

Merging of single-particle levels in finite Fermi systems

V. A. Khodel^{+,1)}, J. W. Clark^{*}, Haochen Li^{*}, M. V. Zverev⁺

⁺Russian Research Centre Kurchatov Institute, 123182 Moscow, Russia

^{*}McDonnell Center for the Space Sciences and Department of Physics, Washington University, St. Louis, MO 63130, USA

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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 [1], 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_{\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_{\min} is several times larger than the average distance between neighboring sp levels in non-magic nuclei. This energy spacing provides a shell correction δE_s , lowering the liquid-drop binding energy and rendering the ground states of known magic nuclei

stable with respect to any mode of decay [2]. 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 [3].

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 $\epsilon_s = E_s(A+1) - E_0(A)$ 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 $\varphi_\lambda(\mathbf{r}) = R_{nl}(r)\Phi_{jlm}(\mathbf{n})$ as well, are solutions of equation $[p^2/2M + \Sigma(\mathbf{r}, \mathbf{p})]\varphi_\lambda(\mathbf{r}) = \epsilon_\lambda\varphi_\lambda(\mathbf{r})$, where Σ stands for the self-energy. In even-even spherical nuclei, which have total angular momentum $J = 0$ due to pairing correlations, the energies ϵ_λ are independent of the magnetic quantum number m associated with the total sp angular momentum j . We sup-

¹⁾e-mail: vak@wuphys.wustl.edu

pose that the level $-$ is filled, the level $+$ is empty, and N neutrons are added to the level 0, changing the density by $\delta\rho(r) = NR_{n_0 l_0}^2(r)/4\pi$. We assume that $l_- \neq l_0 \neq l_+ \sim A^{1/3} \gg 1$.

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 Σ and a primary, $\delta(r)$ -like portion of the Landau-Migdal interaction function f . Accordingly, the FL relation between Σ and the density ρ responsible for the variation of $\epsilon_\lambda(n)$ with n is simplified to [1, 4] $\delta\Sigma(r) = f[\rho(r)]\delta\rho(r)$. For the sake of simplicity, the diagonal and nondiagonal matrix elements of f are assigned the respective values

$$u = \int R_{nl}^2(r) f[\rho(r)] R_{nl}^2(r) r^2 dr / 4\pi, \quad (1)$$

$$w = \int R_{n_1 l_1}^2(r) f[\rho(r)] R_{n_1 l_1}^2(r) r^2 dr / 4\pi, \quad (2)$$

independently of the quantum numbers $nl, n_1 l_1$.

A simple estimate of the ratio u/w is obtained using a semiclassical approximation $R_{nl}(r) \sim r^{-1} \cos \int p(r) dr$, with the result $u \simeq 3w/2$. We next observe that $f(\rho)$ is positive at densities close to equilibrium [1], but changes sign as $\rho \rightarrow 0$; 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

$$\epsilon_0(N) = n_0 U, \quad \epsilon_+(N) = \epsilon_-(N) = n_0 W, \quad (3)$$

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 $f p_F M / \pi^2 \sim 1$, where $p_F = \sqrt{2M\epsilon_F}$ and ϵ_F is the Fermi energy, then the integral (2) has a value $u \simeq \epsilon_F/A$ and therefore $|U| \sim 1$, since in spherical nuclei, $D \sim \epsilon_F/A^{2/3}$.

According to Eqs. (3), the distance $\epsilon_+(N) - \epsilon_-(N)$ remains unchanged when N increases. On the other hand, the difference $d_+(N) = 1 + \epsilon_+(N) - \epsilon_0(N)$ decreases with N when $U > W > 0$, as does the distance $d_-(N) = 1 + \epsilon_0(N) - \epsilon_-(N)$ in the opposite case, $U < W < 0$.

Now let us determine what can happen when the functions $d_\pm(N)$ 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 $n_{0c} = 1/(W - U)$, which requires $W - U$ to be greater than 1 to meet the restriction $n < 1$. The usual Hartree-Fock (HF) scenario prescribes that for $n_0 > n_{0c}$, 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 $n_{0c} = 1/(U - W)$, 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 $n_0 > n_{0c}$, 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 $\epsilon_0(N) = \epsilon_0(N_c) + \delta N_c(w - u)$ and $\epsilon_+(N) = \epsilon_0(N_c) + \delta N_c(u - w)$, where δN_c is the number of quasiparticles shifted from level 0 to level $+$. The δ 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 $\delta N_c > 0$, 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

$$E = \epsilon_0(0)N_0 + \epsilon_+(0)N_+ + \frac{1}{2} [u(N_0^2 + N_+^2) + 2wN_0N_+] \quad (4)$$

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

$$\frac{\delta E}{\delta n_{0m}} = \frac{\delta E}{\delta n_{+m_1}} = \mu, \quad \forall m, m_1, \quad (5)$$

where μ is the chemical potential. Such a condition for characterization of a rearranged ground state first appeared in Refs. [5], where homogeneous Fermi systems were addressed, without attention to degeneracy of sp levels. Eqs. (5) are conveniently rewritten as conditions for the coincidence of the sp energies ϵ_0 and ϵ_+ ,

$$\begin{aligned} \epsilon_0(N) &= \epsilon_0(0) + N_0 u + N_+ w = \mu, \\ \epsilon_+(N) &= \epsilon_+(0) + N_0 w + N_+ u = \mu, \end{aligned} \quad (6)$$

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

$$\frac{N_0}{N} = \frac{1}{2} \left(1 + \frac{N_c}{N} \right), \quad \frac{N_+}{N} = \frac{1}{2} \left(1 - \frac{N_c}{N} \right). \quad (7)$$

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

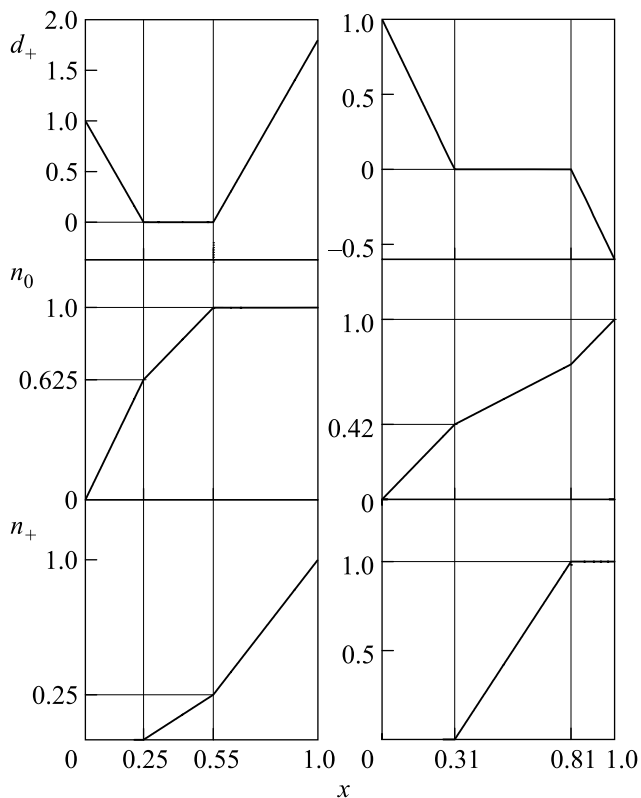


Fig.1. Top panels: Dimensionless distance $d_+ = (\epsilon_+ - \epsilon_0)/D$ between levels $+$ and 0 as a function of the ratio $x = N/(2j_0 + 2j_+ + 2)$. Middle and bottom panels: Occupation numbers n_k for levels 0 and $+$. Input parameters: For the left column, $U = 4.0, W = 2.4$, and the ratio $r \equiv (2j_0 + 1)/(2j_+ + 1) = 2/3$; for the right, $U = 4.0, W = 1.6$, and $r = 3$

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

$$E_M - E_{HF}(N_0=0, N_+=N) = - (u-w)(N-N_c)^2/4 < 0, \quad (8)$$

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 (8) is of the same order as a typical shell correction δE_s in heavy magic nuclei. In such systems, the chemical potential μ lies in the large gap between upper filled and lower unoccupied sp levels, while in the case of merging levels, μ 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_{\min} is played by the pairing gap Δ in the spectrum of sp excitations [6]. 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

$$\Delta = gD \left(\sqrt{n_0(1-n_0)} + \sqrt{n_+(1-n_+)} \right). \quad (9)$$

In so doing we have followed precedent by introducing a common dimensionless pairing matrix element $g = (2j+1)\lambda\epsilon_F/AD$, λ 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 $\epsilon_\lambda = \delta E/\delta n_\lambda$ with E given by Eq. (4), and subtraction of one of Eqs. (6) from the other, leads to the key relation

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

where $R(n_k) = \text{sgn}(1-2n_k)\sqrt{1/[4n_k(1-n_k)]} - 1$. Eqs. (9) and (10), together with the obvious equalities $N_k = n_k(2j_k+1)$, form a closed system determining the occupation numbers n_0, n_+ and the gap value Δ . 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 Δ 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, $\Delta \sim [n_\lambda(1-n_\lambda)]^{1/2}$ shows two humps with a dip in between [6]. As seen in Fig.2, the shrinkage effect fills

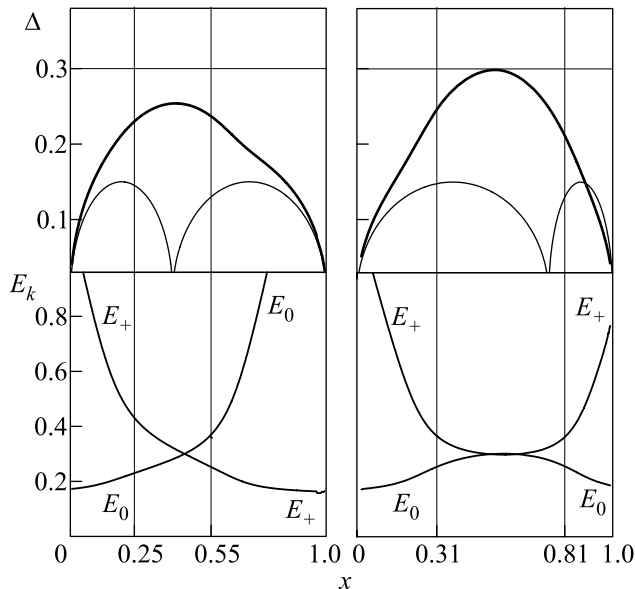


Fig.2. Top panels: Pairing gap Δ (in units of D) plotted versus $x = N/(2j_0 + 2j_+ + 2)$, both accounting for the shrinkage of the interlevel distance (thick line) and neglecting it (thin line). Bottom panels: Energies of Bogoliubov quasiparticles $E_k = \Delta/2[n_k(1 - n_k)]^{1/2}$. Pairing constant: $g = 0.3$. Other input parameters for both columns are the same as in Fig.1

in the dip. This increases the part of the ground-state energy associated with pairing correlations.

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 ϵ_{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 $\delta\rho(\mathbf{r}) = R_{n_0 l_0}^2(r) \sum_m |\Phi_{j_0 l_0 m}^2(\mathbf{n})|^2 n_{0m}$, 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 $\epsilon_k^0 = \sum_m \epsilon_{km}/(2j_k + 1)$ of the levels, since the isotropic part of $\delta\rho$ has the same form $\delta_0\rho = NR_{n_0 l_0}^2(r)/4\pi$ 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 $u > w > 0$ 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, while the others are 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 ρ_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

$$E = \sum \epsilon_k(0)n_{km} + \frac{1}{2} \sum u_{km,k_1 m_1} n_{km} n_{k_1 m_1},$$

wherein the interaction matrix $u_{km,k_1 m_1}$ replaces the matrix element (2) and summation occurs over some states of the last unfilled shell. Results from numerical studies of the variational equations generalizing Eqs. (5), $\mu = \epsilon_k(0) + \sum u_{km,k_1 m_1} n_{k_1 m_1}$, 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 [5, 7]. In any conventional homogeneous Fermi liquid, e.g., liquid ^3He , the momentum \mathbf{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. By contrast, in the case of merging of sp lev-

els, the ground-state features a multitude of quasiparticle terms and therefore exhibits a more complicated 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. In fact, a conventional explanation [8, 9] based on resettling of electrons into the collapsed $4f$ -orbital, framed within the Thomas-Fermi (TF) method for the rare-earth elements having $Z > 60$, is flawed, because the TF self-consistent field, being a universal function of Z , does not change in case quasiparticles resettle from one sp level to another. However, proper accounting for the interaction between resettling electrons within a more sophisticated Landau theory of Fermi liquid demonstrates that the respective change of the self-consistent field exists, and it is large enough to give rise to merging of the collapsed $4f$ -level with others in the open shell and hence level the sp properties of different electron systems that renders merging a complementary reason for the remarkable similarity of chemical properties of rare-earth elements.

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.

In conclusion, our exploration of the mergence of single-particle levels in finite Fermi systems 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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