Kinks in the dispersion of strongly correlated electrons

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The properties of condensed matter are determined by single-particle and collective excitations and their mutual interactions. These quantum-mechanical excitations are characterized by an energy, E, and a momentum, $\hbar\mathbf{k}$, which are related through their dispersion, $E_{\mathbf{k}}$. The coupling of excitations may lead to abrupt changes (kinks) in the slope of the dispersion. Kinks thus carry important information about the internal degrees of freedom of a many-body system and their effective interaction. Here, we report a novel, purely electronic mechanism leading to kinks, which is not related to any coupling of excitations. Namely, kinks are predicted for any strongly correlated metal whose spectral function shows a three-peak structure with well-separated Hubbard subbands and a central peak, as observed, for example, in transition-metal oxides. These kinks can appear at energies as high as a few hundred millielectron volts, as found in recent spectroscopy experiments on high-temperature superconductors[1–4] and other transition-metal oxides[5–8]. Our theory determines not only the position of the kinks but also the range of validity of Fermi-liquid theory.

In systems with strong electron–phonon coupling, kinks in the electronic dispersion at 40–60 meV below the Fermi level are well known[9–11]. Therefore, the kinks that are detected at 40–70 meV in the electronic dispersion of high-temperature superconductors are taken as evidence of phonon-[12,13] or spin-fluctuation-based[14,15] pairing mechanisms. Collective excitations other than phonons, or even an altogether different mechanism, may be the origin of kinks detected at 40 meV in the dispersion of surface states of Ni(110) (ref. 16). Surface states of ferromagnetic Fe(110) show similar kinks at 100–200 meV (ref. 17), and even at 300 meV in Pt(110)—far beyond any phononic energy scale[18]. Kinks at unusually high energies are also found in transition-metal oxides[5–8,19,20], for example, at 150 meV in $SrVO_3$ (ref. 7), where the Coulomb interaction leads to strong correlations. Very recently, kinks were reported at 380 and 800 meV for three different families of high-temperature superconductors[1–4] and at 400–900 meV in graphene[21].

Interactions between electrons or their coupling to other degrees of freedom change the interpretation of $E_{\mathbf{k}}$ as the energy of an excitation with infinite lifetime. Namely, the interactions lead to a damping effect implying that the dispersion relation is no longer a real function. For systems with Coulomb interaction, Fermi-liquid (FL) theory predicts the existence of fermionic quasiparticles[22], that is, exact one-particle states with momentum $\mathbf{k}$ and a real dispersion $E_{\mathbf{k}}$, at the Fermi surface and at zero temperature. This concept can be extended to $\mathbf{k}$ states sufficiently close to the Fermi surface (low-energy regime) and at low enough temperatures, in which case the lifetime is now finite but still long enough for quasiparticles to be used as a concept.

Outside the FL regime, the notion of dispersive quasiparticles is, in principle, inapplicable as the lifetime of excitations is too short. However, it is an experimental fact that $\mathbf{k}$-resolved one-particle spectral functions measured by angle-resolved photoemission spectroscopy often show distinct peaks also at energies far away from the Fermi surface[1–20]. The positions of those peaks change with $\mathbf{k}$, which means that the corresponding one-particle excitations are dispersive, in spite of their rather short lifetime. It turns out that kinks in the dispersion relation are found in this energy region, which is located outside the FL regime.

We describe a novel mechanism leading to kinks in the dispersion of strongly correlated electrons, which does not require any coupling to phonons or other excitations, and which can occur at any energy inside the band. We begin with a discussion of the physics of this microscopic mechanism, which applies to a wide range of correlated metals. Consider first a weakly correlated system and imagine that we inject an electron into the partially filled band at an energy close to the Fermi surface. In this process the entire system becomes excited, leading to the generation of many quasiparticles and quasiholes. In view of their long lifetime, the Coulomb interaction with other quasiparticles or quasiholes modifies their dispersion which, according to FL theory, becomes $E_{\mathbf{k}} = Z_{\mathrm{FL}}\epsilon_{\mathbf{k}}$. Here, Z_{FL} is an FL renormalization factor and $\epsilon_{\mathbf{k}}$ is the bare (non-interacting) dispersion. In contrast, an electron injected at an energy far from the Fermi level leads to excitations with only a short lifetime; their dispersion is hardly affected by the weak interaction, that is, $E_{\mathbf{k}} \approx \epsilon_{\mathbf{k}}$ (see the Supplementary Information). The crossover from the FL dispersion to the non-interacting dispersion can lead to kinks near the band edges, which mark the termination point of the FL regime. However, for weakly correlated metals ($Z_{\mathrm{FL}} \lesssim 1$), the slope of $E_{\mathbf{k}}$ changes only a little; hence the kinks are not very pronounced.

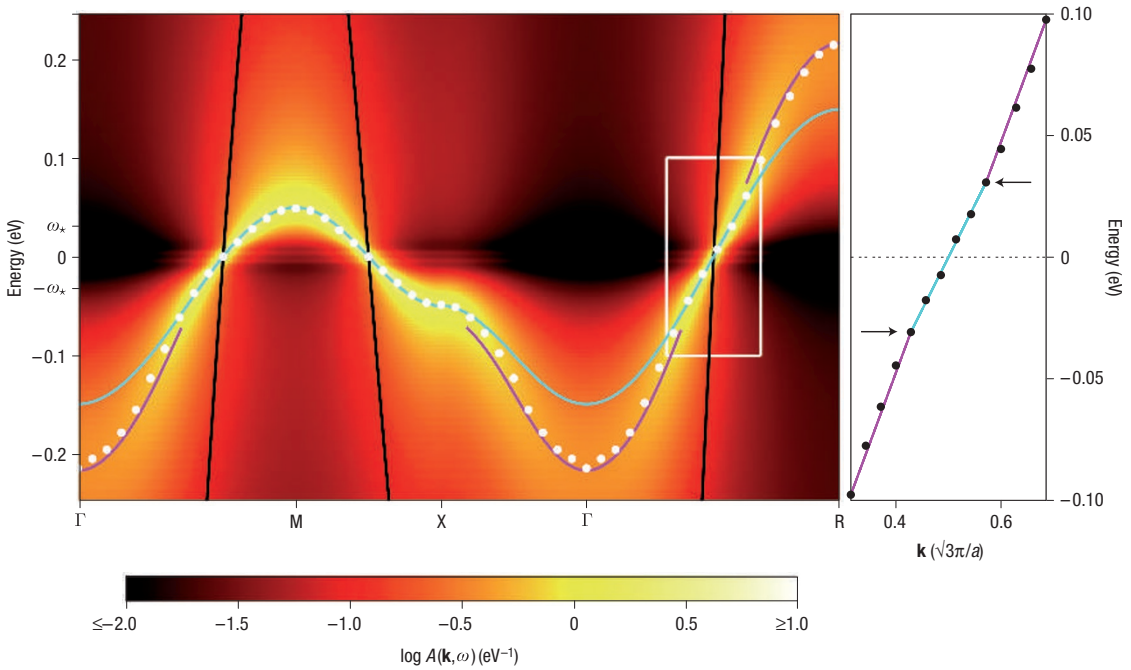

Figure 1 Kinks in the dispersion relation, $E_{\mathbf{k}}$, for a strongly correlated system. The intensity plot represents the spectral function $A(\mathbf{k}, \omega)$ (Hubbard model in DMFT, cubic lattice, interaction $U = 3.5$ eV, bandwidth $W = 3.46$ eV, $n = 1$, $Z_{\mathrm{FL}} = 0.086$, $T = 5$ K). Close to the Fermi energy, the effective dispersion (white circles) follows the renormalized band structure, $E_{\mathbf{k}} = Z_{\mathrm{FL}}\epsilon_{\mathbf{k}}$ (blue line). For $|\omega| > \omega_\star$, the dispersion has the same shape but with a different renormalization, $E_{\mathbf{k}} = Z_{\mathrm{CP}}\epsilon_{\mathbf{k}} - c\,\mathrm{sgn}(E_{\mathbf{k}})$ (pink line). Here, $\omega_\star = 0.03$ eV, $Z_{\mathrm{CP}} = 0.135$ and $c = 0.018$ eV are all calculated (see the Supplementary Information) from Z_{FL} and $\epsilon_{\mathbf{k}}$ (black line). A subinterval of Γ–R (white frame) is plotted on the right, showing kinks at $\pm\omega_\star$ (arrows).

The situation is very different in strongly correlated metals, where Z_{FL} can be quite small such that kinks can be well pronounced. The strong interaction produces a strong redistribution of the spectral weight in the one-particle spectral function. Namely, the conduction band develops so-called Hubbard subbands, whose positions are determined by the atomic energies. For metallic systems, a resonant central peak emerges around the Fermi level that lies between these subbands. The central peak of this so-called three-peak structure is often interpreted as a 'quasiparticle peak', but it will be shown below that genuine FL quasiparticles exist only in a narrow energy range around the Fermi level. Outside this FL regime, but still inside the central peak, we identify a new intermediate-energy regime, where the dispersion is given by $E_{\mathbf{k}} \approx Z_{\mathrm{CP}}\epsilon_{\mathbf{k}}$. Here, Z_{CP} is a new renormalization factor, given by the weight of the central peak, which differs significantly from Z_{FL}. At these intermediate energies, which are much smaller than the interaction strength, an injected electron or hole is still substantially affected by the other electrons in the system. Therefore, its dispersion is neither that of a free system, nor that of the (strongly renormalized) FL regime, but rather corresponds to a moderately correlated system ($Z_{\mathrm{FL}} < Z_{\mathrm{CP}} < 1$). As a consequence, a crossover occurs at an intermediate energy $\pm\omega_\star$ inside the central peak from Z_{FL} renormalization to Z_{CP} renormalization, which is visible as kinks in the dispersion. These observations apply to any correlated metal. As shown below, in a microscopic theory the position of those kinks are located at the termination point of the FL regime. We emphasize that this mechanism yields kinks but does not involve coupling of electrons and collective modes; only strong correlations between electrons are required.

For a microscopic description of these electronic kinks, we use the Hubbard model, which is the generic model for strongly correlated electrons, and solve it by many-body dynamical mean-field theory[23–26] (DMFT), using the numerical renormalization group as an impurity solver. DMFT is known to provide the correct behaviour of local observables in the limit of large coordination numbers, and is used here to quantitatively support the physical mechanism discussed above. We focus on a single band with particle–hole symmetry and discuss the asymmetric case in the Supplementary Information. For the strongly correlated Hubbard model (interaction $U \approx$ bandwidth), the dispersion relation is shown in Fig. 1 and the spectral function is shown in Fig. 2a. The dispersion relation, $E_{\mathbf{k}}$, crosses over from the FL regime (blue line in Fig. 1) to the intermediate-energy regime (pink line in Fig. 1), as described above, and shows pronounced kinks at the energy scale $\omega_\star = 0.03$ eV. In some directions in the Brillouin zone these kinks may be less visible because the band structure is flat (for example, near the X point in Fig. 1). The behaviour of $E_{\mathbf{k}}$ is now analysed quantitatively.

The physical quantity describing properties of one-particle excitations in a many-body system is the Green function or 'propagator' $G(\mathbf{k}, \omega) = (\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, \omega))^{-1}$, which characterizes the propagation of an electron in the solid[22]. Here ω is the frequency, μ is the chemical potential, $\epsilon_{\mathbf{k}}$ is the bare dispersion relation and $\Sigma(\mathbf{k}, \omega)$ is the self-energy, a generally complex quantity describing the influence of interactions on the propagation of the one-particle excitation, which vanishes in a non-interacting system. The effective dispersion relation, $E_{\mathbf{k}}$, of the one-particle excitation is determined by the singularities of $G(\mathbf{k}, \omega)$, which give rise to peaks in the spectral function $A(\mathbf{k}, \omega) = -\mathrm{Im}\,G(\mathbf{k}, \omega)/\pi$. If the damping given by the imaginary part of $\Sigma(\mathbf{k}, \omega)$ is not too large, the effective dispersion is thus determined by $E_{\mathbf{k}} + \mu - \epsilon_{\mathbf{k}} - \mathrm{Re}\,\Sigma(\mathbf{k}, E_{\mathbf{k}}) = 0$. Any kinks in $E_{\mathbf{k}}$ that do not originate from $\epsilon_{\mathbf{k}}$ must therefore be due to slope changes in $\mathrm{Re}\,\Sigma(\mathbf{k}, \omega)$.

In many three-dimensional physical systems, the $\mathbf{k}$ dependence of the self-energy is less important than the ω dependence and can be neglected to a good approximation. Then, the DMFT self-consistency equations can be used to express $\Sigma(\mathbf{k},\omega) = \Sigma(\omega)$ as $\Sigma(\omega) = \omega + \mu - 1/G(\omega) - \Delta(G(\omega))$, where $G(\omega) = \int G(\mathbf{k},\omega)\,\mathrm{d}\mathbf{k}$ is the local Green function (averaged over $\mathbf{k}$) and $\Delta(G)$ is an energy-dependent hybridization function, expressed here as a function of $G(\omega)$. In DMFT, $\Delta(G)$ is determined by the requirement $G(\omega) = G_0(\omega + \mu - \Sigma(\omega))$, that is, $G_0(\Delta(G) + 1/G) = G$. Here, $G_0(\omega)$ is the local Green function in the absence of interactions. The hybridization function describes how the electron at a given lattice site is quantum-mechanically coupled to the other sites in the system. It plays the role of a dynamical mean-field parameter and its behaviour is strongly dependent on the electronic correlations in the system. Figure 2a shows a typical result for the integrated spectral function $A(\omega) = -\mathrm{Im}\,G(\omega)/\pi$ with the aforementioned three-peak structure. The corresponding real parts of the local propagator, $G(\omega)$, and self-energy, $\Sigma(\omega)$, are shown in Fig. 2b and c, respectively.

Kinks in $\mathrm{Re}\,\Sigma(\omega)$ appear at a new small energy scale that emerges quite generally for a three-peak spectral function $A(\omega)$. Kramers–Kronig relations imply that $\mathrm{Re}\,[G(\omega)]$ is small near the dips of $A(\omega)$, located at $\pm\Omega$. Therefore, $\mathrm{Re}\,[G(\omega)]$ has a maximum and a minimum at $\pm\omega_{\max}$ inside the central spectral peak (Fig. 2b). This directly leads to kinks in $\mathrm{Re}\,\Sigma(\omega)$ for the following reason. There are two contributions to $\Sigma(\omega)$: $\omega + \mu - 1/G(\omega)$ and $-\Delta(G(\omega))$. The first contribution $\mathrm{Re}\,[\omega + \mu - 1/G(\omega)]$ is linear in the large energy window $|\omega| < \Omega$ (Fig. 2d); this is due to Kramers–Kronig relations (see the Supplementary Information) and is not particular to DMFT. On the other hand, the term $-\mathrm{Re}\,[\Delta(G(\omega))]$ is approximately proportional to $-\mathrm{Re}\,[G(\omega)]$ (at least to first order in a moment expansion), and thus remains linear only in a much narrower energy window $|\omega| < \omega_{\max}$. The sum of these two contributions produces pronounced kinks in the real part of the self-energy at $\pm\omega_\star$, where $\omega_\star = (\sqrt{2}-1)\omega_{\max}$ is the energy where $\mathrm{Re}\,[G(\omega)]$ has maximum curvature (marked by blue circles in Fig. 2c). The FL regime with slope $\partial\,\mathrm{Re}\,\Sigma(\omega)/\partial\omega|_{\omega=0} = 1 - 1/Z_{\mathrm{FL}}$ thus extends only throughout a small part of the central peak ($|\omega| < \omega_\star$). At intermediate energies ($\omega_\star < |\omega| < \Omega$), the slope is then given by $\partial\,\mathrm{Re}\,\Sigma(\omega)/\partial\omega|_{\omega=0} = 1 - 1/Z_{\mathrm{CP}}$. The kinks at $\pm\omega_\star$ mark the crossover between these two slopes. As a consequence there is also a kink at $\omega_\star$ in the effective band structure $E_{\mathbf{k}}$.

The above analysis also explains why outside the FL regime $E_{\mathbf{k}}$ still follows the uncorrelated dispersion, albeit with a different renormalization Z_{CP} and a small offset c. This behaviour is due to $\omega + \mu - 1/G(\omega)$, the main contribution to the self-energy inside the central peak for $\omega_\star < |\omega| < \Omega$. In particular, our analysis explains the dependence of $E_{\mathbf{k}}$ on $\mathbf{k}$ that was observed in previous DMFT studies of $SrVO_3$ (ref. 27; see the Supplementary Information).

The FL regime terminates at the kink energy scale $\omega_\star$, which cannot be determined within FL theory itself. The quantities $\omega_\star$, Z_{CP} and c can nevertheless all be expressed in terms of Z_{FL} and the bare density of states alone; explicitly, we find $\omega_\star = Z_{\mathrm{FL}}(\sqrt{2}-1)D$, where D is an energy scale of the non-interacting system, for example, D is approximately given by half the bandwidth (see the Supplementary Information for details). For weak correlations ($Z_{\mathrm{FL}} \lesssim 1$), the kinks in $E_{\mathbf{k}}$ thus merge with the band edges and are almost undetectable, as discussed above. On the other hand, for increasingly stronger correlations ($Z_{\mathrm{FL}} \ll 1$), the kinks at $\omega_\star/D \propto Z_{\mathrm{FL}}$ move closer to the Fermi energy and deeper inside the central peak, whose width diminishes only as $\Omega/D \propto \sqrt{Z_{\mathrm{FL}}}$ (ref. 28).

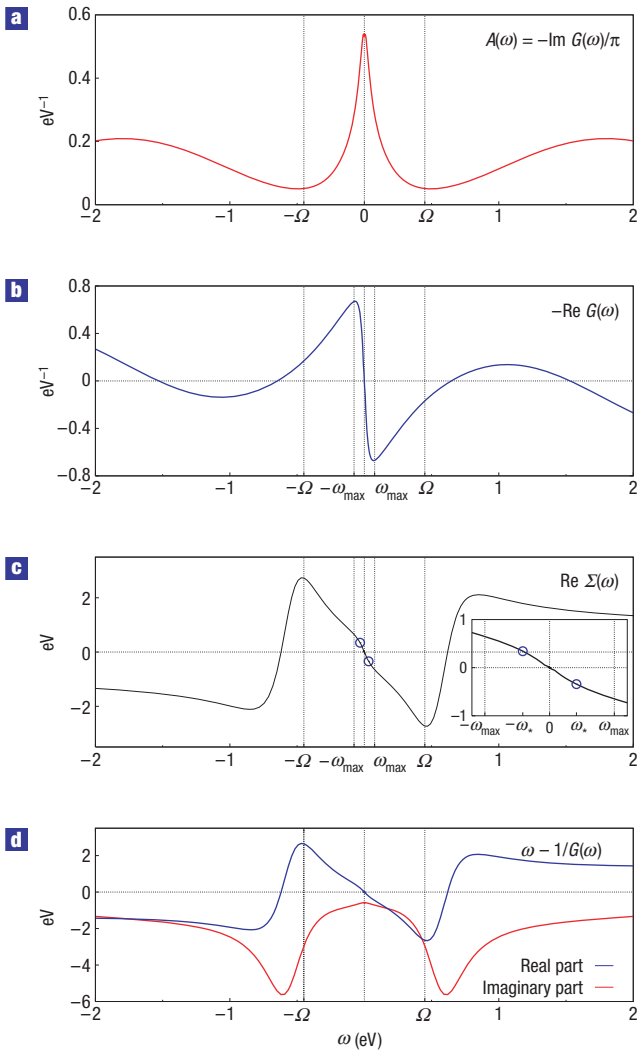

Figure 2 Local propagator and self-energy for a strongly correlated system. The parameters are the same as those in Fig. 1. **a**, Correlation-induced three-peak spectral function $A(\omega) = -\mathrm{Im}\,G(\omega)/\pi$ with dips at $\pm\Omega = 0.45$ eV. **b**, Corresponding real part of the propagator, $-\mathrm{Re}\,G(\omega)$, with minimum and maximum at $\pm\omega_{\max}$ inside the central spectral peak. **c**, Real part of the self-energy with kinks at $\pm\omega_\star$ (blue circles), located at the points of maximum curvature of $\mathrm{Re}\,G(\omega)$, ($\omega_\star = 0.4\omega_{\max} = 0.03$ eV). **d**, $\omega - 1/G(\omega)$ contributes to the self-energy. In general $\mathrm{Re}\,[\omega - 1/G(\omega)]$ (blue line) is linear in $|\omega| < \Omega$. The other contribution to the self-energy is $-\Delta(G(\omega)) \approx -(m_2 - m_1^2)\,G(\omega)$ (to lowest order in the moments m_i of $\epsilon_{\mathbf{k}}$; here $m_2 - m_1^2 = 0.5$ eV^2). Therefore, the nonlinearity of $-\mathrm{Re}\,[G(\omega)]$ at $\pm\omega_\star$ determines the location of kinks.

The energy scale $\omega_\star$ involves only the bare band structure, which can be obtained, for example, from band-structure calculations, and the FL renormalization $Z_{\mathrm{FL}} = 1/(1 - \partial\,\mathrm{Re}\,\Sigma(\omega)/\partial\omega)|_{\omega=0} \equiv m/m^*$ known from, for example, specific-heat measurements or many-body calculations. We note that because phonons are not involved in this mechanism, $\omega_\star$ shows no isotope effect. For strongly interacting systems, in particular close to a metal–insulator transition[26], $\omega_\star$ can become quite small, for example, smaller than the Debye energy.

The mechanism discussed here applies to systems with partially occupied d or f orbitals, where the local interaction is strong. An analysis similar to the one presented above also holds for

systems with strong hybridization such as the high-temperature superconductors, where the overlap between d and oxygen p states is important. The assumption of a **k**-independent self-energy may also be relaxed: if a correlation-induced three-peak spectral function, $A(\mathbf{k}, \omega)$, is present for a certain range of momenta, **k**, the corresponding self-energies, $\Sigma(\mathbf{k}, \omega)$, and effective dispersion, $E_{\mathbf{k}}$, will also develop kinks, as can be proved formally using cluster extensions to DMFT. Kinks in the dispersion are thus a robust many-body feature of correlated metals with a three-peak spectral function, independent of the computational approach.

The energy of electronic kinks is a quantitative measure of electronic correlations in many-body systems; they mark the termination point of the FL regime and can be as high as several hundred millielectron volts. Angle-resolved photoemission spectroscopy experiments at such high binding energies can thus provide new, previously unexpected information about strongly correlated electronic systems. Electronic kinks are a fingerprint of a strongly correlated metal and are expected to be observable in many materials, including high-temperature superconductors.

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Competing financial interests

The authors declare that they have no competing financial interests.