Dynamical mean-field theory of electron-phonon interaction in correlated electron materials: general results and application to doped Mott insulators

Andreas Deppeler\textsuperscript{1} and Andrew J. Millis\textsuperscript{2}

\textsuperscript{1}Center for Materials Theory, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854  
\textsuperscript{2}Department of Physics, Columbia University, 538 W 120th St, New York, New York 10027

(February 25, 2002)

The dynamical mean-field method is used to formulate a computationally tractable theory of electron-phonon interactions in systems with arbitrary local electron-electron interactions in the physically relevant adiabatic limit of phonon frequency small compared to electron bandwidth or interaction scale. As applications, the phonon contribution to the effective mass of a carrier in a lightly doped Mott insulator is determined and the phase separation boundary is discussed.

There is to date no systematic theoretical extension to correlated materials of the successful Migdal-Eliashberg (ME) theory\textsuperscript{1}, which describes electron-phonon interactions in weakly correlated materials. Electron-phonon interactions in one-dimensional systems have been studied by renormalization group methods\textsuperscript{2}, and recent improvements in numerical techniques have for example allowed the spin-phonon dynamics of insulating quasi-one-dimensional Peierls systems to be determined in considerable detail\textsuperscript{10}. Concerning higher-dimensional, metallic systems, Kim and co-workers\textsuperscript{11} argued that near a Mott transition a decrease in electron-phonon coupling was compensated by an increase in carrier mass, leading to electron-phonon effects unrenormalized by proximity to the Mott transition. Our results, to be presented below, disagree with this conclusion. Several authors have used direct numerical simulation [e.g., quantum Monte Carlo (QMC) techniques] of models of electrons interacting both with each other and with lattice vibrations\textsuperscript{12,14}. However, the present limitations of memory size and algorithms have restricted these works mainly to the calculation of static properties, especially phase boundaries and transition temperatures and to the ‘antiadiabatic’ limit of phonon frequency comparable to electronic energy scale.

The development of the dynamical mean-field (DMF) method\textsuperscript{15} has opened an important avenue for progress, by showing that if (as occurs for the electron-phonon interaction) the momentum dependence of the electron self-energy is negligible then a good approximation to the correlation physics can be obtained from the solution of a numerically tractable quantum impurity problem plus a self-consistency condition. Unfortunately the straightforward inclusion of the electron-phonon coupling in the DMF formalism is difficult because the mismatch between the typical phonon frequency scale $\omega_0 \lesssim 0.1$ eV and electron energy scale $t \gtrsim 1$ eV renders conventional numerical approaches to the impurity problem prohibitively expensive, except in the ‘antiadiabatic’ limit\textsuperscript{14} of relevance to rather few materials. In this paper we present a practical implementation of an adiabatic expansion of the DMF formalism and show how it may be used to determine the phonon contribution to electronic properties of correlated systems. The work reported here builds on previous papers, which introduced the adiabatic expansion\textsuperscript{16} and applied it to models involving only electron-lattice interactions\textsuperscript{17,18}. As an application we answer the long-standing question of the electron-phonon contribution to the carrier self-energy in a lightly doped Mott insulator. Our methods may easily be extended, e.g., to heavy fermion materials and may be combined with recent extensions of the DMF method\textsuperscript{19,20}.

We consider the single-site DMF approximation to a general Hamiltonian of the form $H = H_{\text{band}} + H_{\text{el-el}} + H_{\text{ph}} + H_{\text{el-ph}}$, where $H_{\text{band}}$ and $H_{\text{el-el}}$ describe electrons moving in some band structure and interacting via some local interaction. We model the phonons as dispersionless quantum oscillators with instantaneous displacement...
Dispersion may be approximately included by treating $M, K$ as Brillouin-zone averages of phonon dispersions or via the more sophisticated techniques of Refs. [21, 22]. Anharmonic terms such as those considered in Ref. [21] can be easily added and will be seen to be generated.

The electron-phonon coupling is again taken to be local. It is cumbersome to write in general. We illustrate the issues via the physically relevant example of the pseudocubic manganese perovskites. Here the relevant electrons are $e_g$-symmetry Mn-O hybrid states. The generalized phonon field $q$ encompasses (i) a ‘breathing’ mode (symmetric distortion of the Mn-O$_6$ octahedron) coupling via a constant $g_{0h}$ to the total on-site charge density and (ii) a one-parameter family of Jahn-Teller modes (even-parity, volume-preserving distortions of the Mn-O$_6$ octahedron) coupling via a matrix element $g_{JT}$ to appropriate differences of occupancy between different orbitals (for a more detailed discussion of the couplings and notation see, e.g., Ref. [3]). These two distortions will be labeled by a scalar coordinate $x$ and a two-component vector $\vec{Q} = (Q_x, 0, Q_z)$, respectively. The coupling term reads (repeated indices are summed)

$$
H_{el-ph} = \frac{1}{2} \sum_i [g_{0h} x_i (n_i - n) + g_{JT} \vec{Q}_i \cdot \vec{c}^\dagger \gamma_{ph} \vec{c}_i],
$$

where $\vec{r} = (\tau_x, \tau_y, \tau_z)$ are Pauli matrices acting in orbital space, $n_i = \sum_a c^\dagger_{i\alpha} c_{i\alpha}$ is the local electron density, and $\langle x_i \rangle = 0$ is defined to be the equilibrium phonon state for a uniform distribution of electrons.

Within the single-site DMF approximation [13] the properties of $H$ may be obtained from the solution of an impurity model specified by the action

$$
S[c, \bar{c}, q, a] = S_0[q] + S_1[c, \bar{c}, q, a], \quad S_0[q] = \frac{1}{2} \sum_{k} q_{k}^{2} (K_{z} + M_{a}\omega_{k}^{2}) q_{-k}^{2} \quad \text{and} \quad S_1[c, \bar{c}, q, a] = S_{el-cl}[c, \bar{c}] + S_{el-ph}[c, \bar{c}, q] - \sum_{\alpha, n} \bar{c}_{\alpha n} c_{\alpha n} a_{n}.
$$

Here the terms $S_{el-cl}$ and $S_{el-ph}$ are obtained in the usual way from the interaction terms listed above, and $S$ is a functional of a mean-field function $a$, which may depend on spin and orbital indices and expresses the effect of the rest of the lattice upon the single site. It is fixed by equating the impurity Green function $G_{imp}[a]_{n} = \delta \ln Z[a] / \delta a_{n}$ to the local Green function $\Gamma_{loc}[a]_{n} = \int d^{3}p / (2\pi)^{3} (\omega_{n} + \mu - \Sigma[a]_{n} - H_{band})^{-1}$ with $\Sigma[a]_{n} = a_{n} - G_{imp}[a]_{n}^{-1}$. The fields $c, \bar{c}$ and $q$ represent local electronic and phonon degrees of freedom and have been Fourier transformed according to $q(\tau) = \sum_{k} \exp(-i \omega_{k} \tau) q_{k}$ etc. We will index bosonic Matsubara frequencies $\omega_{k} = 2k\pi T$ by integers $k$ and fermionic Matsubara frequencies $\omega_{n} = (2n + 1)\pi T$ by integers $n$, i.e., $q_{k} \equiv q(\omega_{k})$ and $a_{n} \equiv a_{n}^{\dagger}(i\omega_{n})$.

To analyze the effect of phonons on electronic physics [14, 17] we integrate out the electron fields and work with an effective action $S[q, a] = S_0[q] + S_1[q, a]$, which we expand about the values $\bar{q}$ that extremize $S$. We introduce an electronic bandwidth or interaction scale $t$ and define the parameters

$$
\lambda = \frac{g_{0h}^{2}}{K T}, \quad \gamma = \frac{(K/M)^{1/2}}{t} = \frac{\omega_{0}}{t},
$$

Crucial objects in the expansion are the vertices

$$
\Gamma_{N}[a]_{k_{1}, \ldots, k_{N}} = -\frac{1}{(N - 1)!} \frac{\delta S_{1}[q, a]}{\delta q_{k_{1}} \cdots \delta q_{k_{N}}},
$$

which are connected correlation functions of the electrons-only theory. The adiabatic parameter $\gamma$ controls the expansion because each phonon loop involves a sum over frequencies of order $\omega_{n} \sim \gamma$, while the vertices $\Gamma$ vary with frequency on the scale $t$. If terms of order $\gamma^{3/2}$ and higher are neglected, the $\Gamma_{N>4}$ may be dropped and $\Gamma_{3,4}$ may be approximated by their static value computed using $a$ at $\gamma = 0$. With suitably rescaled fields and frequencies (for details see Ref. [10]) we may write

$$
S[q, a] = \frac{1}{2} \sum_{k} q_{k} D_{k}^{a-1} q_{-k}
- \frac{\lambda^{3/2} \gamma^{1/2} T^{1/2}}{3} \sum_{k_{1}, k_{2}} \Gamma_{3}[a]_{k_{1}, k_{2}} q_{k_{1}} q_{k_{2}} q_{-k_{1} - k_{2}}
- \frac{\lambda^{2} \gamma T}{4} \sum_{k_{1}, k_{2}, k_{3}} q_{k_{1}} q_{k_{2}} q_{k_{3}} q_{-k_{1} - k_{2} - k_{3}},
$$

where $D_{k}$ is the phonon propagator, equal for scalar phonons to $1 / (1 + \omega_{n}^{2} / \omega_{0}^{2} - \lambda \Gamma_{2}[a]_{k, -k})$, renormalized by electron-electron interaction effects contained in $\Gamma_{2}$. Note that $O(\gamma)$ corrections to $a$, as well as the leading frequency dependence, must be included in $\Gamma_{2}$.

We used the Hirsch-Fye [24] algorithms distributed with Ref. [14] and routines to compute the connected correlation functions for a single-band Hubbard model. Computations were performed on a Sun workstation; the longest computation $\Gamma_{2}$ at larger $U$ took ~40 minutes. Errors (estimated by comparison to exact solution and scaling with system sizes) were less than 2% for parameters shown. Fig. 4 shows that near half filling and for scalar phonons the Hubbard-U strongly decreases $\Gamma_{2}$, thereby suppressing the polaronic instability occurring at $\lambda \Gamma_{2} = 1$. Although the polaronic instability is suppressed a phase separation instability is found for $\lambda \gtrsim 1$ and $n$ near 1; details will be presented elsewhere. For comparison and to demonstrate the power of the method we also present in the right-hand panel results for a model of ‘colossal magnetoresistance’ manganites in which orbitally degenerate electrons are coupled to Jahn-Teller (JT) phonons via the second term in Eq. (4) and also feel both a Hubbard-U and a ‘double-exchange’ interaction arising from a strong coupling to core spins (i.e., the
model defined in Ref. 3 but with a Hubbard-U added). The $U$ is seen to enhance the effect of JT phonons. Fig. 2 shows that for the Hubbard model $\Gamma_3$ and $\Gamma_4$ are even more rapidly suppressed by $U$ so repulsive interactions effectively decouple electrons from scalar phonons.

The calculation is simplified and made more physically transparent if the action is viewed as a functional of the full electron propagator $G$ rather than as a functional of $\alpha$. The key object is then the ‘local Luttinger-Ward functional’ $\phi[G]$ defined as the sum of all vacuum-to-vacuum skeleton diagrams and related to the self-energy via $\Sigma = \delta \phi[G]/\delta G$. Within DMF theory, $\phi$ may be found from the local thermodynamic potential $\Omega_{\text{imp}} = -T \ln Z$ (see Refs. 13 and 28) so may be computed by an adiabatic expansion. We find $\phi[G] = \phi^{\text{el-ph}}[G] + \phi^{\text{ph}}[G] + O(\gamma^2)$ with $\phi^{\text{ph}}[G] = \frac{1}{2} \sum_k \ln D_k^{-1}$. Therefore

$$\Sigma_n^{\text{ph}} = -\frac{\lambda}{2} \sum_k D_k \frac{\delta \Gamma_2[G]_{k,-k}}{\delta G_n} + O(\gamma^2). \quad (6)$$

In general $\Gamma_2$ and thus $\delta \Gamma_2/\delta G$ vary on the scale of $t$ so $\Sigma_n^{\text{ph}} \sim \gamma$, an unimportant correction to the bare frequency or electron-electron contribution. However, if $\delta \Gamma/\delta G$ is singular at low frequencies, as in Fermi liquids, then $\delta \Sigma/\delta \omega$ may be of order unity. To investigate this we note that $\Gamma_2[G]_{k,-k} = -2t^2 \sum_n G_n G_{n+k} (1 + 2t \sum_n A_{n,n+k}^4 G_n G_{n+k}),$ where the particle-hole reducible vertex $\Lambda^R$ is given in terms of the particle-hole irreducible vertex $\Lambda^I$ via the Dyson equation shown in Fig. 3.

The standard analysis implies that $\Lambda^I$ is a smooth function of its arguments, so the required singular behavior can only occur if we differentiate on one of the explicit $G$ factors. Further, to $O(\gamma)$ we may neglect the frequency dependence of the vertices leading to

$$\Sigma_n^{\text{ph}} = \lambda t \sum_k D_k G_{n+k} \Lambda^2 + \Sigma_n^{\text{ph,reg}} \quad (7)$$

with $\Sigma_n^{\text{ph,reg}}$ varying with $\omega_n$ on the scale of $t$ and

$$\Lambda = 1 + 2t \sum_n \Lambda_{0n}^R G_n^2 + O(\gamma). \quad (8)$$

If the ground state is a Fermi liquid then $G(\nu) = -i \pi \text{sign}(\nu) \rho(\mu) + G^{\text{inc}}$, where $G^{\text{inc}}$ is nonsingular at small frequencies [27]. The leading contribution in $\gamma$ to $m^*/m$ is then $m^*/m_{\text{ph}} = 1 + \lambda \rho(\mu) \Lambda^2 + O(\gamma)$, where $\lambda = \lambda/(1 - \Gamma_2)$. 

$\Lambda$ is a vertex function of the underlying electron-electron theory, determined in general by solving the vertex equation shown in Fig. 3. However, to the order to which we work it is simpler to note that in a Fermi liquid the leading low-frequency behavior of the density-density correlation function is $\chi(\omega) = \chi(0) + i A |\omega|$ with
\[ A = \Lambda^2 \partial \chi^0 / \partial \omega \text{ and } \chi^0_k = -2\tau T \sum_n G_n G_{n+k} \] is the function obtained by convolving two exact Green functions with no vertex corrections. Thus

\[ \Lambda^2 = \frac{\partial \chi_k / \partial (i\omega_k)|_{k=0}}{\partial \chi^0_k / \partial (i\omega_k)|_{k=0}}. \tag{9} \]

The right hand side of Eq. \eqref{eq:9} can be calculated numerically by QMC in the time domain because the leading long-time behavior comes from the first frequency derivative and is \( \chi(0 \ll \tau \ll \beta) = (\pi/\beta)\partial \chi_k / \partial (i\omega_k)|_{k=0}/\sin^2(\pi\tau/\beta) \). For \( \beta \gtrsim 4 \) we find \( \chi(\tau)/\chi^0(\tau) \) is very flat in the center region of the interval \((0, \beta)\) (see inset to Fig. \ref{fig:4}). The rapid decrease of \( \Lambda \) again shows that the electron-phonon mass enhancement and scattering rate are ‘turned off’ near half filling and for strong correlations, in disagreement with the authors of Ref. \cite{11} who found a weaker decrease in the matrix element, which was moreover cancelled by an increase in effective mass.

We summarize the main results of this paper. We have studied a general electron-phonon model in a new approach that combines the adiabatic expansion in \( \gamma \ll 1 \) of the conventional Migdal-Eliashberg theory with a dynamical mean-field treatment of electron correlations. Our main finding is an effective phonon action correct to \( O(\gamma^{N/2}) \) with static coefficients \( \Gamma_N \) \((N = 2, 3, 4)\) and vertex \( \Lambda \), which are easy to compute numerically for various models. For the Holstein-Hubbard model we have shown that the electron-phonon coupling is strongly suppressed by Hubbard-\( U \) effects in systems near Mott transitions. Extension of our results to other correlated systems such as heavy fermions would be worthwhile.

We thank S. Blawid for useful discussions, H. Monien and J. Freericks for critical reading of the manuscript, and NSF DMR00081075 and the University of Maryland/Rutgers MRSEC for support.
[26] U. Brandt and C. Mielsch, Z. Phys. 82, 37 (1991)

[27] M. J. Rozenberg, G. Kotliar, and X. Y. Zhang, Phys. Rev. B 49, 10181 (1994)