Fermi-condensate phase transition in a low-density electron gas

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Arguments presented here indicate that a phase transition associated with the formation of a fermion condensate occurs near $r_s \simeq 10$–15 in an electron gas.

The fact that the ground-state energy E_0 of a Fermi system is a functional of its quasiparticle distribution $n(p)$ has been widely used in the theory of Fermi fluids since the days of Landau[1,2] In homogeneous systems with a weak interaction, the Pauli principle dictates the choice of distribution: a Fermi step $n_F(p) = \theta(p - p_F)$. This step is stable as long as the following condition holds for an arbitrary variation $\delta n(p)$:

$$\delta E_0 = \Sigma(\epsilon(p; n_F(p)) - \mu)\delta n(p) > 0, \tag{1}$$

where $\epsilon(p)$ is the quasiparticle energy, and $\mu = \epsilon(p_f)$. If, on the other hand, the function $s(p) = 2M[\epsilon(p) - \epsilon(p_F)]/(p^2 - p_F^2)$ changes sign at a point p_c upon a change in the coupling constant g or the density of the system, then the distribution $n_{F(p)}$ changes.[3,4] If $s(p)$ first vanishes at $p = p_F$, then the equalities $s(p_F) = M/p_F(\partial\epsilon/\partial p)_{p_F} = M/M^*$ tell us that at the transition point we have $M^* = \infty$ and $(\partial/\partial p)_{p_F} = 0$. It has been customary to assume that the new quasiparticle distribution $n(p)$ is again a Fermi sphere, but now in the space of the new one-particle energies $\tilde{\epsilon}$: $\tilde{n}_F(p) = \theta\{\tilde{\epsilon}[p;\tilde{n}_F(p)] - \mu\}$. However, there is another possibility, which was discussed first in Refs. 3 and 4 and later in Ref. 5. In the terminology of contemporary social sciences, this other possibility can be summarized as follows: The totalitarian solution $\tilde{n}_F(p)$ dictated by the Pauli principle does not lead to a minimum of E_0 away from the point of the phase transition. If $E_0(n_F)$ decreases upon the appearance of at least one particle-hole pair, then the new quasiparticle distribution $n(p)$ is found through democratic elections from the condition for a minimum:

$$\mu = \delta E/\delta n(p), \qquad p_i < p < p_f. \tag{2}$$

Outside the interval p_i, p_f, the old solution remains in power: $n(p) = n_F(p)$. The actual boundaries of the region with the new distribution are found from (2). This point was confirmed in Refs. 3 and 4 for several models used as examples. This phase transition was called "fermion condensation," since the realization of (2) implies the appearance of a plateau in the spectrum of one-particle excitations and the appearance of a sharp peak in the density of states of the system. These effects are characteristic of a Bose fluid below the point of the condensate transition.

In which systems, and under which conditions, can this phase transition occur? These questions can be answered by analyzing a known identity of the theory of Ref. 1:

$$\frac{\partial \epsilon(p)}{\partial p} = \frac{p}{M} + \int \mathcal{F}(p, p_1, \vartheta) \frac{\partial n(p_1)}{\partial p_1} p_1^2 dp_1 \cos\vartheta d\Omega / 4\pi^3. \tag{3}$$

In particular, we see that $s(p = p_F)$ changes sign where the first harmonic $b_1^0 = \mathcal{F}_1(p_F M/\pi^2)$ is positive and equal to 3 (note that it is M, not M^*, which appears here!). Such a large positive value of b_1^0 would be possible only in systems with a strong effective repulsion: in dense media with a repulsive core or in a low-density Coulomb gas. In liquid ^{3}He, one of the densest Fermi systems, we have $b_1^0 \simeq 2$.

In the present letter we take the approach developed in Refs. 6–9 to calculate the quasiparticle spectrum $\epsilon(p;n_F)$ of a homogeneous electron gas in the jellium model. We find that the Fermi-condensate phase transition occurs in this gas at $\alpha_c \sim 2$ ($\alpha = e^2/v_F^0$). The energy $\epsilon(p;n_F) = \delta E_0/\delta m^0(\mathbf{p})$ is found by varying the energy $E_0 = \tau + W$, where τ is the kinetic energy of the Fermi gas ($\delta\tau/\delta n(\mathbf{p}) = \epsilon_p^0 = p^2/2M$. The interaction energy W is expressed in terms of the linear-response function of the system, $\chi(q)$, by[10]

$$W = \frac{1}{2}\rho^2 V(0) - \frac{1}{2}\int\int\int V(q)(\chi(q) + 2\pi\rho\delta(q_0))d\tau dq_0 dg_1/2\pi g_1. \tag{4}$$

Here $d\tau = d^3p/(2\pi)^3$, $q = (\mathbf{q}, q_0)$, and $V(\mathbf{q})$ is the interaction potential of the particles. The integral over q_0 is along the imaginary axis from $-i\infty$ to $+i\infty$. The response functions—the exact function $\chi(q)$ and the function of the noninteracting particles, $\chi_0(q)$—are related through the effective interaction potential of the particles, $R(q) = \delta^2 W/\delta\rho(q)\delta\rho(-q)$:

$$\chi(q) = \chi_0(q)\phi(q) = \chi_0(q)(1 - R(q)\chi_0(q))^{-1}. \tag{5}$$

Landau's theory postulates that the minimum E_0 is always reached at a corner point n_F of the $[n]$ functional space. In this case we have

$$\chi_0(q) = 2\int \frac{n(\vec{p}) - n(\vec{p} + \vec{q})d^4p}{\epsilon_{\vec{p}}^0 - \epsilon_{\vec{p}+\vec{q}}^0 + \omega(2\pi)^4 i}, \tag{6}$$

where $n(p) = \theta(p - p_F)$. From the definition of R, along with (4) and (5), we find a closed functional equation for R:

$$R(k) = V(k) - \frac{1\delta^2}{2\delta\rho(\vec{k})\delta\rho(-\vec{k})}\int\int\int V(q)\chi(q)d\tau dq_0 dg_1/2\pi g_1. \tag{7}$$

This equation can be solved by using as a zeroth approximation the local approximation[6–9] in which the derivative $\delta F(k)/\delta\rho(q)$ of the operator F is replaced by partial derivative $\partial F(k-q)/\partial\rho$. This is a fairly accurate approximation: It reproduces Monte Carlo calculations of the energies of model systems within 3–5%.

We turn now to the calculation of the spectrum $\epsilon(p, n_F(p))$. Varying (4), we find

$$\epsilon(p) = \epsilon_{\vec{p}}^0 - \frac{1}{2}\int\int\int V(\vec{q})\left(\phi(q)\frac{\delta\chi_0(q)}{\delta n(\vec{p})}\phi(q) + \chi(q)\frac{\delta R(q)}{\delta n(\vec{p})}\chi(q)\right) d\tau dq_0 dg_1/2\pi g_1. \tag{8}$$

For $M(\mathbf{p},k) = \delta R(k)/\delta n(\mathbf{p}) = \delta^3 W/\delta\rho(k)\delta\rho(-k)\delta n(\mathbf{p})$ we find from (7) a functional equation[8,9] which can again be solved through the use of the local approximation: $M^0(\mathbf{p},k) = \partial^2\epsilon(\mathbf{p}-\mathbf{k})/\partial\rho^2$. With $k=0$, this equation is the same as the exact equation $M(\mathbf{p},0) = \partial^2\epsilon(\mathbf{p})/\partial\rho^2$. A direct calculation of $\delta\chi_0(q)/\delta n(\mathbf{p})$ yields[11]

$$\frac{1}{2}\frac{\partial\chi_0(q)}{\partial n(\vec{p})} = (1 - n_F(\vec{p}-\vec{q}))\theta(\omega_{pq}) + n_F(\vec{p}-\vec{q})\theta(-\omega_{pq}) + \frac{\epsilon_{\vec{p}}^0 - \epsilon_{\vec{p}-\vec{q}}^0}{(\epsilon_{\vec{p}}^0 - \epsilon_{\vec{p}-\vec{q}}^0)^2 - q_0^2}. \tag{9}$$

Here $\omega_{pq} = \epsilon_{\mathbf{p}}^0 - \epsilon_{\mathbf{p}-\mathbf{q}}^0$. Numerical calculations[6] show that at $r_s < 20$ the amplitude $R(g,q = 2p_F t)$ is a linear function of g:

$$R(t,g) = \pi g\left(1/t^2 - \frac{1}{3}(1 + \frac{1}{t}\ln|\frac{1+t}{1-t}| + t^2\ln(1-t^{-2})\right). \tag{10}$$

We can thus integrate some of the terms in (8) over g analytically. Using the results of Ref. 11, we now rewrite (8) as follows:

$$\epsilon(p) = \epsilon_p^0 + \epsilon_{RPA}^{(1)}(p) + \epsilon_{RPA}^{(2)}(p) + \epsilon_{RPA}^{(3)}(p) + \delta\epsilon_{corr}(p), \tag{11}$$

where $\delta\epsilon_{\rm corr}(p)$ is given by the last term in (8), and

$$\epsilon_{RPA}^{(1)}(p) = -\int_{1<p} V(\vec{p}-\vec{l})d\tau_{\vec{l}}\ ,$$

$$\epsilon_{RPA}^{(2)}(p) = -\int_{1>p} V(\vec{p}-\vec{l})\phi(\vec{p}-\vec{l},\omega_{pl})n_F(\vec{l})d\tau_1 + \int_{1<p} V(\vec{p}-\vec{l})\phi(\vec{p}-\vec{l},\omega_{pl})(1-n_F(\vec{l}))d\tau_{\vec{l}}\ ,$$

$$\epsilon_{RPA}^{(3)}(p) = -\int\int\int V(\vec{q})(\phi(q)-1)\frac{\epsilon_{\vec{p}}^0 - \epsilon_{\vec{p}-\vec{q}}^0}{(\epsilon_{\vec{p}}^0 - \epsilon_{\vec{p}-\vec{q}}^0)^2 + w^2}d\tau dw/2\pi\ . \tag{12}$$

Here $w = iq_0$. The only distinction between (12) and the Gell-Mann–Galitskiĭ formulas[11,12] is that the effective potential R in ϕ acquires (in addition to V) an exchange component [see (10)].

We can evaluate α_c by writing $\chi_0 = p_F M\tilde{\chi}_0/\pi^2$ and by using for $\tilde{\chi}_0$ the interpolation formula $\tilde{\chi}_0(z,t) \simeq (1 + 3z^2 + 3t^2)^{-1}$, where $z = wM/(qp_F)$. In taking this approach, we can avoid lengthy numerical calculations almost completely. Most of the difference between this formula and the exact $\tilde{\chi}_0$ occurs at $z \simeq t \leqslant 1$, and it amounts to less than 25–30%. We see that $\alpha_c \simeq 2$. At these values of α, the component $\delta\epsilon_{\rm corr}$ as estimated in the local approximation is less than 10–15%. An evaluation of the other terms in (12) shows that with increasing α the spectrum $\epsilon(p)$ becomes deformed in

such a way that $s(p)$ changes sign first at the Fermi surface. From (12) we find

$$s^{(3)}(p_F) = -\frac{\alpha}{\pi}\int_0^\infty\int_{-\infty}^{\infty}\left(\frac{t+1}{(t+1)^2+z^2}+\frac{t+1}{(t-1)^2+z^2}\right.$$
$$\left.-\frac{1}{2}\ln\frac{(t+1)^2+z^2}{(t-1)^2+z^2}\right)(\phi-1)dtdz.$$

After we substitute ϕ and χ_0 into this expression and integrate over z analytically, we are left with the task of evaluating a single integral. As a result, we find

$$s^{(1)}(p_F,\alpha) = -\alpha\,,$$

$$s^{(2)}(p_F,\alpha) = \alpha\int_0^1\frac{(1-2t^2)}{t}\phi(t,0)dt\,,$$

$$s^{(3)}(p_F,\alpha) = -\frac{\alpha}{3}\int\left(\ln\left(\frac{(t+1)+(t^2+1/3+f/3)^{1/2}}{|t-1|+(t^2+1/3+f/3)^{1/2}}\right)\right.$$
$$-\frac{1}{t+1+(t^2+1/3+f/3)^{1/2}}$$
$$\left.+\frac{\operatorname{sgn}(1-t)}{|t-1|+(t^2+1/3+f/3)^{1/2}}\right)\frac{f(t)dt}{(t^2+1/3+f/3)^{1/2}}. \qquad (13)$$

The calculations show that the term $s^{(3)}$, like $s^{(1)}$, increases nearly linearly with α, while $s^{(2)}$ drops out of the picture quite early, at $\alpha\simeq 1$. We find $s(p_F,1)=0.4$, $s(p_F,2)=-0.001$, and $s(p_F,3)=-0.2$; $s(p_F,\alpha)$ changes sign at $\alpha_c=2$—near $r_s\simeq 12$. In view of the calculation errors, we conclude that this value could change by $\approx 30\%$. Here we should bear in mind that the quantity $s(0,\alpha)$ also falls off rapidly with increasing α. We thus cannot rule out the possibility that the long-wavelength part of the distribution $n_F(p)$ may also undergo a restructuring beyond the transition point.

How are we to describe the system beyond the phase-transition point? For this case we need to refine nearly all the equations written above to deal with the multiple degeneracy of the one-particle levels of the condensate. Specifically, we are dealing here, as in the theory of a Bose fluid,[15] with two subsystems, one of which—the condensate—is degenerate. When the particle–particle channel is dominated by an effective attraction, the wave function of the condensate has a simple structure, and the problem can be solved by the known methods of superconductivity theory.[3] If, on the other hand, there is no coherence in the binary correlations, the situation becomes much more complex. By generalizing the Hohenberg–Kohn theorem, one can then show that beyond the transition point the energy E_0 becomes a functional of two densities: the ordinary density ρ and the condensate density $k=\Sigma n_\lambda\varphi_\lambda(r)\cdot\varphi_\lambda^*(r)$. The occupation numbers n_λ are found from the condition for a minimum in (2).

Expression (4) is now applicable only to the contribution of the above-conden-

sate particles. To deal with the contribution of the condensate particles, we need to use the methods of the theory of degenerate systems which have been worked out in nuclear physics. The degeneracy is lifted as a result of correlation effects. As a result, the δ-function peak in the density of states of the system becomes broader. These correlation contributions are generally different for the condensate particles and the above-condensate particles, so a gap appears in the spectrum of one-particle excitations. These questions will be examined in more detail in a separate paper; at this point we would simply like to point out that a suitable setting for studying the effects discussed here might be electrons on the surface of liquid helium, in which case the density can be varied over a fairly wide range.

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