Equation of motion approach to the Anderson-Holstein Hamiltonian

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In this work we present an equation of motion approach to analyze the electronic properties of a small system coupled to metallic electrodes in which electron-phonon interaction is present. As a simple model, we consider the single-level Anderson-Holstein Hamiltonian. Two versions of this Hamiltonian, namely, spinless electrons and interacting electrons in the infinite-U limit, are studied in equilibrium and at zero temperature. Differently from previous approaches to the same problem using this method, we do not decouple electronic and vibronic degrees of freedom and keep quantum coherence between the electron at the localized level and the phonons. Also, we improve the method by including corrections that are important for a better description of Kondo physics. We focus in the analysis of the evolution of the resonances with the electron-phonon coupling parameter λ. We find that charge and spin resonances experience very different reduction in their widths, owing to their different physical origins, with the spin resonance being more robust than the charge one to increasing values of λ. This is at variance from the results of simple polaronic approaches to this problem, which treat both kinds of resonances on a similar footing. We expect that our approach is more appropriate to investigate the region of energies near the Fermi level in cases when the Kondo effect is strong.

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I. INTRODUCTION

Recent advances in the field of molecular electronics[1] have renovated the interest in the problem of electron-phonon interaction. It is now possible to fabricate devices in which small molecules are connected to macroscopic charge reservoirs (leads) to realize the ideal system of an "impurity" with quantum energy levels coupled to a continuum of states. Experiments on such systems give evidence that electron-vibrational coupling within the molecule plays an important role in its charge transport properties. This was first found by Park *et al.*[1] on C_{60}. In other cases, the excitation spectra show features that could be ascribed to sidebands formed by the presence of strong electron-phonon interactions.[2–4] In some cases, the Kondo effect has been observed,[5] indicating that both the coupling of the molecules to the leads and the electron-electron interaction are strong. More recently an anomalous dependence of the Kondo temperature with an applied gate voltage has been attributed to the presence of a strong electron-phonon interaction.[6]

From the theoretical point of view, the problem of the interaction of a localized level with a field of bosons can be traced back to the small polaron model of Holstein.[7] The model was applied to analyze the properties of mixed-valence systems coupled to lattice vibrations by Sherrington and von Molnar[8,9] and also used in other contexts. In x-ray photoemission spectroscopy, the photoemission spectra of a core-hole show satellites associated with absorption and emission of plasmons.[10] In this case, the bosons are plasmons and a formally identical problem was studied in Refs. 11 and 12. Most of these works assumed spinless electrons. Later, the extensive analysis performed by Hewson and Newns[13–15] in a series of papers pointed out the importance of Fermi-edge effects. Formally, this problem is exactly soluble only in the case of pure spinless electrons: the electron spin has to be neglected even in the distribution function of the system.[12,14,16,17] It is then equivalent to that of a single electron (or hole) since the presence of the Fermi sea is ignored and it is called the single-particle approximation (SPA).

The case of a spinless electron in a localized level, coupled to a local phonon and immersed in a Fermi sea, has frequently been considered in the literature and analyzed by means of different techniques, depending on the different regimes determined by the parameters: the temperature T, the coupling of the localized level to the leads V, the coupling of the localized level to phonons λ, and the phonon frequency ω_0. The classical regime, defined by $T \gg V$, can be approached from a master-equation point of view.[18,19] In the quantum regime $T \ll V$, the ratio λ/V distinguishes between the weak- and strong-coupling regimes. The weak-coupling regime $\lambda/V \ll 1$ can be approached by a variety of methods with the common characteristic of being perturbative in λ/V such as the Born approximation or the self-consistent Born approximation,[20–23] perturbative renormalization theory,[24] or diagrammatic techniques.[19,25] The quantum strong-coupling regime $\lambda/V \gg 1$ for which perturbation theory breaks down is much more difficult to analyze, with the SPA having been commonly used in this case.[26–28] Another important parameter is the ratio λ/ω_0, with $(\lambda/\omega_0)^2 = g$ being proportional to the mean number of excited phonons. A large value of g is characteristic of a strong polaronic system (see Ref. 29 for a review). The case of interacting electrons with a not too large value of the intrasite Coulomb repulsion energy U has been approached using the numerical renormalization-group (NRG) method.[30–34] This is a numerically exact technique, valid only in equilibrium and appropriate for analyzing the spectral region of energies around the Fermi level. It has been used to study the change in the linear transport properties of the system when going from a weak-coupling regime (characterized by spin fluctuations) to a strong-coupling polaronic regime dominated by charge fluctuations.

In this work we approach the problem of spinless or interacting electrons in the infinite-U limit, coupled to leads and to a local phonon. We apply an equation of motion (EOM) method for the calculation of the Green's function associated to the localized level in equilibrium with the leads, a previous step necessary to approach real nonequilibrium transport problems. The EOM method has been widely

used in the absence of electron-phonon interactions[35–40] in and out of equilibrium. The method consists in creating a hierarchy of the Green's functions by application of their EOM. At a given step, the generated Green's functions have to be approximated to produce a closed system of equations. The simpler and more usual form of the method decouples operators of the localized level and the leads at the second step obtaining in this way an approximation exact to the order $O(V^2)$. While this approximation produces very accurate values of the level occupancy, it is rather inaccurate to describe the properties of the system near the Fermi level. Recently, we have demonstrated how further steps in the procedure of the EOM clearly improve the description of Kondo physics.[41] In the last few years, the EOM method has also been applied to cases with a nonzero electron-phonon interaction for spinless electrons in Refs. 42 and 43 and for interacting electrons in Refs. 44 and 45. In all of these works, the decoupling of the localized level and the leads, leading to an approximation valid to the order $O(V^2)$, is performed. Moreover, decoupling of electrons and phonons is also present in Ref. 44 and also to some extent in Refs. 43 and 45. Our procedure is similar to that of Ref. 42 in that we keep quantum coherence between electrons and phonons but we improve upon it by going beyond the $O(V^2)$ approximation along the lines of Ref. 41. We apply an identical procedure to the case of interacting electrons in the infinite-U limit coupled to a local phonon, obtaining in this way a very good description of the excitation spectra near the Fermi level.

In this paper, we will concentrate on the strong-coupling regime where quantum polaronic effects are most important. The paper is organized in the following way. We first analyze the simplest case of the spinless Anderson-Holstein Hamiltonian in Sec. II. This case is interesting because it has exact solutions in particular limits and we show that our approach recovers all of them. We concentrate in an electron-hole symmetric situation as an intermediate case for which there is no exact solution and compare the results of the EOM method with a recent interpolative self-energy approximation (ISA), which interpolates between the atomic and the perturbative limits.[46] We specially analyze the reduction in width of the spectral density associated to charge fluctuations. Then in Sec. III, we approach the case of interacting electrons in the infinite-U limit, using a slave-boson technique. We chose this limit mainly because of its relative simplicity since all of the states implying double occupancy of the level are projected out of the Hilbert space. Here, we show that the Kondo resonance and the charge resonance experience very different polaronic reduction factors of their widths due to their different physical origins: spin versus charge fluctuations. This behavior is different from what is obtained in simple "polaronic approaches" to the problem. Since our approximation does not decouple electrons and phonons, we expect this method to be more appropriate to describe the Kondo spectral density at the Fermi level. This region of energies is the most important to describe transport properties of these systems. Finally, our conclusions are expounded in Sec. IV.

II. SPINLESS HAMILTONIAN

Our model system consists of a localized electron in a level of energy ϵ_0, coupled to a field of phonons of frequency ω_0. The localized level is also coupled to a continuum of states representing the leads to which it is connected. This is the Anderson-Holstein Hamiltonian which reads,

$$\hat{H} = \sum_{\sigma} \epsilon_0 \hat{n}_{0\sigma} + U\hat{n}_{0\uparrow}\hat{n}_{0\downarrow} + \sum_{k\sigma} \epsilon_{k\sigma}\hat{n}_{k\sigma} + \sum_{k\sigma} V_k(\hat{c}_{0\sigma}\hat{c}^{\dagger}_{k\sigma} + \hat{c}_{k\sigma}\hat{c}^{\dagger}_{0\sigma}) + \omega_0 b^{\dagger}b + \lambda(b^{\dagger} + b)\sum_{\sigma} \hat{n}_{0\sigma}. \quad (1)$$

In Eq. (1), $\hat{c}^{\dagger}_{0,\sigma}$ ($\hat{c}_{0,\sigma}$) are the operators which create (annihilate) an electron of spin σ in the localized level, $\hat{c}^{\dagger}_{k\sigma}$ ($\hat{c}_{k\sigma}$) creates (annihilates) an electron of energy $\epsilon_{k\sigma}$, momentum k, and spin σ in the leads, and $b^{\dagger}$ (b) are the creation (annihilation) operators for phonons. The number operators for electrons are $\hat{n}=\hat{c}^{\dagger}\hat{c}$. U is the value of the intra-atomic Coulomb repulsion, while V_k and λ represent the couplings of the localized level to the leads and to the phonon field, respectively. This is the simplest model Hamiltonian to study electron-vibration interactions even though other effects such as relaxation of the vibrons due to their coupling to another system (i.e., a phonon bath) are disregarded.[18,21,43,45]

We first concentrate on the spinless version of Hamiltonian (1) which is

$$\hat{H} = \epsilon_0\hat{n}_0 + \sum_{k} \epsilon_k\hat{n}_k + \sum_{k} V_k(\hat{c}_0\hat{c}^{\dagger}_k + \hat{c}_k\hat{c}^{\dagger}_0) + \omega_0 b^{\dagger}b + \lambda(b^{\dagger} + b)\hat{n}_0. \quad (2)$$

In the quantum strong-coupling regime we are interested in, defined by $\omega_0 \gg V_k$ and $\lambda \gg V_k$, it is convenient to apply to Hamiltonian (2) the canonical transformation $\tilde{H}=\hat{S}\hat{H}\hat{S}^{-1}$ with $\hat{S}$ given by[10]

$$\hat{S} = \exp\left[\frac{\lambda}{\omega_0}(b^{\dagger} - b)\hat{n}_0\right] \quad (3)$$

which transforms electronic and bosonic operators as

$$\tilde{c}_0 = \hat{S}\hat{c}_0\hat{S}^{-1} = \hat{c}_0 \exp\left[-\frac{\lambda}{\omega_0}(b^{\dagger} - b)\right],$$

$$\tilde{c}_k = \hat{S}\hat{c}_k\hat{S}^{-1} = \hat{c}_k,$$

$$\tilde{b} = \hat{S}b\hat{S}^{-1} = b - \frac{\lambda}{\omega_0}\hat{n}_0. \quad (4)$$

Since operators $\tilde{c}_0$ and $\tilde{c}^{\dagger}_0$ do not commute with operators b and $b^{\dagger}$, the following relations are useful for the derivation of the EOM:

$$\tilde{c}_0 b^{\dagger n} = \left(b^{\dagger} + \frac{\lambda}{\omega_0}\right)^n \tilde{c}_0$$

$$b^n\tilde{c}_0 = \tilde{c}_0\left(b - \frac{\lambda}{\omega_0}\right)^n \quad (5)$$

Note that Eq. (4) implies that the number operators for electrons in the level and in the leads remain unchanged. Then, the transformed Hamiltonian reads

$$\tilde{H} = \tilde{\epsilon}_0 \hat{n}_0 + \sum_k \epsilon_k \hat{n}_k + \sum_k V_k (\tilde{c}_0 \hat{c}_k^\dagger + \hat{c}_k \tilde{c}_0^\dagger) + \omega_0 b^\dagger b \tag{6}$$

with $\tilde{\epsilon}_0 = \epsilon_0 - \lambda^2/\omega_0$ representing the renormalization of the energy level due to its coupling with the local phonon.

The transport properties through the localized level can be generally expressed in terms of the spectral function $\rho_0(\omega)$ defined as

$$\rho_0(\omega) = -\frac{1}{\pi} \mathrm{Im} \langle\langle \hat{c}_0; \hat{c}_0^\dagger \rangle\rangle_\omega \tag{7}$$

With $\langle\langle \hat{c}_0; \hat{c}_0^\dagger \rangle\rangle_\omega$ being the Fourier transform of the retarded Green's function of the localized level $\langle\langle \hat{c}_0(t); \hat{c}_0^\dagger(t') \rangle\rangle$. These Green's functions are also to be evaluated after the canonical transformation is applied; namely, we calculate

$$\langle\langle \tilde{c}_0(t); \tilde{c}_0^\dagger(t') \rangle\rangle = -i\theta(t-t') \langle \tilde{c}_0(t) \tilde{c}_0^\dagger(t') + \tilde{c}_0^\dagger(t') \tilde{c}_0(t) \rangle_{\tilde{H}} \tag{8}$$

and its Fourier transformed function $\langle\langle \tilde{c}_0; \tilde{c}_0^\dagger \rangle\rangle_\omega$. The symbol $\langle \cdots \rangle_{\tilde{H}}$ means that the average should be taken with respect to the transformed Hamiltonian $\tilde{H}$.

Frequently in the literature, electrons and phonons are decoupled at this level of the derivation already by factorizing operators involving electrons with that of phonons on the right-hand side of Eq. (8).[43–45] Instead of doing that, we calculate all of the coupled Green's functions by using the EOM method, which we describe in what follows.

We first write the EOM of $\langle\langle \tilde{c}_0(t); \tilde{c}_0^\dagger(t') \rangle\rangle$ as

$$\frac{d\langle\langle \tilde{c}_0(t); \tilde{c}_0^\dagger(t') \rangle\rangle}{dt} = -i\delta(t-t') - i\theta(t-t') \times \langle [i[\tilde{H}, \tilde{c}_0](t), \tilde{c}_0^\dagger(t')]_+ \rangle_{\tilde{H}} \tag{9}$$

which, when Fourier transformed, yields the following equation:

$$(\omega - \tilde{\epsilon}_0) \langle\langle \tilde{c}_0; \tilde{c}_0^\dagger \rangle\rangle_\omega = 1 + \lambda \langle\langle \tilde{c}_0 b; \tilde{c}_0^\dagger \rangle\rangle_\omega + \lambda \langle\langle b^\dagger \tilde{c}_0; \tilde{c}_0^\dagger \rangle\rangle_\omega + \sum_k V_k \langle\langle \hat{c}_k; \tilde{c}_0^\dagger \rangle\rangle_\omega. \tag{10}$$

From now on, the argument (ω) of all the Green's functions will be dropped for simplicity. The Green's functions appearing on the right-hand side of Eq. (10) are also calculated by means of their respective EOMs, yielding

$$(\omega - \epsilon_k) \langle\langle \hat{c}_k; \tilde{c}_0^\dagger \rangle\rangle = -V_k \langle\langle \tilde{c}_0; \tilde{c}_0^\dagger \rangle\rangle, \tag{11}$$

$$(\omega - \tilde{\epsilon}_0 - \omega_0) \langle\langle \tilde{c}_0 b; \tilde{c}_0^\dagger \rangle\rangle = \left\langle b + \tilde{c}_0 \tilde{c}_0^\dagger \frac{\lambda}{\omega_0} \right\rangle_{\tilde{H}} + \lambda \langle\langle \tilde{c}_0 b^2; \tilde{c}_0^\dagger \rangle\rangle + \lambda \langle\langle b^\dagger \tilde{c}_0 b; \tilde{c}_0^\dagger \rangle\rangle - \sum_k V_k \left\langle \left\langle \hat{c}_k \left(b + \frac{\lambda}{\omega_0} \tilde{c}_0 \tilde{c}_0^\dagger \right); \tilde{c}_0^\dagger \right\rangle \right\rangle, \tag{12}$$

$$(\omega - \tilde{\epsilon}_0 + \omega_0) \langle\langle b^\dagger \tilde{c}_0; \tilde{c}_0^\dagger \rangle\rangle = \left\langle b^\dagger - \tilde{c}_0^\dagger \tilde{c}_0 \frac{\lambda}{\omega_0} \right\rangle_{\tilde{H}} + \lambda \langle\langle b^{\dagger 2} \tilde{c}_0; \tilde{c}_0^\dagger \rangle\rangle + \lambda \langle\langle b^\dagger \tilde{c}_0 b; \tilde{c}_0^\dagger \rangle\rangle - \sum_k V_k \left\langle \left\langle \left(b^\dagger - \frac{\lambda}{\omega_0} \tilde{c}_0^\dagger \tilde{c}_0 \right) \hat{c}_k; \tilde{c}_0^\dagger \right\rangle \right\rangle. \tag{13}$$

The Green's functions $\langle\langle \tilde{c}_0 b^2; \tilde{c}_0^\dagger \rangle\rangle$, $\langle\langle b^\dagger \tilde{c}_0 b; \tilde{c}_0^\dagger \rangle\rangle$, and $\langle\langle b^{\dagger 2} \tilde{c}_0; \tilde{c}_0^\dagger \rangle\rangle$ on the right-hand side of Eqs. (12) and (13) are also expressed by their EOM. Proceeding in this way an infinite set of Green's functions $\langle\langle b^{\dagger n} \tilde{c}_0 b^m; \tilde{c}_0^\dagger \rangle\rangle$ are produced, which are linked by their EOM. The general equation is

$$\begin{aligned}(\omega - \tilde{\epsilon}_0 + (n-m)\omega_0) \langle\langle b^{\dagger n} \tilde{c}_0 b^m; \tilde{c}_0^\dagger \rangle\rangle &= \left\langle \left(b^\dagger - \frac{\lambda}{\omega_0} \right)^n \tilde{c}_0^\dagger \tilde{c}_0 b^m \right\rangle_{\tilde{H}} + \left\langle b^{\dagger n} \tilde{c}_0 \tilde{c}_0^\dagger \left(b + \frac{\lambda}{\omega_0} \right)^m \right\rangle_{\tilde{H}} \\ &+ \lambda \langle\langle b^{\dagger (n+1)} \tilde{c}_0 b^m; \tilde{c}_0^\dagger \rangle\rangle + \lambda \langle\langle b^{\dagger n} \tilde{c}_0 b^{m+1}; \tilde{c}_0^\dagger \rangle\rangle \\ &- \sum_k V_k \left(\left\langle \left\langle \left(b^\dagger - \frac{\lambda}{\omega_0} \right)^n \tilde{c}_0^\dagger \tilde{c}_0 \hat{c}_k b^m; \tilde{c}_0^\dagger \right\rangle \right\rangle \right. \\ &\left. + \left\langle \left\langle b^{\dagger n} \tilde{c}_0 \tilde{c}_0^\dagger \hat{c}_k \left(b + \frac{\lambda}{\omega_0} \right)^m; \tilde{c}_0^\dagger \right\rangle \right\rangle \right).\end{aligned} \tag{14}$$

The Green's functions appearing in the last term on the right-hand side of Eq. (14), involving operators $\hat{c}_k$, are also calculated by means of their respective EOMs which are the following:

$$\begin{aligned}(\omega - \epsilon_k + (n-m)\omega_0) \langle\langle b^{\dagger n} \tilde{c}_0^\dagger \tilde{c}_0 \hat{c}_k b^m; \tilde{c}_0^\dagger \rangle\rangle &= -\left\langle b^{\dagger n} \tilde{c}_0^\dagger \hat{c}_k \left(b + \frac{\lambda}{\omega_0} \right)^m \right\rangle_{\tilde{H}} \\ &- \sum_{k'} V_{k'}' \left(\left\langle \left\langle \left(b^\dagger + \frac{\lambda}{\omega_0} \right)^n \tilde{c}_0 \hat{c}_{k'}^\dagger \hat{c}_k b^m; \tilde{c}_0^\dagger \right\rangle \right\rangle \right. \\ &\left. + \left\langle \left\langle b^{\dagger n} \tilde{c}_0^\dagger \hat{c}_{k'} \hat{c}_k \left(b + \frac{\lambda}{\omega_0} \right)^m; \tilde{c}_0^\dagger \right\rangle \right\rangle \right)\end{aligned} \tag{15}$$

and

$$\begin{aligned}(\omega - \epsilon_k + (n-m)\omega_0) \langle\langle b^{\dagger n} \tilde{c}_0 \tilde{c}_0^\dagger \hat{c}_k b^m; \tilde{c}_0^\dagger \rangle\rangle &= \left\langle \left(b^\dagger - \frac{\lambda}{\omega_0} \right)^n \tilde{c}_0^\dagger \hat{c}_k b^m \right\rangle_{\tilde{H}} - V_k \left\langle \left\langle b^{\dagger n} \tilde{c}_0 \left(b - \frac{\lambda}{\omega_0} \right)^m; \tilde{c}_0^\dagger \right\rangle \right\rangle \\ &+ \sum_{k'} V_{k'}' \left(\left\langle \left\langle \left(b^\dagger - \frac{\lambda}{\omega_0} \right)^n \tilde{c}_0^\dagger \hat{c}_{k'} \hat{c}_k b^m; \tilde{c}_0^\dagger \right\rangle \right\rangle \right. \\ &\left. + \left\langle \left\langle b^{\dagger n} \tilde{c}_0 \hat{c}_{k'}^\dagger \hat{c}_k \left(b - \frac{\lambda}{\omega_0} \right)^m; \tilde{c}_0^\dagger \right\rangle \right\rangle \right).\end{aligned} \tag{16}$$

To approximate $\langle\langle \tilde{c}_0; \tilde{c}_0^\dagger \rangle\rangle$ to order the $O(V^2)$, we now decouple the localized level and the leads by contracting pairs of operators $\hat{c}_k$ and $\hat{c}_{k'}^\dagger$ where possible in the right hand-side of Eqs. (15) and (16), in order to obtain a closed system of equations. Then, all of the Green's functions having the combination $\hat{c}_k \hat{c}_{k'}$ are neglected. This decoupling is traditionally performed when using the EOM method and assumes that

the leads are not affected by the vibrational mode. However, the electrons at the localized level and the phonons keep coupled in all of the Green's functions. Thus, Eqs. (15) and (16) are approximated as

$$(\omega-\epsilon_k+(n-m)\omega_0)\langle\langle b^{\dagger n}\tilde{c}_0^\dagger\tilde{c}_0\hat{c}_k b^m;\tilde{c}_0^\dagger\rangle\rangle = -\left\langle b^{\dagger n}\tilde{c}_0^\dagger\hat{c}_k\left(b+\frac{\lambda}{\omega_0}\right)^m\right\rangle_{\tilde{H}} - V_k\langle n_k\rangle\left\langle\left\langle\left(b^\dagger+\frac{\lambda}{\omega_0}\right)^n\tilde{c}_0 b^m;\tilde{c}_0^\dagger\right\rangle\right\rangle \tag{17}$$

and

$$(\omega-\epsilon_k+(n-m)\omega_0)\langle\langle b^{\dagger n}\tilde{c}_0\tilde{c}_0^\dagger\hat{c}_k b^m;\tilde{c}_0^\dagger\rangle\rangle = \left\langle\left(b^\dagger-\frac{\lambda}{\omega_0}\right)^n\tilde{c}_0^\dagger\hat{c}_k b^m\right\rangle_{\tilde{H}} - V_k\langle 1-n_k\rangle\left\langle\left\langle b^{\dagger n}\tilde{c}_0\left(b-\frac{\lambda}{\omega_0}\right)^m;\tilde{c}_0^\dagger\right\rangle\right\rangle, \tag{18}$$

respectively, with $\langle n_k\rangle$ being the Fermi-Dirac distribution function of the electrons of the reservoir. Substituting Eqs. (17) and (18) into Eqs. (15) and (16), a closed system of linear equations for the unknowns $\langle\langle b^{\dagger n}\tilde{c}_0 b^m;\tilde{c}_0^\dagger\rangle\rangle$ is obtained which can be solved numerically. Such a solution is exact to the order $O(V^2)$ and to all order in λ. From now on we will use the notation $\omega_{nm}=\omega+(n-m)\omega_0$.

The expectation values of the different operators appearing as independent terms on the right-hand side of Eqs. (14)–(18) should, in principle, be calculated self-consistently with the Green's functions. As an example, one can prove the following relation:

$$\langle b^{\dagger n}\tilde{c}_0\hat{c}_k^\dagger b^m\rangle_{\tilde{H}} = V_k\int_{-\infty}^{+\infty}-\frac{d\omega}{\pi}\langle n_k\rangle\mathrm{Im}\frac{\langle\langle b^{\dagger n}\tilde{c}_0 b^m;\tilde{c}_0^\dagger\rangle\rangle(\omega)}{\omega-\epsilon_k+i\eta}. \tag{19}$$

However, we have checked by explicit calculations that all of these expectation values can be neglected at zero temperature and they will not be shown hereafter. Other expectation values such as $\langle b^{\dagger n}\tilde{c}_0^\dagger\tilde{c}_0 b^m\rangle_{\tilde{H}}$ have been approximated assuming that electronic and bosonic subsystems can be separated, as it happens in the atomic limit. That is, at zero temperature, we take

$$\langle b^{\dagger n}\tilde{c}_0^\dagger\tilde{c}_0 b^m\rangle_{\tilde{H}} \cong \delta_{m0}\delta_{n0}\langle\tilde{c}_0^\dagger\tilde{c}_0\rangle. \tag{20}$$

That these approximations are not too severe can be judged by the fact that our results fulfill the Fridel-Langreth sum rule[33] with an accuracy of a few percents. Finally, the following system of equations is solved at zero temperature:

$$\begin{aligned}(\omega_{nm}-\tilde{\epsilon}_0-\Delta_{nm})\langle\langle b^{\dagger n}\tilde{c}_0 b^m;\tilde{c}_0^\dagger\rangle\rangle &= \delta_{n0}\left(\frac{\lambda}{\omega_0}\right)^m\langle\tilde{c}_0\tilde{c}_0^\dagger\rangle+\delta_{m0}\left(-\frac{\lambda}{\omega_0}\right)^n\langle\tilde{c}_0^\dagger\tilde{c}_0\rangle\\ &+\lambda\langle\langle b^{\dagger n}\tilde{c}_0 b^{m+1};\tilde{c}_0^\dagger\rangle\rangle+\lambda\langle\langle b^{\dagger(n+1)}\tilde{c}_0 b^m;\tilde{c}_0^\dagger\rangle\rangle\\ &+\sum_{l=0}^{m-1}\left(-\frac{\lambda}{\omega_0}\right)^{m-l}\langle\langle b^{\dagger n}\tilde{c}_0 b^l;\tilde{c}_0^\dagger\rangle\rangle\sum_{l'=l}^{m}(-1)^{m-l'}\binom{m}{l'}\binom{l'}{l}\\ &\times\sum_k\frac{V_k^2\langle 1-n_k\rangle}{\omega_{nl'}-\epsilon_k}+\sum_{l=0}^{n-1}\left(\frac{\lambda}{\omega_0}\right)^{n-l}\langle\langle b^{\dagger l}\tilde{c}_0 b^m;\tilde{c}_0^\dagger\rangle\rangle\\ &\times\sum_{l'=l}^{n}(-1)^{n-l'}\binom{n}{l'}\binom{l'}{l}\sum_k\frac{V_k^2\langle n_k\rangle}{\omega_{l'm}-\epsilon_k}\end{aligned} \tag{21}$$

with $\binom{n}{l}=\frac{n!}{l!(n-l)!}$ and $\Delta_{nm}=\Sigma_k\frac{V_k^2}{\omega_{nm}-\epsilon_k}$.

We should point out that this procedure does not decouple electrons and phonons, as it has been frequent in the literature. Rather, quantum coherence is preserved in all of the Green's functions $\langle\langle b^{\dagger n}\tilde{c}_0 b^m;\tilde{c}_0^\dagger\rangle\rangle$ which involve emission of n and absorption of m phonons. A similar procedure was used in Ref. 42; the main difference with our treatment is that the Green's functions were expanded in the basis of phonon states. We think that our procedure is more convenient since it requires the evaluation of a shorter number of Green's functions. We should mention that this approximation reproduces all the known exact limits of the spinless Anderson-Holstein Hamiltonian, namely, (a) the atomic limit ($V_k=0$), (b) the limit of electrons uncoupled to phonons ($\lambda=0$), (c) the limit of having just one electron (or just one hole) in the system $\langle n_k\rangle=0$ or $1-\langle n_k\rangle=0$,[14,15] and (d) the limits of a full ($\langle\hat{n}_0\rangle\to 1$) or an empty ($\langle\hat{n}_0\rangle\to 0$) orbital.[17] In these cases, one obtains the SPA for the Green's function of the localized level as follows:

$$\langle\langle\tilde{c}_0;\tilde{c}_0^\dagger\rangle\rangle = e^{-(\lambda/\omega_0)^2}\sum_{n=0}^{\infty}\left(\frac{\lambda}{\omega_0}\right)^{2n}\frac{1}{n!}\times\left(\frac{1-\langle\hat{n}_0\rangle}{\omega-\tilde{\epsilon}_0-n\omega_0+i\Delta}+\frac{\langle\hat{n}_0\rangle}{\omega-\tilde{\epsilon}_0+n\omega_0+i\Delta}\right) \tag{22}$$

with $\Delta_{nm}\equiv -i\Delta$ in the wide-band limit.

The right-hand side of Eq. (21) shows logarithmic singularities associated with the terms

$$\Delta_{ij}^{(e)}(\omega+(i-j)\omega_0)=\sum_k V_k^2\frac{\langle n_k\rangle}{\omega_{ij}-\epsilon_k}, \tag{23}$$

$$\Delta_{ij}^{(h)}(\omega+(i-j)\omega_0)=\sum_k V_k^2\frac{1-\langle n_k\rangle}{\omega_{ij}-\epsilon_k} \tag{24}$$

at ω near any multiple of the phonon frequency ω_0. This is a consequence of the approximation of Eqs. (15) and (16) to the order $O(V^2)$. Therefore, a correct regularization of this kind of term requires going beyond this order. To do that, and following along the lines of Ref. 41, the Green's functions appearing on the right-hand side of Eqs. (15) and (16) are to be calculated by means of their EOM. The decoupling of the localized level and leads, by contraction of operators $\hat{c}_k$ and $\hat{c}_{k'}^\dagger$, is then done in the resulting equation. This procedure, which is described in the Appendix, will provide a solution for $\langle\langle\tilde{c}_0;\tilde{c}_0^\dagger\rangle\rangle$ to the order $O(V^4)$ and to all order in λ. How-

ever, it is very demanding from a computational point of view. At the moment we are interested in the regularization of the functions defined by Eqs. (23) and (24) and this can be done analytically. Details are given in the Appendix. The result is that the structure of Eq. (21) remains the same except for the denominators of Eqs. (23) and (24), which change as

$$\omega_{ij} - \epsilon_k \rightarrow \omega_{ij} - \epsilon_k - \Sigma_{ij}^{(e,h)}(\omega_{ij} - \epsilon_k) \tag{25}$$

for electrons (e) and holes (h), respectively. The self-energy $\Sigma_{ij}^{(e)}(x)$ is given by

$$\begin{aligned}\Sigma_{ij}^{(e)}(x) = e^{-(\lambda/\omega_0)^2} \sum_{l=0}^{i} \frac{(-1)^{i-l}}{l!}\left(\frac{\lambda}{\omega_0}\right)^{2l} \sum_{m=0}^{\infty} \frac{1}{m!}\left(\frac{\lambda}{\omega_0}\right)^{2m} \\ \times \sum_{n=0}^{i} (-1)^n \binom{i}{n}\binom{n+m}{i-l} \\ \times \sum_{k'} \frac{V_{k'}^2 \langle 1 - n_k' \rangle}{x - \tilde{\epsilon}_0 + \epsilon_k' + (n+m-i)\omega_0} + e^{-(\lambda/\omega_0)^2} \\ \times \sum_{l=0}^{j} \frac{(-1)^{j-l}}{l!}\left(\frac{\lambda}{\omega_0}\right)^{2l} \sum_{m=0}^{\infty} \frac{1}{m!}\left(\frac{\lambda}{\omega_0}\right)^{2m} \\ \times \sum_{n=0}^{j} (-1)^n \binom{j}{n}\binom{n+m}{j-l} \\ \times \sum_{k'} \frac{V_{k'}^2 \langle 1 - n_k' \rangle}{x + \tilde{\epsilon}_0 - \epsilon_k' - (n+m-j)\omega_0}\end{aligned} \tag{26}$$

and the expression for $\Sigma_{ij}^{(h)}(x)$ is identical to Eq. (26) by changing $\tilde{\epsilon}_0$ by $-\tilde{\epsilon}_0$ everywhere.

We have already mentioned that Eq. (21) is exact in the limit of having only one electron.[12,14,15] The effects of having a many electron system, and therefore a sharp Fermi level at zero temperature, are more important in the case $\tilde{\epsilon}_0 \simeq \epsilon_F$, where ϵ_F is the Fermi energy which we will take as our zero of energy. Moreover, since the exact solutions in the limits of the localized level being completely occupied or empty are also recovered, the electron-hole symmetric case $\tilde{\epsilon}_0 = 0$, for which $\langle \hat{n}_0 \rangle = 0.5$, seems to be the most interesting one. For this special case $\Sigma_{ij}^{(e)}(x) = \Sigma_{ij}^{(h)}(x) \equiv \Sigma_{ij}(x)$. Also, in all the calculations to be presented in this paper, we use constant values of the couplings V_k and the electronic structure of the leads is described by a flat band of large half width D with a constant density of states, in such a way that the half widths Δ_{nm} are constant and equal to $\Delta_{nm} = -i\pi V^2 \Sigma_k \delta(\omega_{nm} - \epsilon_k) \equiv -i\Delta$.

Figure 1 shows $-\mathrm{Im}\,\Sigma_{ii}(x)$, as a function of the generic variable x, for several values of i. Note that this function is always finite; the smallest values are obtained at $x \simeq 0$ for $i = 0$. For $i \gg 1$ one can appreciate that $-\mathrm{Im}\,\Sigma_{ii}(x) \simeq \Delta$ for all x. Then the denominators of Eqs. (23) and (24) are regularized by $i\Delta$, except for the smallest values of i, j and $\omega \simeq 0$. However, in the calculations to be presented next, we use the functions $\Delta_{ij}^{(e,h)}$ exactly renormalized by $\Sigma_{ij}(x)$.

We now proceed to present our results for the density of states, comparing them to a recent ISA,[46] which interpolates between the atomic and the perturbative ($\lambda \ll \omega_0$ and $\lambda \ll \Delta$) limits. This approximation is shown to be very good by comparison to exact results obtained for small cluster systems.

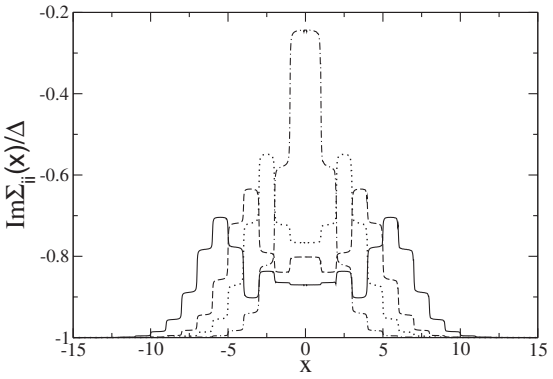

FIG. 1. The imaginary part of the self-energies defined by Eq. (26) as a function of the generic variable x, for $\tilde{\epsilon}_0 = 0$, $\omega_0 = 1$, and $\lambda/\omega_0 = 1.2$, for $i = j = 0$ (dotted-dashed line), 2 (dotted line), 4 (dashed line), and 8 (continuous line).

Figure 2 shows the densities of states for the case $\omega_0 = 1$, $\lambda/\omega_0 = 0.6$, and $\Delta = 0.2\omega_0$. Also shown in this figure are the results of a perturbative calculation of the self-energy to the order $O(\lambda^2)$. For this relatively small value of λ, both the EOM and ISA methods give very similar results which begin to exhibit features different from the perturbative solution. A main difference is in the sidebands, which are displaced and neatly narrowed from the perturbative result.

In Fig. 3 the densities of states for $\omega_0 = 1$, $\lambda/\omega_0 = 1.2$, and $\Delta = 0.2\omega_0$ are compared to the SPA [Eq. (22)] since this is clearly a strong-coupling nonperturbative case. The narrowing of the central resonance and the first sidebands at $\omega \simeq \pm\omega_0$ with respect to the SPA is evident in this figure. Both calculations manifest this consequence of a sharp Fermi level in the same way in the first sidebands but present differences for the higher ones. While the EOM method still narrows the second sidebands at $\omega \simeq \pm 2\omega_0$ and tends to approach the SPA at high ω, the ISA actually widens all of these sidebands.

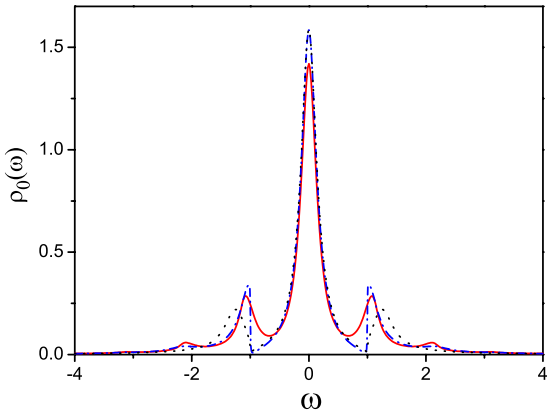

FIG. 2. (Color online) The spectral density as a function of ω for $\tilde{\epsilon}_0 = 0$, $\omega_0 = 1$, $\lambda/\omega_0 = 0.6$, and $\Delta = 0.2\omega_0$. Continuous red line: EOM, dashed-dotted blue line: ISA, and dotted black line: perturbative approximation.

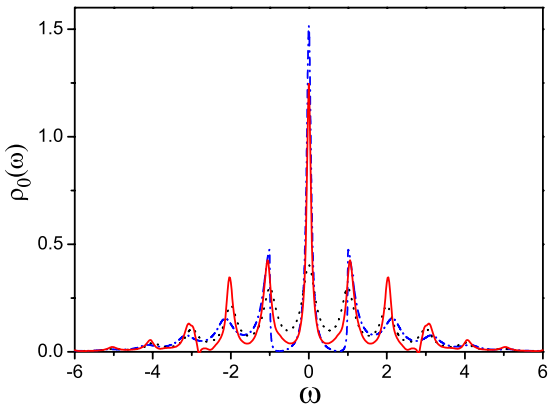

FIG. 3. (Color online) The spectral density as a function of ω for $\tilde{\epsilon}_0=0$, $\omega_0=1$, $\lambda/\omega_0=1.2$, and $\Delta=0.2\omega_0$. Continuous red line: EOM, dashed-dotted blue line: ISA, and dotted black line: SPA [Eq. (22)].

This is more clearly seen in Fig. 4 where we present the same results as in Fig. 3 but for a higher value of Δ ($\Delta=0.5\omega_0$). Then, while both methods give rise to a narrowing of the central resonance and the first sidebands, they describe the rest of the spectrum differently, with the SPA being in between. The narrowing of the central resonance can be understood as an effect of the Friedel-Langreth sum rule that, for the particle-hole symmetric case $\tilde{\epsilon}_0=0$ ($\langle\hat{n}_0\rangle=0.5$), pins $\rho_0(0)$ at the value $\frac{1}{\pi\Delta}$ for all λ. Now, when λ/ω_0 increases, the Franck-Condon factors $e^{-g}\frac{g^n}{n!}, g=(\lambda/\omega_0)^2$ shift the weight of the spectrum toward sidebands at $\omega\simeq\pm g\omega_0$. Consequently, the width of the central resonance has to decrease. Holstein already pointed out that a reduction factor of the width should apply for $g>\frac{\Delta}{\omega_0}$. We indeed find the polaronic exponential reduction factor $\Delta_r=\Delta e^{-g}$ of the resonance at the Fermi level in the range of values investigated, $\Delta<\omega_0$ and $0\leq\lambda/\omega_0\leq1.5$. The question remains on how the spectrum is modified at energies $|\omega|\geq\omega_0$. It is also interesting to note that the solution tends to the SPA, even for $\langle\hat{n}_0\rangle=0.5$, in the extreme polaronic regime $\lambda/\omega_0\gg1$. This is illustrated in Fig. 5, where we show that the results of the ISA are nearly identical to the SPA for $\Delta=0.2\omega_0$ and $\lambda/\omega_0=2.5$. This is a case in which the density of states at the Fermi level is extremely narrow and one is again left with a system of single particles.

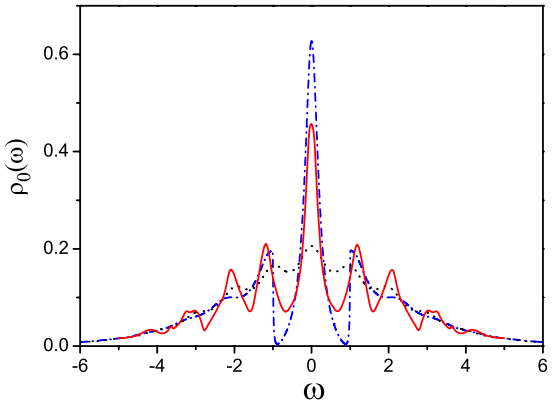

FIG. 4. (Color online) The spectral density as a function of ω for $\tilde{\epsilon}_0=0$, $\omega_0=1$, $\lambda=1.2/\omega_0$, and $\Delta=0.5\omega_0$. Continuous red line: EOM, dashed-dotted blue line: ISA and dotted black line: SPA [Eq. (22)].

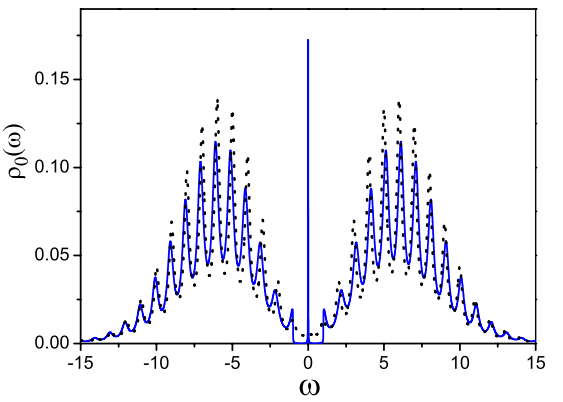

FIG. 5. (Color online) The spectral density as a function of ω in the extreme polaronic regime for $\tilde{\epsilon}_0=0$, $\omega_0=1$, $\lambda/\omega_0=2.5$, and $\Delta=0.2\omega_0$. Continuous blue line: ISA and dotted black line: SPA [Eq. (22)].

III. INTERACTING ELECTRONS IN THE INFINITE-U LIMIT

In this section we start with the Anderson-Holstein Hamiltonian for arbitrary U [Eq. (1)] and apply the canonical transformation $\tilde{H}=\hat{S}\hat{H}\hat{S}^{-1}$ with $\hat{S}$ given by $\hat{S}=\exp[\frac{\lambda}{\omega_0}(b^\dagger-b)\Sigma_\sigma\hat{n}_{0\sigma}]$. The transformed operators for electrons and bosons have the same expressions defined by Eq. (4) but with $\hat{n}_0$ substituted for $\Sigma_\sigma\hat{n}_{0\sigma}$ and the transformed Hamiltonian reads

$$\tilde{H}=\sum_\sigma\tilde{\epsilon}_0\hat{n}_{0\sigma}+\tilde{U}\hat{n}_{0\uparrow}\hat{n}_{0\downarrow}+\sum_{k\sigma}\epsilon_k\hat{n}_{k\sigma}+\sum_{k\sigma}V_k(\tilde{c}_{0\sigma}\hat{c}_{k\sigma}^\dagger+\hat{c}_{k\sigma}\tilde{c}_{0\sigma}^\dagger)+\omega_0b^\dagger b \tag{27}$$

with $\tilde{U}=U-2\lambda^2/\omega_0$. This Hamiltonian will be analyzed in the limit of infinite values of U (or $\tilde{U}$). We choose this limit because, as stated in Sec. I, it is a physically relevant one that has been extensively investigated using the EOM method in the absence of electron-phonon interactions. Moreover, the problem in the presence of the electron-phonon interaction is relatively simpler in this limit since all the states in which the localized level is doubly occupied are projected out of the Hilbert space. We use a slave-boson technique[47] and use auxiliary bosons operators $\hat{a}^\dagger,\hat{a}$ (which commute with the real phonon operators $b^\dagger,b$) and write the Hamiltonian (27) in the equivalent form

$$\tilde{H}=\sum_\sigma\tilde{\epsilon}_0\hat{n}_{0\sigma}+\sum_{k\sigma}\epsilon_k\hat{n}_{k\sigma}+\sum_{k\sigma}V_k(\hat{a}^\dagger\tilde{c}_{0\sigma}\hat{c}_{k\sigma}^\dagger+\hat{c}_{k\sigma}\tilde{c}_{0\sigma}^\dagger\hat{a})+\omega_0b^\dagger b \tag{28}$$

with the constraint relation

$$\hat{a}^\dagger\hat{a}+\sum_\sigma\hat{c}_{0\sigma}^\dagger\hat{c}_{0\sigma}=\hat{Q} \tag{29}$$

with $\hat{Q}=\hat{1}$ for $s=1/2$ spin electrons. The constraint relation ensures that no more than one electron will occupy the lo-

calized level in the infinite-U limit. Within the formalism of slave bosons, the physical operators are those which commute with $\hat{Q}$.[48] For $\lambda=0$, the physical operators associated with creation (annihilation) of electrons in the localized level are not $\hat{c}^{\dagger}_{0\sigma}$ ($\hat{c}_{0\sigma}$) themselves but the combinations $\hat{\chi}^{\dagger}_{\sigma}=\hat{c}^{\dagger}_{0\sigma}\hat{a}$ ($\hat{\chi}_{\sigma}=\hat{a}^{\dagger}\hat{c}_{0\sigma}$). The canonical transformation transforms $\hat{\chi}^{\dagger}_{\sigma}$ and $\hat{\chi}_{\sigma}$ as $\tilde{\chi}^{\dagger}_{\sigma}=\tilde{c}^{\dagger}_{0\sigma}\hat{a}$ and $\tilde{\chi}_{\sigma}=\hat{a}^{\dagger}\tilde{c}_{0\sigma}$, respectively and it can be easily proved that these operators commute with $\hat{Q}$. Then our Hamiltonian (28) is written in terms of physical operators as

$$\tilde{H}=\sum_{\sigma}\tilde{\epsilon}_0\hat{n}_{0\sigma}+\sum_{k\sigma}\epsilon_k\hat{n}_{k\sigma}+\sum_{k\sigma}V_k(\tilde{\chi}_{\sigma}\hat{c}^{\dagger}_{k\sigma}+\hat{c}_{k\sigma}\tilde{\chi}^{\dagger}_{\sigma})+\omega_0 b^{\dagger}b \tag{30}$$

Hamiltonian (30) together with the constraint relation (29) defines our problem. The physical (retarded) Green's function of the localized level is then defined as[39,48]

$$\langle\langle\tilde{\chi}_{\sigma}(t);\tilde{\chi}^{\dagger}_{\sigma}(t')\rangle\rangle=-i\theta(t-t')\langle\tilde{\chi}^{\dagger}_{\sigma}(t')\tilde{\chi}_{\sigma}(t)+\tilde{\chi}_{\sigma}(t)\tilde{\chi}^{\dagger}_{\sigma}(t')\rangle_{\tilde{H}} \tag{31}$$

and its Fourier transform $\langle\langle\tilde{\chi}_{\sigma};\tilde{\chi}^{\dagger}_{\sigma}\rangle\rangle_{\omega}$ will be calculated using the EOM method following a procedure analogous to that of the spinless case. The only difference with that case is that the constraint relation (29) is imposed every time the combinations $\hat{a}^{\dagger}\hat{a}$ and $\hat{a}\hat{a}^{\dagger}$ appear in the process of generating the Green's functions. Thus, starting with $\langle\langle\tilde{\chi}_{\sigma};\tilde{\chi}^{\dagger}_{\sigma}\rangle\rangle$, we obtain an infinite set of Green's functions $\langle\langle b^{\dagger n}\tilde{\chi}_{\sigma}b^{m};\tilde{\chi}^{\dagger}_{\sigma}\rangle\rangle$ which are linked by their EOM, with the general equation being:

$$\begin{aligned}(\omega_{nm}-\tilde{\epsilon}_0)\langle\langle b^{\dagger n}\tilde{\chi}_{\sigma}b^{m};\tilde{\chi}^{\dagger}_{\sigma}\rangle\rangle&=\left\langle\left(b^{\dagger}-\frac{\lambda}{\omega_0}\right)^{n}\hat{n}_{0\sigma}b^{m}\right\rangle_{\tilde{H}}+\left\langle b^{\dagger n}\left(1-\sum_{\sigma}\hat{n}_{0\sigma}\right)\left(b+\frac{\lambda}{\omega_0}\right)^{m}\right\rangle_{\tilde{H}}+\lambda\langle\langle b^{\dagger(n+1)}\tilde{\chi}_{\sigma}b^{m};\tilde{\chi}^{\dagger}_{\sigma}\rangle\rangle\\&+\lambda\langle\langle b^{\dagger n}\tilde{\chi}_{\sigma}b^{m+1};\tilde{\chi}^{\dagger}_{\sigma}\rangle\rangle-\sum_{k}V_k\left(\left\langle\left\langle\left(b^{\dagger}-\frac{\lambda}{\omega_0}\right)^{n}\tilde{c}^{\dagger}_{0-\sigma}\tilde{c}_{0\sigma}\hat{c}_{k-\sigma}b^{m};\tilde{\chi}^{\dagger}_{\sigma}\right\rangle\right\rangle\right.\\&\left.+\left\langle\left\langle\left(b^{\dagger}-\frac{\lambda}{\omega_0}\right)^{n}\hat{n}_{0\sigma}\hat{c}_{k\sigma}b^{m};\tilde{\chi}^{\dagger}_{\sigma}\right\rangle\right\rangle\right)-\sum_{k}V_k\left\langle\left\langle b^{\dagger n}\hat{a}^{\dagger}\hat{a}\hat{c}_{k\sigma}\left(b+\frac{\lambda}{\omega_0}\right)^{m};\tilde{\chi}^{\dagger}_{\sigma}\right\rangle\right\rangle.\end{aligned} \tag{32}$$

The different Green's functions on the right-hand side of Eq. (32), involving annihilation of electrons in the leads, are also calculated from their EOM. At this point, it is possible to contract pairs of operators $\hat{c}^{\dagger}_{k\sigma}$ and $\hat{c}_{k'\sigma'}$, like in the spinless case [Eqs. (15) and (16)]. This procedure gives the following approximate equations:

$$\begin{aligned}(\omega_{nm}-\epsilon_k)\langle\langle b^{\dagger n}\tilde{c}^{\dagger}_{0-\sigma}\tilde{c}_{0\sigma}\hat{c}_{k-\sigma}b^{m};\tilde{\chi}^{\dagger}_{\sigma}\rangle\rangle&\simeq-\left\langle b^{\dagger n}\tilde{\chi}^{\dagger}_{-\sigma}\hat{c}_{k-\sigma}\left(b+\frac{\lambda}{\omega_0}\right)^{m}\right\rangle_{\tilde{H}}\\&-V_k\langle n_{k-\sigma}\rangle\left\langle\left\langle\left(b^{\dagger}+\frac{\lambda}{\omega_0}\right)^{n}\tilde{\chi}_{\sigma}b^{m};\tilde{\chi}^{\dagger}_{\sigma}\right\rangle\right\rangle,\end{aligned} \tag{33}$$

$$\begin{aligned}(\omega_{nm}-\epsilon_k)\langle\langle b^{\dagger n}\hat{n}_{0\sigma}\hat{c}_{k\sigma}b^{m};\tilde{\chi}^{\dagger}_{\sigma}\rangle\rangle&\simeq-\left\langle b^{\dagger n}\tilde{\chi}^{\dagger}_{\sigma}\hat{c}_{k\sigma}\left(b+\frac{\lambda}{\omega_0}\right)^{m}\right\rangle_{\tilde{H}}\\&-V_k\langle n_{k\sigma}\rangle\left\langle\left\langle\left(b^{\dagger}+\frac{\lambda}{\omega_0}\right)^{n}\tilde{\chi}_{\sigma}b^{m};\tilde{\chi}^{\dagger}_{\sigma}\right\rangle\right\rangle,\end{aligned} \tag{34}$$

$$\begin{aligned}(\omega_{nm}-\epsilon_k)\langle\langle b^{\dagger n}\hat{a}^{\dagger}\hat{a}\hat{c}_{k\sigma}b^{m};\tilde{\chi}^{\dagger}_{\sigma}\rangle\rangle&\simeq\left\langle\left(b^{\dagger}-\frac{\lambda}{\omega_0}\right)^{n}\tilde{\chi}^{\dagger}_{\sigma}\hat{c}_{k\sigma}b^{m}\right\rangle_{\tilde{H}}\\&-V_k\langle 1-n_{k\sigma}\rangle\left\langle\left\langle b^{\dagger n}\tilde{\chi}_{\sigma}\left(b-\frac{\lambda}{\omega_0}\right)^{m};\tilde{\chi}^{\dagger}_{\sigma}\right\rangle\right\rangle.\end{aligned} \tag{35}$$

Equations (33)–(35) are then substituted into Eq. (32) producing a closed system of equations for the unknowns $\langle\langle b^{\dagger n}\tilde{\chi}_{\sigma}b^{m};\tilde{\chi}^{\dagger}_{\sigma}\rangle\rangle$. As in the spinless case, all the expectation values will be calculated assuming that electrons and phonons can be separated in the ground state at zero temperature. We have also checked in this case with explicit calculations that this does not alter the results. The resulting system of equations can be written as

$$\begin{aligned}&\left(\omega_{nm}-\tilde{\epsilon}_0-\Delta_{nm}-\sum_{k}\frac{V_k^2\langle n_k\rangle}{\omega_{nm}-\epsilon_k}\right)\langle\langle b^{\dagger n}\tilde{\chi}_{\sigma}b^{m};\tilde{\chi}^{\dagger}_{\sigma}\rangle\rangle\\&=\delta_{n0}\left(\frac{\lambda}{\omega_0}\right)^{m}\left\langle 1-\sum_{\sigma}\hat{n}_{0\sigma}\right\rangle+\delta_{m0}\left(-\frac{\lambda}{\omega_0}\right)^{n}\langle\hat{n}_{0\sigma}\rangle+(-1)^{n}\\&\times\left(\frac{\lambda}{\omega_0}\right)^{n+m}\sum_{k}V_k\langle\tilde{\chi}^{\dagger}_{-\sigma}\hat{c}_{k-\sigma}\rangle\left(\frac{2}{\omega_{0m}-\epsilon_k}-\frac{1}{\omega_{n0}-\epsilon_k}\right)\\&+\lambda\langle\langle b^{\dagger n}\tilde{\chi}_{\sigma}b^{m+1};\tilde{\chi}^{\dagger}_{\sigma}\rangle\rangle+\lambda\langle\langle b^{\dagger(n+1)}\tilde{\chi}_{\sigma}b^{m};\tilde{\chi}^{\dagger}_{\sigma}\rangle\rangle\\&+\sum_{l=0}^{m-1}\left(-\frac{\lambda}{\omega_0}\right)^{m-l}\langle\langle b^{\dagger n}\tilde{\chi}_{\sigma}b^{l};\tilde{\chi}^{\dagger}_{\sigma}\rangle\rangle\sum_{l'=l}^{m}(-1)^{m-l'}\binom{m}{l'}\\&\times\binom{l'}{l}\sum_{k}\frac{V_k^2\langle 1-n_k\rangle}{\omega_{nl'}-\epsilon_k}+2\sum_{l=0}^{n-1}\left(\frac{\lambda}{\omega_0}\right)^{n-l}\langle\langle b^{\dagger l}\tilde{\chi}_{\sigma}b^{m};\tilde{\chi}^{\dagger}_{\sigma}\rangle\rangle\\&\times\sum_{l'=l}^{n}(-1)^{n-l'}\binom{n}{l'}\binom{l'}{l}\sum_{k}\frac{V_k^2\langle n_k\rangle}{\omega_{l'm}-\epsilon_k}.\end{aligned} \tag{36}$$

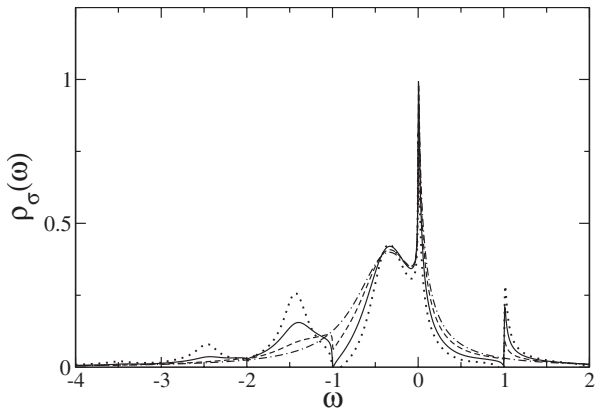

FIG. 6. The spectral density per spin as a function of ω, calculated by the EOM method to the order $O(V^2)$ for $\omega_0=1$, $\Delta=0.2\omega_0$, $\tilde{\epsilon}_0=-3\Delta$, and several values of λ/ω_0. $\lambda/\omega_0=0$ (dotted-dashed line), 0.3 (dashed line), 0.5 (continuous line), and 0.7 (dotted line).

The system of equations (36) reproduces the atomic limit ($V_k=0$) and in the limit $\lambda=0$ recovers the Green's function for interacting electrons approximated to $O(V^2)$, namely,

$$\langle\langle \hat{\chi}_\sigma;\hat{\chi}_\sigma^\dagger\rangle\rangle = \frac{1-\langle \hat{n}_{0-\sigma}\rangle + \sum_k \frac{V_k\langle \hat{\chi}_{-\sigma}^\dagger \hat{c}_{k-\sigma}\rangle}{\omega-\epsilon_k}}{\omega-\epsilon_0+i\Delta-\sum_k \frac{V_k^2\langle \hat{n}_k\rangle}{\omega-\epsilon_k}}. \tag{37}$$

In the Kondo regime, defined by $\epsilon_0\langle 0,|\epsilon_0|\rangle\Delta$, the self-energy $\Sigma_k \frac{V_k^2\langle n_k\rangle}{\omega-\epsilon_k}$ appearing in the denominator of Eq. (37) introduces two typical signatures of the electron-electron interaction: (i) a Kondo peak at the Fermi level, characteristic of spin fluctuations, although it is too narrow at this order of approximation when compared to exact results obtained from NRG calculations[41] and (ii) a shift in the position of the charge resonance from the one-electron value ϵ_0 to the renormalized value $\epsilon_0^*=\epsilon_0+\frac{\Delta}{\pi}Ln\frac{\pi D}{2\Delta}$. When the electron-phonon interaction is also connected, the structure of the left-hand side of Eq. (36) suggests that similar characteristics will appear at energies displaced from the $\lambda=0$ values by multiples of ω_0, with ϵ_0 changed to $\tilde{\epsilon}_0$ by virtue of the electron-phonon interaction. Figure 6 shows that this is indeed the case. In this figure we plot the density of states for $\tilde{\epsilon}_0=-3\Delta$ (Kondo regime) and $\Delta=0.2\omega_0$ for several values of λ. The $\lambda=0$ curve shows the charge resonance at $\epsilon_0^*\simeq-1.8\Delta$ and the Kondo peak at $\omega\simeq 0$. When λ increases, these two structures decrease in width accompanying the clear appearance of logarithmic singularities at $\omega\simeq\pm\omega_0$ and phonon sidebands. Clear Kondo sidebands appear only at positive frequencies in this completely asymmetric infinite-U model. The sidebands at negative frequencies correspond to the charge resonance displaced from $\tilde{\epsilon}_0{}^*$ by multiples of ω_0. In this calculation keeping $\tilde{\epsilon}_0$ fixed, the occupancy of the localized level does not change much with λ, tending to increase slightly with increasing λ. This means that the spectral weight below and above the Fermi level remains nearly constant since $\langle \hat{n}_{0\sigma}\rangle = \int_{-\infty}^0 d\omega\, \rho_\sigma(\omega)$ and $1-2\langle \hat{n}_{0\sigma}\rangle=\int_0^\infty d\omega\, \rho_\sigma(\omega)$. Therefore, the formation of sidebands at negative frequencies comes along with the reduction in spectral weight of the charge resonance at $\tilde{\epsilon}_0$ while Kondo sidebands grow basically from the main Kondo peak at $\omega\simeq 0$. However, the different physical origin of both kinds of resonances, namely, charge versus spin fluctuations, makes a different reduction factor for their widths. This point will be discussed later on.

The logarithmic singularities producing the Kondo sidebands and the appearance of the functions $\Delta_{ij}^{(e,h)}$ on the right-hand side of Eq. (36) call again for renormalization. This has been frequently done by considering in the problem a small value of the temperature.[25,44] Here, we will proceed like in the spinless case, that is, by taking a further step in the EOM method and keeping only those terms leading to regularization of these singularities. The result is that Eqs. (33)–(35) are modified as

$$\begin{aligned}(\omega_{nm}-\epsilon_k-\Sigma_{nm}^{(e)}(\omega_{nm}-\epsilon_k))\langle\langle b^{\dagger n}\tilde{c}_{0-\sigma}^\dagger \tilde{c}_{0\sigma}\hat{c}_{k-\sigma}b^m;\tilde{\chi}_\sigma^\dagger\rangle\rangle \\ \simeq -\left\langle b^{\dagger n}\tilde{\chi}_{-\sigma}^\dagger \hat{c}_{k-\sigma}\left(b+\frac{\lambda}{\omega_0}\right)^m\right\rangle_{\tilde{H}} \\ - V_k\langle n_{k-\sigma}\rangle\left\langle\left\langle\left(b^\dagger+\frac{\lambda}{\omega_0}\right)^n\tilde{\chi}_\sigma b^m;\tilde{\chi}_\sigma^\dagger\right\rangle\right\rangle,\end{aligned} \tag{38}$$

$$\begin{aligned}(\omega_{nm}-\epsilon_k-\Sigma_{nm}^{(e)}(\omega_{nm}-\epsilon_k))\langle\langle b^{\dagger n}\hat{n}_{0\sigma}\hat{c}_{k\sigma}b^m;\tilde{\chi}_\sigma^\dagger\rangle\rangle \\ \simeq -\left\langle b^{\dagger n}\tilde{\chi}_\sigma^\dagger \hat{c}_{k\sigma}\left(b+\frac{\lambda}{\omega_0}\right)^m\right\rangle_{\tilde{H}} \\ - V_k\langle n_{k\sigma}\rangle\left\langle\left\langle\left(b^\dagger+\frac{\lambda}{\omega_0}\right)^n\tilde{\chi}_\sigma b^m;\tilde{\chi}_\sigma^\dagger\right\rangle\right\rangle,\end{aligned} \tag{39}$$

$$\begin{aligned}(\omega_{nm}-\epsilon_k-2\Sigma_{nm}^{(h)}(\omega_{nm}-\epsilon_k))\langle\langle b^{\dagger n}\hat{a}^\dagger\hat{a}\hat{c}_{k\sigma}b^m;\tilde{\chi}_\sigma^\dagger\rangle\rangle \\ \simeq \left\langle\left(b^\dagger-\frac{\lambda}{\omega_0}\right)^n\tilde{\chi}_\sigma^\dagger\hat{c}_{k\sigma}b^m\right\rangle_{\tilde{H}} \\ - V_k\langle 1-n_{k\sigma}\rangle\left\langle\left\langle b^{\dagger n}\tilde{\chi}_\sigma\left(b-\frac{\lambda}{\omega_0}\right)^m;\tilde{\chi}_\sigma^\dagger\right\rangle\right\rangle\end{aligned} \tag{40}$$

with $\Sigma_{ij}^{(e,h)}(x)$ defined in Eq. (26). The lack of electron-hole symmetry in this infinite-U limit manifests itself in the factor of 2 multiplying the hole self-energy $\Sigma_{ij}^{(h)}(x)$ with respect to the electron self-energy $\Sigma_{ij}^{(e)}(x)$. Finally the set of linear equations we have to solve in this limit is

$$(\omega_{nm}-\tilde{\epsilon}_0-\Delta_{nm}-\Sigma_{nm}(\omega_{nm}))\langle\langle b^{\dagger n}\tilde{\chi}_\sigma b^m;\tilde{\chi}_\sigma^\dagger\rangle\rangle=\delta_{n0}\left(\frac{\lambda}{\omega_0}\right)^m\left\langle 1-\sum_\sigma \hat{n}_{0\sigma}\right\rangle+\delta_{m0}\left(-\frac{\lambda}{\omega_0}\right)^n\langle\hat{n}_{0\sigma}\rangle+(-1)^n\left(\frac{\lambda}{\omega_0}\right)^{n+m}\sum_k V_k\langle\tilde{\chi}_{-\sigma}^\dagger\hat{c}_{k-\sigma}\rangle$$
$$\times\left(\frac{2}{\omega_{0m}-\epsilon_k-\Sigma_{nm}^{(e)}(\omega_{0m}-\epsilon_k)}-\frac{1}{\omega_{n0}-\epsilon_k-2\Sigma_{nm}^{(h)}(\omega_{n0}-\epsilon_k)}\right)+\lambda\langle\langle b^{\dagger n}\tilde{\chi}_\sigma b^{m+1};\tilde{\chi}_\sigma^\dagger\rangle\rangle$$
$$+\lambda\langle\langle b^{\dagger(n+1)}\tilde{\chi}_\sigma b^m;\tilde{\chi}_\sigma^\dagger\rangle\rangle+\sum_{l=0}^{m-1}\left(-\frac{\lambda}{\omega_0}\right)^{m-l}\langle\langle b^{\dagger n}\tilde{\chi}_\sigma b^l;\tilde{\chi}_\sigma^\dagger\rangle\rangle\sum_{l'=l}^{m}(-1)^{m-l'}\binom{m}{l'}\binom{l'}{l}$$
$$\times\Delta_{nl'}^{(h)}(\omega_{nl'})+2\sum_{l=0}^{n-1}\left(\frac{\lambda}{\omega_0}\right)^{n-l}\langle\langle b^{\dagger l}\tilde{\chi}_\sigma b^m;\tilde{\chi}_\sigma^\dagger\rangle\rangle\sum_{l'=l}^{n}(-1)^{n-l'}\binom{n}{l'}\binom{l'}{l}\Delta_{l'm}^{(e)}(\omega_{l'm}),\quad(41)$$

where we have defined

$$\Sigma_{nm}(\omega_{nm})=\sum_k V_k^2\langle n_k\rangle\left(\frac{2}{\omega_{nm}-\epsilon_k-\Sigma_{nm}^{(e)}(\omega_{nm}-\epsilon_k)}-\frac{1}{\omega_{nm}-\epsilon_k-2\Sigma_{nm}^{(h)}(\omega_{nm}-\epsilon_k)}\right),\quad(42)$$

$$\Delta_{ij}^{(e)}(\omega_{ij})=\sum_k V_k^2\frac{\langle n_k\rangle}{\omega_{ij}-\epsilon_k-\Sigma_{ij}^{(e)}(\omega_{ij}-\epsilon_k)},\quad(43)$$

and

$$\Delta_{ij}^{(h)}(\omega_{ij})=\sum_k V_k^2\frac{1-\langle n_k\rangle}{\omega_{ij}-\epsilon_k-2\Sigma_{ij}^{(h)}(\omega_{ij}-\epsilon_k)}.\quad(44)$$

We first analyze our results in the Kondo regime defined by $\tilde{\epsilon}_0<0$ and $|\tilde{\epsilon}_0|>\Delta$. In Fig. 7 we present the density of states in the region of the Kondo peak for fixed values of Δ, $\tilde{\epsilon}_0=-3\Delta$, and $\frac{\lambda}{\omega_0}=0.6$. For $\omega_0=\Delta$, we show our results calculated to the order $O(V^2)$ [Eq. (36)] and including corrections to the order $O(V^4)$ [Eq. (41)]. We see that the inclusion of these higher-order corrections has two effects: (i) it increases the width of the main Kondo peak through the term $\Sigma_{00}(\omega_{00})$, in agreement with the case of zero electron-phonon interaction discussed in Ref. 41 and (ii) the logarithmic singularity at $\omega\simeq-\omega_0$ is significantly regularized, while leaving the Kondo sidebands essentially unchanged. Results for a value of $\omega_0=0.5\Delta$ are also shown in this figure, which are in partial agreement with those of Ref. 25 obtained for similar values of the input parameters. The main difference from our results is that we find Kondo sidebands only at positive frequencies and ours are of smaller intensity. At negative frequencies and $\omega\simeq-\omega_0$ we always find rather weak features if $\omega_0<\Delta$. Also note in Fig. 7 how the intensity of the Kondo sidebands increases with ω_0, becoming more prominent for $\omega_0>T_K$, with T_K being the width of the Kondo peak. Their intensity is taken from the main Kondo resonance, making it narrower with increasing ω_0 even if $g=(\lambda/\omega_0)^2$ is kept fixed. Therefore, T_K depends not only on g but on ω_0 as well. This was already noted by Hewson and Meyer.[30]

Other works[44] assume the electron-phonon interaction to be stronger than the hopping interaction and perform a polaronic approximation that decouples electrons and phonons directly in the Hamiltonian by substituting $\tilde{c}_{0\sigma}$ by $\hat{c}_{0\sigma}\langle\exp[-\frac{\lambda}{\omega_0}(b^\dagger-b)]\rangle\equiv\hat{c}_{0\sigma}e^{-g/2}$. This is tantamount to substituting the couplings V_k for $\tilde{V}_k=V_ke^{-g/2}$ in Eq. (27) or Eq. (28). Then, defining

$$\Delta_r=\Delta e^{-g}\quad(45)$$

the width of the charge resonance should be about $2\Delta_r$ and the width of the Kondo peak, in the infinite-U limit, scale as[49]

$$T_K=(D\Delta_r)^{1/2}\exp[-\pi|\tilde{\epsilon}_0|/2\Delta_r].\quad(46)$$

This formula implies the very quick narrowing of the Kondo resonance with g seen in Ref. 44 but not in our results of Fig. 6. As we have anticipated, the charge resonance and the Kondo resonance have a different physical origin and they behave differently when g changes. We have checked that T_K, defined as the full width at half maximum of our calculated Kondo peak, follows an exponential decrease with $|\tilde{\epsilon}_0|$ when Δ and $\frac{\lambda}{\omega_0}$ (or Δ_r) are fixed. This result implies that the width of the Kondo peak will depend exponentially on a

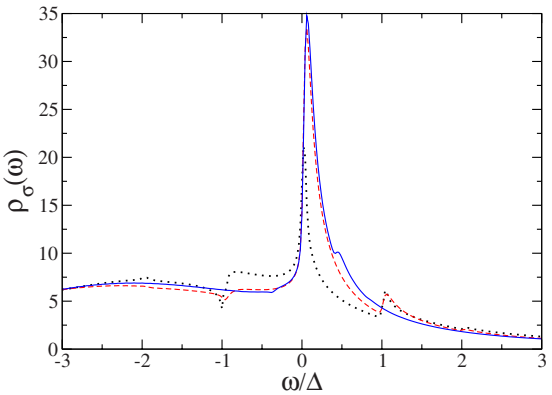

FIG. 7. (Color online) The spectral density per spin as a function of ω/Δ for $\tilde{\epsilon}_0=-3\Delta$ and $\lambda/\omega_0=0.6$ for $\omega_0=\Delta$ calculated to the order $O(V^2)$ (dotted black line) and to the order $O(V^4)$ (dashed red line) and for $\omega_0=0.5\Delta$ calculated to the order $O(V^4)$ (continuous blue line).

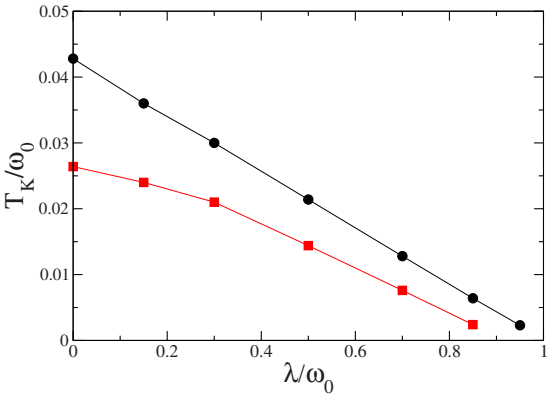

FIG. 8. (Color online) The width of the Kondo resonance as a function of λ/ω_0 for $\omega_0=1$, $\Delta=0.2\omega_0$, and for $\tilde{\epsilon}_0=-3\Delta$ (dots, black line) and $\tilde{\epsilon}_0=-3.5\Delta$ (squares, red line).

gate voltage applied to the localized level for $\frac{\lambda}{\omega_0}\leq 1$, in agreement with calculations using NRG techniques.[34]

Next we keep $\tilde{\epsilon}_0$ and Δ fixed and change $\frac{\lambda}{\omega_0}$. Figure 8 shows T_K versus $\frac{\lambda}{\omega_0}$ for $\Delta=0.2\omega_0$, $\tilde{\epsilon}_0=-3.5\Delta$, and $\tilde{\epsilon}_0=-3\Delta$, demonstrating that the width of the Kondo resonance decreases rather linearly with $\frac{\lambda}{\omega_0}$ in the range of values $0<\frac{\lambda}{\omega_0}\leq 1$ where the width can be extracted from our calculations with good accuracy. Thus we think that the kind of polaronic decoupling proposed in Ref. 44 is not appropriate, in general, to investigate the vicinity of the Fermi level. We remark that our method, like the one of Ref. 44, is an EOM method, but ours provides a much better description of the Kondo physics for $\lambda=0$ (Ref. 41) and moreover we do not decouple electrons and phonons.

The situation just described changes if we are interested in the width of the charge resonance at $\tilde{\epsilon}_0$. Figure 9 shows the evolution of this resonance with $\frac{\lambda}{\omega_0}$ for $\tilde{\epsilon}_0=-4\Delta$ and $\Delta=0.2\omega_0$. It is interesting to note how the transfer of spectral weight to the sidebands of lower energy causes the decrease in width of the resonance and the formation of a pseudogap at $\omega=-\omega_0$.

We roughly measure the half width of the charge resonance as the half width at half maximum on the left hand-

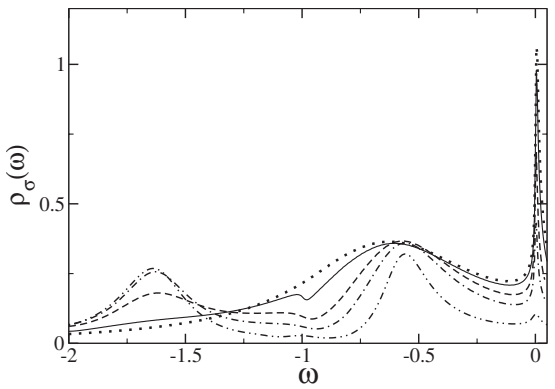

FIG. 9. The spectral density per spin as a function of ω, for $\omega_0=1$, $\tilde{\epsilon}_0=-4\Delta$, and $\Delta=0.2\omega_0$, for several values of λ: $\lambda/\omega_0=0$ (dotted line), 0.3 (continuous line), 0.6 (dashed line), 0.8 (dotted-dashed line), and 1.2 (dotted-dotted-dashed line).

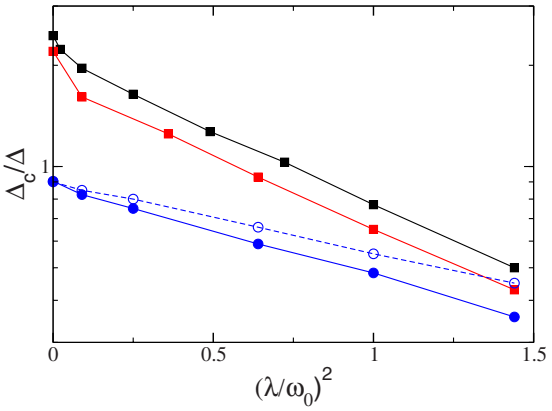

FIG. 10. (Color online) The half width of the charge resonance Δ_c (in units of the single-particle width Δ) as a function of $(\lambda/\omega_0)^2$ in the Kondo regime, with $\omega_0=5\Delta$ and $\tilde{\epsilon}_0=-3\Delta$ (black squares) and $\tilde{\epsilon}_0=-3.5\Delta$ (red squares). Also shown is the mixed-valence case of $\tilde{\epsilon}_0=0$ and two values of ω_0: $\omega_0=5\Delta$ (blue full circles) and $\omega_0=2\Delta$ (blue empty circles).

side of the maximum since these resonances are asymmetric in the Kondo regime. The half width of the charge resonance as a function of $\frac{\lambda}{\omega_0}$ is represented in Fig. 10 for two values of $\tilde{\epsilon}_0$ in the Kondo regime and also for the value $\tilde{\epsilon}_0=0$, characteristic of the mixed-valence regime. An exact exponential decrease with $(\lambda/\omega_0)^2$ is found, which is the same result predicted by Eq. (45) and already discussed in the spinless case. However, the slope depends on $\tilde{\epsilon}_0$ and also on ω_0, as it is evident in the figure. This again points out to the inaccuracy of simple polaronic approximations to the problem. We should comment that, since the calculations presented here are also approximated, it may happen that a better solution will change the linear scaling of the Kondo width with λ/ω_0, presented in Fig. 8. However, this calculation shows that the Kondo resonance is more robust that the charge resonance for increasing electron-phonon coupling since the latter decreases exponentially while the decrease in width of the former is certainly weaker.

Figure 11 shows the density of states for $\tilde{\epsilon}_0=0$ typical of

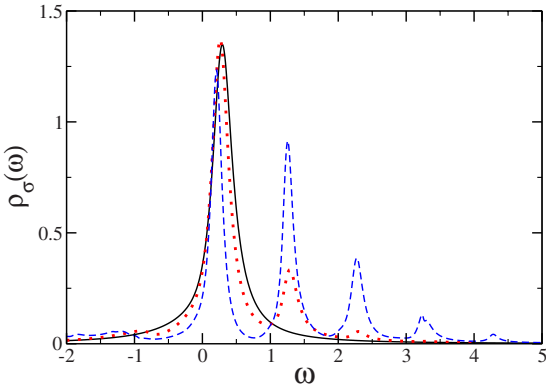

FIG. 11. (Color online) The spectral density per spin as a function of ω, for $\omega_0=1$, $\tilde{\epsilon}_0=0$ and $\Delta=0.2\omega_0$, for several values of λ: $\lambda/\omega_0=0$ (continuous black line), 0.5 (dotted red line), and 1.0 (dashed blue line).

the mixed-valence regime. In this case the spectral weight is predominantly on the positive frequency side and presents similar features to the ones discussed for charge fluctuations in the Kondo regime, with the more interesting one being the formation of pseudogaps at nearly all positive multiples of ω_0. The same situation appears in the empty orbital regime $\epsilon_0 \geq \Delta$ and we will not discuss it further. Finally, we mention here that, even for $\frac{\lambda}{\omega_0} > 1$, where there is not a single-charge resonance but a series of sidebands, the transfer of spectral weight from negative to positive frequencies is very quick when ϵ_0 changes from the Kondo to the empty orbital regime. This is because the occupancy of the level changes very quickly from $\langle \hat{n}_{0\sigma} \rangle \simeq 0.5$ to $\langle \hat{n}_{0\sigma} \rangle \simeq 0$, in agreement with the NRG calculations of Refs. 32 and 34, even though we analyze the infinite-U limit.

IV. CONCLUSIONS

In this work we present an EOM method to analyze the electronic properties of a small system consisting of a localized level coupled to metallic electrodes and to a local phonon. This is modeled by the Anderson-Holstein Hamiltonian. Two versions of this Hamiltonian, namely, spinless electrons and interacting electrons in the infinite-U limit, are studied in equilibrium and at zero temperature, as a previous step to address more realistic and out of equilibrium problems. Differently from previous approaches to the same Hamiltonian using the EOM, in which the electronic and vibronic degrees of freedom are decoupled, we keep quantum coherence between the electron at the localized level and the phonons. Another difference we present in this work is to go beyond the usual decoupling of the localized level and the leads, leading to an approximation valid to the order $O(V^2)$, by including further order corrections which are important for a better description of Kondo physics.

We are interested in the quantum strong-coupling regime $\lambda \gg \Delta$ and focus our study in the evolution of the charge and spin resonances with increasing values of the electron-phonon coupling parameter λ. We systematically find that the width of the charge resonances decreases exponentially with $(\lambda/\omega_0)^2$, both for spinless and interacting electrons. This fact is corroborated by the comparison with the results obtained using the ISA method, in the spinless case. However, the spin (Kondo) resonances are reduced in width linearly with λ/ω_0. We find this behavior to be different from simple polaronic approximations based on decoupling of electrons and phonons, which treat both kinds of resonances on a similar footing. Since electrons and phonons are not decoupled, we expect our approximation to be more appropriate to investigate the region of energies near the Fermi level in cases when the Kondo effect is strong. The method can be straightforwardly generalized to finite temperatures, even though this will be computationally more demanding because a much larger number of the Green's functions should be evaluated. It can also be generalized to nonequilibrium cases where a bias voltage is applied to the leads, in the same way it has already done in the absence of the electron-phonon interaction.[41]

ACKNOWLEDGMENTS

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APPENDIX: EOM BEYOND $O(V^2)$

In this appendix we give details of the EOM method presented in this work and also indicate how the self-energies $\Sigma_{ij}^{(e,h)}$ are obtained. The first step of the method has been explained in the text. The next step consists of calculating the Green's functions $\langle\langle b^{\dagger i}\tilde{c}_0\hat{c}_{k'}^{\dagger}, \hat{c}_k b^j; \tilde{c}_0^{\dagger}\rangle\rangle$ and $\langle\langle b^{\dagger i}\tilde{c}_0^{\dagger}\hat{c}_{k'}, \hat{c}_k b^j; \tilde{c}_0^{\dagger}\rangle\rangle$, appearing on the right-hand side of Eqs. (15) and (16), by means of their EOM. For $\langle\langle b^{\dagger i}\tilde{c}_0\hat{c}_{k'}^{\dagger}, \hat{c}_k b^j; \tilde{c}_0^{\dagger}\rangle\rangle$ we get

$$
\begin{aligned}
&(\omega_{ij} - \tilde{\epsilon}_0 + \epsilon_k' - \epsilon_k)\langle\langle b^{\dagger i}\tilde{c}_0\hat{c}_{k'}^{\dagger}, \hat{c}_k b^j; \tilde{c}_0^{\dagger}\rangle\rangle \\
&\quad = \left\langle \left(b^{\dagger} - \frac{\lambda}{\omega_0}\right)^i \tilde{c}_0^{\dagger}\tilde{c}_0\hat{c}_{k'}^{\dagger}\hat{c}_k b^j \right\rangle_{\tilde{H}} \\
&\quad + \left\langle b^{\dagger i}\tilde{c}_0\tilde{c}_0^{\dagger}\hat{c}_{k'}^{\dagger}\hat{c}_k\left(b + \frac{\lambda}{\omega_0}\right)^j \right\rangle_{\tilde{H}} \\
&\quad + \lambda\langle\langle b^{\dagger(i+1)}\tilde{c}_0\hat{c}_{k'}^{\dagger}, \hat{c}_k b^j; \tilde{c}_0^{\dagger}\rangle\rangle + \lambda\langle\langle b^{\dagger i}\tilde{c}_0\hat{c}_{k'}^{\dagger}, \hat{c}_k b^{j+1}; \tilde{c}_0^{\dagger}\rangle\rangle \\
&\quad - \sum_{k''} V_{k''}\left(\left\langle\left\langle\left(b^{\dagger} - \frac{\lambda}{\omega_0}\right)^i \tilde{c}_0^{\dagger}\tilde{c}_0\hat{c}_{k''}\hat{c}_{k'}^{\dagger}, \hat{c}_k b^j; \tilde{c}_0^{\dagger}\right\rangle\right\rangle\right. \\
&\quad \left. + \left\langle\left\langle b^{\dagger i}\tilde{c}_0\tilde{c}_0^{\dagger}\hat{c}_{k'}^{\dagger}\hat{c}_k\hat{c}_{k''}\left(b + \frac{\lambda}{\omega_0}\right)^j; \tilde{c}_0^{\dagger}\right\rangle\right\rangle\right).
\end{aligned}
\tag{A1}
$$

Next, in the last two terms of Eq. (A1) we perform all possible contractions of operators $\hat{c}_{k'}^{\dagger}$ and $\hat{c}_k$ as

$$
\begin{aligned}
&\left\langle\left\langle\left(b^{\dagger} - \frac{\lambda}{\omega_0}\right)^i \tilde{c}_0^{\dagger}\tilde{c}_0\hat{c}_{k''}\hat{c}_{k'}^{\dagger}, \hat{c}_k b^j; \tilde{c}_0^{\dagger}\right\rangle\right\rangle \\
&\quad \simeq \langle n_k\rangle\delta_{k,k'}\left\langle\left\langle\left(b^{\dagger} - \frac{\lambda}{\omega_0}\right)^i \tilde{c}_0^{\dagger}\tilde{c}_0\hat{c}_{k''}b^j; \tilde{c}_0^{\dagger}\right\rangle\right\rangle \\
&\quad + \langle 1 - n_k'\rangle\delta_{k'k''}\left\langle\left\langle\left(b^{\dagger} - \frac{\lambda}{\omega_0}\right)^i \tilde{c}_0^{\dagger}\tilde{c}_0\hat{c}_k b^j; \tilde{c}_0^{\dagger}\right\rangle\right\rangle
\end{aligned}
\tag{A2}
$$

and

$$
\begin{aligned}
&\left\langle\left\langle b^{\dagger i}\tilde{c}_0\tilde{c}_0^{\dagger}\hat{c}_{k'}^{\dagger}\hat{c}_k\hat{c}_{k''}\left(b + \frac{\lambda}{\omega_0}\right)^j; \tilde{c}_0^{\dagger}\right\rangle\right\rangle \\
&\quad \simeq \langle n_k\rangle\delta_{k,k'}\left\langle\left\langle b^{\dagger i}\tilde{c}_0\tilde{c}_0^{\dagger}\hat{c}_{k''}\left(b + \frac{\lambda}{\omega_0}\right)^j; \tilde{c}_0^{\dagger}\right\rangle\right\rangle \\
&\quad - \langle n_k'\rangle\delta_{k',k''}\left\langle\left\langle b^{\dagger i}\tilde{c}_0\tilde{c}_0^{\dagger}\hat{c}_k\left(b + \frac{\lambda}{\omega_0}\right)^j; \tilde{c}_0^{\dagger}\right\rangle\right\rangle.
\end{aligned}
\tag{A3}
$$

Equations (A2) and (A3) can now be substituted into Eq. (A1). However, the correction we are looking for is more conveniently calculated in terms of the difference of operators $\hat{c}_{k'}^{\dagger}\hat{c}_k-\langle n_k\rangle\delta_{kk'}$. Then, the use of these three equations together with the general equation (14) yields

$$\begin{aligned}(\omega_{ij}-\tilde{\epsilon}_0+\epsilon_k'-\epsilon_k)\langle\langle b^{\dagger i}\tilde{c}_0(\hat{c}_{k'}^{\dagger}\hat{c}_k-\langle n_k\rangle\delta_{k,k'})b^j;\tilde{c}_0^{\dagger}\rangle\rangle \\ \simeq \lambda\langle\langle b^{\dagger(i+1)}\tilde{c}_0(\hat{c}_{k'}^{\dagger}\hat{c}_k-\langle n_k\rangle\delta_{k,k'})b^j;\tilde{c}_0^{\dagger}\rangle\rangle \\ +\lambda\langle\langle b^{\dagger i}\tilde{c}_0(\hat{c}_{k'}^{\dagger}\hat{c}_k-\langle n_k\rangle\delta_{k,k'})b^{j+1};\tilde{c}_0^{\dagger}\rangle\rangle \\ -V_k'\langle 1-n_k'\rangle\left\langle\left\langle\left(b^{\dagger}-\frac{\lambda}{\omega_0}\right)^i\tilde{c}_0^{\dagger}\tilde{c}_0\hat{c}_k b^j;\tilde{c}_0^{\dagger}\right\rangle\right\rangle \\ +V_k'\langle n_k'\rangle\left\langle\left\langle b^{\dagger i}\tilde{c}_0\tilde{c}_0^{\dagger}\hat{c}_k\left(b+\frac{\lambda}{\omega_0}\right)^j;\tilde{c}_0^{\dagger}\right\rangle\right\rangle. \end{aligned} \tag{A4}$$

Using identical procedure we also obtain

$$\begin{aligned}(\omega_{ij}-\tilde{\epsilon}_0-\epsilon_k'-\epsilon_k)\langle\langle b^{\dagger i}\tilde{c}_0^{\dagger}\hat{c}_{k'}\hat{c}_k b^j;\tilde{c}_0^{\dagger}\rangle\rangle \\ \simeq -\lambda\langle\langle b^{\dagger(i+1)}\tilde{c}_0^{\dagger}\hat{c}_{k'}\hat{c}_k b^j;\tilde{c}_0^{\dagger}\rangle\rangle-\lambda\langle\langle b^{\dagger i}\tilde{c}_0^{\dagger}\hat{c}_{k'}\hat{c}_k b^{j+1};\tilde{c}_0^{\dagger}\rangle\rangle \\ +V_k'\langle n_k'\rangle\left\langle\left\langle\left(b^{\dagger}+\frac{\lambda}{\omega_0}\right)^i\tilde{c}_0\tilde{c}_0^{\dagger}\hat{c}_k b^j;\tilde{c}_0^{\dagger}\right\rangle\right\rangle \\ -V_k\langle n_k\rangle\left\langle\left\langle\left(b^{\dagger}+\frac{\lambda}{\omega_0}\right)^i\tilde{c}_0\tilde{c}_0^{\dagger}\hat{c}_{k'}b^j;\tilde{c}_0^{\dagger}\right\rangle\right\rangle \\ -V_k'\langle 1-n_k'\rangle\left\langle\left\langle b^{\dagger i}\tilde{c}_0^{\dagger}\tilde{c}_0\hat{c}_k\left(b-\frac{\lambda}{\omega_0}\right)^j;\tilde{c}_0^{\dagger}\right\rangle\right\rangle \\ +V_k\langle 1-n_k\rangle\left\langle\left\langle b^{\dagger i}\tilde{c}_0^{\dagger}\tilde{c}_0\hat{c}_{k'}\left(b-\frac{\lambda}{\omega_0}\right)^j;\tilde{c}_0^{\dagger}\right\rangle\right\rangle. \end{aligned} \tag{A5}$$

Equations (A4) and (A5) can now be substituted into Eqs. (15) and (16), producing a closed system of equations which will provide a solution for $\langle\langle\tilde{c}_0;\tilde{c}_0^{\dagger}\rangle\rangle$ to the order $O(V^4)$ and all order in λ. However, the structure of Eqs. (A4) and (A5) is similar to that of Eq. (14) in that all of the Green's functions $\langle\langle b^{\dagger i}\hat{O}b^j;\tilde{c}_0^{\dagger}\rangle\rangle$ for varying i and j are linked. Here $\hat{O}$ denotes operators $\tilde{c}_0(\hat{c}_{k'}^{\dagger}\hat{c}_k-\langle n_k\rangle\delta_{k,k'})$ and $\tilde{c}_0^{\dagger}\hat{c}_{k'}\hat{c}_k$ in Eqs. (A4) and (A5), respectively. Moreover, note that these operators involve creation/annihilation of any state in the leads. Therefore a full solution is too demanding. At the moment we shall be interested in the renormalization of the denominators appearing in the functions $\Delta_{ij}^{(e,h)}$ and this can be done analytically. We illustrate the procedure in the following.

Consider Eq. (15) rewritten in terms of the difference of operators $\hat{c}_{k'}^{\dagger}\hat{c}_k-\langle n_k\rangle\delta_{kk'}$,

$$\begin{aligned}(\omega-\epsilon_k+(n-m)\omega_0)\langle\langle b^{\dagger n}\tilde{c}_0^{\dagger}\tilde{c}_0\hat{c}_k b^m;\tilde{c}_0^{\dagger}\rangle\rangle \\ =-\left\langle b^{\dagger n}\tilde{c}_0^{\dagger}\hat{c}_k\left(b+\frac{\lambda}{\omega_0}\right)^m\right\rangle_{\tilde{H}}-V_k\langle n_k\rangle \\ \times\left\langle\left\langle\left(b^{\dagger}+\frac{\lambda}{\omega_0}\right)^n\tilde{c}_0\hat{c}_{k'}^{\dagger}\hat{c}_k b^m;\tilde{c}_0^{\dagger}\right\rangle\right\rangle \\ -\sum_{i=0}^{n}\binom{n}{i}\left(\frac{\lambda}{\omega_0}\right)^{n-i} \\ \times\sum_{k'}V_{k'}'\langle\langle b^{\dagger i}\tilde{c}_0(\hat{c}_{k'}^{\dagger}\hat{c}_k-\langle n_k\rangle\delta_{kk'})b^m;\tilde{c}_0^{\dagger}\rangle\rangle \\ -\sum_{j=0}^{m}\binom{m}{j}\left(\frac{\lambda}{\omega_0}\right)^{m-j}\sum_{k'}V_{k'}'\langle\langle b^{\dagger n}\tilde{c}_0^{\dagger}\hat{c}_{k'}\hat{c}_k b^j;\tilde{c}_0^{\dagger}\rangle\rangle, \end{aligned} \tag{A6}$$

where the Green's functions of the last two terms on the right-hand side of Eq. (A6) have to be found from Eqs. (A4) and (A5), respectively. These equations are of the general form

$$\begin{aligned}(\omega_{ij}-E)\langle\langle b^{\dagger i}\hat{O}b^j;\tilde{c}_0^{\dagger}\rangle\rangle \\ =\lambda\langle\langle b^{\dagger(i+1)}\hat{O}b^j;\tilde{c}_0^{\dagger}\rangle\rangle+\lambda\langle\langle b^{\dagger i}\hat{O}b^{j+1};\tilde{c}_0^{\dagger}\rangle\rangle+S_{ij} \end{aligned} \tag{A7}$$

which has the formal solution

$$\begin{aligned}\langle\langle b^{\dagger i}\hat{O}b^j;\tilde{c}_0^{\dagger}\rangle\rangle=\sum_{l=0}^{\infty}\frac{1}{l!}\left(\frac{\lambda}{\omega_0}\right)^l\sum_{l'=0}^{\infty}\frac{1}{l'!}\left(-\frac{\lambda}{\omega_0}\right)^{l'}S_{i+l,j+l'} \\ \times\sum_{m=0}^{l}(-1)^m\binom{l}{m}\sum_{m'=0}^{l'}(-1)^{m'}\binom{l'}{m'} \\ \times\frac{1}{\omega+(i+m-j-m')\omega_0-E}. \end{aligned} \tag{A8}$$

For $\hat{O}=\tilde{c}_0(\hat{c}_{k'}^{\dagger}\hat{c}_k-\langle n_k\rangle\delta_{kk'})$, the "source" function given in Eq. (A4) is

$$\begin{aligned}S_{ij}=V_k'\langle 1-n_k'\rangle\left\langle\left\langle\left(b^{\dagger}-\frac{\lambda}{\omega_0}\right)^i\tilde{c}_0^{\dagger}\tilde{c}_0\hat{c}_k b^j;\tilde{c}_0^{\dagger}\right\rangle\right\rangle \\ +V_k'\langle n_k'\rangle\left\langle\left\langle b^{\dagger i}\tilde{c}_0\tilde{c}_0^{\dagger}\hat{c}_k\left(b+\frac{\lambda}{\omega_0}\right)^j;\tilde{c}_0^{\dagger}\right\rangle\right\rangle. \end{aligned} \tag{A9}$$

When Eq. (A9) is first substituted into Eq. (A8) and then into Eq. (A6), we get terms proportional to $\langle\langle b^{\dagger n'}\tilde{c}_0^{\dagger}\tilde{c}_0\hat{c}_k b^{m'};\tilde{c}_0^{\dagger}\rangle\rangle$ and to $\langle\langle b^{\dagger n'}\tilde{c}_0\tilde{c}_0^{\dagger}\hat{c}_k b^{m'};\tilde{c}_0^{\dagger}\rangle\rangle$, with all possible values of m' and n', which render a full solution difficult to obtain. Since we want to renormalize denominators, we only keep the term strictly proportional to $\langle\langle b^{\dagger n}\tilde{c}_0^{\dagger}\tilde{c}_0\hat{c}_k b^m;\tilde{c}_0^{\dagger}\rangle\rangle$. This term is

$$\begin{aligned}\sum_{i=0}^{n}\binom{n}{i}\sum_{l=n-i}^{\infty}\frac{(-1)^l}{l!}\binom{i+l}{n}\left(\frac{\lambda}{\omega_0}\right)^{2l}\sum_{m'=0}^{l}(-1)^{m'}\binom{l}{m'} \\ \times\sum_{k'}V_{k'}^2\frac{1-\langle n_{k'}\rangle}{\omega-E+(n-i+m'-m)\omega_0}. \end{aligned} \tag{A10}$$

Finally, by making use of the identity

$$\sum_{i=0}^{\infty}(-1)^i\left(\frac{\lambda}{\omega_0}\right)^{2(i+l)}\frac{(i+n)!}{i!}\sum_{j=0}^{i+l}\frac{(-1)^j}{j!\,(i+l-j)!}\frac{1}{w+(n-l+j)\omega_0}$$
$$=(-1)^{n-l}\left(\frac{\lambda}{\omega_0}\right)^{2l}e^{-(\lambda/\omega_0)^2}\sum_{j=0}^{\infty}\frac{1}{j!}\left(\frac{\lambda}{\omega_0}\right)^{2j}\sum_{m=0}^{n}(-1)^m\binom{n}{m}$$
$$\times\frac{(j+m)!}{(j+m-n+l)!}\frac{1}{w+(j+m)\omega_0}, \tag{A11}$$

we obtain the first term of $\Sigma_{ij}^{(e)}$ in Eq. (26). The second term of Eq. (26) is obtained from the same analysis of the Green's function $\langle\langle b^{\dagger n}\tilde{c}_0^{\dagger}\hat{c}_{k'}\hat{c}_k b^j;\tilde{c}_0^{\dagger}\rangle\rangle$ [Eq. (A5)] for which the source term is

$$S_{ij}=V_k'\langle 1-n_k'\rangle\left\langle\left\langle b^{\dagger i}\tilde{c}_0^{\dagger}\tilde{c}_0\hat{c}_k\left(b-\frac{\lambda}{\omega_0}\right)^j;\tilde{c}_0^{\dagger}\right\rangle\right\rangle$$
$$+V_k'\langle n_k'\rangle\left\langle\left\langle\left(b^{\dagger}+\frac{\lambda}{\omega_0}\right)^i\tilde{c}_0\tilde{c}_0^{\dagger}\hat{c}_k b^j;\tilde{c}_0^{\dagger}\right\rangle\right\rangle. \tag{A12}$$

Finally, repeating the procedure in Eq. (16), one obtains $\Sigma_{ij}^{(h)}$.

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