Merging of single-particle levels in finite Fermi systems

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Properties of the distribution of single-particle levels adjacent to the Fermi surface in finite Fermi systems are studied, focusing on the case in which these levels are degenerate. The interaction of the quasiparticles occupying these levels lifts the degeneracy and affects the distance between the closest levels on opposite sides of the Fermi surface, as the number of particles in the system is varied. In addition to the familiar scenario of level crossing, a new phenomenon is uncovered, in which the merging of single-particle levels results in the disappearance of well-defined single-particle excitations. Implications of this finding are discussed for nuclear, solid-state, and atomic systems.

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Advanced technologies seek to exploit the properties of objects of nanometer size in the design of new materials and devices. The behavior of the electronic system within such a nanoscale object is largely determined by the structure of individual single-particle (sp) levels. It therefore seems opportune to revive the fundamental study of single-particle aspects of finite Fermi systems as developed many years ago for atomic nuclei in the expectation that the findings may also be of value for electronic systems of current technological importance.

In homogeneous matter, all the relevant measurable quantities, such as various susceptibilities, are functions of a single momentum transfer variable $q$. Inhomogeneous systems with a uniform distribution of sp levels possess basically the same properties. However, the situation changes when the spectrum of their sp excitations is degenerate. This degeneracy implies the existence of a new energy scale $D_{\text{min}}$, given by the difference between the energies of the closest sp levels lying on opposite sides of the Fermi surface. The properties of such systems exhibit striking departures from what is found in homogeneous matter.

To offer a prominent example, consider the ground-state energy $E_0(A)$ of atomic nuclei as a function of mass number $A$. For most nuclei, this quantity is well described by the Bethe-Weizsäcker liquid-drop formula. However, nuclei with a magic number of protons or neutrons have spherical form, and the relevant energy scale $D_{\text{min}}$ is several times larger than the average distance between neighboring sp levels in non-magic nuclei. This energy spacing provides a shell correction $\delta E_s$, lowering the liquid-drop binding energy and rendering the ground states of known magic nuclei stable with respect to any mode of decay. Another example is associated with the degeneracy of the sp spectrum of the two-dimensional electron gas in an external magnetic field. In this case, the degeneracy gives rise to a step-like behavior of the chemical potential $\mu(A)$, triggering oscillations of thermodynamic properties.

Customary explanations of such extraordinary behavior do not take account of the alteration of key quantities due to interactions between added particles under variation of their number. In many cases such an approximation is justified, since these interactions do not affect the deviations mentioned above, even if the sp levels cross one another. However, we shall demonstrate that the dependence of sp energies $\epsilon_\lambda = E_n(A+1) - E_0(A)$ on quasiparticle occupation numbers $n$, inherent in Fermi-liquid (FL) theory, allows for an alternative scenario. The familiar crossing of sp levels is replaced by a merging of these levels, a new phenomenon that leads to the disappearance of well-defined sp excitations and drastic departures from predictions of standard FL theory.

To gain insight into this unconventional scenario, we first consider a schematic model involving three neutron levels in an open shell of a spherical nucleus. The levels are denoted $-$, 0, and $+$, in order of increasing energy, and the distance between $-$ and 0 and between 0 and $+$ has the same value $D$. As usual, the sp energies and wave functions $\varphi_\lambda(r) = R_{\lambda n}(r)\Phi_{\lambda jm}(n)$ as well, are solutions of equation $[p^2/2M + \Sigma(r, p)]\varphi_\lambda(r) = \epsilon_\lambda \varphi_\lambda(r)$, where $\Sigma$ stands for the self-energy. In even-even spherical nuclei, which have total angular momentum $J = 0$ due to pairing correlations, the energies $\epsilon_\lambda$ are independent of the magnetic quantum number $m$ associated with the total sp angular momentum $j$. We suppose that the level $-$ is filled, the level $+$ is empty, and $N$ neutrons are added to the level 0, changing the density by $\delta \rho(r) = N R_{\text{min}}^2(r)/4\pi$. We assume that $l_\lambda \neq l_0 \neq l_+ \sim A^{1/3} \gg 1$.

It is our goal here to explore the consequences of the dependence of the sp energies $\epsilon_\lambda(n)$ on the distribution $n$. In what follows, we shall retain only a major, spin- and momentum-independent part of the self-energy $\Sigma$ and a primary, $\delta(r)$-like portion of the Landau-Migdal interaction function $f$. Accordingly, the FL relation between $\Sigma$ and the density $\rho$ responsible for the variation of $\epsilon_\lambda(n)$ with $n$ is simplified to $\delta \Sigma(r) = f[\rho(r)]\delta \rho(r)$. For the sake of simplicity, the diagonal and nondiagonal matrix elements of $f$ are assigned the respective values

$$u = \int R_{nl}^2(r) f[\rho(r)] R_{nl}^2(r) r^2 dr / 4\pi,$$  

(1)
\begin{equation}
 w = \int R_{nl}^2(r) f(\rho(r)) R_{n'l'}^2(r)r^2 dr / 4\pi,
 \end{equation}

independently of the quantum numbers \( n_l, n_{l'} \).

A simple estimate of the ratio \( u/w \) is obtained using a semiclassical approximation \( R_{nl}(r) \sim r^{-1} \cos \rho(r) dr \), with the result \( u \approx 3w/2 \). We next observe that \( f(\rho) \) is positive at densities close to equilibrium, but changes sign as \( \rho \to 0 \); hence the signs of \( u \) and \( w \) may depend on the quantum numbers of the sp levels in play.

Based on these results, the dimensionless shift \( \epsilon_k(N) = [\epsilon_k(N) - \epsilon_k(0)]/D \) for \( k = 0, +, - \) is given by

\begin{equation}
 \epsilon_0(N) = n_0U, \quad \epsilon_+(N) = \epsilon_-(N) = n_0W,
 \end{equation}

where \( n_k = N_k/(2j_k + 1) \) is the occupation number of level \( k \), \( U = u(2j_0 + 1)/D \), and \( W = w(2j_0 + 1)/D \). It is readily verified that if \( fpF/\pi^2 \sim 1 \), where \( pF = \sqrt{2M\epsilon_F} \) and \( \epsilon_F \) is the Fermi energy, then the integral \( \rho(k) \) has a value \( u \approx \epsilon_F/A \) and therefore \( \rho(U) \sim 1 \), since \( D \sim \epsilon_F/A^{2/3} \) in spherical nuclei.

According to Eqs. (3), the distance \( \epsilon_+(N) - \epsilon_-(N) \) remains invariant when \( N \) increases. On the other hand, the difference \( d_+(N) = \epsilon_+(N) - \epsilon_0(N) \) decreases with \( N \) when \( U > W > 0 \), as does the distance \( d_-(N) = \epsilon_0(N) - \epsilon_-(N) \) in the opposite case, \( U < W < 0 \).

Now let us determine what can happen when the functions \( d_+(N) \) change their signs before the sp level 0 is completely filled. We first examine the case \( U < W < 0 \). According to Eqs. (3), the sign of \( d_-(N) \) changes at \( n_0 = 1/(W - U) \), which requires \( W - U \) to be greater than 1 to meet the restriction \( n < 1 \). The usual Hartree-Fock (HF) scenario prescribes that for \( n_0 > n_{qc} \), quasiparticles must leave the occupied level and resettle into the unfilled level 0. Further, when the dependence \( \epsilon_\lambda = \epsilon_\lambda(n) \) from Eqs. (3) is brought into the picture, this effect is seen to promote the HF rearrangement.

In the opposite case, \( U > W > 0 \), the function \( d_+(N) \) changes sign at \( n_{qc} = 1/(U - W) \), implying \( U - W > 1 \). In order to satisfy this inequality, the repulsive part of the interaction \( f \) has to be sufficiently large, or else the scale \( D \) must be rather small. At \( n_0 > n_{qc} \), the HF scenario requires the quasiparticles to leave the unfilled level 0 and move into the empty level +. Were this scenario the correct one, the rearranged sp energies would obey the equations \( \epsilon_0(N) = \epsilon_0(N_0) + \delta N_0(w - u) \) and \( \epsilon_+(N) = \epsilon_+(N_0) + \delta N_0(u - w) \), where \( \delta N_0 \) is the number of quasiparticles shifted from level 0 to level +. The \( \delta \) term in each of these equations arises due to the feedback of the immigrating quasiparticles. Upon subtracting one equation from the other, we find that \( \epsilon_+(N) - \epsilon_0(N) > 0 \) for any \( \delta N_0 > 0 \), which says that the level + lies above rather than below the level 0. We thus arrive at a contradiction that excludes the HF scenario in the case \( U > W > 0 \).

Under these conditions, a new ground state must form, denoted henceforth by \( M \). As will now be shown, in the state \( M \) both of the levels 0 and + are partially occupied. Solution of the problem for this case reduces to finding the minimum of the relevant energy functional

\begin{equation}
 E = \epsilon_0(0)N_0 + \epsilon_+(0)N_+ + \frac{1}{2} [u(N_0^2 + N_+^2) + 2wN_0N_+] \end{equation}

with \( N_k = \sum_m n_{km} \), through the variational conditions

\begin{equation}
 \frac{\delta E}{\delta n_{0m}} = \frac{\delta E}{\delta n_{m_1+}} = \mu, \quad \forall m, m_1,
 \end{equation}

where \( \mu \) is the chemical potential. Such a condition for characterization of a rearranged ground state first appeared in Refs. 3, where homogeneous Fermi systems were addressed, without attention to degeneracy of sp levels. Eqs. (5) are conveniently rewritten as a conditions for the coincidence of the sp energies \( \epsilon_0 \) and \( \epsilon_+ \),

\begin{align}
 \epsilon_0(N) &= \epsilon_0(0) + N_0u + N_+w = \mu, \\
 \epsilon_+(N) &= \epsilon_+(0) + N_0w + N_+u = \mu,
 \end{align}

which, at \( N > N_c = (2j_0 + 1)/(U - W) \), yield

\begin{equation}
 \frac{N_0}{N} = \frac{1}{2} \left( 1 + \frac{N_c}{N} \right), \quad \frac{N_+}{N} = \frac{1}{2} \left( 1 - \frac{N_c}{N} \right).
 \end{equation}

\begin{figure}[h]
\begin{center}
\includegraphics[width=\textwidth]{fig1.png}
\caption{Top panels: Dimensionless distance \( d_+ = (\epsilon_+ - \epsilon_0)/D \) between levels + and 0 as a function of the ratio \( x = N/(2j_0 + 2j_+ + 2) \). Middle and bottom panels: Occupation numbers \( n_k \) for levels 0 and +. Input parameters: \( U = 4.0, W = 2.4 \). For the left column, the ratio \( r = (2j_0 + 1)/(2j_+ + 1) = 2/3 \); for the right, \( r = 3.0 \).
\end{center}
\end{figure}

Results from numerical calculations are plotted in Fig. 1, which consists of two columns, each made up of three plots. The uppermost panels show the dimensionless ratio \( d_+(N) = (\epsilon_+(N) - \epsilon_0(N))/D \). The middle and
lower panels give, respectively, the occupation numbers \( n_0 \) and \( n_+ \). We observe that there are three different regimes: in two of them there exist well-defined sp excitations, and \( d_+ \neq 0 \), and in the third, the energies of the levels 0 and + coincide at zero. Passage through the three regimes can be regarded as a second-order phase transition, with the occupation number \( n_+ \) treated as an order parameter.

Inserting the above results into Eq. (4), we find

\[
E_M - E_{HF}(N_0=0,N_+=N) = -(u-w)(N-N_f)^2/4 < 0 ,
\]

thereby verifying that the \( M \) state, having occupation numbers \( 0 < n < 1 \) for both of the levels 0 and +, has lower energy than any HF state. Significantly, the difference is of the same order as a typical shell correction \( \delta E_s \) in heavy magic nuclei. In such systems, the chemical potential \( \mu \) lies in the large gap between upper filled and lower unoccupied sp levels, while in the case of merging levels, \( \mu \) is located at the place where the density of states attains its maximum.

The 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 then under further increase of \( N \), quasiparticles fill the level +, signaling that the distance \( d_+(N) \) again becomes positive. This behavior resembles the repulsion of two levels of the same symmetry in quantum mechanics, although here one deals with sp levels of different symmetry. In the opposite case where level + becomes fully occupied before level 0, as in the right column, the distance \( d_+(N) \) 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. The role of \( D_{\text{min}} \) is played by the pairing gap \( \Delta \) in the spectrum of sp excitations. To illustrate this situation, we make BCS calculations in the above two-level model, under the assurance that realistic pairing forces are weak enough that the gap value remains smaller than the distance between neighboring sp levels in magic nuclei.

This two-level BCS problem is set up and solved as follows. First we rewrite the BCS gap equation as

\[
\Delta = gD \left( \sqrt{n_0(1-n_0)} + \sqrt{n_+(1-n_+)} \right). \tag{9}
\]

In so doing we have followed precedent by introducing a common dimensionless pairing matrix element \( g = (2j + 1)\lambda e_F/AD \), \( \lambda \) being a dimensionless pairing constant. A straightforward derivation, based on the BCS identity \( 4n_k(1-n_k) = \Delta^2/(\epsilon_k^2 + \Delta^2) \), the definition \( \epsilon_k = \sqrt{\delta E/\delta n_k} \) with \( E \) given by Eq. (4), and subtraction of one of Eqs. (6) from the other, leads to the key relation

\[
1 + (U-W)(N_0 - N_+) = \frac{\Delta}{D} \left[ R(n_+) - R(n_0) \right], \tag{10}
\]

where \( R(n_k) = \text{sgn}(1-2n_k)\sqrt{1/\left[4n_k(1-n_k)\right]} - 1 \). and

\[
\Omega, \tag{11}
\]

1), form a closed system determining the occupation numbers \( n_0, n_+ \) and the gap value \( \Delta \). This set of equations must be solved numerically; some results are given in Fig. 2. The inclusion of pairing correlations does indeed lift the degeneracy of the sp levels. However, the value of lowest of the energies \( E_k \) of the Bogoliubov quasiparticles remains markedly less than \( D \).

It is instructive to compare the structure of the pairing gap \( \Delta \) in two cases: when the above shrinkage of the distance between the sp levels + and 0 is taken into account, and when it is not. In the latter case, \( \Delta \sim |n_-(1-n_\lambda)|^{1/2} \) shows two humps with a dip in between. As seen in Fig. 2 the shrinkage effect fills in the dip. This increases the part of the ground-state energy associated with pairing correlations.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2}
\caption{Top panels: Pairing gap \( \Delta \) (in units of \( D \)) plotted versus \( x = N/(2j_0 + 2j_k + 2) \), both accounting for the shrinkage of the interlevel distance (solid line) and neglecting it (dashed line). Bottom panels: Energies of Bogoliubov quasiparticles \( E_k = \Delta/2|n_k(1-n_k)|^{1/2} \). Pairing constant: \( g = 0.3 \). Other input parameters for both columns are the same as in Fig. 1.

Let us now address the case \( u > w > 0 \) without pairing, existing for example in atoms and quantum dots. In this case, a pair of particles added to any sp level with \( l \neq 0 \) always have total angular momentum \( J \neq 0 \) (Hund’s rule), in principle destroying spherical symmetry and lifting the \( m \)-degeneracy of the sp energies \( \epsilon_{km} \). This gives rise to spreading of the levels, the magnitudes of which are proportional to \( u \) for the level 0, and \( w \) for the level +. If the interaction function \( f \) has long-range character, we have \( u/w \gg 1 \), and hence the spread of level 0 is much larger than that of level +. For the density \( \delta \rho \) associated with the added quasiparticles, we may write \( \delta \rho(x) = R^2_{\text{adj}}(x) \sum_m |\tilde{\Phi}(x)^2| n_m^2 \), which is applicable at least until the crossing of relevant orbitals begins. Upon inserting this formula into the relation \( \delta \Sigma = (f \delta \rho) \), it is found that the spread does not affect the evolution of the centers of gravity \( \epsilon_k = \sum_m \epsilon_{km}/(2j_k + 1) \) of the levels, since the isotropic part of \( \delta \rho \) has the same form.
\[ \delta \rho = N R_{\omega \rho}^2(r) / 4 \pi \] as if the degeneracy of the sp level were still in effect. This circumstance is especially important at the stage when the two families of sp levels begin to cross each other. Since at \( u > v > 0 \) the center of the gravity of the level \( + \) gets stuck close to the Fermi surface, our results provide a simple mechanism for pinning of the narrow bands in solids to the Fermi surface.

To exemplify this point, let us consider a model where the sp spectrum in local-density approximation (LDA) is exhausted by (i) a wide band, which disperses through the Fermi surface, and (ii) a narrow one, placed below the Fermi surface at a distance \( D_n \). We assume that only the diagonal matrix element \( f_{nn} \) of the interaction function \( f \) referring to the narrow band is significant, the others being negligible. The shift \( \delta \epsilon_n \) in the location of the narrow band due to switching on the intraband interactions is given by a formula analogous to Eq. (3), namely \( \delta \epsilon_n = f_{nn} \rho_n \), where \( \rho_n \) is the density of the band. If the correction \( \delta \epsilon_n \) exceeds the distance \( D_n \), then the HF scenario calls for the narrow band to be completely emptied; but then the shift \( \delta \epsilon_n \) must vanish. To eliminate this inconsistency, only a fraction of the particles leave the narrow band, in just the right proportion to equalize the chemical potentials of the two bands. The feedback mechanism we have described positions the narrow band exactly at the Fermi surface, resolving a long-standing problem with the LDA scheme.

In atoms, remnants of an accidental degeneracy of the Coulomb problem persist in the formation of electronic shells for which the distance between sp levels with different orbital momenta \( l \) is rather small. Recalling that matrix elements of the electron-electron interaction are quite sensitive to the \( l \) value, mergence of definite sp levels cannot be excluded. To elucidate this situation, one needs to analyze the energy functional \( E = \sum \epsilon_k(0)n_{km} + \frac{1}{2} \sum u_{km,k_1m_1} n_{km} n_{k_1m_1} \), wherein the interaction matrix \( u_{km,k_1m_1} \) replaces the matrix element and summation occurs over some states of the last unfilled shell. Results from numerical studies of the variational equations generalizing Eqs. (2), \( \mu = \epsilon_k(0) + \sum u_{km,k_1m_1} n_{k_1m_1} \), will be given elsewhere.

The new many-body effect uncovered in the foregoing analysis resembles a previously studied phenomenon, called fermion condensation, which involves wholesale mergence of sp levels in homogeneous Fermi fluids. In any conventional homogeneous Fermi liquid, e.g., liquid \(^3\)He, the momentum \( p \) of an added particle can be associated with a certain quasiparticle. Similarly, in most spherical odd-\( A \) nuclei, the total angular momentum \( J \) in the ground state is carried by an odd quasiparticle. In atomic physics, the electronic configuration of ions of elements belonging to the principal groups of the periodic table repeats that of preceding atoms. From the microscopic perspective, in all such “open-shell” systems conforming to standard FL theory, the single quasiparticle term \( a_+^\dagger \Psi_0 \) assumes a special role in the ground-state wave function, where \( \Psi_0 \) represents the ground state of a parent system. By contrast, in the case of merging of sp levels, the ground-state features a multitude of quasiparticle terms and therefore exhibits a more complicated, yet more balanced character — as in the comparison of a chorus with a dominant soloist. This implication of our analysis offers a qualitative explanation of the fact that the chemical properties of rare-earth elements differ little, in spite of marked variation in atomic numbers. Such an explanation may or may not be at variance with the textbook arguments that the relative squeezing of \( f \) and \( d \) orbitals is responsible for the remarkable similarity.

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 the 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 \( u \) and \( w \) are equal to each other, implying zero energy gain due to the rearrangement when velocity-dependent forces are absent. We point out that the study of level mergence in finite systems has the advantage of transparency, in that (i) it is free of the complicated issue of damping sp excitations, and (ii) it gives access to the precursor stage of the effect.

Our exploration of the mergence of single-particle levels in a finite Fermi system with degeneracy has revealed a phenomenon that entails the disappearance of well-defined low-lying single-particle excitations, with important implications in diverse physical settings.

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