Dynamical screening effects from first principles: implications for low-energy models and application to the iron pnictides

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The discovery, in 2008, of superconductivity above 50K in the iron pnictides has opened a new playground in condensed matter physics. The theoretical description of their electronic properties, even in the normal phase, poses a challenge to theory, emphasizing the need of determining many-body models entirely from first principles. A proper ab-initio derivation of low-energy correlated Hamiltonians, based on the constrained RPA method, produces a frequency dependent Coulomb interaction U, as it is dynamically screened by the higher-energy degrees of freedom. We present new methods to include these screening effects in an extended dynamical mean field theory (DMFT) framework[1,2]. We demonstrate that the frequency dependence of U brings in additional features, such as the correlation satellites seen in photoemission spectroscopy together with a renormalization of the low-energy properties[3]. Our first application of the dynamically screened U to the iron pnictides indicates that $BaFe_2As_2$ is a strongly correlated compound with strongly doping- and temperature-dependent properties. In the hole-overdoped region an incoherent metal is found, whereas Fermi-liquid behaviour is recovered in the undoped compound[4]. In the intermediate-doping regime, a fractional power-law behavior of the self energy is observed for the first time in a realistic modelization of materials. The resulting spectral function is in an overall agreement with the most recent ARPES data, and provides a theoretical support to their interpretation.

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