Path integral approach to the Anderson-Holstein model

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The Anderson-Holstein model is studied in the framework of the semiclassical approximation. Analytical results for the Kondo temperature renormalized by a weak electron-phonon interaction and for the phonon Green function are obtained, and they are interpreted from the viewpoint of dynamical mean field theory. In particular, the isotope effect of the effective electron mass is discussed in the presence of strong electron correlation. The results are also compared with those obtained by numerical renormalization group and other related work, and they are consistent with each other in their common domain of validity.

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I. INTRODUCTION

Both electron correlation and lattice dynamics are important in understanding the physical properties of many condensed matter systems.1 But the interplay between them has not been studied in detail owing to the lack of reliable calculation methods. Conceptually this problem is difficult to handle due to the absence of suitable expansion parameters.

Impurity problems have been relatively well studied compared to problems on the lattice, mainly because of diverse analytic and numerical nonperturbative techniques. With the recent advent of the dynamical mean field theory2 (DMFT) various lattice problems can be mapped (or approximated) to impurity problems. The mapping can be justified rigorously in the limit of infinite spatial dimensions. Once the mapping to a certain impurity problem is accomplished, the powerful techniques of impurity problems can be employed to understand lattice problems.

In the perspective of DMFT, the problem of the interplay between electron correlation and lattice dynamics can be mapped to an impurity problem with both electron and phonon degrees of freedom. One of the simplest models with both degrees of freedom is the Anderson-Holstein (AH) model.3 4 The AH model is a single-impurity Anderson model with a linear coupling to a local phonon mode as in the Holstein model.5

Our goal is to understand the physical properties of the AH model in the light of the interplay of electron correlation and lattice dynamics. Recently, the numerical renormalization group (NRG) method has been successfully applied to the AH model,3 4 and almost exact results on the electron and phonon spectral functions have been obtained. However, it is still desirable to develop an analytical scheme in spite of its approximate nature, since it helps us to understand the underlying physics in a more clear and intuitive way. Of course, a systematic analytical approach to a model like the AH model does not exist in general. But by restricting our focus to a certain parameter regime we can develop an approximation scheme which captures the essential features of the interplay between electron correlation and phonons. We will be mostly interested in the regime where the electron correlation effects are much stronger (large local Coulomb repulsion $U$) than the electron-phonon coupling. If the electron-phonon coupling is omitted (Anderson model) it is well known that the ground state is the Kondo singlet state. Our main focus is on understanding how the spin fluctuation processes responsible for the Kondo ground state are influenced by the weak electron-phonon interaction. We have developed a semiclassical approximation scheme in the context of the path integral approach where the spin fluctuations are represented by instantons (or kinks).6 9 In this scheme, phonons can be naturally incorporated and the features of interplay can be clearly exhibited.

The isotope effect is a suitable physical property for addressing the issue of the interplay of electron correlation and phonons. In conventional metals, where the Midal-Eliashberg (ME) theory7 of electron-phonon interaction applies, the isotope effect appears to be very small. This is because ME theory keeps only the diagrams of zeroth order in $\Omega/t$, where $\Omega$ is the phonon frequency and $t$ is the bandwidth of the conduction electron.8 The omission of diagrams of higher order in $\Omega/t$ is justified by the Migdal theorem on the electron-phonon vertex function, which is the key element of ME theory. Presumably the ME theory cannot be employed for systems with strong electron correlations since vertex corrections are not expected to be small for such systems in general. We can compute the isotope effect for strongly correlated systems by studying how the Kondo temperature of the impurity model is modified by (local) electron-phonon interactions [see Eq. (44)].

There is a caveat in directly translating the results obtained for the impurity model to those of the corresponding lattice model. The lattice model with a Lorentzian density of states (DOS) is formally identical with the impurity model since there is no need for solving a self-consistency relation. Thus for the lattice model with a Lorentzian DOS the results obtained for the impurity model can be directly applied. However, the Lorentzian DOS is not physical in many aspects, but it is expected to be valid for systems with a finite DOS at the Fermi surface.5 The constraint of a finite DOS at

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the Fermi surface restricts the applicability of our results to the metallic regime. For the lattice Hubbard model, this implies that the system should be away from half filling or $U_c > U > \pi \Delta$ at half filling (see Ref. 2 for details). In addition, our results are not relevant for insulating regimes such as the small polaron regime.\(^9\)

We point out that Deppeler and Millis addressed a similar issue using the adiabatic expansion of DMFT without assuming any specific ground state.\(^8\,10\) They identified a class of electron-phonon diagrams missed in previous studies but they treated electron correlations in the scheme of the Hartree-Fock approximation. Our approach treats the strong electron correlation more accurately; thus it provides more accurate electron correlation dependences of the physical properties.

In a single-band model without extra orbital degrees of freedom, the Holstein phonon interaction acts in the charge channel, while the electron correlation effect, represented by local Coulomb repulsion, acts via the spin channel at low energy. Due to this apparent “spin-charge separation,” the interplay of electron correlation and electron-phonon interaction first appears in the second order expansion with respect to the phonon field in our treatment. For a multiband model where the orbital degrees of freedom are active, the electron-phonon dynamics becomes much richer as exemplified by the phase diagrams of colossal magnetoresistance (CMR) materials.\(^1,11\) We have compared our results with those of the spin-polarized Jahn-Teller model studied in the context of CMR manganites.\(^12\) The only formal difference between the two models lies in the structure of the coupling of the phonon modes, but this difference brings about drastic differences in physical properties such as isotope effects.

Our main results are the following. (1) The electron-phonon interaction increases the Kondo energy scale in the regime of strong electron correlation. The explicit results are given in Eqs. (36) and (39). (2) The isotope effect of the effective electron mass is given by Eq. (44). (3) The phonon spectral function is computed in the fugacity expansion scheme, Eq. (56).

This paper is organized in the following way. In Sec. II we introduce the AH model and present it in a form suitable for semiclassical approximation. In Sec. III we develop an instanton expansion of the partition function and its renormalization group (RG) flow. In Sec. IV the phonon Green function is calculated in the fugacity expansion scheme. We conclude this paper in Sec. V with a discussion and summary. Some details of the calculations can be found in the Appendices.

II. FORMULATION

The AH model is defined by the following Hamiltonian:\(^3\)

\[
\mathcal{H}_{AH} = \mathcal{H}_{el} + \mathcal{H}_{ph} + \mathcal{H}_{el-ph},
\]

\[
\mathcal{H}_{el} = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + E_{j} \sum_{\sigma} f_{\sigma}^\dagger f_{\sigma} + U \sum_{\sigma\sigma'} f_{\sigma}^\dagger f_{\sigma}^\dagger f_{\sigma'} f_{\sigma'},
\]

\[
+ \sum_{k,\sigma} \frac{1}{N_{lat}} (V_{k\sigma} f_{\sigma}^\dagger c_{k\sigma} + V_{k\sigma}^* c_{k\sigma}^\dagger f_{\sigma}),
\]

where $\sigma = \uparrow, \downarrow$ is the spin index, and $V_{k\sigma}$ is the hybridization matrix element. $f_{\sigma}$ is the impurity electron operator, and $c_{k\sigma}$ is the conduction electron operator. $Q$ is the local phonon coordinate. $P$ is the conjugate momentum of $Q$ satisfying $[Q, P] = i\hbar$. $M$ is the ion mass and $\Omega$ is the oscillator frequency of dispersionless (Einstein) phonons. $N_{lat}$ is the number of lattice sites for the conduction electrons. We will consider the symmetric AH model specified by the relation $\epsilon_f + U/2 = 0$.

The conduction electrons $c_k$ can be integrated out exactly, yielding the local impurity action

\[
S_{imp} = -T \sum_{i,\sigma} f_{i\sigma}^\dagger G_0^{-1}(i\epsilon_f) f_{i\sigma} + \int_0^\beta d\tau U f_{i\sigma}^\dagger f_{i\sigma} + \int_0^\beta d\tau \left[ \frac{M}{2} (\partial_\tau Q)^2 + \frac{\hbar^2}{2} Q^2 + gQ(n - 1) \right],
\]

where $n_{\sigma} = f_{i\sigma}^\dagger f_{i\sigma}$, $n = n_{\uparrow} + n_{\downarrow}$, and

\[
G_0^{-1}(i\epsilon_f) = i\epsilon_f - \Sigma(i\epsilon), \quad \Sigma(i\epsilon) = \frac{1}{N_{lat}} \sum_k \frac{|V_k|^2}{i\epsilon + \mu - \epsilon_k}.
\]

For the hybridization matrix elements weakly dependent on momentum near the Fermi surface, $G_0^{-1}(i\epsilon_f)$ can be approximated by

\[
G_0^{-1}(i\epsilon_f) = i\epsilon_f - \epsilon_f + i\Delta \sigma\text{sgn}(\epsilon),
\]

where $\Delta$ is the hybridization energy scale

\[
\Delta = \pi |\langle V_k |^2 \delta(\omega - \epsilon_k) \rangle_{av}|.
\]

The average is done on the Fermi surface of the conduction electron. We are interested in the strongly correlated regime $U \gg \Delta$. The charge fluctuations at an energy scale of order $U/\Delta$ can be neglected in considering the low energy physics. To separate out the charge fluctuations at high energy it is convenient to introduce the Hubbard-Stratonovich (HS) transformation for the Hubbard $U$ interaction. Two HS fields $\phi_c$ and $\phi_s$ are introduced to decouple the on-site repulsion $U$ into charge and spin channels, respectively.

\[
e^{-U n_1 n_\downarrow} = e^{-U(n_\uparrow^2 - n_\downarrow^2)/4}.
\]

\[
= \int D[\phi_c, \phi_s] \exp \left[ -\frac{\phi_c^2}{U} - \frac{\phi_s^2}{U} + i\phi_c n + i\phi_s S_z \right].
\]

$S_z = n_\uparrow - n_\downarrow$ is the $z$ component of the impurity spin. Then we choose the mean value of the charge HS field $\phi_c$ which can be absorbed into $G_0^{-1}(i\epsilon_f)$ (canceling $-\epsilon_f$) and neglect its high energy fluctuations.\(^3\) Then the electron-electron interaction (valid only at low energy) acts only in the spin
channel, while the phonon couples only in the charge channel. Consequently, in the leading approximation, electron-electron interaction and electron-phonon interaction seem to decouple; however, the interplay can be seen from the second order in the expansion with respect to the phonon fields (see below).

The resulting local action in imaginary time is

\[ S_{\text{imp}} = -\int d\tau d\tau' \sum_{\sigma} f_\sigma^d(\tau') G_0^{-1}(\tau' - \tau) f_\sigma(\tau) \]
\[ + \int d\tau \left[ \frac{1}{U} \partial^2_\tau - \phi_\sigma(n_1 - n_{\bar{1}}) + gQ(n_1 + n_{\bar{1}} - 1) \right] \]
\[ + \frac{M}{2} (\partial_\tau \phi_\sigma)^2 + \frac{M \Omega^2}{2} \phi_\sigma^2 \].

The bare Green function \( G_0(\tau' - \tau) \) is given by

\[ G_0(\tau' - \tau) = T \sum_{i \omega_n} e^{-i \omega_n (\tau' - \tau)} \] (10).

The impurity electron \( f \) can be integrated out exactly for an action of the type of Eq. (10):

\[ Z = \int D[f, \phi_\sigma, Q] e^{-S_{\text{imp}}} = \int D[\phi_\sigma, Q] e^{-S[\phi_\sigma, Q]}, \]

where \( S = S_p + S_K \) is given by

\[ S_p = \int_0^\beta d\tau \left[ \frac{\phi_\sigma^2}{U} + \frac{M}{2} \Omega^2 Q^2 \right] \]
\[ + \sum_\sigma \frac{\Delta}{\pi} \left[ -\xi_\sigma \tan^{-1} \xi_\sigma + \frac{1}{2} \ln \left( 1 + \xi_\sigma^2 \right) \right] \].

\[ S_K = \int_0^\beta d\tau \frac{M}{2} (\partial_\tau \phi_\sigma)^2 + \sum_\sigma \frac{1}{2 \pi^2} P \int_0^\beta d\tau d\tau' \frac{\partial_\tau \phi_\sigma(\tau')}{\partial_\tau' \phi_\sigma(\tau)} \]
\[ \times \frac{1}{\xi_\sigma^2(\tau') - \xi_\sigma^2(\tau)} \ln \left( 1 + \xi_\sigma^2(\tau) \right) + \frac{1}{\xi_\sigma^2(\tau) - \xi_\sigma^2(\tau')}, \] (13)

where \( \xi_\sigma(\tau) = [-\sigma \phi_\sigma(\tau) + gQ(\tau)]/\Delta \). \( S_p \) and \( S_K \) are the potential and the kinetic terms, respectively. It is convenient to define an energy scale \( E_L \) associated with lattice relaxation (or equivalently polaron energy):

\[ E_L = \frac{g^2}{2M \Omega^2}. \]

(15)

Following Refs. 8 and 10 we define dimensionless variables

\[ X = \frac{\phi_\sigma}{\Delta}, \quad Y = \frac{gQ}{\Delta}, \quad u = \frac{U}{\Delta}, \quad \lambda = \frac{E_L}{\Delta}, \quad \gamma = \frac{\Omega}{\Delta}. \]

(16)

To develop the semiclassical approximation we first need to locate the classical minima of the potential term \( S_p \). When \( u \gg \lambda \) and \( u \gg \pi \), \( S_p \) has two degenerate minima \((X^*, Y^*) = (\pm \eta_0, 0)\), where \( \eta_0 \sim u/2 \). We also assume \( \gamma \ll 1 \), even though the adiabatic expansion is not systematically employed in our study. Our main interest resides in the case with strong electron correlation and weak electron-phonon interaction. Accordingly, we restrict our attention to the regime \( u \gg 1 \gg \lambda \), so that the phonon part can be treated perturbatively.

There can exist other minima in the regime \( \lambda \gg u \). This regime is essentially similar to the original Holstein model and has been studied in Ref. 13 in the semiclassical approximation scheme. Since we have treated the charged HS field \( \phi_\sigma \), which couples to charged density like phonons, only in a mean field approximation, our present approach does not apply to the regime \( \lambda \gg u \). Furthermore, the polaron state that is likely to occur in the regime \( \lambda \gg u \) cannot be described within the DMFT scheme with a Lorentzian DOS.

The quantum tunnelings between two minima \((X^*, Y^*) = (\pm \eta_0, 0)\) are nothing but the spin flip processes in the path integral framework.6,13 The tunneling amplitude is determined by the kinetic term \( S_K \). The key is to understand how the presence of weak electron-phonon interaction influences the spin flip processes which are responsible for strongly correlated states. To this end we integrate out the phonon field \( Y \) in the second order. There are no parts linear in \( Y \). They vanish upon spin summation. This integration over the phonon field is justified since the phonon field has a trivial minimum at the origin, so that we can employ the harmonic approximation at low energy. Concretely, we have to expand the action Eqs. (13) and (14) as a power series in \( Y \) up to the second order. The action \( S = S_p + S_K \) expanded in \( Y \) can be written as

\[ S \approx S_X + S_Y + S_{XY}. \] (17)

\( S_X \) is just the action Eqs. (13), (14) with \( Q = 0 \), and it is the starting point of Hamann’s original analysis.6

\[ S_X = \frac{P}{\pi^2} \int_0^\beta \frac{d\tau d\tau'}{\tau - \tau'} \left[ \frac{X(\tau)}{d\tau} \frac{dX(\tau')}{d\tau'} \right] \]
\[ \times \ln \left[ \frac{[1 + X^2(\tau)]/[1 + X^2(\tau')]}{X^2(\tau) - X^2(\tau')} \right] \]
\[ + \int_0^\beta d\tau \left[ \frac{X^2}{u} + \frac{2}{\pi} \left( -X \tan^{-1} X + \frac{1}{2} \ln [1 + X^2] \right) \right]. \]

(18)

\( S_Y \) is the phonon part of Eq. (10) written in terms of \( Y \):

\[ S_Y = \int_0^\beta d\tau \left[ \frac{1}{4 \Delta \lambda} \left( \frac{dY}{d\tau} \right)^2 + \frac{\Delta}{4 \lambda} Y^2(\tau) \right]. \] (19)

\( S_{XY} \) embodies the interplay of spin fluctuation and the electron-phonon interaction, and has a very complicated structure. The explicit expressions for the terms of \( S_{XY} \) are listed in Appendix A. A typical term of \( S_{XY} \) looks as follows:
We note two new terms coming from \( S_{XY} \) in \( S_{ph} \). From the action \( S_{ph} \) in Eq. (22), the phonon propagator in the absence of instantons is easily obtained:

\[
\langle Y(i\omega)Y(-i\omega) \rangle_{N=0} = \left( \frac{g^2}{\Delta} \right)^2 \left[ \frac{1}{|\omega|^2 + E^*|\omega| + \omega_0^2} \right]^{M-1}.
\]  

where (the condition \( \eta_0 \ll 1 \) is used)
where  

\[ \lambda = \frac{g^2}{2M \omega_0 \Delta} \]  

(31)

The corrections in Eqs. (28) and (30) \([\lambda \gamma / 2 \eta_0]\) reveal the expansion parameters as noted by Deppeler and Millis.\(^\text{10}\) The influences of phonons are reflected in the \(K_2\) term of the energy \(V(t_i)\) and in the change of initial values from those without phonons. The most drastic difference of the \(K_2\) term from \(K_1\) is the absence of the alternating factor \((-1)^{y-l}\). This absence of the alternating factor indirectly demonstrates the fact that the phonon interacts with the electron via the charge channel not the spin channel.

The renormalization group equation (RGE) of the instanton gas Eq. (25) can be derived by following the procedure of Ref. 14 (for details, see Appendix B):

\[ \frac{dx}{dl} = x \left[ 1 - \frac{K_1}{2} + 2x^2 K_2 g_2 \right], \]  

(32)

\[ \frac{dK_1}{dl} = -4K_1x^2, \quad \frac{dK_2}{dl} = 0, \]  

(33)

where \(dl = d\tau_0 / \tau_0\), \(x = z \tau_0\). \(g_2\) is defined in Eq. (B10). At the present level of approximation the influence of phonon coupling is manifest only in the renormalization of the fugacity \(x\). For the sake of comparison with the original Kondo model, it is convenient to introduce a new variable \(y = 2 - K_1\). The initial value of \(y\) is smaller than 1 as can be seen in Eq. (28). Using the result Eq. (B14), the RGE’s (32) and (33) can be reexpressed as

\[ \frac{dx}{dl} = \frac{x}{2} \left[ y + x^2 \alpha e^{-\omega_0 \tau_0} \right], \]  

\[ \frac{dy}{dl} = 8x^2 - 4yx^2 - 8x^2, \quad \frac{dK_2}{dl} = 0. \]  

(34)

\(\alpha\) is defined in Eq. (24). Since the phonons have been treated perturbatively from the outset we are not far from the original Kondo physics, which does not have phonons. Thus, even if the SU(2) spin symmetry is not manifest in our approximate RGE, we can trace the isotropic ray \(y = 4x\) of Eq. (34) in approaching the strong coupling regime. Due to the presence of the explicit energy scale \(\omega_0\) in Eq. (34), two energy scales \(T_K^{(0)}\), \(\omega_0\) should be taken into account in the analysis of Eq. (34). \(T_K^{(0)} \sim D e^{-\omega_0 / \Delta}\) is the Kondo temperature in the absence of phonons. \(D\) is an energy cutoff.

First consider the case of \(\omega_0 \ll T_K^{(0)}\). Then the scaling should stop near \(l_K = \ln (D / T_K^{(0)}) \approx \ln (D / \omega_0) = l_{\omega_0}\). This is because beyond \(l_K\) the RG flow begins to enter the strong coupling regime where our perturbative scaling equations do not apply. In this region of \(l < l_K\), \(e^{-\omega_0 \tau_0} \approx 1\) holds. Integrating the RG equation until \(x\) becomes of order unity we obtain

\[ T_K \sim D e^{\lambda / 2(0)} \times e^{\lambda / \omega_0 \tau_0} \approx T_K^{(0)} e^{\lambda / 2 \omega_0 \tau_0} \left( 1 + \alpha \ln \eta_0 / 8 \right). \]  

(35)

According to the result Eq. (35) the electron-phonon interaction increases the Kondo energy scale, and this is in agreement with the results of NRG studies.\(^\text{34}\) The amount of increase is given by

\[ \delta T_K \sim \left( \frac{\lambda}{2 \eta_0} + \frac{\alpha}{8} \ln \eta_0 \right) T_K^{(0)}. \]  

(36)

Second, consider the case of \(T_K^{(0)} \ll \omega_0\). In this case, the RG flow evolves until \(l = l_{\omega_0} = \ln (D / \omega_0)\), and then the second term of \(dx / dl\) in Eq. (34) becomes completely negligible beyond \(l_{\omega_0}\). In the region \(l > l_{\omega_0}\), \(x(l_{\omega_0})\) plays the role of a new initial value. Integrating the RG equation starting from \(l = l_{\omega_0}\) until \(x\) becomes of the order of unity, we obtain the Kondo temperature for the second case.

\[ T_K \sim \omega_0 e^{-1/2(\omega_0 / \gamma_0)}. \]  

(37)

The direct evaluation of \(x(l_{\omega_0})\) gives

\[ T_K \sim \left( \frac{\lambda}{2 \eta_0} + \frac{\alpha}{2 \eta_0} \ln \frac{1}{\gamma_0} \right) T_K^{(0)}. \]  

(39)

Note that the results Eqs. (35) and (38) are obtained in the regime of strong electron correlation where ME theory does not apply. Both results Eqs. (35) and (38) show that the electron-phonon interaction increases the Kondo temperature but by rather a small amount. The increase of Kondo temperature can be heuristically understood in the somewhat unphysical adiabatic limit \(\Omega \gg \Delta\) [see Eqs. (61) and (62)]. This point will be elaborated further in Sec. V. In the adiabatic limit the retardation effects of phonons are negligible. Our results for the Kondo temperature are valid for strong electron correlation and fully incorporate the retardation effects of phonons.

The results Eqs. (35) and (38), can be interpreted in the light of a lattice system within the context of DMFT. The Kondo singlet state of the impurity problem corresponds to the Fermi liquid in the original (large-\(d\)) lattice system (see Sec. VII of Ref. 2). Here the momentum dependence of the electron self-energy is neglected, and the effect of correlation is encapsulated in the wave-function renormalization \(Z\):

\[ Z(z) = 1 - \frac{\partial \Sigma(z)}{\partial z} \bigg|_{z = -i\omega}, \]  

(40)

which gives the residue of the quasiparticle. \(Z\) is related to the mass enhancements of quasiparticles as

\[ Z^{-1} = m_b / m_b, \]  

where \(m_b\) is the bare mass and \(m_b\) is the effective mass given by band theory. The Kondo temperature itself can be identified with the effective bandwidth \(B_{eff}\) of the lattice system. Then the mass enhancement can be estimated to be
where $m^* = m_b \sim D/T_K$. 

\[ Z^{-1} = m^* / m_b \sim D / T_K. \]  

(42)

$D$ is of the order of half the bandwidth. In the DMFT with Lorentzian DOS it can be identified with $\Delta$. The above estimate follows from the observation $B_{eff} \sim \frac{p_F}{m^*}$, $D \sim \frac{p_F^2}{m}$. $p_F$ is the Fermi momentum. Combining Eq. (42) with our results Eqs. (35), (38), the issue of the isotope effect on the mass enhancement can be addressed. The ratio of mass enhancements in the presence and absence of phonons is given by

\[ \frac{m^*/m}{m^*/m_b} \sim \frac{T_{K0}}{T_K} \sim 1 - \delta T_K / T_{K0}. \]

(43)

where $m^*/m_b$ is the effective mass in the presence of phonons. Thus, the isotope effect is negative in that the electron-phonon interaction which depends on ion masses decreases the effective mass of electrons. This isotope effect manifests itself in the specific heat coefficient, the $T^2$ coefficient of low temperature resistivity, the Drude weight of optical conductivity, and in other physical quantities which depend on the effective bandwidth $B_{eff}$ in a crucial way. Our results show that the isotope effect is very small in the regime of strong electron correlation:

\[ \frac{m^*/m}{m^*/m_b} \sim 1 - E_L \Delta / U^2. \]

(44)

The proof of Eq. (44) is beyond the validity of ME theory, however.

IV. PHONON CORRELATION FUNCTION

The phonon correlation function is defined by

\[ D(t-t') = \int D[X,Y] e^{-S} Y(t) Y(t') / D[X,Y] e^{-S}. \]

(45)

The correlation function of the original phonon coordinate $Q$ is related to Eq. (45) by

\[ \langle Q(t) Q(t') \rangle = \left( \frac{\Delta}{8} \right)^2 D(t-t'). \]

(46)

The denominator of the right hand side of Eq. (45) is just the partition function studied in the previous section and will be written as $Z = Z_0 (Z / Z_0)$.

We will compute the phonon correlation function in the framework of the fugacity expansion. The phonon correlation function in the absence of the instanton is given by Eq. (23). As discussed in Sec. III, the fugacity is relevant at low energy; thus our result for the phonon correlation is expected to be valid only in the high frequency/temperature regime ($|\omega| / T > T_K$).

The first nontrivial contribution comes from the trajectories with an instanton–anti-instanton pair. We rewrite Eq. (45) as

\[ D(t-t') = \frac{Z_{ph}^{-1} \int D[X,Y] e^{-S + S[\eta_0]} Y(t) Y(t')} {Z / Z_0}. \]

(47)

where $Z_{ph} = \int D[Y] e^{-S_{ph}[Y]}$ [see Eq. (22)]. Let us write the exponent of Eq. (47) in the form

\[ - S + S_X[\eta_0] = - S_{ph} - \delta S_X - \delta S_{XY}, \]

(48)

where

\[ \delta S_X = S_X[X] - S_X[X = \eta_0], \]

\[ \delta S_{XY} = S_{XY}[X,Y] - S_{XY}[X = \eta_0,Y]. \]

(49)

By construction $\delta S_X$ and $\delta S_{XY}$ vanish in the absence of instantons. Now the structure of the fugacity expansion is manifest in the form of Eq. (47):

\[ D(t-t') = D_0(t-t') + D_2(t-t') + \cdots, \]

(50)

where $D_n$ is proportional to $\zeta^n$. Since we are interested in only the connected diagrams, we have to select the connected components among the contributions to $D_2(t-t')$.

The structure of $\delta S_{XY}$ is very complicated, and a typical term (which, in fact, will give the most dominant contribution) looks like

\[ \delta S_{XY,2} = - \frac{1}{\pi^2} \int d\tau d\tau' \ln |\tau - \tau'| \dot{Y}(\tau) \dot{Y}(\tau') \]

\[ \times \int_0^1 d\xi \left[ \frac{1}{1 + \xi X^2(\tau)} \frac{1}{1 + \xi X^2(\tau')} - \frac{1}{(1 + \xi \eta_0^2)^2} \right] \]

\[ + \frac{1}{\pi^2} \int d\tau d\tau' \ln |\tau - \tau'| \dot{Y}(\tau) \dot{Y}(\tau') \]

\[ \times \int_0^1 d\xi \left[ \frac{2 \xi X^2(\tau)}{(1 + \xi X^2(\tau))^2[1 + \xi X^2(\tau')]} \right] \]

\[ - \frac{2 \xi \eta_0^2}{(1 + \xi \eta_0^2)^3}. \]

(51)

Next we need to evaluate the actions $\delta S_X$ and $\delta S_{XY}$ in the subspace of two instantons which are parametrized by their locations $t_1, t_2$. Then the connected component of $D_2(\tau - \tau')$ can be written

\[ D_2(t-t') = \frac{\zeta^2}{Z_{ph}} \int D[Y] e^{-S_{ph}} \int_{t_2}^{t_1} dt_2 \]

\[ \times \int_{t_2}^{t_2 - \tau_0} dt_1 \exp \left( - K_1 \ln \frac{t_2 - t_1}{\tau_0} \right) \]

\[ \times e^{-\delta S_{XY}(t_1,t_2)} Y(t) Y(t'). \]

(52)

We will treat $\delta S_{XY}(t_1,t_2)$ perturbatively as in the evaluation of the partition function. In the expansion $e^{-\delta S_{XY}} = 1 - \delta S_{XY} + \cdots$, the first term cancels the disconnected piece coming from the denominator $Z / Z_0$. Among various contri-
butions to $D_2(t-t')$, the term containing two time derivatives of $Y, \delta S_{XY,2}$, gives the most dominant one. The calculation of $D_2(t-t')$ can be cast into the following form:

$$D_2(t-t') = D_0(t-t') + \int dt_1 dt_2 D_0(t-t_1) \times \Sigma(t_1-t_2) D_0(t_2-t').$$

(53)

The function $\Sigma(t_1-t_2)$ plays the role of the self-energy. The explicit form of the self-energy is

$$\Sigma(t_1-t_2) \sim z^2 \frac{\alpha^2}{\eta_0} \ln \left( 1 \right)$$

(54)

In frequency space it becomes

$$\Sigma(i\omega) \sim z^2 \frac{\alpha^2}{\eta_0} |\omega|^{\xi_{1-1}} \ln \left( 1/|\omega| \right).$$

(55)

Thus the phonon correlation function, which is accurate up to the second order of $z^2$, is

$$D(i\omega) = \frac{2\lambda \gamma^2 \Delta}{\omega^2 + E^*|\omega| + \omega_0^2 + z^2 \gamma^2 E^*|\omega|^{1-1}} \ln \left( 1/|\omega| \right).$$

(56)

Apparently the self-energy term behaves as if very singular at low energy, but we have to keep in mind that Eq. (56) was derived in the high temperature/frequency regime $(|\omega|/T) > T_K$.

Let us compare our results with those obtained by NRG. The NRG calculation of the phonon Green function by Hewson and Meyer was improved in Ref. 4. The imaginary part of the phonon Green function in the regime of large $U$ has the following features: (1) a decrease of phonon frequency with increasing phonon coupling, (2) a broadened phonon peak, and (3) the absence of a peak near zero frequency. These features are consistent with our results. First, the renormalized phonon frequency

$$\omega_0 \sim \Omega \left( 1 - \frac{2}{\pi} \frac{E_L \Delta}{U^2} \right)$$

(57)

clearly shows the decrease of phonon frequency with increasing $\lambda$.

This result can be compared with that derived in the weak coupling random phase approximation (RPA) type perturbative calculation.

$$\omega_0 \sim \Omega \left( 1 - \frac{E_L}{\pi \Delta} \right).$$

(58)

Second, the renormalization of the phonon propagator can be reliably discussed if the energy scale of interest is larger than the Kondo temperature. If $\omega_0 \approx T_K$ our result for the phonon Green function can be applied in the neighborhood of $\omega_0$. The broadening is basically determined by the energy scale $E^*$, which increases with increasing electron-phonon coupling. This feature is also consistent with the NRG result. In the perturbative RPA approach, the broadening width is predicted to be linear in $\omega$ while our results predict a sublinear dependence of width $\omega^{1-1}$, which is stronger at low energy. Notice that the anomalous self-energy term represents strongly temperature dependent broadening since it originates from the electronic processes happening near the Fermi energy. This feature can be checked in principle by a NRG calculation at finite temperature.

V. DISCUSSION AND SUMMARY

Antidiabatic limit

Our results can be compared with those obtained in the antidiabatic limit. In fact, the antidiabatic limit is relevant to rather few materials, but theoretically it provides a convenient benchmark. The antidiabatic limit can be easily taken by integrating out phonons. The integration results in an effective retarded and attractive interaction between electrons:

$$S_{ee, eff} = - \int d\tau d\tau' \frac{g^2}{2M} \left[ T \sum_{n} \frac{e^{-i\omega(l-\tau')}}{\omega^2 + \Omega^2} \right] n(\tau - 1)$$

(59)

$$\times [n(\tau') - 1].$$

If the phonon frequency $\Omega$ is larger than the typical electronic energy scale such as $\Delta$, then the frequency dependence in the denominator of $e^{-i\omega(l-\tau')/(\omega^2 + \Omega^2)}$ can be neglected. The summation over frequency gives a $\delta$ function in imaginary time, and Eq. (59) becomes

$$S_{ee, eff} = - 2 E_L \int d\tau n_{1+1}, \Omega \gg \Delta.$$  

(60)

Now $S_{ee, eff}$ can be combined with the on-site Coulomb repulsion $U$ term, leading to

$$U_{eff} = U - 2 E_L.$$  

(61)

Note that this effective Anderson model is valid only in the limit $U \gg \Delta$. In our regime of interest $U \gg E_L$, $U_{eff}$ is sufficiently large that the physics in the Kondo regime applies. One can expect a qualitative change of behavior if $U_{eff} = U - 2 E_L$ becomes negative. This is indeed confirmed by NRG studies. The treatment is not applicable to those regimes, and the polaron physics describes the regime adequately. The Kondo temperature of this effective Anderson model in the limit $U \gg E_L$ is given by

$$T_{K, eff} \sim \sqrt{\frac{U_{eff} \Delta}{2}} \exp \left[ \frac{-\pi U_{eff}}{8 \Delta} \right].$$

(62)

The change of Kondo temperature due to electron-phonon interaction is given by

$$\delta T_{K, eff} \sim T_K^{(0)} \left( \frac{\pi}{4} \frac{\lambda}{\Delta} - \frac{\lambda}{u} \right).$$

(63)
in the limit of small $\lambda$. Equation (63) appears to be much larger than Eqs. (36) and (39). This also demonstrates that the physics in our regime is essentially different from that of the antiadiabatic limit.

**Adiabatic expansion**

Deppeler and Millis studied the problem of electron-phonon interactions in correlated systems using an adiabatic expansion of DMFT without any specific ground state being assumed.\(^8,^{10}\) They obtained the phonon Green function

$$D^{-1}(i\omega) = 1 - \frac{\lambda}{\lambda_c} + \omega^2 + \lambda \gamma \alpha_p |\omega| + o(\gamma^2). \quad (64)$$

The factor $1 - \lambda/\lambda_c$ represents the softening of phonon frequency in our notation. At half filling and in the Hartree-Fock approximation, they obtained $\lambda_c \approx 1/\mu^3$, while our result is $\lambda_c \approx 1/\mu^2$. This is not a real contradiction since our result does not apply to the half-filling case in the limit of large $U$. They also identified the renormalized expansion parameters

$$\tilde{\gamma} = \gamma(1 - \lambda/\lambda_c)^{1/2}, \quad \tilde{\lambda} = \frac{\lambda}{1 - \lambda/\lambda_c}, \quad (65)$$

which coincide with our results. In this regime, we obtain the expansion parameters through

$$\int \frac{d\omega}{2\pi} (Y(-i\omega)Y(+i\omega))_{\nu=0} = \frac{1}{2}\tilde{\gamma}/\tilde{\lambda}. \quad (66)$$

In Ref. 8 the isotope effect on the effective electron mass was investigated. Away from half filling and in the absence of strong electron correlation with a semicircular DOS they authors obtained a positive mass enhancement which increases with decreasing phonon frequency and decreases with increasing $\tilde{\lambda}$. This should also be compared with our negative mass enhancement [see Eq. (44)], where the strong electron correlation plays an essential role.

**Role of the orbital degrees of freedom**

It should be pointed out that our results depend very crucially on the detailed structure of the electron-phonon coupling. We wish to illustrate this point by an example from a DMFT study on CMR manganese oxides in the metallic regime, such as La$_{0.7}$Sr$_{0.3}$MnO$_3$.\(^{11,12}\) The local action of this system is

$$S_{imp} = -\int d\tau d\tau' \sum_{\sigma} f_{\sigma}^{\dagger}(\tau') G^{-1}_0(\tau' - \tau)f_{\sigma}(\tau)$$

$$+ \int d\tau \left[ \frac{1}{U} \phi_x^2 - \phi_x(n_{\uparrow} - n_{\downarrow}) + gQ(n_{\uparrow} - n_{\downarrow}) \right]$$

$$+ M \left( \frac{\partial_t Q}{} + \frac{M\Omega^2}{2} \right). \quad (67)$$

In this system the real spin is fully polarized, and the index $\sigma$ denotes the orbital degrees of freedom of the $d$ band. $\uparrow$

$= d_{x^2-y^2} \propto d_{3z^2-r^2}$. Here $Q$ is one of the Jahn-Teller phonons (the third component). In spite of the similarity of the local action Eq. (67) with Eq. (10) except for the difference in the electron-phonon coupling, the outcomes are drastically different. For the model Eq. (67), the phonon frequency is hard-ened $\omega_0 = \sqrt{\frac{U + 4E_L}{U}}$, and the Kondo temperature decreases as follows:

$$T_K \sim \frac{1}{\Delta} \exp \left[ - \frac{U + 4E_L}{\Delta} \right], \quad R \gg 1. \quad (68)$$

The reduction factor $R$ is related to the overlap of the phonon wave functions in the process of instanton tunneling. In fact, the major results are just opposite to ours. This indicates that the orbital degrees of freedom, being associated with diverse forms of coupling with electrons, exhibit rather rich physics.

**Summary**

We studied the AH model in the framework of the semiclassical approximation, and interpreted the results in the light of DMFT. We obtained analytical results for the Kondo temperature, which are renormalized by weak electron-phonon interaction, and for the phonon Green function, which are valid at frequencies higher than Kondo temperature. We compared our results with the existing NRG results and other related work, and they are consistent with each other in their common regime of validity.

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**APPENDIX A: THE DETAILED FORM OF $S_{XY}$**

In this section we exhibit all the terms comprising $S_{XY}$. The expansion of the action as a power series in $Y$ is facilitated by utilizing the following parametric integral:

$$I_0 = \int_0^1 \frac{\xi}{\xi^2 + 1 + \xi^2 \xi^2} \frac{d\xi}{\xi^2 + 1 + \xi^2 \xi^2}$$

$$= \frac{1}{\xi^2 \xi^2} \ln \frac{1 + \xi^2 \xi^2}{1 + \xi^2 \xi^2}. \quad (A1)$$

$S_{XY}$ consists of ten terms which are numbered as $S_{XY,i}$, $i=1, \ldots, 10$. Every term contains two time derivatives except for $S_{XY,1}$:

$$S_{XY,1} = -\frac{\Delta}{\pi} \frac{1}{1 + X^2(\tau)}. \quad (A2)$$
\[ S_{XY,2} = -\frac{1}{\pi^2} \int d\tau d\tau' \ln |\tau - \tau'| \bar{Y}(\tau) \bar{Y}(\tau') \]
\[ \times \left( \int_0^1 d\xi \left[ \frac{1}{1 + \xi X^2(\tau)} + \frac{1}{1 + \xi X^2(\tau')} - \frac{1}{1 + \xi \eta_0^2} \right] \right) \]

\[ S_{XY,3} = -\frac{1}{\pi^2} \int d\tau d\tau' \ln |\tau - \tau'| \bar{X}(\tau) \bar{X}(\tau') \]
\[ \times \left( \int_0^1 d\xi \left[ \frac{2\xi X^2(\tau)}{[1 + \xi X^2(\tau)]^2} - \frac{2\xi \eta_0^2}{(1 + \xi \eta_0^2)^3} \right] \right) \]

\[ S_{XY,4} = -\frac{1}{\pi^2} \int d\tau d\tau' \ln |\tau - \tau'| \bar{X}(\tau) X(\tau) \]
\[ \times \left[ \int_0^1 d\xi \frac{d}{d\tau} \left( \frac{3X^2(\tau)\xi^2 - \xi}{[1 + \xi X^2(\tau)]^3} \right) \frac{Y^2(\tau)}{[1 + \xi X^2(\tau')]} \right] \]
\[ + \int_0^1 d\xi \frac{d}{d\tau} \left( \frac{1}{1 + \xi X^2(\tau)} \right) \left( 3X^2(\tau)\xi^2 - \xi \right) Y^2(\tau') \]
\[ + \int_0^1 d\xi \frac{d}{d\tau} \left( \frac{4\xi X(\tau)X(\tau')Y(\tau)Y(\tau')}{[1 + \xi X^2(\tau)]^2 [1 + \xi X^2(\tau')]^2} \right) \]

\[ S_{XY,5} = -\frac{1}{\pi^2} \int d\tau d\tau' \ln |\tau - \tau'| \bar{X}(\tau') Y(\tau) \]
\[ \times \left[ \int_0^1 d\xi \frac{d}{d\tau} \left( \frac{X(\tau)}{[1 + \xi X^2(\tau)]^2} \right) \frac{Y(\tau)}{[1 + \xi X^2(\tau')]} \right] \]
\[ + \int_0^1 d\xi \frac{d}{d\tau} \left( \frac{1}{1 + \xi X^2(\tau)} \right) X(\tau') Y(\tau') \]

**APPENDIX B: DERIVATION OF RG EQUATIONS**

We will closely follow the original work by Anderson, Yuval, and Hamann,\(^\text{14}\) so that only the major steps will be described below. First, the trajectories with instanton--anti-instanton pairs in the interval \([\tau_0, \tau_0 + d\tau_0]\) are to be integrated out. Let \(dZ\) be the part of the partition function containing only one close pair. The trajectories containing two or more pairs are accompanied by a factor of \((d\tau_0)^2\) and are neglected in our (essentially one-loop) approximation:
\[ \delta Z = \prod_i \left[ 1 + z^2 \int_{t_i+1-\tau_0}^{t_i+\tau_0} dt' \int_{t_i}^{t_i-\tau_0} dt'' \times \exp \left[ \delta V(t' - t_1, \ldots, t' - t_n) \right] \right]. \]  

(B1)

\( t', t'' \) denote the locations of the close pair. Writing out the exponent \( V \) in detail,

\[ \delta V = K_1 \sum_j (-)^{i+j} \ln \left| \frac{t'' - t_j}{\tau_0} \right| + K_2 \sum_j (-)^{i+j+2} \ln \left| \frac{t' - t_j}{\tau_0} \right| \]

\[ + K_2 \sum_j \ln \left| \frac{t' - t_j}{\tau_0} \right| d(t' - t_j) + K_2 \sum_j \ln \left| \frac{t'' - t_j}{\tau_0} \right| d(t'' - t_j) \]

(B2)

The last line of Eq. (B2) can be neglected since \( t' - t'' \) is of the order of the cutoff \( \tau_0 \). The most important difference between the \( K_1 \) part and the \( K_2 \) part of Eq. (B2) is the absence of an alternating sign factor in the \( K_2 \) part. With the mean value theorem applied for the integration over \( t'' \) of Eq. (B1), one can effectively impose the relation \( t'' = t' - \tau_0 \) in other parts of the integrand, and then one factor of \( d \tau_0 \) is multiplied. Now the exponent \( V \) becomes

\[ \delta V = K_1 \sum_j (-)^{i+j} \ln \left| \frac{t' - t_j}{\tau_0} \right| - \ln \left| \frac{t' - \tau_0 - t_j}{\tau_0} \right| \]

\[ + K_2 \sum_j \ln \left| \frac{t' - t_j}{\tau_0} \right| d(t' - t_j) \]

\[ + \ln \left| \frac{t' - \tau_0 - t_j}{\tau_0} \right| d(t' - \tau_0 - t_j) \]. \]

(B3)

We proceed by expanding \( e^{\delta V} \sim 1 + \delta V \). The Taylor expansion of the second term of the \( K_2 \) part of Eq. (B3) with respect to \( \tau_0 \) gives

\[ \sum_j \int dt' \partial_{\tau_0} d(t' - t_j) = \sum_j \left[ d(t_{i+1} - t_j) - d(t_i - t_j) \right], \]

which vanishes upon the summation over \( i \) of the following approximation:

\[ \prod_i \left[ 1 + d \tau_0 a_i \right] \sim 1 + \sum_i \tau_0 a_i + o((\tau_0)^2). \]

(B4)

Collecting the remaining factors, we obtain

\[ \delta Z = \prod_i \left[ 1 + z^2 d \tau_0 \left( t_{i+1} - t_i - 3 \tau_0 \right) \right. \]

\[ + \int_{t_i+1-\tau_0}^{t_i+\tau_0} dt' \left[ K_1 \sum_j (-)^{i+j} \frac{\tau_0}{t' - t_j} \right. \]

\[ + 2 K_2 \sum_j \ln \left| \frac{t' - t_j}{\tau_0} \right| d(t' - t_j) \right] \]. \]

(B5)

Reexponentiating the expression in the large square brackets of Eq. (B5), the correction to the partition function becomes

\[ \delta Z \sim \exp \left[ z^2 d \tau_0 \sum_i \left( t_{i+1} - t_i - 3 \tau_0 \right) \right. \]

\[ + z^2 d \tau_0 K_1 \sum_i (-)^{i+j+2} \ln \left| \frac{t' - t_j}{\tau_0} \right| \]

\[ + 2 z^2 d \tau_0 K_2 \sum_i \int_{t_i}^{t_i-\tau_0} dt' \sum_j \ln \left| \frac{t' - t_j}{\tau_0} \right| d(t' - t_j) \]. \]

(B6)

The first term in the exponent of Eq. (B6) contributes to the normalization of free energy \( e^{\Delta g d \tau_0} \). The \( K_1 \) and \( K_2 \) parts of Eq. (B6) behave very differently owing to the presence/absence of the oscillating factor:

\[ \delta Z \sim \exp \left[ z^2 d \tau_0 (K_1 \tau_0 \sum_i (-)^{i+j+1} (1 - 2) \ln |t_i - t_j| \right. \]

\[ \times \exp \left[ z^2 d \tau_0 \left( \int_{0}^{\beta} dt' \sum_j 2 K_2 \ln \left| \frac{t' - t_j}{\tau_0} \right| d(t' - t_j) \right) \right]. \]

(B7)

The \( K_2 \) part of Eq. (B7), in fact, does not depend on \( t_j \) owing to the integration over the whole range of imaginary time. Thus, the \( K_2 \) part of Eq. (B7) is proportional to the number of instantons, and consequently it contributes only to the fugacity correction. From the structure of Eq. (B7), the renormalization of \( K_1 \) is easily found:

\[ \tilde{K}_1 = K_1 - 4 K_1 \tau_0^2 \frac{d \tau_0}{\tau_0}. \]

(B8)

The renormalization of fugacity is given by

\[ (\tau_0 + d \tau_0) \tilde{\zeta} = (\tau_0 \tilde{\zeta}) \frac{\tau_0 + d \tau_0}{\tau_0} \exp \left[ - \frac{K_1}{2} \ln \frac{\tau_0 + d \tau_0}{\tau_0} \right. \]

\[ + z^2 d \tau_0 (2 K_2 g_2) \], \]

(B9)

where \( g_2 \) is

\[ g_2 = \int \frac{dt'}{\tau_0} \ln \left| \frac{t'}{\tau_0} \right| d(t'). \]

(B10)

The dependence of \( d(t') \) is far stronger than \( \ln |t'|/\tau_0 \); thus we neglect the logarithmic factor up to logarithmic accuracy. The explicit expression for \( d(t') \) is

\[ d(t') = \frac{2 \lambda \gamma^2 \Delta}{\omega_0^2} \int_{-\infty}^{\infty} \frac{d \omega}{\omega^2} \frac{e^{-i \omega t}}{\omega^2 + E} . \]

(B11)
\[ d(t') = -\frac{2\lambda \gamma^2 \Delta}{\omega_0^2} \int d\omega \frac{(E^*|\omega| + \omega_0^2) e^{-i\omega t'}}{\omega^2 + E^*|\omega| + \omega_0^2}. \] 

(B12)

\[ E^*|\omega| \] is a small perturbation at both high and low energy. The correction coming from \( E^*|\omega| \) is of the order of \( E^*/\omega_0 \ll 1 \). In leading approximation we can disregard \( E^* \).

Explicit evaluation gives

\[ d(t') = -\frac{\lambda \gamma^2 \Delta}{\omega_0^2} e^{-\omega_0 t'}. \] 

(B13)

The evaluation of \( g_2 \) gives

\[ g_2 \sim -\frac{\lambda \gamma^2 \Delta}{\omega_0 \tau_0} e^{-\omega_0 \tau_0}. \] 

(B14)

The scaling equation of fugacity is

\[ \frac{d(z\tau_0)}{d\tau_0} = \left( z\tau_0 \right) \left[ 1 - \frac{K_1}{2} + (z\tau_0)^2 (2Kg_2) \right]. \] 

(B15)

It is convenient to introduce variables which are more suitable in the context of the original Kondo model:

\[ dl = d\tau_0 / \tau_0, \quad x = z\tau_0, \quad K_1 = 2 - y, \quad y \ll 1. \] 

(B16)

In terms of these variables Eq. (B15) can be written as

\[ \frac{dx}{dl} = \frac{x}{2} \left[ y + xe^{-\omega_0 \tau_0} \right]. \] 

(B17)

In Eq. (B17) the short time cutoff was identified with \( 1/\Delta \), while for the path integral approach the apparent cutoff is \( 1/U \). This ambiguity has already been discussed in detail by Hamann in Sec. IV B of Ref. 6, and it was argued that the ambiguity does not give rise to any significant errors.