Dynamical Screening in Correlated Electron Materials

Philipp Werner[1] and Andrew J. Millis[2]

[1] *Theoretische Physik, ETH Zurich, 8093 Zürich, Switzerland*
[2] *Columbia University, 538 West, 120th Street, New York, NY 10027, USA*
(Dated: January 8, 2010)

We present an efficient method for incorporating the dynamical effects of the screening of the Hubbard U by electronic degrees of freedom in the solid into the single site dynamical mean field approximation. The formalism is illustrated by model system calculations which capture the essential features of the frequency dependent interactions proposed for Gd, Ni, SrVO$_3$ and other compounds. Screening leads to shifts in the metal-insulator phase boundary, changes in the spectral function near the Mott-Hubbard gap edge and to a renormalization of the quasiparticle weight. Hubbard bands are generically neither separated by the screened nor the unscreened interaction energy, implying that the common practice of extracting the Hubbard U from the energies of features in photoemission and inverse photoemission spectra requires reexamination.

PACS numbers: 71.27.+a,71.30.+h,71.10.Fd

'Strongly correlated electron systems' are a central topic in electronic condensed matter physics [1]. The low energy physics of these systems is typically described by an effective Hamiltonian which models the behavior of relatively localized d or f orbitals and is obtained (at least notionally) via a "downfolding" procedure in which other degrees of freedom are integrated out. A crucial aspect of the effective Hamiltonian is an interaction which acts to suppress local number fluctuations. This interaction is typically parametrized by a number, the "Hubbard U". However, U is generically dynamical: a density fluctuation in a correlated orbital produces electric fields, which other degrees of freedom will act to screen, resulting in a frequency-dependent renormalization. Screening has been observed as a shift in excitation energies in experiments comparing the surface of solid C$_{60}$ to C$_{60}$ films on silver [2] and has been computed using variations of the 'random phase approximation' (RPA) [3–5]. The renormalizations are found to be strong in many cases. In Gd, $U(\omega)$ rises from a static value of about 6.5 eV to about 17 eV as the frequency ω is raised from 0 to ~ 3 eV, while in Ce, $U(\omega)$ changes from ~ 3.5 eV to ~ 7 eV as ω is increased from 0 to ~ 4 eV [4].

While the study of the strong correlation effects induced by an instantaneous interaction is well advanced thanks to the development of dynamical mean field theory (DMFT) [6], our ability to treat frequency dependent interactions has been limited. The most widely used method for solving the DMFT equations has been the Hirsch-Fye algorithm [7], which is based on a time-discretization and decoupling of interaction terms by auxiliary fields. Frequency dependent interactions lead to a proliferation of decoupling fields which become prohibitively expensive to sample. A treatment of screening effects within exact diagonalization, numerical renormalization group and other Hamiltonian based methods requires the explicit introduction of many bosonic modes, leading to a Hilbert space which is too large to be handled

numerically. Considerations of this sort have led to the belief (see e.g. Ref. [3]) that DMFT simulations with frequency dependent interactions are exceedingly difficult.

Here we show that this is not the case: the recently developed 'hybridization expansion' diagrammatic quantum Monte Carlo method [8, 9] can be used to treat models with an arbitrary frequency dependence of the on-site repulsion $U(\omega)$ at negligible additional computational cost, opening the door to a systematic investigation of screening effects in correlated electron materials. We begin our discussion by recalling that the downfolded models used to describe the correlated degrees of freedom in a transition metal or actinide involve a one electron part and an interaction part. The parameters describing the one-electron physics are obtained by projecting a band theory calculation onto a set of distinguished ("d") orbitals and are in principle energy dependent. If the d orbitals are correctly chosen the energy dependence is negligible [10, 11] so the one electron part may be modelled as a tight-binding-like Hamiltonian $H_{\rm band}$.

The interaction part is obtained (see, e.g. Ref. 3) by screening the bare Coulomb interaction $e^2/|r-r'|$ with real and virtual transitions involving the orbitals which are integrated out, projecting the result onto the d manifold and retaining only the fully site-diagonal terms. One finds two kinds of terms: an instantaneous interaction and a screening contribution. The instantaneous interaction may be represented as a Hamiltonian term $H_{\rm int}$ which takes the usual Slater-Kanamori form $H_{\rm int} = \sum_i \frac{1}{2} U \hat{N}_i^2 + ...$ with $\hat{N}_i$ the number operator for electrons in the d manifold on site i and the ellipsis denoting exchange, 'pair hopping' and other terms which involve operators such as the spin and angular momentum which commute with $\hat{N}$. The screening contribution couples the site densities at different times and is expressed as a contribution $S_W = \frac{1}{2} \int d\tau d\tau' N(\tau) W(\tau-\tau') N(\tau')$ to the effective action. The screening function $W(\tau)$ is negative, depends only on one time (or frequency) argu-