Normal Helium 3: a Mott-Stoner liquid.

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A physical picture of normal liquid $^3$He, which accounts for both “almost localized” and “almost ferromagnetic” aspects, is proposed and confronted to experiments.

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Helium 3 is a liquid of strongly interacting fermionic atoms. As pressure is increased between $p = 0$ and 34 bars, the compressibility is drastically reduced from $\kappa/\kappa_0 \simeq .27$ to $\kappa/\kappa_0 \simeq .066$, while the effective mass (specific heat coefficient) and magnetic susceptibility are enhanced from $m^*/m \simeq 2.8$, $\chi/\chi_0 \simeq 9.2$ to $m^*/m \simeq 5.8$, $\chi/\chi_0 \simeq 24$ ($m$ is the mass of free $^3$He atoms, and $\kappa_0$, $\chi_0$ refer to the free Fermi gas at the same pressure) . This is clearly the signal of the increasingly important effect of the interatomic interaction, which has a strong repulsive hard-core. Given the difficulties of a full quantitative treatment of such a problem, more phenomenological theoretical descriptions have been sought.

There are mainly two different, and seemingly contradictory, physical pictures that have emerged over the years. In the “almost ferromagnetic” approach , the liquid is viewed as being increasingly close to a ferromagnetic instability as pressure is increased and the large susceptibility is explained as a Stoner enhancement $\chi = \chi_0/(1 - I \chi_0)$. Being very close to an instability, critical spin-fluctuation modes (“paramagnons” (PM)) must be taken into account beyond the mean-field Stoner description. These modes have been claimed to be essential to explain, for example, the low-temperature dependence of the susceptibility . They also provide a logarithmic increase of the effective mass (though in rather mediocre quantitative agreement with experimental values). The “almost ferromagnetic” PM picture has some severe limitations however, particularly in failing to explain the strong reduction of compressibility .

This reduction is one of the main motivation for viewing instead the liquid as “almost localized”, i.e becoming more and more “solid-like” with pressure, as first proposed by Anderson and Brinkman and extensively developed by Vollhardt. The essential physics behind that picture is that of localization by repulsive interactions, in the sense of Mott. As explained below however, the simplest implementation of the quasi-localized picture leads to an incorrect description of the magnetic correlations and spin-fluctuation properties.

In this letter, we would like to propose a novel description of liquid $^3$He, which retains the proximity to Mott localization as a central notion, but reintroduces a more accurate description of the spin-spin correlations, of dominantly ferromagnetic nature. In our picture, in addition to being “almost localized”, the liquid is also close to a ferromagnetic instability (see also ), but not in a critical regime (contrary to PM theory). For this reason, liquid $^3$He is viewed in our picture as a “Mott-Stoner” liquid.

The quasi-localized picture was first implemented quantitatively by considering a lattice-gas model and modeling the hard-core repulsion as a Hubbard interaction:

$$H_1 = - \sum_{ij, \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

(1)

This model was then treated using the Gutzwiller approximation (GA), which yields a Mott transition at half-filling ($n = 1$) between a Fermi-liquid phase for $U < U_c$ and a localized Mott insulating phase for $U > U_c$. Close to the transition, the compressibility vanishes as $U_c - U$ and the effective mass diverges as $1/(U_c - U)$, in qualitative similarity with the behavior of liquid $^3$He for increasing pressure. In the simplest description, the lattice-gas is constrained to be at half-filling, and the GA expression for $m^*/m$ can be fitted to the experimental result in order to extract the single parameter $u(p) = U(p)/U_c$, with $u(p)$ an increasing function of $p$. (More refined formulations also allow a variable filling factor, and consider a trajectory $u = u(p)$, $n = n(p)$ in the $(u, n)$ plane). Given $u(p)$, the calculated GA compressibility is found to be in reasonable agreement with experiment. It is interesting in this respect to consider the dimensionless ratio $R_\kappa \equiv (\kappa/\kappa_0)(m^*/m)$, which is predicted to reach a finite value at the transition $R_\kappa^{GA}(U_c) \simeq .25$. Experimentally, this ratio does saturate at high pressure at a value $R_\kappa^{exp} \simeq .38$.

Turning to magnetic properties, the GA also leads to a divergent susceptibility $\chi \sim 1/(U_c - U)$, and thus to a finite “Wilson ratio” $R_W \equiv 1/(1 + F^2_W) = (\chi/\chi_0)/(m^*/m)$. Experimentally, this ratio has a very weak dependence on pressure, with $R_W^{exp}(p = 34\text{bars}) \simeq 4.1$, close to $R_W^{GA}(U_c)$. This agreement was originally viewed as one of the
main success of the approach and interpreted as evidence that the susceptibility enhancement could be entirely due to the incipient localization \[\tilde{\rho}\], responsible for the effective mass enhancement. However, we would like to point out that this divergence of the uniform susceptibility is an artefact of the GA, rather than a genuine feature of the Hubbard model. Indeed, in this model, the superexchange mechanism produces a nearest-neighbor antiferromagnetic exchange (of order \(J \simeq \tilde{\rho}^2/2U\) \[\tilde{\rho}\] for large enough \(U\)). On physical grounds, one expects this magnetic exchange to cutoff the divergence of the uniform susceptibility, which should remain finite, of order \(\chi \simeq 1/J\) through the transition and in the localized phase. More accurate treatments of the Mott transition within a dynamical mean-field of the Hubbard model based on the limit of large lattice coordination fully support this view \[\tilde{\rho}\]. Given the Fermi energy of liquid \(^3\)He, the magnetic superexchange would induce antiferromagnetic correlations on the scale of \(J \simeq 350\) mK, which is physically unrealistic and yields a too small susceptibility enhancement \(\chi/\chi_0 \simeq \epsilon_F/J \leq 7\). This has actually an even more drastic consequence, namely that the groundstate of the half-filled Hubbard model is in fact an antiferromagnetic insulating solid, rather than a paramagnetic liquid (except if a very large lattice frustration is introduced \[\tilde{\rho}\]). In the GA, the superexchange is neglected altogether so that these difficulties are simply overlooked. The overestimate of short-range antiferromagnetic correlations is actually not entirely due to the lattice description of the system. Variational treatments in continuum space using Jastrow-Slater wave functions and a realistic interatomic potential, also suffer from similar problems (when confronted, e.g. to neutron data) \[\tilde{\rho}\]. This is because, as in the Hubbard model, the emphasis is put mainly on only one of the effects of the hard-core, namely the avoidance of double occupancy.

Here, we suggest that the original formulation of the quasi-localized picture must be modified in order to account for the correct scale and type of magnetic correlations in the liquid. A very simple way to achieve this, while remaining in the framework of a lattice-gas model as above, is to introduce explicitly an additional nearest-neighbor ferromagnetic exchange, leading to the two-parameter model:

\[
H_2 = -\sum_{ij,\sigma} J_{ij} c_{i\sigma}^+ c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \frac{t}{2} \sum_{<ij>} \mathbf{S}_i \cdot \mathbf{S}_j \tag{2}
\]

The overall magnetic exchange \(\tilde{I} \equiv I - J \simeq I - \tilde{\rho}^2/2U\), can have a priori an arbitrary sign, and will be determined below from experimental considerations. We shall use the dynamical mean-field approximation, formally exact in the limit of large lattice coordination \(z \to \infty\), to analyze the behavior of this model (for an extensive review and technical details see Ref. \[\tilde{\rho}\]). In this limit, the inter-site magnetic interaction can be treated at the (static) mean-field level (in contrast, the local Hubbard interaction requires a full dynamical treatment). Hence, the dynamical magnetic susceptibility \(\chi(q, \omega)\) is readily obtained from that of the Hubbard model \(\chi_H(q, \omega)\) at the same value of \(U\) as:

\[
\chi(q, \omega)^{-1} = \chi_H(q, \omega)^{-1} - I \Delta(q) \tag{3}
\]

where \(\Delta(q)\) is the Fourier transform of the nearest-neighbor connectivity matrix:

\[
\Delta(q) = \frac{1}{V} \sum_{j=1}^V \exp(iq \cdot \mathbf{R}_j).
\]

In Fig. 1, we display the zero-temperature phase diagram of this model at half-filling, in the \((U, I)\) plane \[\tilde{\rho}\]. We shall mainly focus in the following on the Fermi liquid phase which is found when the Hubbard repulsion is smaller than a critical value associated with Mott localization \((U < U_c \simeq 3.7\epsilon_F)\), and the ferromagnetic exchange \(I\) is in the intermediate range \(I_{c}^{AF} < I < I_{c}^{F}(U)\). We emphasize that this phase does not display any kind of magnetic long-range order (the overall magnetic exchange \(\tilde{I}\) being in an intermediate coupling regime, it is always successfully opposed by kinetic energy effects). Stabilizing such a phase is one of the primary motivation of our approach. (Note that, as expected, the half-filled pure Hubbard model \((I = 0)\) is ordered antiferromagnetically for all values of \(U\) at \(T = 0\) in our treatment). When \(I\) is too small \((I < I_{c}^{AF}(U))\), the antiferromagnetic superexchange induced by the Hubbard repulsion takes over, and the liquid orders antiferromagnetically, while for large \(I > I_{c}^{F}(U)\), it orders ferromagnetically. The Mott localized state for \(U > U_c\) is always magnetically ordered at \(T = 0\), either antiferromagnetically for \(I < I_{c}^{AF}\) or ferromagnetically for \(I > I_{c}^{F}\), with
Inserting those into Eq. (3), one obtains for small energy effective Fermi scale well approximated by the form [10]:

$$U_{\text{eff}}(U) = I_{\text{eff}}(U) = J \cong \epsilon_F^2/2U$$

for $U > U_c$. Simple estimates of the critical couplings $I_{\text{eff}}, I_{\text{AF}}$ can be obtained for small $U$, and $U$ close to $U_c$. To first order in $U$, the Hubbard model static susceptibility reads: $\chi_H(q = 0) = 1 - U \equiv \epsilon_F - U$, and $\chi_H(Q) = U$ for the antiferromagnetic wavevector $Q = (\pi, \cdots, \pi)$. Inserting those into Eq.(3), one obtains for small $U$: $I_{\text{eff}} = \epsilon_F - U + O(U^2)$ and $I_{\text{AF}} = U + O(U^2)$. Close to the Mott transition, the static susceptibility of the Hubbard model in the dynamical mean-field approach is

$$\epsilon_F - U + O(U^2)$$

closest to the Mott transition, the static susceptibility of the Hubbard model in the dynamical mean-field approach is well approximated by the form [10]: $\chi_H(q, \omega = 0) = 1 \cong \lambda(q)\epsilon_F + J\Delta(q)$. In this expression, $\lambda(q)$ has a rather weak $\vec{q}$-dependence (with $\lambda(0) = 1$), while $\epsilon_F$ is the low-energy effective Fermi scale $\epsilon_F \cong 0.66 Z\epsilon_F$, with $Z$ the quasi-particle residue which vanishes as the Mott transition is reached at half-filling: $Z \cong 0.5(1 - U/U_c)$. Hence, the static $\vec{q}$-dependent susceptibility of (2) is reasonably approximated for $U \approx U_c$ by:

$$\chi(q, \omega = 0) = 1 \cong \lambda(q)\epsilon_F + (J - I)\Delta(q)$$

Using this expression, one obtains the estimates for $U$ close to $U_c$: $I_{\text{eff}} = J + \epsilon_F \approx J + 0.16(U_c - U)$, $I_{\text{AF}} = J - \lambda(Q)\epsilon_F$.

We now focus on the behavior of various physical quantities in the strongly correlated liquid phase, and on the application to the physics of liquid $^3$He. In this phase, the single-particle self-energy, and the density-density response function are unaffected by the coupling $I$ within the dynamical mean-field treatment, so that the effective mass and compressibility are functions of $U$ only and coincide with those of the pure Hubbard model. Close to the Mott transition, the effective mass diverges as $m^*/m = 1/Z \cong 1.1/(1 - U/U_c)$, while the compressibility vanishes as $\kappa/\kappa_0 \cong 66(1 - U/U_c)$, which is qualitatively similar to the GA (in contrast with $\chi \cong 1/(\epsilon_F + J - I)$).

Following the original phenomenological spirit of the quasi-localized approach [1], one can determine the pressure dependence of the two effective parameters $U(p)$, $I(p)$ by fitting the experimental results for two physical quantities. We have chosen to use the effective mass (specific heat) data to determine $U(p)$, and then to extract $I(p)$ from the susceptibility. For each pressure, liquid $^3$He thus corresponds to a point indicated on the phase diagram of Fig.1. The resulting trajectory is seen to approach both Mott localization $U = U_c$, and the ferromagnetic phase boundary $I = I_{\text{eff}}(U)$. While the effective mass enhancement is entirely associated with the on-site repulsion $U$, the proximity of the ferromagnetic phase boundary is crucial to account for the observed magnitude of the susceptibility enhancement: at the value of $U$ corresponding to the highest pressures, the susceptibility enhancement of the pure Hubbard model would be $\chi_H/\chi_0 \cong 5.4$, about 4.5 times too small. In the present approach, the saturation of the Wilson ratio $R_W = 1/(1 + F_n)$ precisely reflects the fact that both instabilities are approached. Indeed, using Eq. (4) we have, close to $U_c$: $\chi/\chi_0 = \epsilon_F/(\epsilon_F + J - I) = \epsilon_F/(I_{\text{AF}} - I)$, so that $R_W = (\chi/\chi_0)/(m^*/m) \cong \epsilon_F/(I_{\text{AF}} - I)$, and hence $U_c - U(p) \cong 4R_W(I_{\text{AF}} - I(p))$, indicating a linear trajectory towards the multicritical point at the highest pressure. The total magnetic exchange $I \equiv I - J \cong (0.66R_W - 1)/\chi \cong 1.6/\chi$ obtained from our approach is ferromagnetic ($I > 0$) and of the order of 300mK. This is precisely the typical energy gained by including short-range magnetic correlations in variational calculations [11]. The ferromagnetic sign is consistent with an instability of the liquid towards a triplet superfluid phase at low temperature. Having determined $U(p), I(p)$, we have compared the compressibility computed for our model to experiment. Excellent agreement is found at low pressure, while calculated values at high pressure are too large by approximately a factor of 2. The ratio $R_\kappa \equiv (\kappa/\kappa_0)(m^*/m)$ is predicted to saturate at high pressure as observed experimentally (with $R_\kappa(U_c) \approx .73$, while $R_\kappa^{exp}(p = 34\text{bars}) \approx .38$).

We would now like to compare and contrast the physical picture proposed here to that of the “almost ferromagnetic” PM description [2,3]. We first evaluate the dimensionless parameter $r \equiv (1 - I_c)/I_{\text{eff}}$ measuring the distance to the ferromagnetic critical boundary. From above, we find $r \cong 1.5/R_{W}$, which varies from $r \cong .46$ at low pressure to $r \cong .36$ at high pressure and is thus never very small in the present approach (in contrast $r \cong .11$ to .042 in PM theory). Hence, the ferromagnetic exchange may be treated within Stoner mean-field theory, with no significant effect of the long-wavelength PM fluctuations. This justifies a posteriori our treatment of this coupling within the large-connectivity limit. At low-energy, we have a liquid of quasi-particles characterized by the effective Fermi scale $\epsilon_F$. In the absence of any magnetic exchange ($I = 0$), the susceptibility of this gas would be of order $\chi_{qp} \cong 1/\epsilon_F$. The actual susceptibility $\chi = 1/\epsilon_F$ is correctly given by Stoner expression, with an effective Stoner enhancement $S_{eff} = \chi/\chi_{qp} \cong 0.66R_W$. $S_{eff}$ depends weakly on pressure, and measures the fraction of the total susceptibility enhancement due to the exchange (in contrast, $S \equiv \chi/\chi_0 = 1.55S_{eff}(m^*/m)$ is a combination of exchange and localization effects and strongly depends on pressure). These remarks also imply that there is no significant enhancement of the effective mass due to ferromagnetic spin fluctuations (in contrast with the logarithmic effect of PM theory), which leaves the estimate $m^*/m \cong 1.1/(1 - U/U_c)$ used above essentially unaffected. From Eq.(4) and the fact that $I > 0$, one sees that the susceptibility is peaked around $\vec{q} = 0$. For low $\vec{q} \equiv q \ll k_F$ and $\omega \ll qv_F^p$ (with $v_F^p = Zv_F$ the effective Fermi velocity), we can approximate the dynamical susceptibility by (neglecting all other residual interactions between quasiparticles apart from the exchange):
\[
\chi(q, \omega)^{-1} \simeq \epsilon^*_F \left(1 - \frac{i}{\epsilon^*_F} + \frac{q^2}{k_F^2} - \frac{i\omega}{qv_F^*} \right) \tag{5}
\]

From this expression, we see that there is a spin-fluctuation peak in \(\text{Im} \chi\) at a frequency \(\omega_{\text{max}}(q) \simeq qv_F^*/S\). The peak height is of order \(\text{Im} \chi_{\text{max}} \simeq S/\epsilon_F\). These estimates coincide with those found in conventional PM theory, and are in reasonable agreement with the available neutron data [14]. In contrast, the correlation length of the ferromagnetic fluctuations is found in our approach as a way to discriminate between the "almost ferromagnetic" and "almost localized" approaches [3]. Recently, a magnetic field dependence of the magnetization, which has been proposed to allow for a small concentration of vacancies \(\delta \sim 8\%\) (in the spirit of Ref. [3]) allows a reasonable description of the experimental magnetization curve \(m(h)\).

In conclusion, we have proposed a physical picture of normal \(^3\)He as a "Mott-Stoner" liquid, which seems in qualitative agreement with several experimental aspects.

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1. For a recent review and references on liquid \(^3\)He, see e.g. C. Lhuillier in "Strongly Interacting Fermions and High \(T_c\) Superconductivity", B. Douçot and J. Zinn-Justin eds., (Elsevier Science Pub. 1994).

2. For a review and references on the paramagnon approach, see e.g. K. Levin and O. T. Valls, Phys. Rep. 98, 1 (1983) and M. T. Béal-Monod, Proceedings of the International Workshop on 3d Metallic Magnetism, p.279, 1983.

3. For a critical review, see P. Nozières, Lecture Notes at Collège de France, unpublished, 1986.

4. M. T. Béal-Monod, S. K. Ma and D. R. Fredkin, Phys. Rev. Lett. 20, 929 (1968).

5. P. W. Anderson and W. F. Brinkman, in The Helium Liquids, J. G. M. Armitage and I. E. Farquhar eds, Academic, New York, 1975, and in The Physics of Liquid and Solid Helium, Part II, K. H. Bennemann and J. B. Ketterson eds (Wiley, New York, 1978).

6. D. Vollhardt, Rev. Mod. Phys. 56, 99 (1984).

7. M. T. Béal-Monod, Phys. Rev. B 31, 1647 (1985).

8. K. Seiler, C. Gros, T. M. Rice, K. Ueda and D. Vollhardt, J. Low. Temp. Phys. 64, 195 (1986).

9. Throughout this paper, the energy scale \(\epsilon_F\) stands for the inverse of the non-interacting susceptibility \(\epsilon_F \equiv 1/\chi_0\). It is related to the \(^3\)He Fermi energy by: \(E_F(\(^3\)He) = 3\epsilon_F/2\).

10. For a recent review, see A. Georges, G. Kotliar, W. Krauth and M. Rozenberg, Rev. Mod. Phys. 68, 13 1996.

11. J.P. Bouchaud and C. Lhuillier, Z.Phys.B 75, 283 (1989).

12. Quantitative calculations are made here for a semi-circular d.o.s: \(D(\epsilon) = \sqrt{1 - (\epsilon / 4\epsilon_F)^2} / (2\epsilon_F)\)

13. The detailed topology of the phase diagram near the triple point (e.g. possible first-order transitions) will not be investigated in detail in this paper.

14. K. Sköld, C.A. Pelizzari, R. Kiehl and G. E. Ostrowski, Phys. Rev. Lett 37, 842, (1976); B. Fäk, K. Guckelberger, R. Scherm and A. Stunault, J. Low. Temp. Phys. 97, 445 (1994); M. T. Béal-Monod, J. Low. Temp. Phys. 37, 123 (1979).

15. S.A.J. Wiegers, P.E. Wolf and L. Puech, Phys. Rev. Lett 66, 2895 (1991)

16. L. Laloux, A. Georges and W. Krauth, Phys. Rev. B 50, 3092 (1994).