Kinks in the dispersion of strongly correlated electrons

Authors: K. Byczuk, M. Kollar, K. Held, Y.-F. Yang, I. A. Nekrasov, Th. Pruschke and D. Vollhardt

arXiv:cond-mat/0609594

Nature Physics **3,** 168 (2007).

Recommended and Commentary by Peter Wölfle, Universität Karlsruhe, Germany

As first discussed by Mott and Hubbard the energy spectrum of strongly correlated electrons on a lattice is characterized by two "Hubbard bands" , separated approximately by an energy of the order of the onsite Coulomb interaction. In the metallic phase a third spectral peak appears in the middle, near or at the Fermi level [see e.g. G. Kotliar and D. Vollhardt, Physics Today **57**, 53 (2004)] . Single particle spectral functions showing these features may be quantitatively calculated using the Dynamical Mean Field Theory (DMFT), when it is applicable, i.e. when the relevant physics is local [W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62,** 324 (1989); A. Georges et al., Rev Mod Phys. **68,** 13 (1996)]. This generic structure of the spectrum gives rise to surprising consequences, as discussed in the paper by Byczuk et al. The existence of pronounced minima between the central peak and the Hubbard side peaks leads to a new energy regime above the usual low energy Fermi liquid regime, in which relatively well defined fermionic excitations are found. In the new energy regime excitations acquire a different and in general larger weight factor z_{CP} (here CP stands for "central peak "), as compared to the weight factor z_{FL} in the Fermi liquid regime. One readily observable consequence is a change in slope in the energy dispersion curve, which is proportional to the weight factor z, a phenomenon usually referred to as a "kink" .

In their detailed qualitative analytic analysis Byczuk et al. show that a local spectral function $\mathrm{Im}G(\omega)$ characterized by three peaks leads via the DMFT self-consistent equations to a specific form of the real part of the self energy $\mathrm{Re}\Sigma(\omega)$ (note that in DMFT the self-energy is momentum independent). The quasiparticle weight factor follows as $z = [1 - \partial \mathrm{Re}\Sigma(\omega)/\partial\omega]^{-1}$. One part derives from the energy dependent hybridization function,

which near the Fermi energy is approximately proportional to $t^2 \mathrm{Re}G(\omega)$, is responsible for the large renormalization by the factor $z_{FL} << 1$ in the Fermi liquid regime (here t is the hopping amplitude). Indeed, if one models the central peak of a particle-hole symmetric model by the Lorentzian form $G_{CP}(\omega) = z_{CP}/(\omega + i\gamma)$, where γ is of the order of the Kondo temperature of the DMFT quantum impurity problem, one finds $z_{FL} \propto z_{CP}^{-1}(\gamma/t)^2$, which is small if $\gamma/t << 1$. The latter regime extends up to the renormalized Fermi energy $\omega_* = z_{FL}D$, where D is the bare half band width (assuming an approximately half filled band). The second contribution to $\mathrm{Re}\Sigma(\omega)$ is proportional to $\mathrm{Re}[\omega - G^{-1}(\omega)]$, and is approximately linear up to a much higher energy, defined by the minima in the spectral function. The slope of this linear segment is $1 - z_{CP}^{-1}$, significantly smaller than the slope in the Fermi liquid regime. Within the approximation of a momentum-independent self-energy the quasiparticle dispersion is given by $E_p = z\epsilon_p$, with ϵ_p the "bare" dispersion as calculated, e.g., in density functional theory. As argued by Byczuk et al. the appearence of kinks of this type is a generic feature of strongly correlated electron systems, at least within the class of single band models.

These qualitative considerations are backed up by a full numerical solution of the DMFT equations, using the numerical renormalization method as an impurity solver . Results are shown for the spectral intensity of the Hubbard model at $U \simeq W$ and filling $n = 0,8$, demonstrating the kink in the spectrum above the Fermi energy, but not below, as in this case the lower Hubbard band is not well separated from the central peak. Also shown are the dispersion curves of $SrVO_3$, where kinks are found at 220 and -240 meV as compared to 150 meV observed in experiment.

Kinks in the electronic dispersion have long been associated with a coupling of electrons to a collective mode, e.g. phonons. In recent years many observations of kinks deduced from photoemission spectra and other sources in particular of transmission-metal oxides have been reported. Some of these kinks appear at rather high energy, up to 900 meV, clearly outside the range of phonon effects. Examples are the transition-metal oxides $SrVO_3$ (150 meV), and high temperature superconducting compounds (380 and 800 meV) and graphene (400-900 meV). The intrinsic mechanism for kink formation proposed by Byczuk et al. offers a natural explanation for these observations at least in systems that may be described by a single self-energy as in a single-band model or in materials with several degenerate bands.