present descriptions are consistent with previous investigations of spin-polarized helium in the frame of theories of Fermi liquids.[12,19,29]

In view of the most recent experimental results regarding the magnetic behavior of the liquid,[15–18] we believe that the present density-functional description, in particular, the BHN2 parametrization, can be safely adopted to describe this system up to magnetizations not higher than 30%. A detailed investigation of the dynamical response of weakly spin-polarized liquid helium anticipated in Ref. 28 is in progress and will be presented elsewhere.

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