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INTERPLAY BETWEEN FERMION CONDENSATION AND DENSITY-WAVE-INSTABILITY

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It is shown that the phase transition in homogeneous liquids related to the density waves origin is preceded by the fermion condensation. Thus, the fermion condensation may be observed in a low density electron liquid, neutron stars, and in a liquid He^3. The three-dimensional (3D) and the two-dimensional (2D) liquids are considered.

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Several years ago an extremely powerful method of measuring the electronic structure close to the Fermi level was developed [1], that is angle- resolved photoemission spectroscopy (ARPES). ARPES measurements of electronic spectra in the vicinity of the Fermi level exhibit the dispersionless sharp peak, i.e., extended Van Hove singularity (VHS). Recently measured ARPES data from single-crystalline Sr_2RuO_4 reveal VHS with an extension in both directions in contrast to usual case when saddle point extends only in one direction [2, 3]. Thus, it turns out that there is a broad plateau in spectrum $\varepsilon(p_x, p_y)$, which lies at or less then 17 meV from the Fermi level. It is worth to note that the observed Fermi surface is in contrast to the LDA calculations [1, 2]. We propose that such a behavior of electronic spectra ε(p) can be understood within the frameworks of the theory of fermion condensation, based on the Landau theory of Fermi liquid [4]. Landau postulated that entropy S, as well as the other thermodynamical functions, being a functional of the quasiparticle distribution $n(p)$, is of the form,

$$S = -\int [n(p,T)\ln(n(p,T)) + (1-n(p,T))\ln(1-n(p,T))]\frac{d^3p}{(2\pi)^3}.$$

Then, the variational condition for the free energy, $F = E_0 - TS$, is to produce such a relation,

$$\frac{\delta(F-\mu N)}{\delta n(p)} = \varepsilon(p,T) - \mu(T) - T\ln\frac{1-n(p,T)}{n(p,T)} = 0, \tag{1}$$

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where T is a temperature, μ is a chemical potential. Eq. (1) is usually rewritten in the Gibbs form,

$$n(p) = \frac{1}{1 + e^{(\varepsilon(p,T)-\mu)/T}}, \tag{2}$$

with $\varepsilon(p)$ given by [4],

$$\frac{\delta E_0}{\delta n(p,T)} = \varepsilon(p,T), \tag{3}$$

where E_0 is the ground state energy functional. Eq. (2) is a compact form of eq. (1) rather than its solution, since the quasiparticle energy $\varepsilon(p)$ apperaing in eq. (2) is a nontrivial functional of $n(p)$.

Landau suggested that the derivative, $d\varepsilon(p)/dp$, is positive and finite at the Fermi level, that immediately produces $n(p, T{=}0)$ to coincide with the Fermi step function. But the former solution of eq. (1) is not the only one. There exist "anomalous" solutions [5-10] of eq. (1) associated with a so-called fermion condensation [5]. Being continuous within the Ω region in p, such a solution $n(p)$ admits a finite limit for the logarithm in eq. (1) at $T \to 0$, yielding [8]

$$\varepsilon(p) = \frac{\delta E_0}{\delta n(p)} = \mu, \; p_i \le p \le p_f. \tag{4}$$

Thus, within the region $p_i, p_f \in \Omega$, the solution $n(p)$ deviates from the Fermi step function $n_F(p)$ in such a way that the energy $\varepsilon(p)$ stays constant, while outside this region, $n(p)$ coincides with $n_F(p)$. Therefore, the occupation numbers $n(p)$ serve as variational parameters for the energy E_0 can be reduced by varying them. Since the single particle energy $\varepsilon(p)$ stays constant at exactly the chemical potential, eq. (4), one can conclude, $p_i < p_F < p_f$, where p_F is the Fermi momentum. When the condensation is only starting the momenta $p_i = p_f = p_F$. This fact means that the effective mass M^*, given by the formula,

$$\frac{1}{M^*} = \frac{1}{p_F}\frac{d}{dp}\varepsilon(p)\mid_{p=p_F}, \tag{5}$$

$M^* \to \infty$. So we can conclude that the beginning of the fermion condensation phase transition manifests itself by the absolute growth of the effective mass.

In this Letter we show that unlimited growth of the effective mass has to precede the appearance of the density-wave-instability in a homogeneous Fermi liquid. Thus, the fermion condensation can be thought of as widely spread effects rather then the uncommon and "anomalous" solution of eq. (2).

Let us briefly outline the main points of calculations of the effective mass [9, 11]. The energy E_0 is given by the equation,

$$E_0 = T - \int \left[\mathrm{Im}\left(\frac{\chi_0(q,\omega)}{1 - R(q,\omega,g)\chi_0(q,\omega)} \right) + 2\pi\rho\delta(\omega) \right] v(q) \frac{d^3q\, d\omega\, dg}{(2\pi)^4}, \tag{6}$$

where T is the kinetic energy of noninteracting particles, $\chi_0(q,\omega)$ is the linear response function of noninteracting particles depending on momentum q and frequency ω. The effective interaction R tends to the bare interparticle interaction $g\,v(q)$ when the coupling constant $g \to 0$. The integration over frequency ω goes along the real axis from 0 to $+\infty$, while the integration over g goes from 0 to a real value of g_0. Substituting eq. (6) into eq. (3) and upon using eq. (5) and some tedious algebra, we get,

$$\frac{1}{M^*} = \frac{1}{M} -$$

$$-\frac{d}{2p_F\, dp}\int\left[\frac{\frac{\delta\chi_0(q,\omega)}{\delta n(p)}}{(1-R(q,\omega,g)\chi_0(q,\omega))^2}\right]v(q)\frac{d^3q\, d\omega\, dg}{(2\pi)^4 i} -$$

$$-\frac{d}{2p_F\, dp}\int\left[\frac{\frac{\delta R(q,\omega,g)}{\delta n(p)}\chi_0^2(q,\omega)}{(1-R(q,\omega,g)\chi_0(q,\omega))^2}\right]v(q)\frac{d^3q\, d\omega\, dg}{(2\pi)^4 i}. \tag{7}$$

Here M is the bare mass of the particle of a system under consideration, and the integration over ω goes along the imaginary axis. We remember that the derivative d/dp is taken at $p = p_F$. One can calculate the function

$$I_0(p_F, q, \omega) = \frac{d}{dp}\frac{\delta}{\delta n_p}\chi_0(q,\omega)\,|_{p=p_F},$$

upon taking into account the explicit form of χ_0 [12],

$$\chi_0(q,\omega) = -\sum_k n_k(1-n_{k+q})\frac{2\omega_{kq}}{\omega^2+\omega_{kq}^2}. \tag{8}$$

Here $\omega_{kq} = (\mathbf{k}+\mathbf{q})^2/(2M) - \mathbf{k}^2/(2M)$. Now the calculations of the derivatives is performed directly,

$$\frac{d}{dp}\frac{\delta}{\delta n_p}\chi_0(q,\omega)\,|_{p\to p_F} \simeq I_0(p_F, q, \omega) =$$

$$= -\frac{4\pi}{p_F^2}\delta(p_F - |\,\mathbf{p}+\mathbf{q}\,|)\delta(\omega)\mathbf{p}(\mathbf{p}+\mathbf{q})\,|_{p=p_F}\,. \tag{9}$$

It is seen from eq. (9) that I_0 is the singular function. But this singular function will make a main contribution to the effective mass M^* if it meets another singular function. Otherwise, the four-dimensional integral takes away the two-dimensional singularity, and the first term on the right hand side of eq. (7) will be finite and quite comparable to the second one. Let us consider a homogeneous Fermi system located in the vicinity of the density-wave-instability, that is close by the phase transition when the system in question possesses the density wave characterized by the momentum q_c. The instability threshold is reached when the linear response function χ,

$$\chi(q,\omega) = \frac{\chi_0(q,\omega)}{1-R(q,\omega,g)\chi_0(q,\omega)}, \tag{10}$$

of the system possesses a pole at,

$$q = q_c; \;\; p_F = p_{Fc} = (3\pi^2\rho_c)^{1/3},$$

and at frequency, $\omega = 0$, or the denominator of the terms on the right hand side of eq. (7) vanishes [12]. Here ρ_c is the critical density at that the density-wave-instability sets in, while p_{Fc} is the corresponding Fermi momentum. So, the wanted singular function can be delivered by the denominator of the first term integrand, provided the system is nearby the instability. While in that case the integrand of the second term on the right hand side of eq. (7) has only two-dimensional singularity and therefore its contribution to the effective mass can be omitted. Now, we can simplify eq. (7), keeping the main contribution which comes from the function I_0, given by eq. (9),

$$\frac{1}{M^*}=\frac{1}{M}+$$

$$+\frac{p_F}{4\pi^2}\int_{-1}^{1}\int_{0}^{g_0}\frac{v(p_F\sqrt{2(1-x)})\,x\,dx\,dg}{\left[1-R(p_F\sqrt{2(1-x)},\omega=0,g)\chi_0(p_F\sqrt{2(1-x)},\omega=0)\right]^2}. \quad (11)$$

It is worth to note that $p_F\sqrt{2(1-x)}$ is the transferred momentum q. Below we adopt the shorthand, $p_F\sqrt{2(1-x)}=q(x)$. It is seen from eq. (11) that the integral, being negative, is logarithmically divergent in the limit $p \rightarrow p_{Fc}$. Of course, we suppose $q_c \simeq 2p_{Fc}$ since there is no the other vector but $\mathbf{p}_F$. On the hand, in the case of an electron gas, the direct calculations of the effective interaction R [9], including ones basing on the Monte Carlo calculations [13−15], showed that R becomes negative at $q \simeq 2p_F$. We remark, that $\chi_0(q,\omega=0)$ is negative, hence $R(q,\omega=0)$ must be negative to deliver the pole to the linear response function, eq. (10). The fermion condensation occurs when the effective mass becomes infinite, i.e. the condensation is started as soon as the integral on the r.h.s. of eq. (11) cancels the term $1/M$. It is clear that it must take place long before the density-wave-instability displays itself.

Now let us consider 2D liquid. The transportation from 3D liquid to 2D one is clear since the form of the singular function I_0 is preserved for we do not take into account the dimension calculating this function. We can arrive at the final result, bearing in mind that instead of dx we have to write $dx/\sqrt{1-x^2}$:

$$\frac{1}{M^*}=\frac{1}{M}+$$

$$+\frac{1}{4\pi^2}\int_{-1}^{1}\int_{0}^{g_0}\frac{v(q(x))}{\left[1-R(q(x),\omega=0,g)\chi_0(q(x),\omega=0)\right]^2}\frac{x\,dx\,dg}{\sqrt{1-x^2}}. \quad (12)$$

The fermion condensation "more easy" occurs in 2D liquid compared to the 3D case. To see this, we remark that the integrand of eq. (12) is multiplied by a factor $1/\sqrt{1-x^2}\geq 1$. On the other hand, the density-wave- instability in the 2D case is also expected to take place "more easy" as compared to the 3D case, see below.

Consider a particular kind of a liquid which are two and three-dimensional electron gas. In the case of 3D electron gas the bare interaction $gv(q)$ is of the form,

$$gv(q)=\frac{4\pi^2e^2}{q^2}, \quad (13)$$

and the effective mass M^*, when system under consideration being not far from the instability point, can be directly got upon putting eq. (13) into eq. (11),

$$\frac{1}{M^*}=\frac{1}{M}+$$

$$+\frac{e^2}{p_F\pi}\int_{-1}^{1}\int_{0}^{1}\frac{x\,dx\,dg}{(1-x)\left[1-R(q(x),\omega=0,g)\chi_0(q(x),\omega=0)\right]^2}. \tag{14}$$

One can get the well-known Gell-Mann result for the effective mass of a dense electron gas [16] by putting $R=4\pi e^2/q^2$, as it should be in the low coupling limit. It was shown that the charge-density-wave-instability takes place in 3D gas at $r_s\simeq 30$, and $q_c\simeq 2p_F$ [17, 14, 18]. While a Wigner crystallization was predicted by the Monte Carlo calculations at $r_s\sim 100$ [19].

In the case 2D electron gas one gets,

$$\frac{1}{M^*}=\frac{1}{M}+$$

$$+\frac{e^2}{p_F\pi}\int_{-1}^{1}\int_{0}^{1}\frac{x\,dx\,dg}{(1-x)\sqrt{2(1+x)}\left[1-R(q(x),\omega=0,g)\chi_0(q(x),\omega=0)\right]^2}. \tag{15}$$

Here we put $gv(q)=2\pi e^2/q$. We stress that the effective interaction R of both 2D and 3D electron systems tends to the Coulomb interaction when $q\to 0$, and integrands of eqs. (14), (15) have no singularities at $x=1$. The Monte Carlo calculations of the ground state properties of an electron gas predicted a Wigner crystallization at the density $r_s\simeq 37$ in the 2D electron gas [20]. But before crystallization the density waves should take place, and that is the case: the charge-density-wave-instability is shown to occur at $r_s=(10\div 5)$, and $q_c\simeq 2p_F$, in parallel electron layers separated by potential barriers [13, 15]. Thus, as we have shown above, the fermion condensation will inevitably arise, being produced by the possibility of the charge-density-wave-instability. Our calculations predict the fermion condensation in 3D electron gas at $r_s\simeq 21$ [11], while calculations in the 2D case give the value of $r_s\simeq 8$, and will be published elsewhere.

Wigner crystallization have been also predicted to occur for dense neutron matter [21]. Different calculations yield varying values for the solidification density of neutron matter in the interior of neutron stars [22]. One can imagine that before forming crystal structures a liquid becomes unstable against small amplitude density fluctuations, i.e., the linear response function has a pole for q_c [12, 17]. We suppose the same is true for the solidification of liquid ^{3}He. Therefore, we can conclude that the fermion condensation should display itself in such liquids.

In summary, we have shown that the fermion condensation could take place in any Fermi liquid (electron gas, nuclear matter, neutron matter and liquid ^{3}He), which undergoes the density-wave-instability under some conditions.

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