Merging of single-particle levels and non-Fermi-liquid behavior of finite Fermi systems

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We examine the problem of finite Fermi systems having a degenerate single-particle spectrum and show that the Landau approach, applied to such a system, admits the possibility of merging single-particle levels. It is demonstrated that the opportunity for this behavior is widespread in quantum many-body systems. The salient feature of the phenomenon is the occurrence of nonintegral quasiparticle occupation numbers, leading to a radical alteration of the standard quasiparticle picture. Implications of this alteration are considered for nuclear, atomic, and solid-state systems.

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Landau Fermi-liquid theory (FL) is recognized as one of the foundation stones of our understanding of the properties of condensed matter. When adapted to finite Fermi systems in nuclear and atomic physics, the standard FL quasiparticle picture prescribes that the total angular momenta of the ground states of odd nuclei must be carried by a single quasiparticle, and that the electronic configurations of ions of elements of the periodic table must repeat those of preceding atoms. Its iconic stature notwithstanding, the standard FL picture sometimes fails. Currently, the origin of non-Fermi-liquid (NFL) behavior of homogeneous Fermi systems is one of the central issues of condensed-matter physics. Inhomogeneous, finite Fermi systems, although unburdened by the damping of single-particle (sp) excitations cited as the source of failure of the Landau quasiparticle picture [2], are also known to exhibit violations of FL theory. For example, the total angular momenta of the ground states of many odd-A nuclear isotopes in the transition region cannot be attributed to a sp state, and the electronic configurations of elements not belonging to principal groups differ from those expected in FL theory.

Here we focus attention on finite Fermi systems whose sp spectrum has a degeneracy and show that, rather surprisingly, NFL behavior can arise within the Landau approach [1] itself, with the merging of sp levels lying on opposite sides of the Fermi surface. This phenomenon, almost never addressed in condensed-matter physics, stems from the variation of sp energies under change of the occupation of the last unfilled sp level due to the interaction between quasiparticles. In the systems to be studied, the energetic distance between a sp level being filled and the nearest empty level shrinks progressively as the former level is filled, leading to a crossing of the levels in cases where standard FL theory is obeyed. However, in the case of interest, the levels do not cross one another; instead, they merge. As will be seen, a primary condition for merging to occur is that the Landau-Migdal interaction function is repulsive in coordinate space, which holds for the interactions between particles of the same kind in the nuclear interior and for electron-electron interactions in atoms.

We begin the analysis of this phenomenon by considering two neutron levels in an open shell of of a schematic model of a spherical nucleus of mass number A and radius \( R = r_0 A^{1/3} \). The levels are denoted by 0 and +, in order of increasing energy. As usual, the sp energies \( \varepsilon_\lambda \) and wave functions \( \varphi_\lambda(r) = R_{nl}(r)\lambda_j\ell(k) \) are solutions of equation \( [p^2/2M + \Sigma(r,p)]\varphi_\lambda(r) = \varepsilon_\lambda\varphi_\lambda(r) \), where \( \Sigma \) stands for the quasiparticle self-energy. In a spherical nucleus with even numbers of neutrons and protons, which has zero total angular momentum in its ground state due to pairing correlations, the sp energies \( \varepsilon_\lambda \) are independent of the magnetic quantum number \( m \). We suppose that the orbital angular momenta of levels 0 and + obey \( l_0 \neq l_+ \gg 1 \) and follow the variation of the distance between these levels, as \( N \gg 1 \) neutrons are added to the level 0, changing the density \( \rho(r) \) by \( \delta \rho(r) = N R_{n=0}^2(r)/4\pi \). We neglect self-interaction corrections and retain only a major, spin- and momentum-independent part \( V(r) \) of the self-energy \( \Sigma \) and a primary, \( \delta(r) \)-like portion of the Landau-Migdal interaction function \( f \). In this case, the FL relation between the self-energy and the density that is responsible for the variation of \( \varepsilon_\lambda \) simplifies to [3, 4]

\[
\delta V(r) = f[\rho(r)] \delta \rho(r) .
\]  

The interaction matrix elements

\[
f_{kk'} = \int R_k^2(r)f[\rho(r)]R_{k'}^2(r)\frac{r^2 dr}{4\pi}
\]  

are assigned values \( f_{00} = u, f_{++} = v, \) and \( f_{0+} = w \). In a semiclassical approximation where \( R_k(r) \sim r^{-1}R^{-1/2}\cos \int p_k(r) dr, \) one has \( u v = 3w/2 \).

Based on these assumptions, the dimensionless energy shifts \( \xi_k(N) = [\varepsilon_k(N) - \varepsilon_k(0)]/D \) are given by

\[
\xi_k(N) = n_k U \quad \text{and} \quad \xi_k(N) = n_k W ,
\]  

where \( n_k = N_k/(2j_k + 1) \) is the occupation number of level \( k, D \) is the initial distance between levels + and 0,
$U = u(2j_0 + 1)/D$, and $W = w(2j_0 + 1)/D$. We have neglected second-order corrections that have little effect on the results since they are almost independent of the sp quantum numbers.

According to Eqs. (3), the dimensionless distance $d(N) = [\epsilon_+(N) - \epsilon_0(N)]/D = 1 + \xi_+(N) - \xi_0(N)$ changes sign at $N_c = D/(u - w)$. This always occurs before filling of the level 0 is complete if the distance $D$ is rather small. For $N$ above some critical value $N_c$, Eqs. (3) become inapplicable, since the pattern of orbital filling must change. In the standard FL picture, which allows only for crossing of sp levels, all the added $N > N_c$ quasiparticles must settle into the empty sp level $+$, which entails a change of the relevant sp energies. The sign of the difference $\epsilon_+(N) = \delta \epsilon_+(N) - \delta \epsilon_0(N)$ of the shifts of the sp energies $\epsilon_+$ and $\epsilon_0$ due to total migration of the quasiparticles from level 0 into level $+$ is crucial. With the help of Eq. (1), it is seen that

$$\epsilon_+(N) = N(u - 2w + v) \ . \ (4)$$

In our model, $\epsilon_+(N) \simeq 2Nu/3$ is positive. The positivity of this key quantity means that level $+$ remains above level 0 upon the migration. The standard FL scenario must then encounter a catastrophe at $N > N_c$: on the one hand, quasiparticles must leave level 0; on the other, their total migration into level $+$ is prohibited. To end the deadlock, both levels must be partially occupied, in contradistinction to FL theory where one and only one level can be partially occupied. Such dual partial occupation is possible only if the sp energies $\epsilon_0$ and $\epsilon_+$ coincide with the chemical potential $\mu$. If so, at $N > N_c$, Eqs. (3) becomes

$$\epsilon_0(0) + N_0u + N_+w = \epsilon_+(0) + N_0w + N_+v , \ (5)$$

which has the solution

$$N_+ = (N - N_c)(u - w)(u + v - 2w)^{-1} . \ (6)$$

Significantly, a resolution of the dilemma has been found within the Landau approach itself. To understand the consistency of this resolution, recall that the occupation numbers of Landau quasiparticles are given by

$$n_\lambda(T) = [1 + e^{(\lambda - \mu)/T}]^{-1} . \ (1)$$

At $T = 0$, this formula guarantees that occupation numbers are restricted to the values 0 and 1, but only for those sp levels with energies $\epsilon_\lambda \neq \mu$; otherwise the index of the exponent is uncertain. As seen above, the merging of two (or more) sp levels drives the levels exactly to the Fermi surface. Solution of equations of merging such as (5) removes the residual uncertainty at the expense of introducing fractional occupation numbers $n_\lambda$, violating what would appear to be an elementary truth of FL theory, but in fact maintaining consistency. The sp Green function in the presence of merging has the familiar form

$$G(\mathbf{r}, \mathbf{r}', \epsilon) = \sum_{k=0,+} \left( \frac{1 - nk}{\epsilon - \epsilon_k + i\delta} + \frac{nk}{\epsilon - \epsilon_k - i\delta} \right) \varphi_k(\mathbf{r}) \varphi_k^*(\mathbf{r}) ,$$

but be

![FIG. 1: Top panels: Dimensionless distance $d = (\epsilon_+ - \epsilon_0)/D$ between levels $+$ and 0 as a function of the ratio $x = N/(2j_0 + 2j_+, 2)$. Lower panels: Occupation numbers $n_k$ for levels 0 and $. Input parameters: $U = V = 3, W = 1$. For the left column, the ratio $r = (2j_0 + 1)/(2j_+, 1) = 2/3$; for the right, $r = 3$. Results from numerical calculations are plotted in Fig. 1 which consists of two columns, each made up of two plots. The upper panels show the dimensionless ratio $d(x) = |\epsilon_+(x) - \epsilon_0(x)|/D$ versus $x = N/(2j_0 + 2j_+, 2)$, which runs from 0 to 1. The lower panels give the occupation numbers $n_+(x)$ and $n_0(x)$, which, in the range of $x$ where $d(x) = 0$, behave as $n_+(x) = x(1 + r)/2 - r/(2(U - W))$ and $n_0(x) = x(1 + r)/(2r) + 1/(2(U - W))$, with $r = (2j_0 + 1)/(2j_+, 1)$.

In the variable $x$, the model exhibits three distinct regimes. In two of them, $d \neq 0$ and the standard FL picture holds. It fails in the third region, where $d = 0$ and integration of Eq. (1) over $\epsilon$ yields the density $\rho(\mathbf{r}) = \sum_{k=0, +} n_k \varphi_k(\mathbf{r}) \varphi_k^*(\mathbf{r})$ for the added quasiparticles. This result cannot be attributed to a single sp level, implying that well-defined sp excitations in the familiar Landau sense no longer exist. Passage through the three regimes can be regarded as a second-order phase transition, with the occupation number $n_+(x)$ treated as an order parameter.

The two sp levels remain merged until one of them is completely filled. If the level 0 fills first, as in the left column of Fig. 1 the episode of merging is ended by repulsion of the two levels, as if they possess the same symmetry – despite the fact that in the open shell, they always have different symmetries. In another case where
level + becomes fully occupied before level 0, as in the right column, the distance \( d(x) \) becomes negative, and the two levels just cross each other at this point.

In the nuclear many-body problem, both types of sp level degeneracy – either initially present or arising in the scenario described above – are lifted when pairing correlations are explicitly involved [3, 4, 5]. In atomic nuclei, realistic pairing forces are so weak that in nuclei with closed shells, pairing correlations are completely suppressed, with the effect that the nuclear pairing energy becomes a part of a shell correction to the Bethe-Weizsäcker liquid-drop formula. A model calculation [6] shows that merging of even two sp levels approximately doubles the gap value and drastically increases the pairing energy. More realistic calculations are needed to determine whether this enhancement is enough to promote the existence of a new minimum in the ground-state energy functional of superheavy nuclei.

We turn now to the merging of sp levels in atoms. In fact, it was in atomic physics that one of the first models of NFL behavior involving nonintegral occupation numbers was developed by Slater et al. [7]. This model is based on the observation that results of Hartree-Fock (HF) calculations for atoms of intermediate groups are often based on the observation that results of Hartree-Fock (HF) calculations for atoms of intermediate groups are often improved if, in an extended HF energy functional, contributions of two leading Slater configurations are included additively with factors 0 < \( x < 1 \) and 1 – x. The best choice for \( x \) is found from a minimization procedure, yielding equations similar to Eqs. [8], which naturally entail fractional occupation numbers \( n_A \). As we have already seen within the framework of the non-perturbative Landau approach, this feature is not a prerogative or artifact of the HF method: nonintegral occupation numbers may legitimately come into play provided the sign of the key quantity \( \delta c \), from Eq. [4] is positive, and, hence, the criterion for merging of sp levels is met. It therefore comes as no surprise that the conditions for merging of sp levels are satisfied in certain strongly correlated Fermi systems [9, 10] for which the HF method is inapplicable.

Two circumstances complicate the analysis of merging electron sp levels in atoms. First, the sp energies \( \epsilon_{njlm} \) cease to be \( m \)-independent due to the absence of Cooper pairing. Difficulties stemming from this fact can be avoided if, following Ref. [3] one tracks the center-of-gravity \( \epsilon_k = \sum_m \epsilon_{km}/(2j + 1) \) energies of levels, rather than individual \( m \)-levels or a band. Then one only has to deal with the spherically symmetric part of \( \delta \rho_0(r) \), as in the nuclear case. Second, the self-energy \( \Sigma \) has a nonlocal character due to the presence of long-range Coulomb interactions. In another respect, the treatment of merging sp levels in atomic systems is much simpler than in the nuclear case, because the space parameter \( r_o = r_0/a_B \) is less than unity (\( r_0 \) being the radius of the volume per electron and \( a_B \), the Bohr radius). This implies that correlation contributions to the electron-electron interaction function \( f_{ee} \) are rather small compared to exchange [8], so that \( f_{ee} \) takes the Hartree-Fock form. Carrying out the same operations that led to the necessary condition [4], we readily arrive at the corresponding condition

\[
\begin{align*}
 f_{nl} &+ f_{nl'} - 2f_{nl'nl''} > 0
\end{align*}
\]

(8)

for the merging of two electron sp levels with quantum numbers \( n, l \) and \( n', l' \). Introducing \( R_{nl}(r) = rR_{nl}(r) \), the interaction matrix elements are constructed as

\[
\begin{align*}
 f_{nl'} &= c^2 \int |\mathcal{R}_{nl}^2(r_1)|^{1/2} dr_1 \int |\mathcal{R}_{nl'}(r_2)|^{1/2} dr_2, \\
-(2j+1)^{-1}R_{nl}'(r_1)R_{nl'}(r_1)R_{nl'}(r_2) &= \frac{1}{r_>} dr_1 dr_2,
\end{align*}
\]

(9)

where \( r_> \) is the greater of \( r_1, r_2 \). In obtaining Eq. [9], we have neglected insignificant contributions to the exchange part of \( f_{ee} \) coming from multipole moments created by electrons moving in the open shell. Semiclassical estimates along the same lines as before confirm that the nondiagonal matrix elements of \( f_{ee} \) are of much smaller size than the diagonal ones. We may then conclude that the difference on the l.h.s. of inequality [8] is positive independently of the quantum numbers, so that the necessary condition for merging of the sp levels is met.

It is instructive to compare the values of the basic parameter \( N_c \) that governs the merging phenomenon in nuclear and atomic systems. In the nuclear problem, the neutron-neutron interaction is characterized by the dimensionless constant \( F_{NN} = f_{NN}N_F M/\pi^2 \approx 1 \); from Eq. [2] one then obtains \( u \approx e_F^0 A/2M \), where \( e_F^0 = p_F^0/2M \) is the Fermi energy. On the other hand, the distance \( D \) between sp levels in spherical nuclei with closed shells is of order of \( e_F^0 A^{2/3} \). Consequently, the critical particle number \( N_c = D/(u - w) \) must be of order of \( A^{1/3} \), which in turn means that not every pair of nuclear sp levels adjacent to the Fermi surface is susceptible to merging.

The situation in heavy atoms is quite different: the diagonal matrix elements of the electron-electron interaction in the open shell are of order several eV, markedly enhanced in the event \( f \)-orbital collapse, as occurs in rare-earth and transuranic elements [11, 12, 13, 14, 15]. The distance \( D \) between the sp levels adjacent to the Fermi surface in atoms with closed electron shells is known to be some 1–2 eV as well, so the critical number \( N_c \) in atoms is of order of unity. Consequently, in elements with nuclear charge \( Z > 20 \), the sp Green function has the form [7] – except for elements of principal groups, where the standard FL picture still holds. Furthermore, when \( N \) substantially exceeds \( N_c \), as is the case of many rare-earth and transuranic elements, merging of levels triggered by collapse of the \( f \) orbitals inescapably involves most of the sp levels in the open shell. Fractional occupation numbers become a necessity, with
the result that these elements lose their chemical individuality, a well-known feature of the sequence of rare-earth elements. The veracity of these inferences can be tested by means of precise measurements of the difference $\sigma(Z+1) - \sigma(Z)$ between cross sections for elastic scattering of charged particles by rare-earth or transuranic atoms with atomic numbers differing by unity. In the theory of Goeppert-Mayer [11], this difference is directly expressed in terms of the single $4f$ wave function, whereas if merging occurs, the density change involves all the merged sp levels.

According to the above argument, in systems devoid of pairing the centers of merged sp levels “get stuck” at the Fermi surface. We observe that this could provide a simple mechanism for pinning narrow bands in solids to the Fermi surface. To exemplify this point, consider a model in which the electron sp spectrum, calculated in the local-density approximation (LDA), is exhausted by (i) a wide band that disperses through the Fermi surface, and (ii) a narrow band, placed below the Fermi surface at a distance $D_n$. Turning on the electron-electron interactions produces a change of the sp energies in accordance with the Landau equation

$$\epsilon(p) = \epsilon_{LDA}(p) + \int f(p, p_1)n(\epsilon(p_1))d^3p_1/(2\pi)^3.$$  \(10\)

To proceed, we assume that only matrix elements $f^{(n)}(p, p_1)$ of the interaction function $f$ referring to the narrow band are significant, the others being negligible. If the shift $\delta \epsilon^{(n)}$ in the location of the narrow band due to switching on the intraband interactions exceeds the distance $D_n$, then the standard FL scenario calls for the narrow band to be completely emptied; but then $\delta \epsilon_n$ must vanish, and quasiparticles are obliged to return. To eliminate this mismatch, only a fraction of the particles leave the narrow band, in just the right proportion to equalize the band chemical potentials. The feedback mechanism we have described positions the narrow band exactly at the Fermi surface, resolving a long-standing problem in the LDA scheme.

It is worth noting that the bare narrow-band group velocity, proportional to the corresponding bandwidth $W^{(n)}$, is rather small, whereas the matrix elements $f^{(n)}(p, p_1)$, which do not contain this factor, are not suppressed. Consequently, the group velocity might change its sign when the interaction correction is taken into account, giving rise to the previously studied phenomenon known as fermion condensation, which involves whole-sale merging of sp levels in homogeneous Fermi fluids. In spite of evident commonalities, there is a crucial difference between the conditions for the “level-mergence” phenomenon in homogeneous Fermi liquids and in finite Fermi systems with degenerate sp levels. In the former, the presence of a significant velocity-dependent component in the interaction function $f$ is needed to promote fermion condensation, while in the latter, sp levels can merge even if $f$ is momentum-independent. The reason for this difference is simple. In the homogeneous case, the matrix elements $u, v$, and $w$ are equal to each other, implying zero energy gain due to the rearrangement when velocity-dependent forces are absent. The same is seen from Eq.\(\text{[10]}\): the group velocity, whose sign determines whether the Landau FL state is stable, is unaffected by the momentum-independent part of $f$.

The merging of sp levels quite often violates a symmetry inherent in the initial ground state. In nuclei, for example, the members of pairs of sp levels with quantum numbers $n, l$ and $n \pm 1, l \pm 2$ lie quite close to each other. As the lower of the two levels is being filled, the distance from its neighbor shrinks, resulting in an increase of the nuclear quadrupole moment. If merging occurs, spherical symmetry is broken. This mechanism is presumably responsible for the occurrence of islands of nuclear deformation beyond the mainland of rare-earth elements. Merging can also promote the enhancement of parity violation effects in nuclei and atoms. These issues will be addressed in a future article.

In conclusion, our exploration of the merger of single-particle levels in finite Fermi systems exhibiting degeneracy reveals that if the merging of two or more sp levels occurs, the ground state experiences a rearrangement that introduces a multitude of quasiparticle terms, endowing it with a more complex character, as in the comparison of a chorus with a dominant soloist.

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