Valence bond dynamical mean-field theory of doped Mott insulators with nodal/antinodal differentiation

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Abstract – We introduce a valence bond dynamical mean-field theory of doped Mott insulators. It is based on a minimal cluster of two orbitals, each associated with a different region of momentum space and hybridized to a self-consistent bath. The low-doping regime is characterized by singlet formation and the suppression of quasiparticles in the antinodal regions, leading to the formation of Fermi arcs. This is described in terms of an orbital-selective transition in reciprocal space. The calculated tunneling and photoemission spectra are consistent with the phenomenology of the normal state of cuprates. We derive a low-energy description of these effects using a generalization of the slave-boson method.

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The doping of a Mott insulator is a fundamental problem of condensed-matter physics, relevant to the physics of cuprate superconductors [1]. In the simplest Brinkman-Rice [2] description, the doped metallic state is a Fermi liquid in which quasiparticles are formed with a heavy mass \(m^*/m \sim 1/\delta\) and a reduced weight \(Z \sim \delta\) (\(\delta\) is the doping level). This physical picture can indeed be rationalized using the modern theoretical framework of dynamical mean-field theory (DMFT) [3,4]. It is applicable when spatial correlations are weak, which is favored by high dimensionality and strong competing (e.g. orbital) fluctuations. In cuprates however, which are quasi–two-dimensional materials with low orbital degeneracy, it was pointed long ago by Anderson in a seminal paper [1] that the antiferromagnetic superexchange (\(J\)) plays a key role, leading to strong short-range correlations associated with singlet formation (valence bonds) between nearest-neighbor lattice sites. Slave-boson mean-field theories [5–8], as well as projected variational wave functions [9,10], provide simple theoretical frameworks to incorporate this effect, modifying the Brinkman-Rice picture at small doping \(\delta \lesssim J/t\) and leading, e.g. to a finite effective mass \(m^*/m \sim 1/(J/t + \delta)\), consistent with observations in cuprates. However, these theories fail to describe a key phenomenon in underdoped cuprates, namely the strong differentiation in momentum space observed e.g. by photoemission spectroscopy (ARPES) [11]: Coherent quasiparticle excitations are suppressed in the antinodal regions of the Brillouin zone (BZ) and a pseudogap appears in the normal state. In order to take this phenomenon into account while incorporating short-range correlations, cluster extensions of the DMFT framework have been investigated by several groups [4,12,13]. Most studies have considered clusters of at least four sites (plaquette) and numerical efforts have been devoted to increase the cluster size in order to improve momentum-resolution and get closer to the two-dimensional lattice [14].

In this article, we follow a different route, looking for a description based on the minimal cluster able to successfully describe momentum-space differentiation together with Mott physics. We find that a two-site cluster is sufficient to achieve this goal on a qualitative level, and to a wide extent on a quantitative level when compared to larger cluster calculations. This allows us to construct a valence bond dynamical mean-field theory (VB-DMFT) of nodal/antinodal differentiation, in which this phenomenon is linked to the distinct properties of the orbitals associated with different regions of momentum space.

The main motivation to choose the smallest possible cluster is to advance our qualitative understanding,
Since the theory is based on a two-site Anderson model, results can be interpreted in terms of valence-bond singlet formation and linked to the competition between singlet-formation and individual Kondo screening [15–18]. However, the self-consistency of the bath does bring in novel aspects to this competition in comparison to the non self-consistent two-impurity model. The present VB-DMFT can be viewed as an extension of the static mean-field theories (e.g., slave-boson based) of singlet formation. In contrast to those theories which have a limited number of static variational parameters, it involves a dimer coupled to a self-consistent bath through energy-dependent hybridization functions. This allows for a description of the physics over a wide range of energy scales. At low energy however, the new slave-boson approximation introduced in [19] reproduces several aspects of the full solution with a remarkable accuracy.

We study the Hubbard model on a square lattice, with hopping between nearest-neighbor sites (t) and next-nearest-neighbor sites (t'). In the following, we use $U/t = 10$ and $t'/t = -0.3$, which are values commonly used for modeling hole-doped cuprates in a single-band framework. All energies (and temperatures) are expressed in units of $D = 4t = 1$, and the doping is denoted by $\delta$.

We use a two-site effective Anderson impurity problem, involving the on-site interaction $U$ and two hybridization functions: a local one $\Delta_{11}(\omega) = \Delta_{22}(\omega)$ and an inter-site one $\Delta_{12}(\omega)$, which are self-consistently determined by relating the two-impurity problem to the original lattice one. We have investigated several such embodiments, both of the dynamical cluster approximation (DCA) and cellular-DMFT (CDMFT) type [4,12] with similar results. Here, we focus on a somewhat generalized form of the DCA embedding, which preserves the symmetries of the square lattice, in which the Brillouin zone is decomposed into two patches of equal surface: a central square (denoted $P_{\uparrow}$) centered at momentum (0,0) and the complementary region ($P_{\downarrow}$) extending to the edge of the BZ and containing in particular the ($\pi, \pi$) momentum.

From the lattice Green’s function, two coarse-grained Green’s functions in momentum space are constructed:

$$G_{\pm}(\omega) = \sum_{k \in P_{\pm}} G(k, \omega)$$

(with momentum summations normalized to unity within each patch). Following the DCA construction, the inner (respectively, outer) patch self-energy is associated with the even- (respectively, odd) parity self-energy of the two-impurity effective problem, i.e. to the even (respectively, odd) orbital combinations $(c_1^\dagger \pm c_2^\dagger)/\sqrt{2}$. Indeed, the states close to (0,0) have more bonding character while those close to ($\pi, \pi$) have more antibonding character. The self-consistency condition reads:

$$G_{\pm}^{\prime}(\omega) = \sum_{k \in P_{\pm}} [\omega + \mu - \varepsilon_k - \Sigma_K(\omega)]^{-1}.$$

In this expression, the index $K = \pm$ refers both to the inner/outer patch index and to the even/odd orbital combinations. We solve the self-consistent two-impurity problem using both continuous-time quantum Monte Carlo (CTQMC) [20] which sums the perturbation theory in $\Delta_{ab}(\omega_n)$ on the Matsubara axis, and an approximate method geared at low-energy properties: the rotationally invariant slave-boson formalism (RISB) presented in [19].

In fig. 1, we display the real part of the even- and odd-orbital self-energy at zero frequency, as determined by both methods, as a function of $\delta$. Even though the frequency dependence of the self-energy obtained by CTQMC is non-trivial, its zero-frequency limit is in remarkable agreement with the RISB solution. The two orbitals behave in a similar way at high doping $\delta \gtrsim 25\%$. Below this doping level, we observe an onset of orbital differentiation, which is a manifestation of momentum differentiation in the lattice model. This differentiation increases as $\delta$ is reduced, until a transition is reached at $\delta \approx 16\%$ (in CTQMC). At this characteristic doping, $\mu - \Sigma_-(0)$ reaches the band edge corresponding to the odd orbital, and the latter becomes empty at low energy and remains so for all lower dopings. $G(k, \omega)$ no longer has poles at $\omega = 0$ in the outer patch, and low-energy quasi-particles exist only inside the inner patch. Hence, at low doping, momentum-space differentiation becomes strong and manifests itself as an orbital-selective transition in VB-DMFT.

In order to gain further qualitative insight, we also plot in fig. 1 (right part) the statistical contribution [21] of several cluster eigenstates $|\Gamma\rangle$. This contribution can be compared to a similar quantity obtained within slave bosons. Indeed, the RISB method introduces slave-boson amplitudes $\phi_{\Gamma n}$, a density matrix connecting the eigenstates $|\Gamma\rangle$ of the isolated dimer to the quasiparticle Fock states $|n\rangle$. The quantity $p_{\Gamma} = \sum_n |\phi_{\Gamma n}|^2$ is then interpreted as the statistical weight of $|\Gamma\rangle$ in the groundstate. The agreement between CTQMC and RISB is again very good, and even quantitative for the two states with highest weights. At large doping, the empty state and the two spin-degenerate states with one electron in the even orbital dominate, as expected. As doping decreases, these states lose weight and the intra-dimer singlet prevails, reflecting the strong tendency to valence bond formation.
The states with immediately lower weights are the one-electron states and the valence-bond–breaking triplet excitation which dominates over the empty state. Therefore, the orbital (momentum) differentiation at low doping is governed by intra-dimer singlet formation, reminiscent of the singlet regime of the two-impurity Anderson model.

The gapping of the odd orbital (outer patch) is actually a crude description of the pseudogap phenomenon. To illustrate this, we compute the tunneling conductance $dI/dV$ as a function of voltage $V$. This calculation is made possible by the high quality, low-noise, of the CTQMC results on the Matsubara axis, allowing for reliable analytical continuations to the real axis at low and moderate energy, using simple Padé approximants. The conductance is displayed in fig. 2 together with the gap $\Delta$ in the odd Green’s function, obtained from $\Delta = \Sigma'(\Delta) + \varepsilon_{\text{min}} - \mu$, with $\varepsilon_{\text{min}}$ the lower edge of the band dispersion $\varepsilon_k$ in the outer patch. Note the overall particle-hole asymmetry of $dI/dV$ and the peak at positive voltage. This peak shifts towards higher energy with decreasing doping, as does the gap $\Delta$, and can indeed be traced back to the edge of the unoccupied odd-orbital spectral function. These observations compare favorably to tunneling experiments in the normal state of underdoped cuprates [22].

We now address two related issues: how to reconstruct information in momentum space using our two-orbital description, and how to gauge the reliability of a description based on only two momentum-space components, as compared to calculations with larger cluster sizes and better momentum space resolution. The approximation of lattice quantities from the cluster ones is a central issue in cluster methods. Periodization is crucial in CDMFT to restore translational invariance. In DCA, translational invariance is not broken, but there is still a large freedom when interpolating the self-energy in the BZ from the cluster self-energies. The most local quantity is expected to give the more reliable interpolation. We investigate two possibilities among those that have been discussed in the literature [23]: i) interpolating the self-energy ($\Sigma$-interpolation) as $\Sigma(k, \omega) = \Sigma_+(\omega)\alpha_+(k) + \Sigma_-(\omega)\alpha_-(k)$, with $\alpha_{\pm}(k) = \frac{1}{2}(1 \pm \frac{1}{2}[\cos(k_x) + \cos(k_y)])$; ii) interpolating the cumulant ($M$-interpolation) as $M(k, \omega) = M_+(\omega)\alpha_+(k) + M_-(\omega)\alpha_-(k)$. The cumulant is related to the self-energy by $\Sigma = \omega + \mu - M^{-1}$. It is the dual quantity of the self-energy in an expansion around the atomic limit and a natural measure of how much the hybridization to the self-consistent environment changes the impurity Green’s function as compared to an isolated dimer. Close to the Mott insulator, it is more local than the self-energy and a better quantity to interpolate [23]. Comparing the interpolations on small clusters with direct calculations on larger clusters, having better $k$-resolution, provides a systematic test of cluster schemes and interpolations. As a first step, we compare in fig. 3 the results of VB-DMFT, with $\Sigma$- or $M$-interpolation, to the cluster components $\Sigma_K(\omega)$ of a four-site cluster (plaquette), using the standard DCA embedding (with the BZ divided into 4 patches centered around $K = (0, 0)$, $0, \pi), (\pi, 0), (\pi, \pi)$). The results of fig. 3 reveal two main points: i) the $M$-interpolation of the two-orbital results is clearly superior to the $\Sigma$-interpolation for reconstructing plaquette cluster quantities and ii) when $M$-interpolated, the two-orbital description does quite a remarkable job at capturing the full-frequency dependence of the various cluster components $\Sigma_K(\omega)$ of the plaquette results. Note that the plaquette cluster momentum $K = (\pi, 0)$ is not present as an individual orbital in the two-site description: it is entirely reconstructed by interpolation, and as such is the most direct test of the reconstructed momentum dependence. A distinctive feature of the results depicted in fig. 3 is that the scattering rate near momentum $(\pi, 0)$, proportional to $\text{Im}\Sigma_{\pi0} (\omega^{\pi/2})$, displays a maximum around a doping level $\delta \simeq 8\%$, as previously noted in the plaquette.
resolution (larger clusters) is necessary to obtain reliable results. This limitation is intrinsic to cluster methods, regardless of the interpolation scheme.

VB-DMFT and the (non-self-consistent) two-impurity Anderson model share common features. In both cases, at low-\(\delta\), the singlet state dominates, and the real part of the odd-orbital self-energy is large. These effects are due to the term transferring singlet pairs from the even orbital to the odd orbital, as can be checked by explicitly removing it from the dimer Hamiltonian. Interestingly, strong fluctuations in the singlet pairing channel and momentum-space differentiation appear to be related effects. The key difference between VB-DMFT and the two-impurity model with fixed bath is that the self-consistency leads to the opening of a gap in the odd orbital. This gap reduces the scattering rate of the even orbital, leading to an extremum in \(\text{Im}\Sigma_\phi(i\delta^+\lambda)\) (and also in the reconstructed \(\text{Im}\Sigma_\phi(i\delta^+)\)), which is absent in the non-self-consistent two-impurity model.

To summarize, we have proposed in this article a valence bond dynamical mean-field theory (VB-DMFT) as a minimal cluster-based description of momentum space differentiation in doped Mott insulators. Because of its simplicity, this theory can be investigated with moderate numerical effort and progress in qualitative understanding can be achieved with low-energy methods such as rotationally invariant slave bosons. The calculated STM and ARPES spectra are consistent with the phenomenology of the normal state of cuprates. The low-doping regime is dominated by singlet formation. Mott physics is responsible for the suppression of coherent quasiparticles at the antinodes, in qualitative agreement with other approaches starting from the weak/intermediate-coupling viewpoint [32]. Within VB-DMFT, this suppression is described as an orbital-selective transition in momentum space.

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