Non local theory of excitations applied to the Hubbard model\[1\]

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Abstract. We propose a nonlocal theory of single-particle excitations. It is based on an off-diagonal effective medium and the projection operator method for treating the retarded Green function. The theory determines the nonlocal effective medium matrix elements by requiring that they are consistent with those of the self-energy of the Green function. This allows for a description of long-range intersite correlations with high resolution in momentum space. Numerical study for the half-filled Hubbard model on the simple cubic lattice demonstrates that the theory is applicable to the strong correlation regime as well as the intermediate regime of Coulomb interaction strength. Furthermore, the results show that nonlocal excitations cause sub-bands in the strong Coulomb interaction regime due to strong antiferromagnetic correlations, decrease the quasi-particle peak on the Fermi level with increasing Coulomb interaction, and shift the critical Coulomb interaction $U_{c2}$ for the divergence of effective mass towards higher energies at least by a factor of two as compared with that in the single-site approximation.

The description of single-particle excitations in correlated electron systems has been a challenging problem because new phenomena are observed there and because simple perturbation approaches are not applicable \[1\]. At present, excitations in the systems of infinite dimensions have been clarified by use of the dynamical mean field theory (DMFT) \[2\]. That theory makes use of a momentum-independent self-energy, and determines the energy self-consistently by solving an impurity problem with use of advanced many-body theories. The DMFT can be traced back to the many-body coherent potential approximation (CPA) for magnetic alloys \[3\]. It is also known to be equivalent to the dynamical CPA \[4\] for describing finite-temperature magnetism \[5\]. More recently, we proposed the projection operator method CPA (PM-CPA) \[6\], which is equivalent to the DMFT too. It is based on the projection technique applied to the retarded Green function and on an energy-dependent Liouville operator.

The theories mentioned above are based on a single-site approximation (SSA) which neglects the off-diagonal components of the self-energy. Therefore the momentum dependence of excitations in real systems is described incompletely. In this paper, we propose a nonlocal theory of excitations which extends the PM-CPA, and demonstrate that it describes self-consistently momentum-dependent excitations with high resolution in the strong Coulomb interaction regime as well as in the intermediate regime.

We adopt here the Hubbard Hamiltonian $H$ with nearest-neighbor transfer integral $t$ and intra-atomic Coulomb interaction $U$, and consider the retarded Green function

$$G_{ij\sigma}(z) = \langle a_{i\sigma}^\dagger \frac{1}{z-L} a_{j\sigma}^\dagger \rangle .$$

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Thus, the Green function is expressed as
\begin{equation}
G_{ij\sigma}(z) = [(z - H_0 - \Lambda(z))^{-1}]_{ij\sigma} .
\end{equation}

Here \((H_0)_{ij\sigma}\) is the Hartree-Fock Hamiltonian matrix and \((\Lambda(z))_{ij\sigma}\) is the self-energy matrix defined by \(\Lambda_{ij\sigma}(z) = U^2 G_{ij\sigma}(z)\). The reduced memory function \(\overline{G}_{ij\sigma}(z)\) is given by
\begin{equation}
\overline{G}_{ij\sigma}(z) = \left( A_{i\sigma}^\dagger \right| \frac{1}{z - \overline{L}} A_{j\sigma}^\dagger \right) .
\end{equation}

The operator \(A_{i\sigma}^\dagger\) is defined by \(A_{i\sigma}^\dagger = a_{i\sigma}^\dagger \delta n_{i-\sigma} + \delta n_{i-\sigma} - \langle n_{i-\sigma} \rangle\). \(a_{i\sigma}^\dagger (a_{i\sigma})\) is the creation (annihilation) operator for an electron with spin \(\sigma\) on site \(i\), and \(\langle n_{i\sigma} \rangle\) is the average electron number on site \(i\) for spin \(\sigma\). Moreover, \(\overline{L}\) is a Liouville operator acting on the space orthogonal to the space \(|a_{i\sigma}^\dagger\rangle\); \(\overline{L} = QLQ, Q = 1 - P\), and \(P\) is a projection operator defined by \(P = \sum_{i\sigma} |a_{i\sigma}^\dagger\rangle \langle a_{i\sigma}^\dagger|\).

In our nonlocal theory, we introduce an energy-dependent Liouville operator \(\tilde{L}(z)\) for an effective Hamiltonian \(\tilde{H}_0(z)\) of an off-diagonal medium \(\tilde{\Sigma}_{ij\sigma}(z)\), i.e., \(\tilde{H}_0(z) = H_0 + \sum_{ij\sigma} \tilde{\Sigma}_{ij\sigma}(z) a_{i\sigma}^\dagger a_{j\sigma}\). Here \(H_0\) is the Hartree-Fock Hamiltonian. The retarded Green function \(F_{ij\sigma}(z)\) for the Liouvillean \(\tilde{L}(z)\) is expressed as
\begin{equation}
F_{ij\sigma}(z) = [(z - H_0 - \tilde{\Sigma}(z))^{-1}]_{ij\sigma} ,
\end{equation}
where \(\tilde{\Sigma}(z)_{ij\sigma} = \tilde{\Sigma}_{ij\sigma}(z)\). It should be noted that the Green function \(F_{ij\sigma}(z)\) becomes identical with \(G_{ij\sigma}(z)\) when
\begin{equation}
\tilde{\Sigma}_{ij\sigma} = \Lambda_{ij\sigma}(z) .
\end{equation}

Thus, \(F_{ij\sigma}(z)\) describes properly many-body excitations when the above relation is satisfied.

In order to obtain an explicit expression of the self-energy \(\Lambda_{ij\sigma}(z)\), we separate the Liouvillean \(L\) into \(\tilde{L}(z)\) and the remaining interaction part \(L_I(z)\), i.e., \(L = \tilde{L}(z) + L_I(z)\), and expand the memory function \(G\) by using the incremental method:
\begin{equation}
\overline{G}_{ij\sigma}(z) = \overline{G}^{(ij)}_{ij\sigma}(z) + \sum_{l \neq i,j} \Delta \overline{G}^{(ijl)}_{ij\sigma}(z) + \frac{1}{2} \sum_{l \neq i,j} \sum_{m \neq i,j,l} \Delta \overline{G}^{(ijlm)}_{ij\sigma}(z) + \cdots .
\end{equation}

Here \(\Delta \overline{G}^{(ijl)}_{ij\sigma}(z) = \overline{G}^{(ijl)}_{ij\sigma}(z) - \overline{G}^{(ij)}_{ij\sigma}(z)\), and \(\Delta \overline{G}^{(ijlm)}_{ij\sigma}(z) = \overline{G}^{(ijlm)}_{ij\sigma}(z) - \Delta \overline{G}^{(ijl)}_{ij\sigma}(z) - \Delta \overline{G}^{(ijm)}_{ij\sigma}(z) - \overline{G}^{(ij)}_{ij\sigma}(z)\). These terms are all calculated from cluster memory functions defined by \(\overline{G}^{(c)}_{ij\sigma}(z) = (A_{i\sigma}^\dagger |(z - \overline{L}^{(c)}(z))^{-1} A_{j\sigma}\rangle\). \(\overline{L}^{(c)}(z) = QL^{(c)}(z)Q\) and \(L^{(c)}(z) (c = ij, ijl, \ldots)\) is the Liouvillian for a cluster \(c\) embedded in the medium with off-diagonal matrix elements \(\{\tilde{\Sigma}_{ln\sigma}(z)\}\). Note that a “cluster” \(c = (ij)\), for example, does not mean that sites \((i,j)\) are nearest neighbors. Instead they may be far apart.

When we truncate the expansion at a certain stage in the series of Eq. (6), the self-energy \(\Lambda_{ij\sigma}(z) = U^2 \overline{G}_{ij\sigma}(z)\) depends on the medium \(\tilde{\Sigma}_{ij\sigma}(z)\). We then determine the medium self-consistently from condition (5). Note that the present theory reduces to the PM-CPA (i.e., the DMFT) in infinite dimensions.
In the above self-consistent theory, one needs explicit expressions for the cluster memory functions, for which we apply the renormalized perturbation theory [7].

$G^{(c)}_{ij\sigma}(z) = \left[ G^{(c)}_{0}(z) \cdot (1 - \mathcal{L}^{(c)}_{ij\sigma}(z))^{-1} \right]_{ij\sigma}$.  

(7)

Here $(\mathcal{L}^{(c)}_{ij\sigma}(z))_{ij\sigma} = U(1 - 2\langle n_{i-\sigma} \rangle / \chi_{i\sigma}$, and $\chi_{i\sigma} = \langle n_{i-\sigma} \rangle(1 - \langle n_{i-\sigma} \rangle)$. In the simplest approximation (RPT-0), $(G^{(c)}_{0}(z))_{ij\sigma}(z)$ is given by

$(G^{(c)}_{0}(z))_{ij\sigma}(z) = A_{ij\sigma} \int \frac{\delta \delta' \epsilon' \epsilon''}{z - \epsilon - \epsilon' - \epsilon''} \rho^{(c)}_{ij\sigma}(\epsilon) \rho^{(c)}_{ij-\sigma}(\epsilon') \rho^{(c)}_{ji-\sigma}(\epsilon'') \chi(\epsilon, \epsilon', \epsilon'')$.  

(8)

Here $A_{ij\sigma} = \chi_{i\sigma}/\langle n_{i-\sigma} \rangle_c (1 - \langle n_{i-\sigma} \rangle_c) \delta_{ij} + 1 - \delta_{ij}, \chi(\epsilon, \epsilon', \epsilon'') = (1 - f(\epsilon))(1 - f(\epsilon'))f(\epsilon'') + f(\epsilon)f(\epsilon')(1 - f(\epsilon''))$, $f(\epsilon)$ is the Fermi distribution function, $\langle n_{i\sigma} \rangle_c$ is the electron number for a cavity state defined by $\langle n_{i\sigma} \rangle_c = \int d\epsilon \rho^{(c)}_{i\sigma}(\epsilon)f(\epsilon)$, and $\rho^{(c)}_{ij\sigma}(\epsilon) = -\pi^{-1} \text{Im}[(F^{(c)}_{ij\sigma}(z))^{-1}]_{ij\sigma}$. The coherent cluster Green function $(F^{(c)}_{c}(z))_{ij\sigma} = F_{ij\sigma}(z)$ is given by Eq. (4), and $(\Sigma^{(c)}_{c}(z))_{ij\sigma} = \Sigma_{ij\sigma}(z)$ for sites $(i, j)$ belonging to the cluster $c$.

Finally the momentum dependent excitation spectra are calculated from the Green function

$G_{k\sigma}(z) = \frac{1}{z - \epsilon_{k\sigma} - \Lambda_{k\sigma}(z)}$.  

(9)

Here $\epsilon_{k\sigma}$ is the Hartree-Fock one-electron energy eigen value, and the momentum-dependent self-energy is calculated via Fourier transform of the off-diagonal self-energy as $\Lambda_{k\sigma}(z) = \sum_{j} \Lambda_{j0\sigma}(z) \exp(ik \cdot R_{j})$.

We have performed numerical calculations for the single-particle excitation spectra on a simple cubic lattice at half-filling. In the nonlocal self-energy calculations, we have taken all two-site pairs up to 10-th nearest neighbors, and neglected the clusters beyond the 2 sites. Figure
1 shows an example of the momentum-dependent spectra along high-symmetry lines for $U = 14$ in unit of $|t| = 1$. We find quasiparticle states near the Fermi level, which form a narrow band with averaged quasiparticle weight $Z = 0.21$. On the other hand, the lower (upper) Hubbard band is enhanced around the $\Gamma$ (R) point. It should be noted that the energy splitting between the main peaks of the lower and upper Hubbard bands is about 20, being larger than $U = 14$ as seen in Fig. 2. This seems to be explained by strong antiferromagnetic (AF) correlations. In fact, in the strong AF correlation limit the energy to remove (add) an electron is expected to be $\epsilon_0 - zJ (\epsilon_0 + U + zJ)$ at half filling. Here $\epsilon_0$ is the atomic level and $J$ is the super exchange interaction constant ($J = 4|t|^2/U$). Then the splitting is given by $U + 2zJ$ instead of $U$. The former yields 17.4 for $U = 14$, which is comparable to the calculated splitting 20. We also find sub-peaks around $|\omega| = 8$ in Figs. 1 and 2. These peaks are interpreted as the lower and upper Hubbard peaks in the absence of long-range AF correlations because the splitting is close to $U$. Furthermore, we find weak excitations at $|\omega| \approx 3$, which might correspond to a “shadow band” due to strong AF correlations as found in QMC calculations [8]. We also point out that in the nonlocal theory, the density of states at the Fermi level $\rho(0)$ does not agree with the one in the SSA as seen in Fig. 2.

We have calculated the nonlocal excitation spectra with increasing Coulomb interaction. Self-consistent solutions are found up to $U \approx 21$. In this range, we find that the quasiparticle weights $Z$ are larger than those of the SSA but never vanish. We suggest that the critical Coulomb interaction is $U_{c2}(Z = 0) \approx 30$.

In summary, we have presented a nonlocal theory for excitation spectra by introducing a fully off-diagonal effective medium $\Sigma_{ij\sigma}(z)$ to the projection operator formalism. The theory describes self-consistently the long-range nonlocal excitations in momentum space with high resolution. We verified from the numerical calculations that the present scheme works from the weak to strong Coulomb interaction regime, and found the shadow bands as well as the Hubbard sub-bands due to strong AF correlations.

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References

[1] Fulde P., Thalmeier P., Zwicknagl G. 2006, Solid State Phys. 60 1
[2] Georges A., Kotliar G., Krauth W., Rosenberg M. J. 1996 Rev. Mod. Phys. 68 13
[3] Hirooka S. and Shimizu M. 1977 J. Phys. Soc. Jpn. 43 70
[4] Kakehashi Y. 1992 Phys. Rev. B 45 7196; 2002 Phys. Rev. B 65 184420
[5] Kakehashi Y. 2004 Adv. in Phys. 53 498
[6] Kakehashi Y and Fulde P. 2004 Phys. Rev. B69 045101
[7] Kakehashi Y and Fulde P. 2004 Phys. Rev. B70 195102
[8] Gröber C., Eder R., and Hanke W. 2000 Phys. Rev. B62 4336