Microscopic Theory of a Fully Polarized Model Fermi Liquid

Tai Kai Ng and K. S. Singwi
Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60201
(Received 22 January 1986)

Microscopic calculations of the dynamical properties of a fully polarized model Fermi liquid are presented and compared with those of an unpolarized model liquid. The model system is intended to simulate liquid ^{3}He.

PACS numbers: 67.50.Dg, 61.20.Ne, 67.65.+z

As a result of the pioneering work of Castaing and Nozières,[1] it has now become possible to perform experiments on a very interesting quantum system: a highly polarized ^{3}He liquid. However, microscopic theoretical studies[2-5] on the problem are still at a very preliminary stage. In the absence of any experimental data, it is also hard to construct a phenomenological theory.[5] Very little is known about the dynamical properties of this liquid. In this Letter, we present a microsopic calculation of the dynamical properties of a model system of fully polarized fermions interacting via a potential of the form

$$V(r)=V_0 \quad (V_0\to\infty), \quad r\le a_0,$$
$$V(r)=-\epsilon, \quad a_0<r\le a_1, \tag{1}$$
$$V(r)=0, \quad a_1<r,$$

which includes the two most essential features of a realistic helium-helium potential: a repulsive hard core at short distances and a short-ranged attractive tail.

The microscopic theory we use is the one given by Singwi *et al.*[6] which, although approximate, has been found to be quite successful in its application to Coulombic systems.[7] A recent application[8] of the same theory to the unpolarized system of fermions interacting via potential (1) was also found to give properties qualitatively very similar to what is observed in normal-liquid ^{3}He, including the pressure dependence of these properties. The aim here is to compare our results for the fully polarized and unpolarized systems, hoping that the results can shed some light on the future experimental and theoretical works on the subject. Since the theory is a microscopic one, it enables us to study separately the effects of the hard-core and attractive parts of the bare potential giving us more insight into the behavior of the real system.

In the Singwi-Tosi-Land-Sjölander scheme[6] the density response of the polarized system is given by a generalized random-phase-approximation expression:

$$\chi(k,\omega)=\chi_0(k,\omega)/[1-V_{\rm eff}(k)\chi_0(k,\omega)], \tag{2}$$

where $\chi_0(k,\omega)$ is the Lindhard function for a polarized Fermi liquid and $V_{\rm eff}(k)$ is the Fourier transform of an effective interparticle potential. The latter is given by[6]

$$V_{\rm eff}(r)=-\int_r^\infty g(r')[dV(r')/dr']dr', \tag{3a}$$

where $g(r)$ is the pair-correlation function. In differential form (3a) is

$$\nabla V_{\rm eff}(r)=g(r)\nabla V(r). \tag{3b}$$

In the equation-of-motion approach of Ref. 6, Eq. (3b) follows if the hierarchy of higher-order Wigner distribution functions is truncated by approximating the two-particle Wigner distribution function by the product of two one-particle Wigner distribution functions times the pair-correlation function.

Using (1) and (3), the Fourier transform of the effective potential can be found easily to be

$$V_{\rm eff}(k)=(4\pi/k^3)(V_0+\epsilon)g(a_0)[\sin(ka_0)-(ka_0)\cos(ka_0)]$$
$$-(4\pi/k^3)\epsilon g(a_1)[\sin(ka_1)-(ka_1)\cos(ka_1)], \tag{4}$$

where $g(a_0)$ and $g(a_1)$ are the values of the pair-correlation function at $r=a_0$ and $r=a_1$, respectively. The parameters $(V_0+\epsilon)g(a_0)$ and $\epsilon g(a_1)$ are determined self-consistently by use of fluctuation-dissipation theorem

$$S(k)=-(6\pi/k_{\rm F}^3)\int_0^\infty d\omega\,{\rm Im}\chi(q,\omega), \tag{5}$$

where $S(k)-1$ is the Fourier transform of $g(r)-1$. A similar set of equations is obtained for the density response of the unpolarized liquid except that one has for χ_0 the usual Lindhard function. The resulting 2×2 nonlinear matrix equation was solved in the limit $V_0\to\infty$ (hard core) for various densities using the generalized Newton's method. We have here not written these equations down since the algebra is quite straightforward. The corresponding result with the full Lennard-Jones (L-J) potential will be a $N\times N$ non-

linear matrix equation where $N \simeq 100$–500. At this stage, we felt it was not warranted to embark on such a massive numerical calculation. In our calculation a_0 was chosen to be 0.9σ ($\sigma = 2.556$ Å for helium), and a_1 and ϵ were fixed by our equating the zeroth and first moments of the attractive part of our model potential to the corresponding moments for the L-J potential. This gives us $a_1 = 2.05a_0$ and $\epsilon = 0.46\bar{\epsilon}$ ($\bar{\epsilon}$ is the depth of the L-J potential). a_0 was chosen to be slightly less than σ since the L-J potential is actually weaker than the hard-core potential. We discuss below the results of our self-consistent calculations.

In Fig. 1 the effective potential $V_{\rm eff}(k)$ is plotted as a function of ka_0 for two different densities. The normalization density n_0 is chosen for convenience to be $n_0^{-1} = (4\pi/3)a_0^3$. Notice the qualitative similarity between $V_{\rm eff}(k)$ and the polarization potential $f^s(k)$ of Aldrich and Pines.[9] Also note that the "dip" in the potential at small ka_0 disappears at larger densities. We find that this dip is a result of the attractive part of the bare potential. As the density increases, the effect of the hard core becomes more pronounced leading to the disappearance of the dip in $V_{\rm eff}(k)$. An interesting and quite unexpected consequence of this is that a "plateau" is found in $S(k)$ in the small-k region which weakens and gradually disappears as the density increases. This effect is seen in both unpolarized and polarized liquids in our calculations. Such a plateau has been seen experimentally[10] in normal-liquid ^{3}He at saturated vapor pressure. We also find that the shapes of the structure factors $S(k)$ for the fully polarized and unpolarized liquids are very similar with changes less than 5% in most regions of k. It is worth commenting that most of the properties calculated here are qualitatively insensitive to the changes in the parameters a_0, a_1, and ϵ.

In Fig. 2, the Landau parameter F_0 [$F_0 = N(0) \times V_{\rm eff}(0)$; note that $N(0)$ is the density of states of the noninteracting liquid in the present theory] is shown as a function of density. The Landau parameter F_0^s for the unpolarized system is also shown for comparison. The behavior of both F_0 and F_0^s with density variation is similar except that the magnitude of F_0 is smaller than that of F_0^s. The latter fact results in a larger compressibility ratio κ/κ_0 for the polarized liquid, where κ_0 is the compressibility of the noninteracting polarized Fermi liquid of the same density. Notice the rapid increase of both F_0^s and F_0 with density (or pressure), and that both F_0 and f_0^s become negative at density $n/n_0 \leq 0.4$.

In Fig. 3 is plotted the zero-sound dispersion for density $n/n_0 = 0.69$. Interestingly enough, the zero-sound velocities for the polarized and the unpolarized model liquids are nearly the same in the entire density range considered—the difference is less than 3%. Apparently, the decrease in F_0 from F_0^s is compensated

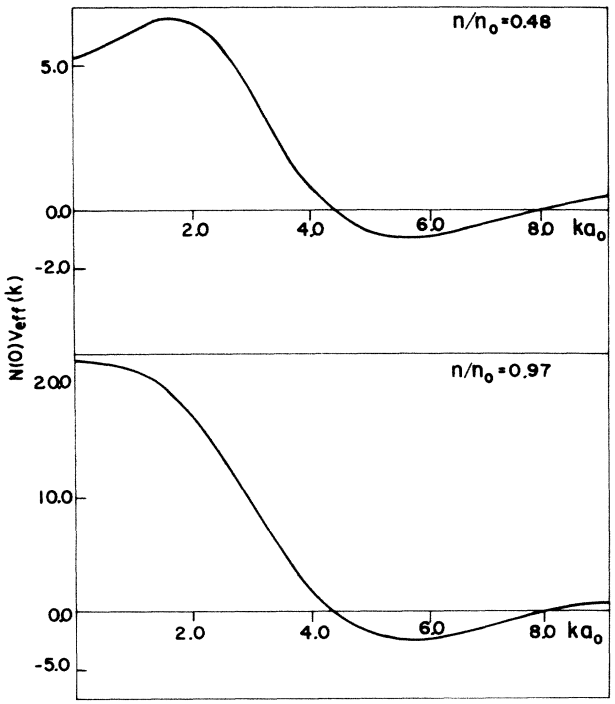

FIG. 1. Effective interaction $V_{\rm eff}(k)$ vs ka_0 for two densities, $n/n_0 = 0.48$ and 0.97.

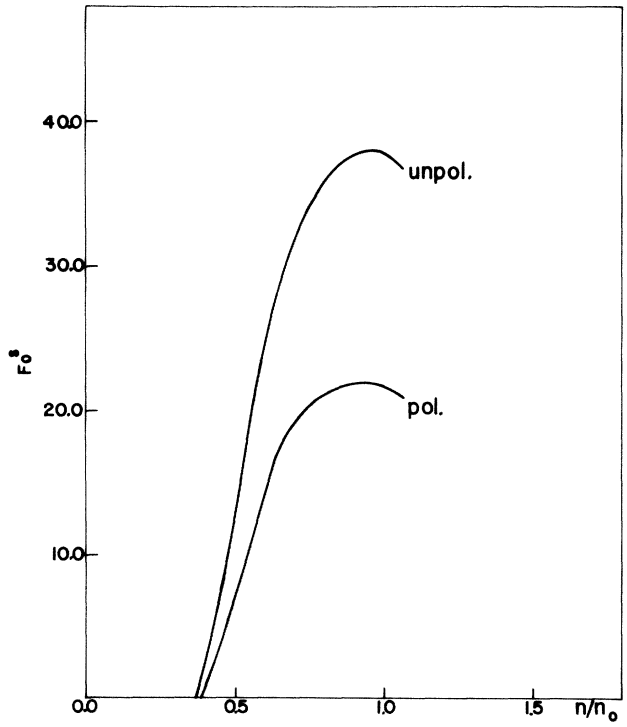

FIG. 2. Landau parameters F_0 (polarized) and F_0^s (unpolarized) vs n/n_0.

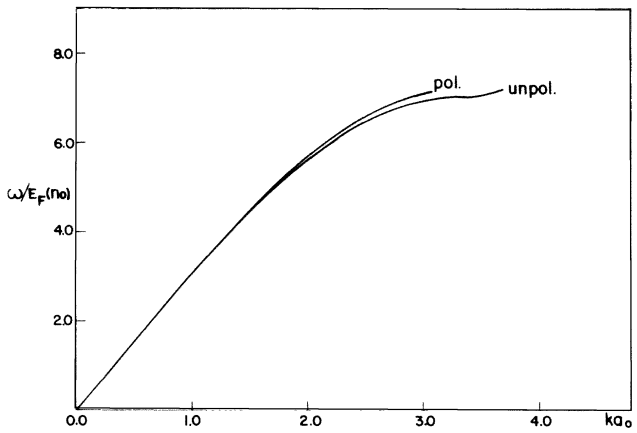

FIG. 3. Zero-sound dispersion, $\omega/E_F(n_0)$ vs ka_0, for the polarized and unpolarized liquids for the density $n/n_0=0.69$. $E_F(n_0)$ is the free-particle Fermi energy for the unpolarized liquid at density $n=n_0$.

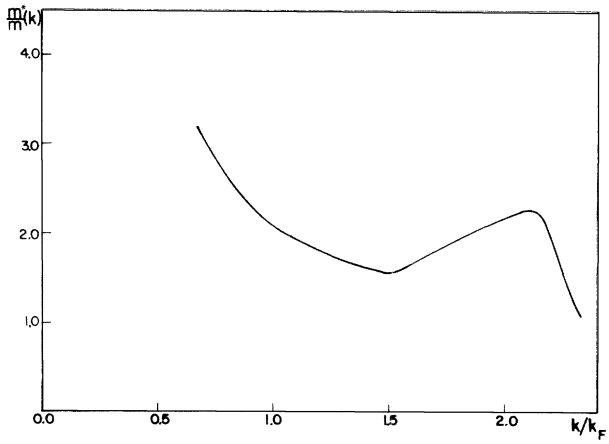

FIG. 4. On-shell effective mass $m^*(k)/m$ vs k/k_F for the fully polarized liquid with density $n/n_0=0.48$.

almost exactly by the increase in the Fermi velocity of the polarized liquid. For the same reason, the absolute value of the compressibility remains about the same in the two cases. However, one notices that in the region of large k, the dispersion in the polarized case is much less flat compared to that in the unpolarized case. It also vanishes at a smaller k because of the higher energy of the particle-hole continuum.

We have also calculated the self-energy using the following expression:

$$\Sigma(k,\omega)=\int[d^3k'/(2\pi)^3]\int[d\omega'/2\pi]G^0(\mathbf{k}-\mathbf{k}',\omega-\omega')\Psi_{\rm eff}(k',\omega'), \tag{6}$$

where

$$\Psi_{\rm eff}(k,\omega)=V_{\rm eff}(k)+[V_{\rm eff}(k)]^2\chi(k,\omega). \tag{7}$$

The above expression is similar to that used by Friman and Krotscheck[11] in their calculation of the effective mass in normal-liquid ^{3}He except that the contribution from the spin-fluctuation term is absent for a fully polarized liquid. We find that the effective mass on the Fermi surface is significantly reduced in the polarized case because of the absence of spin-fluctuation contribution. For example, m^*/m changes from 1.53 in the unpolarized system to 1.30 in the fully polarized system for $n/n_0=0.48$ and from 2.00 to 1.37 at $n/n_0=0.97$. An on-shell calculation of the momentum-dependent effective mass has also been done for $n/n_0=0.48$. The results are shown in Fig. 4. Notice that it is qualitatively very similar to what Friman and Krotscheck[11] obtained for normal ^{3}He when the spin-fluctuation contribution is excluded. For small momentum, m^*/m diverges, which is an artifact of the on-shell calculation when quasiparticle renormalization effect is strong. The large "bump" seen at large momentum $k\geq 1.5k_F$ is a result of the coupling of the single-particle excitations to the zero-sound mode.

In conclusion, using a simple model interaction which contains the two main features of a realistic helium-helium interaction, we have been able to calculate and compare, using a microscopic approach, various properties of an unpolarized and a fully polarized Fermi liquid. In comparing our results with experiments in liquid ^{3}He for which $n/n_0\cong 0.7$, one must bear in mind that ours is a model system. We find that the sound velocities are almost identical in the unpolarized and fully polarized systems, in contrast to what is predicted by Bedell and Quader[3] and Hess, Pines, and Quader,[5] using semiphenomenological theories. We also find that $m^*/m>1$ on the Fermi surface, suggesting that the higher angular momentum ($l\geq 2$) Landau parameters may be more important in a fully polarized Fermi liquid such as ^{3}He because of the scattering amplitude sum rule $\sum_l\{F_l[1+F_l/(2l+1)]^{-1}\}=0$ (Refs. 2 and 3). The Landau parameter F_0 of the polarized system is found to be smaller than the corresponding parameter F_0^s, in agreement with the predictions by other authors.[3,5] Both the parameters are found to increase rapidly with density and change sign at $n/n_0\simeq 0.39$. (The corresponding value of the parameter $c=a_0k_F$ is 1.4. For nuclear matter $c<1$.)

This work has been supported by the Materials Research Center of Northwestern University under a grant from the National Science Foundation.

[1]B. Castaing and P. Nozières, J. Phys. (Paris) **40**, 257 (1979).

[2]H. R. Glyde and S. I. Hernadi, Phys. Rev. B **28**, 141 (1983); see also E. Manousakis, S. Fantoni, V. R. Pandharipande, and Q. N. Usmani, Phys. Rev. B **28**, 2770 (1983); C. Lhuillier and D. Levesque, Phys. Rev. B **23**, 2203 (1981).

[3]K. S. Bedell and K. F. Quader, Phys. Lett. **96A**, 91 (1983).

[4]K. F. Quader and K. S. Bedell, J. Low Temp. Phys. **58**, 89 (1985).

[5]D. Hess, D. Pines, and K. F. Quader, to be published.

[6]K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. **176**, 589 (1968); see also G. D. Mahan, *Many-Particle Physics* (Plenum, New York, 1981), p. 442.

[7]K. S. Singwi and M. P. Tosi, Solid State Phys. **36**, 177 (1981).

[8]Tai Kai Ng and K. S. Singwi, "Model Fermi Liquid Interacting via a Hard-Core Repulsive Potential and an Attractive Tail" (to be published).

[9]C. H. Aldrich, III, and D. Pines, J. Low Temp. Phys. **32**, 689 (1978).

[10]E. K. Achter and L. Meyer, Phys. Rev. **188**, 291 (1969); R. B. Hallock, Phys. Rev. Lett. **26**, 618 (1971).

[11]B. L. Friman and E. Krotscheck, Phys. Rev. Lett. **49**, 1705 (1982). See also E. Krotscheck, J. W. Clarke, and A. D. Jackson, Phys. Rev. B **28**, 5088 (1983).