Hund's Induced Fermi-Liquid Instabilities and Enhanced Quasiparticle Interactions

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Hund's coupling is shown to generally favor, in a doped half-filled Mott insulator, an increase in the compressibility culminating in a Fermi-liquid instability towards phase separation. The largest effect is found near the frontier between an ordinary and an orbitally decoupled ("Hund's") metal. The increased compressibility implies an enhancement of quasiparticle scattering, thus favoring other possible symmetry breakings. This physics is shown to happen in simulations of the 122 Fe-based superconductors, possibly implying the relevance of this mechanism in the enhancement of the critical temperature for superconductivity.

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A wealth of unexpected phenomena have been discovered in strongly correlated materials, and many technological applications are foreseen. At the heart of the observed remarkable behaviors is the many-body physics of the conduction electrons. Indeed, their tendency to avoid each other leads to a complex dynamics with surprising properties, even more so in the typical multiorbital landscape of these systems. In particular, the different repulsion that two electrons feel depending on them being in the same or in different orbitals, or on the alignment of their spins (embodied by the well-known Hund's rules of atomic physics), plays an important role in these materials.

Recently, our understanding of the influence of Hund's coupling on the metallicity properties of correlated materials has drastically improved [1]. Three aspects have been singled out as the most influential. (i) Hund's coupling tunes the splitting of atomic multiplets, which affects the distance in energy between the various sectors of atomic states with a given total charge. This energy is responsible for the local charge fluctuations, in a material, and thus for the ease with which a Mott insulating state can occur. The main outcome is that a Mott insulating state is strongly favored when conduction bands arise from an atomic shell that is half filled. (ii) Hund's coupling typically lowers the overall coherence of conduction electrons, especially for electron densities near half filling. (iii) It also favors the differentiation of the correlation strength among the conduction electrons. This was termed "orbital decoupling" [2,3], since it stems from Hund's coupling suppression of orbital fluctuations, favoring selective Mott physics depending on the orbital character of the conduction electrons. This can cause the coexistence of electrons with different correlation strength.

All of these results have been consistently found in iron-based superconductors and related materials [see, for example, Ref. [4] for (i), Ref. [5] for (ii), and Refs. [6,7] for (iii)], thus testifying to the importance of electronic correlations in these compounds in accord with theoretical studies [6,8,9].

However, these materials are Fermi liquids at low temperature [10], and their instabilities (magnetism, superconductivity) have been consistently modeled within weak-coupling theories [11]. The influence of electronic correlations on the high-T_c superconductivity is at present still not understood.

Here, we show that multiorbital correlations and Hund's coupling, in particular, have another, hitherto undiscovered, influence on these systems, in that not only the quasiparticle weight and masses but also the residual interactions between quasiparticles can be affected in a highly nontrivial way. This happens in the zone of influence of the aforementioned half-filled Mott insulator. We show that Hund's coupling affects these interactions enhancing the compressibility of the electron fluid, up to a point in which the system is unstable towards phase separation. Besides the many implications that an intrinsic instability towards a phase separation can entail [12], it is worth stressing that simply these altered quasiparticle interactions can have direct effects on the interaction vertices with low-energy bosons and radically enhance some bosonic-mediated mechanisms towards long-range ordered phases. We will show that this might be the case for the pairing mechanism for the high-T_c superconductivity in Fe-based superconductors.

We investigate the M-orbital Hubbard model with Hamiltonian $\hat{H} - \mu\hat{N} = \hat{H}_0 + \hat{H}_{\rm int} - \mu\hat{N}$, with

$$\hat{H}_0 = \sum_{i\neq j m m' \sigma} t_{ij}^{mm'} d^\dagger_{im\sigma} d_{jm'\sigma} + \sum_{im\sigma} \epsilon_m n_{im\sigma}, \quad (1)$$

where $d^\dagger_{im\sigma}$ creates an electron with spin σ in orbital $m = 1, \ldots, M$ on site i of the lattice, and

$$\begin{aligned}\hat{H}_{\rm int} = {} & U \sum_m n_{m\uparrow} n_{m\downarrow} \\ & + U' \sum_{m\neq m'} n_{m\uparrow} n_{m'\downarrow} + (U' - J) \sum_{m<m',\sigma} n_{m\sigma} n_{m'\sigma} \\ & + -J \sum_{m\neq m'} d^+_{m\uparrow} d_{m\downarrow} d^+_{m'\downarrow} d_{m'\uparrow} + J \sum_{m\neq m'} d^+_{m\uparrow} d^+_{m\downarrow} d_{m'\downarrow} d_{m'\uparrow}.\end{aligned} \quad (2)$$

The number operator is $n_{im\sigma} = d^{\dagger}_{im\sigma} d_{im\sigma}$, $\hat{N} = \sum_{im\sigma} n_{im\sigma}$, μ is the chemical potential, and customarily we set $U' = U - 2J$ and we drop the last two terms in $\hat{H}_{\rm int}$ (spin flip and pair hopping), which needs extra approximations to be treated within our method of choice (the effect of these terms is addressed in the Supplemental Material [13]). We first study the degenerate model in which we only consider diagonal hopping in orbital space, equal for all orbitals, i.e., $t^{mm'}_{ij} = t_{ij}\delta_{mm'}$ and $\epsilon_m = 0$, as a function of the average density of electrons per lattice site $n = \langle \hat{N} \rangle / \mathcal{N}_{\rm sites}$.

We treat the model in the slave-spin mean-field approximation (SSMF) [24], and we focus on the normal, nonmagnetic, zero-temperature metallic phase. There, the SSMF describes the metal as a Fermi liquid by construction, yielding the following quasiparticle Hamiltonian:

$$H - \mu N = \sum_{km\sigma} (Z\epsilon_{\mathbf{k}} + \lambda - \mu) f^{\dagger}_{km\sigma} f_{km\sigma}, \qquad (3)$$

where $f^{\dagger}_{km\sigma}$ is the creation operator of a quasiparticle with momentum k, orbital (band) character m, and spin σ, and $\epsilon_{\mathbf{k}}$ is the bare electronic dispersion relation, which is the same for all the bands. We customarily choose a semicircular density of states (DOS) $D(\epsilon) \equiv (2/\pi D)\sqrt{1 - (\epsilon/D)^2}$ of bandwidth $W = 2D$ for all bands. The renormalization parameters of the dispersion, Z and λ, are calculated in the self-consistent SSMF scheme as an average on the auxiliary slave-spin Hamiltonian [24], which treats explicitly the interaction term Eq. (2). They thus embody the effect of the electronic interactions determining the quasiparticles: Z is the quasiparticle weight and the inverse of the mass enhancement, while λ is a shift of the bare on-site energy. The Fermi-liquid condition $n_f \equiv \sum_{km\sigma} \langle f^{\dagger}_{km\sigma} f_{km\sigma} \rangle = n$ is built in.

We wish to study the compressibility of the electronic fluid $\kappa_{\rm el} = dn/d\mu$ as a function of Hund's coupling and the number of orbitals in the model. We thus calculate the μ versus n dependence in these models within SSMF. In Fig. 1 (left-hand panel), the result for the 2-orbital Hubbard model at a typical value of Hund's coupling $J/U = 0.25$ is reported for various values of U. Remarkably, approaching the half-filled Mott insulator (that is realized at $n = 2$, for $U > U_c = 1.96D$), the slope of the μ versus n curves vanishes, marking a divergence in the compressibility, and then becomes negative, signaling a sizable zone in the U/doping (from half filling, i.e., $\delta \equiv n - M$) plane, where the system is unstable. A diverging compressibility implies an instability towards phase separation or incommensurate charge ordering [12] and a strong enhancement of the compressibility in the thermodynamically stable zone near the frontier.

This spinodal line marking the phase-separation instability in the $U - \delta$ plane is shown in Fig. 2 (left-hand panel): it departs from the Mott transition and has a nonmonotonic behavior as a function of the interaction strength, so that the unstable zone widens rapidly for $U > U_c$, but at larger interactions (for $U/D > 3.3$ in this case) it narrows again.

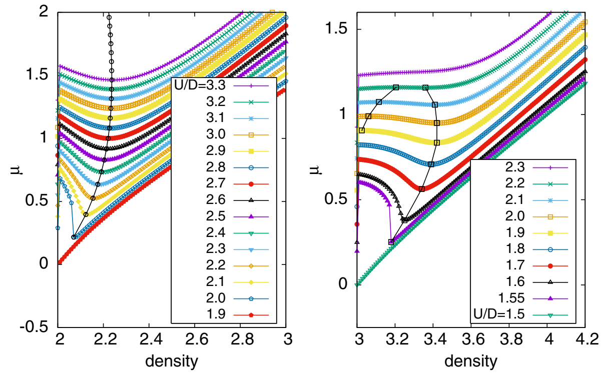

FIG. 1. Degenerate 2-orbital (left-hand panel) and 3-orbital (right-hand panel) Hubbard model with semicircular DOS of half-bandwidth D and Ising-type Hund's coupling $J/U = 0.25$: μ versus n curves for different values of U. In the 2-orbital case for $U_c/D = 1.96$ at half filling ($n = 2$ in this model), the system undergoes a Mott transition. The curves for $U > U_c$ show a negative slope inside a spinodal line departing from the Mott transition that is marked with black circles. In the 3-orbital case most of the μ versus n curves for $U > U_c = 1.515$ show a double change of slope (the same happens in the 5-orbital model [13]), so that the instability zone extends between two spinodal lines (black squares), both at finite doping from half filling ($n = 3$ here).

Hund's coupling is essential for this instability zone to appear; no diverging compressibility is found at $J = 0$. Already at very small J/U a wide zone opens at large U. This zone moves towards lower interaction strengths for increasing J/U, following the position of the Mott transition [2] at half filling, from which the instability frontier always departs. The zone extends, for typical values of J/U, in the range $n = 2$ to $\sim$2.2. The complete study as a function of J/U is presented in the Supplemental Material [13].

A similar behavior is found for the 3-orbital (Fig. 1, right-hand panel) and 5-orbital model (shown in the Supplemental Material [13]). The main difference with the 2-orbital case is, however, that a second frontier can be traced, at smaller doping compared to the first, where the μ vs n curve recovers a positive slope. This signals that the instability due to the compressibility divergence now mostly happens in a range of finite doping. The region (Fig. 2, left-hand panel) still departs from the Mott transition at half filling, but then extends in the U-doping plane until the two lines merge, having thus a "moustache" shape in the $M > 2$ cases, instead of an "onion" shape like in the $M = 2$ case. It is comparatively less extended in U but more extended in doping. In particular, in the 5-orbital model it approaches values close to $n = 6$ densities. At $n = 6$ the system is stable again, but still an evident signature of this physics in terms of enhanced compressibility is present.

Despite a marked difference, then, in the way the instability zone evolves at large U, the common robust

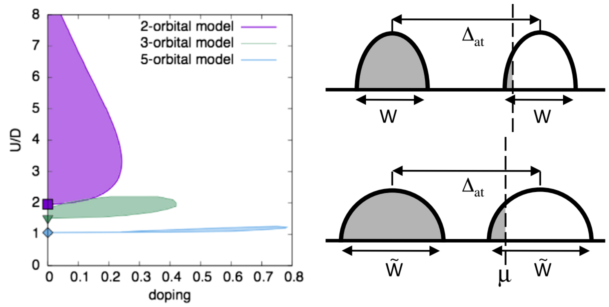

FIG. 2. Left-hand panel: The colored areas are the zones of instability towards phase separation in the U-doping plane for the 2-, 3-, and 5-orbital models, with $J/U = 0.25$. The low-U frontier departs from the Mott transition point at half filling (symbols). For a growing number of orbitals the unstable zone extends to larger and larger doping, albeit narrowing in U. Right-hand panel: A plausible mechanism by which Hund's coupling causes the charge instability. Hund's coupling reduces the width of the Hubbard bands at half filling, through the quenching of orbital fluctuations. Upon doping the quenching is lifted and the Hubbard bands are expected to expand (going from $\sim W$ to some larger value $\tilde{W}$). This makes it possible to have a lower chemical potential at larger particle density, i.e., a charge instability.

feature is that in all these models the onset of Hund's coupling triggers the appearance of a zone departing from the Mott transition at half filling where the system is unstable towards phase separation. The low-U frontier of this zone in all cases is rather horizontal in the U-doping plane; i.e., for $U > U_c$ it moves quickly towards the maximum doping it will reach. This frontier is found to follow a well-known crossover, appearing in these models in several physical quantities. Indeed (see, for instance, Fig. 16 in Ref. [24]), along a line departing from the Mott transition [8,25], at finite doping one observes for increasing U or doping moving towards half filling a quick decrease of the quasiparticle weight Z, an increase of the interorbital spin-spin correlations, and a suppression of the interorbital charge correlations. The crossover is very sharp near the Mott transition, whereas it becomes progressively broader with increasing doping. At finite temperature it is identifiable with the "spin-freezing crossover" [8,26], and the recent successful denomination of "Hund's metal" [9] might be used for the zone at large U-small doping. The three mentioned quantities then have a different, and rather disconnected, evolution in other zones of the phase diagram. This crossover is where the compressibility divergence is empirically found to appear for increasing interaction U in all cases (as explicitly shown for selected cases in the Supplemental Material [13]). The reentrant shape of the instability zone suggests a closer analogy with the zone of reduced interorbital correlations, however, which is the only quantity among the three showing a similar shape in its crossover at large U [24].

Let us now analyze the origin of this behavior. Interestingly, this phase separation arises as an instability of the Fermi liquid, the latter being enforced, within the SSMF method. Indeed, it is worth stressing that the renormalization parameters in the quasiparticle Hamiltonian Eq. (3) depend in an intricate way on all the couplings in the bare Hamiltonian and the chemical potential, so that the effective system described by Eq. (3) is not to be viewed as a simple rigid band picture with an effective dispersion: the dispersion itself changes with the filling instead. Thus, besides the quasiparticle energy (the linear—in the k-resolved density—contribution to the energy of the system), this method also accounts for the effects of quasiparticle interaction, (the quadratic term); i.e., they yield the Landau parameters F_0^s, F_0^a, etc. [27]. Indeed, in an isotropic Fermi-liquid metal the electronic compressibility reads as

$$\kappa_{\rm el} = \frac{D^*(\epsilon_F)}{1 + F_0^s} = \frac{1}{D^*(\epsilon_F)^{-1} + f_0^s}, \qquad (4)$$

where $D^*(\epsilon_F)$ is the total quasiparticle (i.e., renormalized) density of states at the Fermi energy and $F_0^s = D^*(\epsilon_F) f_0^s$ is the isotropic, spin-symmetric Landau parameter. From Eq. (3) one can formally calculate the total density of quasiparticles, $n_f(\mu) = \int d\epsilon D(\epsilon) n_F(Z\epsilon + \lambda - \mu)$ [where $n_F(\epsilon)$ is the Fermi function], and deriving this expression by respect to μ one indeed finds at zero temperature the above expression for the electronic compressibility with $D^*(\mu) = D(\mu_0)/Z$ and $f_0^s = \mu_0(dZ/dn) + d\lambda/dn$. Here, $\mu_0(n)$ is the chemical potential for the noninteracting system with the same particle density ($\mu_0 = 0$ at half filling in our particle-hole symmetric case), entering through the relation $\mu_0 = (\mu - \lambda)/Z$ implied by the Luttinger theorem that holds in our Fermi-liquid framework [13]. Since for the compressibility to diverge when Z is finite (as we indeed find here) it must be $F_0^s < -1$, and thus f_0^s at least negative, this last formula implies that $d\lambda/dn$ has to be negative, since $\mu_0(dZ/dn)$ is always positive (indeed, Z diminishes upon approaching the half-filled Mott insulator, so that its slope always has the sign of μ_0). This is confirmed numerically [13]: the compressibility divergence always happens because $d\lambda/dn$ becomes negative and larger in absolute value than $D^*(\epsilon_F)^{-1} + \mu_0(dZ/dn)$. The last quantity is always small near the Mott insulator (because Z and μ_0 are small there, and dZ/dn is finite), but the question remains of why $d\lambda/dn < 0$.

Indeed, the renormalization parameters Z and λ set, respectively, the width and the position of the quasiparticle band(s), compared to the noninteracting case. In particular, in a doped Mott insulator λ places the quasiparticle band above the charge gap in the so-called Hubbard band [28], the range of the spectrum with delocalized excitations at finite energy. The Hubbard band is centered around the energy of the atomic charge excitation (e.g., $U/2$ in the single-band case), and if its width is fixed one expects λ to grow monotonically when shifting the quasiparticle band within it, upon doping. It has, however, become clear recently that the Hubbard bands can vary in width, for instance, among different models: in the absence of Hund's coupling, their width grows like $\sqrt{M}$ with the number of orbitals [29], while it was shown that the onset of Hund's coupling J reduces their width back to values of the order of the one-band model [24]. Indeed, J quenches the orbital fluctuations responsible for the enhancement of the delocalization energy of the charge excitations, and hence of the width of the Hubbard bands. This quenching is, however, complete only at half filling, while the extra particles introduced by doping necessarily create doubly occupied orbitals, unquenching the orbital degrees of freedom. One can then expect the Hubbard bands to expand again, when doping the half-filled Mott insulator. This gives a plausibility argument for the nonmonotonic behavior of λ with n: if the Hubbard band expands quickly enough with doping, it may happen that for a larger density n the quasiparticle band is located at lower energy than for a smaller n (see Fig. 2, right-hand panel), and, consequently, μ can be lower for the larger n, causing the negative compressibility that we find.

Incidentally, the mechanism reducing the width of the Hubbard bands was shown to coincide [24] with the one causing the "orbital decoupling" (i.e., the suppression of interorbital charge-charge correlations) leading to the selective Mott physics that one finds in these models once the degeneracy of the bands is removed [2,30]. It is not surprising then to find the divergence of the compressibility on the frontier of the crossover towards the orbitally decoupled region.

It is worth stressing that the proximity to such a Fermi-liquid instability has several remarkable consequences [12]. Indeed, a negative F_0^s implies an attractive interaction between quasiparticles in the particle-hole channel, at $q = 0$, $\omega \to 0$. This in general favors superconductivity [31], and critical fluctuations of the order parameter might even directly provide the pairing [32]. But the interaction of quasiparticles with low-energy bosons can also be enhanced. Indeed, Ward identities relate the quasiparticle interaction vertices with the Fermi-liquid parameters. For instance, for the density vertex $\Lambda(q,\omega)$, the following Ward identity holds [33]:

$$Z\Lambda(q \to 0, \omega = 0) = \frac{1}{1 + F_0^s}. \quad (5)$$

This implies an enhancement of this interaction vertex, if $1 + F_0^s$ decreases until vanishing, as in the present case (for a complete plot of $1 + F_0^s$ in the 2-orbital model with $J/U = 0.25$, see the Supplemental Material [13]). In turn, the enhancement of the vertex can favor a symmetry breaking, if a related susceptibility is correspondingly enhanced.

It is tempting to attribute to these effects the enhancement of a number of instabilities of the paramagnetic metallic phase in materials that are dominated by Hund's

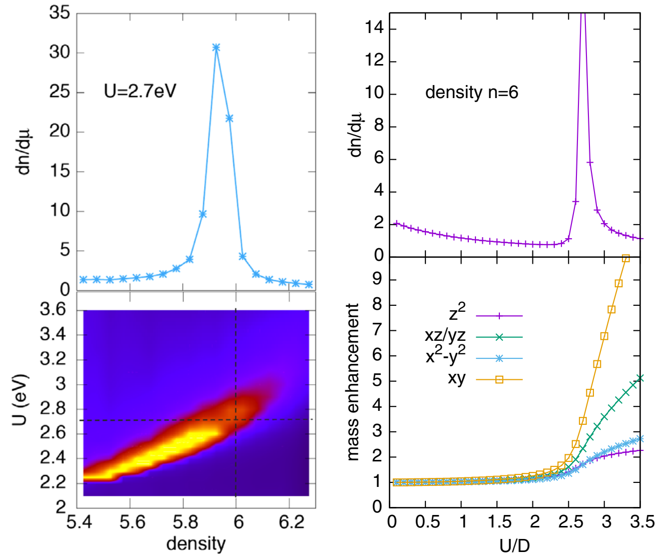

FIG. 3. Lower left-hand panel: Compressibility (color scale) in $BaFe_2As_2$ calculated within DFT + SSMF ($J/U = 0.25$) in the U-density plane. The saturated yellow color corresponds to the unstable region (the pixelation is due to numerical discretization and is unphysical), surrounded by an area of enhanced compressibility (red). Upper panels: Compressibility plotted along the cuts (dashed lines) for constant $U = 2.7$ eV and constant density $n = 6$, relevant values for $BaFe_2As_2$. Lower right-hand panel: Orbitally resolved mass enhancements, showing that the compressibility enhancement happens near the crossover, where correlations become orbitally selective.

many-body physics [1]. Most notably one might speculate that, whatever the mechanism leading to superconductivity in iron-based superconductors, the enhancement of the critical temperature be due to the Fermi-liquid compressibility enhancement outlined in this Letter. Indeed, when modeling doped $BaFe_2As_2$ with density functional theory (DFT) + slave spin, one finds confirmation that the phase separation instability is realized also in this realistic framework, emanates from the half-filled Mott insulator, and reaches the zones in the phase diagram relevant to the iron-based superconductors, as shown in Fig. 3. Remarkably indeed, using the set of interaction parameters ($U = 2.7$ eV, $J/U = 0.25$) that yields the correct Sommerfeld coefficient for all of the 122 family [24,34] one finds that the compressibility is greatly enhanced in the density range 5.75–6.1, coinciding with the zone where doped $BaFe_2As_2$ shows high-T_c superconductivity in the tetragonal phase.

Recently, Misawa and Imada [35] have highlighted a zone of phase separation, in the *ab initio* phase diagram of LaFeAsO [36] studied within a variational Monte Carlo scheme, in proximity of the superconducting phase. The zone of phase separation is compatible with the corresponding zone we find in the present study and with its continuation in terms of enhanced compressibility. What we highlight in the present work is that this phase is a genuine instability of the Fermi-liquid phase even in the absence of all symmetry breaking, it is to be tracked back to Hund's coupling, and it is a universal feature of all Hund's dominated doped half-filled Mott insulators.

Analogously to the model studies, we find that in $BaFe_2As_2$ the instability zone and the zone of enhanced compressibility that continues it is located on the crossover frontier between the normal and the orbitally decoupled (Hund's) metal (Fig. 3, right-hand panels). We suggest that, in general, an enhancement of the compressibility, with the possible related enhancement of superconductive pairing, happens when a material is near the frontier between a normal metal and a Hund's metal. A possible universally detectable sign of this situation is the arising of high-T_c superconductivity in between a phase with (orbitally) selective electronic correlation strength and another, more conventional metallic phase, as it also happens in cuprates [6].

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