Coherent-state functional-integral approach to high-field transport in coupled electron-phonon systems

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Coherent-state functional-integral methods are used to develop approximation schemes for the description of coupled electron-phonon systems far from equilibrium. We consider an interacting-electron system which is coupled to a system of phonons and subjected to an external—not necessarily weak—perturbation. For systems where the electron-phonon interaction is linear in the phonon variables, the phonon degrees of freedom can be accounted for exactly. From a formally exact representation of a suitable generating function for the expectation value of electronic observables, approximation schemes based on mean-field solutions can be derived. Within the lowest order of approximation, the coupled electron-phonon system may be treated as a self-consistent system of indepenent electrons. Higher-order corrections are shown to give a random-phase approximation based on self-consistent mean fields. This approach is applied to electronic two-level systems coupled to phonons under a large external bias. We find that the coupling to acoustical-phonon modes leads to a damping of the quantum beats and drives the system into a new equilibrium state. The coupling to LO phonons is shown to account correctly for resonance effects which arise when the level splitting is close to the LO-phonon energy.

I. INTRODUCTION

It can be shown that a very important class of coupled electron-phonon systems in thermal equilibrium can be conveniently treated by functional-integral techniques.[1] This class of systems is standard in transport theory, as well as the theory of superconductivity, and is characterized by an electron-phonon coupling which is linear in the phonon creation and annihilation operators and quadratic in the corresponding electron operators.[2,3] Here, we extend our approach to treat the nonequilibrium state. We believe that functional integrals offer a physically more transparent approach to many-body problems than the more commonly used diagrammatic techniques. The motivation for this work is to develop a functional-integral formulation of high-field quantum transport in electron-phonon systems. In particular, we are interested in a microscopic formulation which can account for charge transport in solids where the charge carriers (strongly) interact with each other and the lattice ions. Virtually every solid-state problem, of course, is a coupled electron-phonon problem and various quantum transport theories have been formulated in the past.[4] Due to the complexity of the problem, however, either formally exact, but very complicated, or more tractable, but rather phenomenological approaches, have been developed.[5,6] For the former, the Keldysh-Baym-Kadanoff formalism is probably the most widely pursued approach. Progress in this direction has been seriously hampered by its complexity. Without the incorporation of simplifying *ad hoc* assumptions, it seems to be hopeless to apply this formalism to realistic situations as, for example, encountered in microdevices.[7] For a recent review on the problems concerning the Keldysh-Baym-Kadanoff formalism and its application to actual calculations, see, for example, Ref. 8. The latter type of transport models is usually some extrapolation of classical transport theory and/or treats the carrier-lattice interaction on semiclassical grounds. Weak and/or simplified particle-particle interactions and weak external perturbations have frequently been assumed in these models. Interest in quantum theories of transport in dissipative systems which allow actual calculations has recently been revived due to advances in nanostructure fabrication.[9] The geometry of these systems makes quantum-confinement effects important. At the same time, however, inelastic scattering in the form of electron-electron, electron-phonon, and/or electron-impurity scattering is present, at least in the ancillary parts of the structure.

For simplicity, nanostructures have traditionally been investigated on the basis of independent-particle pictures which has led to conceptual difficulties and/or inconsistencies in the treatment of scattering processes and the treatment of structure boundaries.[10] Here, we develop a general approach to transport in dissipative electron systems which is complementary to weak-coupling, small-perturbation models by incorporating particle-particle interactions and external perturbations in a nonperturbative fashion. Our approach is based on an expansion about a mean-field approximation to the coupled electron-phonon system in which the electron-electron and electron-phonon interactions are accounted for up to all orders in the coupling strength. Corrections to the mean-field approximation can be included up to arbitrary order.

As for the system in thermal equilibrium, we resort to a coherent-state functional-integral (CSFI) representation of ensemble averages, integrate over the phonon fields, in-

troduce an auxiliary field, and integrate over the electron fields to arrive at a formally exact representation in the form of a functional integral over the auxiliary field. The stationary-phase approximation (SPA) is then used to derive mean-field equations whose self-consistent solutions are used to derive approximate expressions for the expectation value of electronic observables within, in principle, arbitrary degree of accuracy. However, only the lowest-order corrections are simple enough to be of practical value. It is, therefore, of importance to seek a physically relevant mean-field approximation as the starting point for such an expansion. For simplicity and because of its importance in semiconductor physics, we will here confine ourselves to a derivation of Hartree-type time-dependent mean-field equations.[11]

The paper is organized as follows. In Sec. II, we develop a formally exact representation of a suitable generating function in the form of a CSFI. This generating function is constructed so as to facilitate the calculation of the ensemble average of any normal-ordered n-electron operator as a function of time. In Sec. III, we apply the SPA to the CSFI representation of the generating function to obtain time-dependent mean-field equations for the system. Self-consistent solutions to these equations will be discussed. Approximate expressions for time-dependent quantum-statistical averages will be presented in Sec. IV at several levels of approximation. In Sec. V, the qualitative nature of the approximations involved in this approach will be discussed at the example of an electronic two-level system coupled to phonons. In particular, it will be demonstrated that the theory above provides a term which introduces dissipation and irreversibility into the time evolution of the electron system. Finally, summary and conclusions will be given in Sec. VI.

II. FUNCTIONAL-INTEGRAL REPRESENTATION OF QUANTUM-STATISTICAL AVERAGES OF ELECTRONIC OBSERVABLES

We consider a system of electrons and phonons given by the following Hamiltonian

$$H=H_e+H_{\rm ph}+H_{e\text{-ph}}+U(t) , \tag{1}$$

where

$$H_e=\sum_\alpha \varepsilon_\alpha b_\alpha^\dagger b_\alpha+\tfrac{1}{2}\sum_{\alpha,\gamma,\delta,\rho} v_{\alpha\gamma\delta\rho} b_\alpha^\dagger b_\gamma^\dagger b_\rho b_\delta , \tag{2}$$

$$H_{e\text{ph}}=\sum_q \omega_q a_q^\dagger a_q , \tag{3}$$

$$H_{e\text{-ph}}=\sum_q \sum_{\alpha,\gamma} b_\alpha^\dagger b_\gamma (M_{\alpha\gamma}^{(q)} a_q^\dagger + M_{\gamma\alpha}^{(q)*} a_q) , \tag{4}$$

$$U(t)=\sum_{\alpha,\alpha'} U_{\alpha\alpha'}(t) b_\alpha^\dagger b_{\alpha'} , \tag{5}$$

and b's and a's are electron and phonon operators, respectively. H_e is the electron part which contains a free-electron Hamiltonian and a two-electron interaction v. Here, the phonon part $H_{\rm ph}$ is of simple harmonic oscillator type. The eigenstates of the free-electron system $\{|\alpha\rangle\}$ and the free-phonon system $\{|q\rangle\}$ are assumed to be known. The electron-phonon coupling term $H_{e\text{-ph}}$ is linear in the phonon operators and quadratic in the electron operators with, in general, complex coupling constants $M_{\alpha\gamma}^{(q)}$. $U(t)$ is an external time-dependent perturbation to the system which is zero for times $t\le 0$ and can be of arbitrary strength for $t>0$.

We consider the system to be in thermal equilibrium with a bath for $t\le 0$. For $t>0$, the external perturbation U becomes effective and drives the system out of equilibrium. The state of the complete system can be characterized by a density operator $\rho(t)$ which fulfills the von Neumann equation and evolves in time according to

$$\rho(t)=\mathcal{U}(t,0)\rho_0\mathcal{U}^\dagger(t,0) , \tag{6}$$

where

$$\mathcal{U}(t,0)=\mathcal{T}\left[\exp\left[-\frac{i}{\hbar}\int_0^t H\,dt'\right]\right] \tag{7}$$

is the propagator according to the Hamiltonian operator H and $\mathcal{T}$ is the usual time-ordering operator. ρ_0 is the grand canonical density operator for the system in thermal equilibrium

$$\rho_0=e^{-\beta(H_0-\mu H)} , \tag{8}$$

where

$$H_0=H_e+H_{\rm ph}+H_{e\text{-ph}} ,$$

and

$$N=\sum_\alpha b_\alpha^\dagger b_\alpha .$$

Using the Von Neumann equation implies that the interaction between the system and the bath is neglected as soon as the system evolves in time under the influence of the external perturbation. This issue will be discussed in more detail in Sec. V.

$\rho(t)$ contains the statistical information about the system as it evolves in time. The physical processes, which arise as a consequence of the applied perturbation, can be studied by calculating statistical averages of observables using the ensemble defined by $\rho(t)$. One may express any electronic observable in terms of a normal-ordered Hermitian operator A and write its average at time $t=T$ as

$$\langle A\rangle_T=\frac{1}{Z}\mathrm{Tr}[A\rho(T)] , \tag{9}$$

where $Z=\mathrm{Tr}(\rho_0)$ is the equilibrium grand partition function of the system.

Rather than studying specific observables or Green's functions, we introduce a generating function which allows us to conveniently express the ensemble average for any electron observable,

$$\mathcal{G}(J^*,J)=\left\langle \exp\left[\sum_\alpha b_\alpha^\dagger J_\alpha\right]\exp\left[\sum_\alpha J_\alpha^* b_\alpha\right]\right\rangle_T , \tag{10}$$

where the sources $\{J_\alpha^*,J_\alpha\}$ are Grassmann variables. The quantum-statistical average over any normal-ordered electron operator A can be written as

$$\langle A(b^\dagger,b)\rangle_T = A\left[-\frac{\partial}{\partial J},\frac{\partial}{\partial J^*}\right]\mathcal{G}(J^*,J)\Big|_{J=J^*=0} . \quad (11)$$

The generating function can be conveniently expressed as a CSFI over electron and phonon variables.[12,13] Following Ref. 1, the Trotter formula

$$e^{-\lambda B} = \lim_{M\to\infty}[(e^{-\lambda\epsilon B})^M] \quad (12)$$

with $\epsilon = M^{-1}$ and B an operator, is used to write

$$\mathcal{U}(T,0)\rho_0\mathcal{U}^\dagger(T,0) = \lim_{M\to\infty}\prod_{s=1}^{3M} e^{-\epsilon_s \bar{H}_s} . \quad (13)$$

Here, we have introduced a unified notation for real and imaginary time, where

$$\bar{H}_s = \begin{cases} H, & s=1,2,\ldots,M \\ H_0-\mu N, & s=M+1,\ldots,2M \\ H, & s=2M+1,\ldots,3M , \end{cases} \quad (14)$$

and

$$\epsilon_s = \begin{cases} -\dfrac{i}{\hbar}\dfrac{T}{M}, & s=1,2,\ldots,M \\ \dfrac{\beta}{M}, & s=M+1,\ldots,2M \\ \dfrac{i}{\hbar}\dfrac{T}{M}, & s=2M+1,\ldots,3M . \end{cases} \quad (15)$$

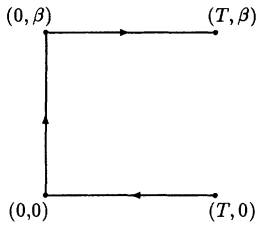

FIG. 1. The integration path in the complex time plane.

Thus $\rho(T)$ has the structure of a propagator for a time-dependent Hamiltonian operator which takes the system along the real-time axis from $(T,0)\to(0,0)$, corresponding to $s=1,2,\ldots,M$, then along the imaginary-time axis from $(0,0)\to(0,\beta)$, corresponding to $s=M+1,\ldots,2M$, and finally from $(0,\beta)\to(T,\beta)$, corresponding to $s=2M+1,\ldots,3M$. This time path is given schematically in Fig. 1. It is similar to the time path introduced by Keldysh.[6]

Equation (10) is formally of the same structure as the generating function previously introduced for coupled electron-phonon systems in thermal equilibrium.[1] The main difference is that here the "Hamiltonian operator" which enters the density operator (13) is explicitly time dependent.

Following Ref. 1, one may write the generating function as a CSFI over a set of electron and phonon variables

$$\mathcal{G}(J^*,J) = \lim_{M\to\infty}\int_{\substack{\psi_{3M}=-\psi_0,\\ \phi_{3M}=\phi_0}}\prod_{s=1}^{3M} d\mu(\psi_s)d\mu(\phi_s)\, e^{-S(\psi^*_{\alpha s},\psi_{\alpha,s-1};\phi^*_{qs},\phi_{q,s-1};J^*,J)} \quad (16)$$

with

$$S(\psi^*_{\alpha s},\psi_{\alpha,s-1};\phi^*_{qs},\phi_{q,s-1};J^*,J) = \sum_{s=1}^{3M}\left[\sum_\alpha(\psi^*_{\alpha s}\psi_{\alpha s}-\psi^*_{\alpha s}\psi_{\alpha,s-1}) + \sum_q(\phi^*_{qs}\phi_{qs}-\phi^*_{qs}\phi_{q,s-1}) + \epsilon_s\bar{H}_s(\psi^*_{\alpha s},\psi_{\alpha,s-1};\phi^*_{qs},\phi_{q,s-1})\right] - \sum_\alpha(J^*_\alpha\psi_{\alpha,3M-1}+\psi^*_{\alpha,3M}J_\alpha) . \quad (17)$$

Due to the linearity of the electron-phonon interaction in the phonon variables, the integral over the phonon fields can be carried out exactly

$$\mathcal{G}(J^*,J) = \lim_{M\to\infty}\left[\frac{Z_{\rm ph}}{Z}\int_{\psi_{3M}=-\psi_0}\prod_{s=1}^{3M} d\mu(\psi_s)\, e^{-S_{\rm eff}(\psi^*_{\alpha s},\psi_{\alpha,s-1};J^*,J)}\right] , \quad (18)$$

where,

$$\begin{aligned} S_{\rm eff}(\psi^*_{\alpha s},\psi_{\alpha,s-1};J^*,J) = {} & \sum_{s=1}^{3M}\sum_\alpha[\psi^*_{\alpha s}\psi_{\alpha s}-\psi^*_{\alpha s}\psi_{\alpha,s-1}(1-\epsilon_s\varepsilon_\alpha)] + \left[\sum_{s=1}^{M}+\sum_{s=2M+1}^{3M}\right]\sum_{\alpha,\alpha'}\epsilon_s U_{\alpha\alpha' s}\psi^*_{\alpha s}\psi_{\alpha',s-1} \\ & - \sum_\alpha\left[\mu\sum_{s=M+1}^{2M}\epsilon_s\psi^*_{\alpha s}\psi_{\alpha,s-1}+J^*_\alpha\psi_{\alpha,3M-1}+\psi^*_{\alpha,3M}J_\alpha\right] \\ & + \tfrac{1}{2}\sum_{s=1}^{3M}\sum_{\alpha,\alpha',\gamma,\gamma'}\epsilon_s v_{\alpha\gamma\alpha'\gamma'}\psi^*_{\alpha s}\psi^*_{\gamma s}\psi_{\gamma',s-1}\psi_{\alpha',s-1} \\ & - \sum_{s,s'=1}^{3M}\sum_q h^*_q[(\psi^*_s,\psi_{s-1})]\epsilon_s\mathcal{F}^{(q)}_{s,s'}\epsilon_{s'}h_q[(\psi^*_{s'},\psi_{s'-1})] , \end{aligned} \quad (19)$$

$$\mathcal{F}^{(q)}_{s,s'}=\begin{cases} e^{\beta\omega_q}n_q, & \text{for } s'=3M \text{ and } s=1 \\ e^{\beta\omega_q}n_q a_{3M}a_{3M-1}\cdots a_{s'+1}, & \text{for } s'<3M \text{ and } s=1 \\ e^{\beta\omega_q}n_q a_{s-1}\cdots a_1 a_{3M}\cdots a_{s'+1}, & \text{for } s-1<s' \text{ and } s>1 \\ e^{\beta\omega_q}n_q, & \text{for } s-1=s' \text{ and } s>1 \\ e^{\beta\omega_q}n_q a_{s-1}\cdots a_{s'+1}, & \text{for } s-1>s' \text{ and } s>1 \end{cases}$$

where $a_s=1-\epsilon_s\omega_q\approx e^{-\epsilon_s\omega_q}$, and n_q is the Planck distribution, $1/(e^{\beta\omega_q}-1)$. Moreover, we use the abbreviation

$$h^*_q[(\psi^*_s,\psi_{s-1})]=\sum_{\alpha,\gamma}M^{(q)*}_{\gamma\alpha}\psi^*_{\alpha s}\psi_{\gamma,s-1}\ ,$$

$$h_q[(\psi^*_s,\psi_{s-1})]=\sum_{\alpha,\gamma}M^{(q)}_{\alpha\gamma}\psi^*_{\alpha s}\psi_{\gamma,s-1}\ .$$

The partition function of the free-phonon system, $Z_{\rm ph}=\prod_q(1-e^{-\beta\omega_q})^{-1}$, which arises from the integral over the phonon variables, cancels with the equivalent term in the partition function Z. Besides the direct electron-electron coupling, an additional electron-electron interaction term due to the phonon coupling appears in the exponent of the integrand of (18). Both prohibit direct integration over the electron fields.

In anticipation of the desired type of mean-field solution, we pair electron variables according to

$$\varphi_{\alpha\gamma s}=\epsilon_s\psi^*_{\alpha s}\psi_{\gamma,s-1}\ .$$

Then we can write the fourth-order terms in the electron fields as

$$\tfrac{1}{2}\sum_{s,s'=1}^{3M}\sum_{\alpha,\alpha',\gamma,\gamma'}\varphi_{\alpha\gamma s}V_{\alpha\gamma s,\alpha'\gamma's'}\varphi_{\alpha'\gamma's'}\ .$$

Here, we have introduced the matrix

$$V_{\alpha\gamma s,\alpha'\gamma's'}=-\frac{1}{\epsilon_{s'}}v_{\alpha\alpha'\gamma\gamma'}\delta_{ss'}+\sum_q\left(M^{(q)*}_{\gamma\alpha}M^{(q)}_{\alpha'\gamma'}\mathcal{F}^{(q)}_{s,s'}+M^{(q)*}_{\gamma'\alpha'}M^{(q)}_{\alpha\gamma}\mathcal{F}^{(q)}_{s',s}\right)\ . \tag{20}$$

The non-Gaussian factors of the integrand in (18) can be rewritten by introducing an auxiliary field $\{x_{\alpha\gamma s}\}$,[1,14,15] to give the integral over the electron variables Gaussian form. Consequently, this integral can be performed analytically and one can give the generating function the form of a functional integral over the auxiliary field x

$$\mathcal{G}(J^*,J)=\lim_{M\to\infty}\left[\frac{Z_{\rm ph}}{Z}(\det V)^{-1/2}\times\int_{\mathcal{U}}d\mu(x)e^{-S'(x,J^*,J)}\right], \tag{21}$$

with

$$S'(x,J^*,J)=\tfrac{1}{2}\sum_{a,b}x_a V^{-1}{}_{ab}x_b-\ln\det[I+\mathcal{D}(x,T,\beta)]+\sum_{\alpha,\gamma}J^*_\alpha[I+\mathcal{D}^{-1}(x,T,\beta)]^{-1}{}_{\alpha\gamma}J_\gamma\ , \tag{22}$$

and

$$\mathcal{D}(x,T,\beta)=\lim_{M\to\infty}\left[\prod_{s=1}^{3M}[I-\epsilon_s\mathcal{A}_s(x)]\right]\approx\lim_{M\to\infty}\left[\prod_{s=1}^{3M}e^{-\epsilon_s\mathcal{A}_s(x)}\right], \tag{23}$$

where the $\mathcal{A}_s$'s are $N\times N$ matrices of the form

$$\mathcal{A}_{\alpha\gamma s}(x)=\begin{cases}\epsilon_\alpha\delta_{\alpha\gamma}+U_{\alpha\gamma s}+x_{\alpha\gamma s}\ , \\ \quad\text{for } 1\le s\le M \text{ or } 2M+1\le s\le 3M \\ (\epsilon_\alpha-\mu)\delta_{\alpha\gamma}+x_{\alpha\gamma s}\ , \\ \quad\text{for } M+1\le s\le 2M\ .\end{cases} \tag{24}$$

The integral boundaries and the normalization are such that

$$\exp\left[\tfrac{1}{2}\sum_{a,b}\varphi_a V_{ab}\varphi_b\right]=(\det V)^{-1/2}\times\int_{\mathcal{U}}d\mu(x)\exp\left[-\tfrac{1}{2}\sum_{a,b}x_a V^{-1}_{ab}x_b+\sum_a\varphi_a x_a\right]$$

is fulfilled. For simplicity, we assume that V is nonsingular and use the abbreviations $a=(\alpha_a,\alpha'_a,s_a)$, $b=(\alpha_b,\alpha'_b,s_b)$. Equations (21)–(24) are an exact representation of the generating function. In the next section, it will be used to develop an approximation scheme for the calculation of ensemble averages.

III. STATIONARY-PHASE APPROXIMATION

Since an exact (numerical) evaluation of the functional integral (21) would be rather difficult, we calculate the generating function within the stationary-phase approximation (SPA).[12] Strictly speaking, there is no large expansion parameter which *a priori* justifies this step. As for any mean-field approximation, its justification is ulti-

mately provided by physical criteria. Mean-field approximations have played a significant role throughout condensed-matter physics. For instance (relativistic) mean-field approximations for fermion-boson couplings have been developed previously in nuclear physics,[12,16] and quantum optics.[17] While they can be obtained within standard diagrammatic techniques, they most directly can be derived from functional-integral representations.[12]

Equation (21) provides an exact representation of the generating function and any expansion, provided that it is either convergent or asymptotic, is legitimate. However, one is, of course, interested in an expansion which provides a good zero-order approximation and, therefore, requires merely a small number of correction terms. Technically, the resulting expansion is directly related to the way in which the fourth-order terms in the electron variables in (19) were regrouped. As the Hartree approximation has a long history of success in connection with semiconductor physics, we follow an approach which gives time-dependent Hartree-type mean-field equations which account for both the two-electron and electron-phonon interactions. In the absence of the electron-phonon coupling, the present resummation gives the well-known time-dependent Hartree equations, except that single-particle states are populated according to a Fermi-Dirac filling factor, rather than being either empty or filled.

An important part of the evaluation of the functional integral is the calculation of the determinant of $[I+\mathcal{D}(x,T,\beta)]$, which can be expressed in terms of the eigenvalues of $\mathcal{D}(x,T,\beta)$, $\{e^{-\beta(\lambda_l-\mu)}, l=1,2,\ldots,N\}$. In general, these eigenvalues are not real and left and right eigenkets of $\mathcal{D}(x,T,\beta)$ are not identical. Resorting to the Dirac notation, we introduce

$$|v_{ls}\rangle = d_s \cdots d_1 |v_{l0}\rangle ,$$

and

$$\langle w_{ls}| = \langle w_{l,3M}| d_{3M} \cdots d_{s+1} ,$$

where

$$d_l(s) \equiv e^{-\epsilon_s \mathcal{A}_s(x)} .$$

Then, the eigenvalue equations for $\mathcal{D}(x,T,\beta)$ are

$$|v_{l,3M}\rangle = \mathcal{D}(x,T,\beta)|v_{l0}\rangle = e^{-\beta(\lambda_l-\mu)}|v_{l0}\rangle ,$$

$$\langle w_{l0}| = \langle w_{l,3M}|\mathcal{D}(x,T,\beta) = \langle w_{l,3M}| e^{-\beta(\lambda_l-\mu)} .$$

It is convenient to introduce a continuum notation in which we write

$$|v_l(t_s,0)\rangle = \lim_{M\to\infty} |v_{l,M-s}\rangle, \quad s=1,2,\ldots,M ;$$

$$|v_l(0,\tau)\rangle = \lim_{M\to\infty} |v_{ls}\rangle, \quad s=M+1,M+2,\ldots,2M ;$$

$$|v_l(t_s,\beta)\rangle = \lim_{M\to\infty} |v_{ls}\rangle, \quad s=2M+1,2M+2,\ldots,3M ;$$

where, $t_s \in [0,T]$ and $\tau \in [0,\beta]$.

The time evolution of these states can be written as

$$i\hbar\frac{\partial}{\partial t}|v_l(t,0)\rangle - \mathcal{A}(x,t,0)|v_l(t,0)\rangle = 0 ,$$

$$\text{as } (T,0)\to(0,0) ; \quad (25)$$

$$\frac{\partial}{\partial \tau}|v_l(0,\tau)\rangle + \mathcal{A}(x,0,\tau)|v_l(0,\tau)\rangle = 0 ,$$

$$\text{as } (0,0)\to(0,\beta) ; \quad (26)$$

$$i\hbar\frac{\partial}{\partial t}|v_l(t,\beta)\rangle - \mathcal{A}(x,t,\beta)|v_l(t,\beta)\rangle = 0 ,$$

$$\text{as } (0,\beta)\to(T,\beta) . \quad (27)$$

These eigenkets fulfill the boundary conditions $|v_l(T,\beta)\rangle = e^{-\beta(\lambda_l-\mu)}|v_l(T,0)\rangle$.

As discussed in our previous paper,[1] strict application of the SPA to the generating function (21) will give stationary solutions which depend on the specific observable under investigation. In particular, application of the SPA to (21) would give a stationary solution x^0 which is J^* and J dependent. Moreover, the statistical average of an observable within the SPA would depend on whether the explicit form or the generating function is used for its calculation. In order to avoid this ambiguity and to make the physical meaning of the mean fields transparent, we expand the integrand in (21) with respect to the auxiliary field x^0 which extremizes only the J^* and J independent terms in $S'(x,J^*,J)$, i.e.,

$$\tfrac{1}{2}\sum_{a,b} x_a V^{-1}{}_{ab} x_b - \ln\det[I+\mathcal{D}(x,T,\beta)] .$$

This stationary field is

$$x^0_{\alpha\gamma s} = -\sum_{l=1}^{N}\sum_{\alpha',\gamma'}\sum_{s'=1}^{3M} \epsilon_{s'} \frac{V_{\alpha\gamma s,\alpha'\gamma' s'}\langle w^0_{ls'}|\alpha'\rangle\langle\gamma'|v^0_{ls'}\rangle}{1+e^{-\beta(\lambda^0_l-\mu)}} . \quad (28)$$

Thus, from Eqs. (25)–(27), the set of equations which specifies the eigenvalues and eigenfunctions of $\mathcal{D}(x^0,T,\beta)$ is

$$\sum_\gamma \left[\left(i\hbar\frac{\partial}{\partial t}-\varepsilon_\alpha\right)\delta_{\alpha\gamma} - U_{\alpha\gamma}(t) - x^0_{\alpha\gamma}(t)\right]\langle\gamma|v^0_l(t,0)\rangle = 0 , \quad (29)$$

$$\sum_\gamma \left[\left(\frac{\partial}{\partial\tau}+\varepsilon_\alpha-\mu\right)\delta_{\alpha\gamma} + x^0_{\alpha\gamma}(\tau)\right]\langle\gamma|v^0_l(0,\tau)\rangle = 0 , \quad (30)$$

$$\sum_\gamma \left[\left(i\hbar\frac{\partial}{\partial t}-\varepsilon_\alpha\right)\delta_{\alpha\gamma} - U_{\alpha\gamma}(t) - x^0_{\alpha\gamma}(t)\right]\langle\gamma|v^0_l(t,\beta)\rangle = 0 . \quad (31)$$

These equations are of Hartree type where the interaction term accounts for all particle interactions within a mean-field picture. Together with the boundary conditions,

$$|v^0_l(T,\beta)\rangle = e^{-\beta(\lambda^0_l-\mu)}|v^0_l(T,0)\rangle ,$$

they must be solved self-consistently. Expansion of the

exponent in (21) around x^0 and subsequent integration over the auxiliary field allows a systematic expansion of the generating function in terms of $\{\lambda_l^0\}$ and $\{|v_l^0(t,\tau)\rangle\}$.

The problem of self-consistently calculating the eigenvalues of $\mathcal{D}(x^0,T,\beta)$ and the functions $\{|v_l^0(t,\tau)\rangle\}$ is nonlinear and one cannot expect a unique solution without implementing further physical constraints. First, it can be shown that choosing $\mathcal{D}(x^0,T,\beta)$ to be Hermitian is consistent with the structure of x^0 (see Appendix). As a consequence, left and right eigenkets of $\mathcal{D}(x^0,T,\beta)$ are identical and fulfill

$$|w_{l,3M-s+1}^0\rangle = |v_{ls}^0\rangle \ . \tag{32}$$

As a consequence, the partition function is real up to any order of approximation. x^0 can now be expressed entirely in terms of right eigenkets

$$x_{\alpha\gamma s}^0 = -\sum_{l=1}^{N}\sum_{\alpha',\gamma'}\sum_{s'=1}^{3M}\epsilon_{s'}\frac{V_{\alpha\gamma s,\alpha'\gamma' s'}\langle v_{l,3M-s'+1}^0|\alpha'\rangle\langle\gamma'|v_{ls'}^0\rangle}{1+e^{-\beta(\lambda_l^0-\mu)}} \tag{33}$$

with $||v_l^0(0)||=1$.

The exact generating function has the property that $\mathcal{G}(J^*=0,J=0)=1$ for any external perturbation U. In other words, $\mathrm{Tr}\{\rho(T)\}=Z$ for arbitrary time T. We require this property to hold within any order of approximation. Imposed upon the lowest order of approximation, in which the integrand in (21) is evaluated for the stationary field x^0 (i.e., the "classical approximation"), one finds that, for $x=x^0$, the first two terms in $S'(x,J^*,J)$, Eq. (22), must cancel with the corresponding terms in the partition function.[1] Therefore, the integrals over the two paths parallel to the real-time axis must cancel each other. This is achieved if

$$|v_l^0(t,\beta)\rangle = e^{-\beta(\lambda_l^0-\mu)}|v_l^0(t,0)\rangle$$

is fulfilled. Due to the properties of x^0, this has

$$x_{\alpha\gamma}^0(t,\beta)=x_{\alpha\gamma}^0(t,0)$$

as a consequence which, in turn, is consistent with the original assumption. Therefore, such a solution is indeed supported by the structure of V, Eq. (20). Now Eqs. (29) and (31) take the form of a generalized Schrödinger equation with a Hermitian Hamiltonian operator and are, in fact, identical to each other. The eigenvalues $\{e^{-\beta(\lambda_l^0-\mu)}\}$ are now solely determined by Eq. (30) with the constraint

$$|v_l^0(0,\beta)\rangle = e^{-\beta(\lambda_l^0-\mu)}|v_l^0(0,0)\rangle \ ,$$

which is identical to the eigenvalue problem for the partition function in thermal equilibrium.[1] In particular, the eigenvectors $\{|v_l^0(0,\tau)\rangle\}$ are identical to the eigenvectors $\{|v_l^0(\tau)\rangle\}$ introduced in Ref. 1 for the partition function.

Finally, any sensible approximation to the exact time evolution of observables must ensure that the system remains in thermal equilibrium in the absence of an external perturbation. In other words, in the absence of an external perturbation, the functions $\{|v_l^0(t,0)\rangle\}$ may only change by a phase factor. This is accomplished by setting

$$|v_l^0(0,\tau)\rangle = e^{-\tau(\lambda_l^0-\mu)}|v_l^0(0,0)\rangle \tag{34}$$

for the eigenvalue problem (30). It should be noted that this property ensures that, in the limit $V\to 0$, the solutions $|v_l^0(t,\tau)\rangle$ reduce to the one-particle states $\{|l\rangle\}$ with $\{\lambda_l^0=\epsilon_l\}$. Moreover, it can be shown that an iterative solution to the eigenvalue problem (30) in powers of V also leads to the solution which fulfills (34).

With these constraints implemented and the introduction of the states

$$|\phi_l^0(t,0)\rangle = |v_l^0(t,0)\rangle, \quad \text{as } (T,0)\to(0,0) \ ;$$

$$|\phi_l^0(0,\tau)\rangle = e^{\tau(\lambda_l^0-\mu)}|v_l^0(0,\tau)\rangle, \quad \text{as } (0,0)\to(0,\beta) \ ;$$

$$|\phi_l^0(t,\beta)\rangle = |v_l^0(t,\beta)\rangle, \quad \text{as } (0,\beta)\to(T,\beta) \ ;$$

the procedure for finding the eigenvalues and mean-field solutions $\{|\phi_l^0(t,\tau)\rangle\}$ can be summarized as follows. First, self-consistently solve the eigenvalue problem

$$\sum_{\gamma}[\epsilon_\alpha\delta_{\alpha\gamma}+x_{\alpha\gamma}^0(0,0)]\langle\gamma|\phi_l^0(0,0)\rangle = \lambda_l^0\langle\alpha|\phi_l^0(0,0)\rangle \tag{35}$$

with

$$x_{\alpha\gamma}^0(0,0)=\sum_{l=1}^{N}\sum_{\alpha',\gamma'}\left[v_{\alpha\alpha'\gamma\gamma'}-\sum_q\frac{M_{\gamma\alpha}^{(q)*}M_{\alpha'\gamma'}^{(q)}+M_{\gamma'\alpha'}^{(q)*}M_{\alpha\gamma}^{(q)}}{\omega_q}\right]\langle\phi_l^0(0,0)|\alpha'\rangle\langle\gamma'|\phi_l^0(0,0)\rangle f_{\mathrm{FD}}(\lambda_l^0) \ , \tag{36}$$

and the normalization $\|\phi_l^0(0,0)\|=1$, with $l=1,\ldots,N$. This problem is identical to the eigenvalue problem which was obtained for the partition function of the system in thermal equilibrium.[1] Subsequently, the functions $|\phi_l^0(t,0)\rangle$ can be found from the time-dependent Schrödinger equations

$$\sum_{\gamma}\left[\left[i\hbar\frac{\partial}{\partial t}-\epsilon_\alpha\right]\delta_{\alpha\gamma}-U_{\alpha\gamma}(t)-x_{\alpha\gamma}^0(t,0)\right]\langle\gamma|\phi_l^0(t,0)\rangle=0 \ , \tag{37}$$

where the eigenfunctions $|\phi_l^0(0,0)\rangle$ from the eigenvalue problem (35) provide the initial conditions and

$$x^0_{\alpha\gamma}(t,0)=\sum_{l=1}^{N}\sum_{\alpha'\gamma'} f_{\mathrm{FD}}(\lambda_l^0)\left[v_{\alpha\alpha',\gamma\gamma'}\langle\phi_l^0(t,0)|\alpha'\rangle\langle\gamma'|\phi_l^0(t,0)\rangle\right.$$
$$-\frac{i}{\hbar}\sum_q\int_0^t dt'\left(M^{(q)*}_{\gamma\alpha}M^{(q)}_{\alpha'\gamma'}e^{-i\hbar^{-1}(t-t')\omega_q}-M^{(q)*}_{\gamma'\alpha'}M^{(q)}_{\alpha\gamma}e^{-i\hbar^{-1}(t'-t)\omega_q}\right)$$
$$\times\langle\phi_l^0(t',0)|\alpha'\rangle\langle\gamma'|\phi_l^0(t',0)\rangle$$
$$-\sum_q\frac{M^{(q)*}_{\gamma\alpha}M^{(q)}_{\alpha'\gamma'}e^{-i\hbar^{-1}t\omega_q}+M^{(q)*}_{\gamma'\alpha'}M^{(q)}_{\alpha\gamma}e^{-i\hbar^{-1}t\omega_q}}{\omega_q}$$
$$\left.\times\langle\phi_l^0(0,0)|\alpha'\rangle\langle\gamma'|\phi_l^0(0,0)\rangle\right] \tag{38}$$

represents the self-consistent mean-field introduced by the electron-electron and electron-phonon interaction. The electron-electron coupling in these equations appears in the form of a Hartree-like potential and has a rather simple interpretation. Each electron is exposed to an instantaneous potential produced by the charge of all electrons in the system. The occupation probability of the one-particle states $\{|\phi_l^0(t,\tau)\rangle\}$ is given by Fermi-Dirac factors $f_{\mathrm{FD}}(\lambda_l^0)=\{1+\exp[\beta(\lambda_l^0-\mu)]\}^{-1}$. The electron-phonon interaction also appears in the form of a Hartree-type potential. However, this potential depends on the previous history of the system. In particular, the last term in (38) represents the influence of the initial state of the system prior to the onset of the external perturbation. The two contributions under the time integral arise from phonon emission and absorption *after* the onset of the external field. Note that these two terms account for modifications in the phonon emission and absorption rates. Phonons emitted or absorbed relative to the equilibrium Planck distribution affect the time evolution of electrons at a later point in time, which causes a non-Markovian form of the time evolution. This is an explicit example for non-Markovian time evolution of a reduced system.[18] Even within the lowest order of approximation, a fully quantum-mechanical treatment of the electronic system is maintained. If the interaction goes to zero, an exact description of the electronic system is provided. This makes the present approach better suited for the study of quantum-confined systems than the conventional Feynman-path integral approach, which, in the lowest approximation, gives a classical description of the system.

In the absence of an external perturbation, it is easy to verify that $\{|\phi_l^0(t,0)\rangle\}$, indeed, changes merely by a phase factor,

$$|\phi_l^0(t,0)\rangle=e^{-i\hbar^{-1}t\lambda_l^0}|\phi_l^0(0,0)\rangle\ . \tag{39}$$

At present, we did not account for phonon decay other than reabsorption and the combined system of electrons and phonons forms a closed system. Finite phonon lifetimes due to phonon-phonon coupling may be incorporated via quadratic and anharmonic terms in the phonon Hamiltonian operator which, however, would greatly complicate the treatment of the functional integrals. Alternatively, finite phonon lifetimes may be incorporated into the self-consistent mean fields on a phenomenological level.[10,19]

IV. THERMAL AVERAGES OF OBSERVABLES WITHIN THE SPA

With the self-consistent solutions from above and $\bar{x}\equiv x-x^0$, the generating function can be written as

$$\mathcal{G}(J^*,J)=\lim_{M\to\infty}\left[\frac{Z_{\mathrm{ph}}}{Z}(\det V)^{-1/2}\int_\Omega d\mu(\bar{x})\exp\left[-S'(x^0,J^*,J)-\sum_{n=1}^{\infty}\frac{1}{n}\frac{\partial^n S'(x,J^*,J)}{\partial x^n}\bigg|_{x^0}\bar{x}^{\,n}\right]\right], \tag{40}$$

with the hope that a small number of terms in the exponent will provide a sufficiently accurate approximation. In this section, we will consider terms up to order $\bar{x}^2$, i.e., the SPA.

The lowest-order contribution to the generating function, which is obtained by evaluating the integrand of (21) at the stationary point, is

$$\mathcal{G}(J^*,J)\approx\exp\left[-\sum_{\alpha,\alpha'}J^*_\alpha[I+\mathcal{D}^{-1}(x^0,T,\beta)]^{-1}_{\alpha\alpha'}J_{\alpha'}\right]. \tag{41}$$

In this approximation, the generating function has an independent-particle form. Approximate expressions for ensemble averages of observables can be obtained via Eq. (11). For a one-particle operator, $A=\sum_{\alpha,\alpha'}\langle\alpha|A|\alpha'\rangle b^\dagger_\alpha b_{\alpha'}$, one obtains

$$\langle A\rangle_T\approx\sum_{l=1}^{N}\langle\phi_l^0(T,0)|A|\phi_l^0(T,0)\rangle f_{\mathrm{FD}}(\lambda_l^0)$$
$$=\mathrm{Tr}\left[A\frac{I}{I+e^{\beta[H_{\mathrm{eff}}(T)-\mu N]}}\right]. \tag{42}$$

This expression has a simple physical interpretation. At time $T=0$, the system is in thermal equilibrium. The occupation probability of state $|\phi_l^0(0,0)\rangle$ is given by the Fermi-Dirac factor $f_{\rm FD}(\lambda_l^0)$. At times $T\geq 0$, the system evolves such that the states $|\phi_l^0(T,0)\rangle$ diagonalize the (effective one-particle) density operator,

$$\rho_{\rm eff}(T)=\frac{I}{I+e^{\beta[H_{\rm eff}(T)-\mu N]}} ,$$

which approximately describes the system at time T. Within this approximation, the statistical average for a general n-body operator can be found via Wick's theorem

$$\langle b_{i_1}^\dagger \cdots b_{i_n}^\dagger b_{j_n} \cdots b_{j_1}\rangle_T \approx \sum_P (-1)^P \langle b_{i_{P_n}}^\dagger b_{j_n}\rangle_T \cdots \langle b_{i_{P_1}}^\dagger b_{j_1}\rangle_T ,$$

where the sum is over all permutations P of $\{i_1,i_2,\ldots,i_n\}$ and $(-1)^P$ is the sign of the permutation. Thus, the interacting-electron system which is coupled to a phonon system is approximated by an independent-electron system for which the individual particles move in an effective, time-dependent (and self-consistently calculated) potential produced by the mutual interactions, as well as the external perturbation. Particle-particle correlations are accounted for only within a mean-field approximation.

It should be noted that the fact that the occupation probabilities $f_{\rm FD}$ do not evolve in time is linked to the fact that, *during* the application of the external field, the coupling to the bath with which the system originally was in thermal equilibrium, is not accounted for when using the Von Neumann equation. Such an approximation can be justified if there is a hierarchy in relaxation processes.

The next-higher approximation is the stationary-phase approximation, which takes into account the quadratic fluctuations around the stationary field x^0 in (40). It introduces particle-particle correlations within the random-phase approximation (RPA). Within this approximation, the generating function takes the form

$$\mathcal{G}(J^*,J)\approx\exp\left[-\sum_{\alpha,\alpha'} J_\alpha^*[I+\mathcal{D}^{-1}(x^0,T,\beta)]^{-1}_{\alpha\alpha'}J_{\alpha'}-\tfrac{1}{2}{\rm Tr}\{\ln[I-(I-V\Gamma^0)^{-1}V\Gamma'(J^*,J)]\}\right.$$
$$\left.+\tfrac{1}{2}\sum_{a,b} S_a^{(1)}(x^0,J^*,J)(\{I-V[\Gamma^0+\Gamma'(J^*,J)]\}^{-1}V)_{ab}S_b^{(1)}(x^0,J^*,J)\right] . \tag{43}$$

Where, with the abbreviations $a=(\alpha_a,\alpha_a',s_a)$ and $b=(\alpha_b,\alpha_b',s_b)$, we have used

$$\Gamma_{ab}^0={\rm Tr}\left[(I+\mathcal{D}_0)^{-1}\left[\frac{\partial^2\mathcal{D}(x,T,\beta)}{\partial x_a\partial x_b}\bigg|_{x^0}-\frac{\partial\mathcal{D}(x,T,\beta)}{\partial x_a}\bigg|_{x^0}(I+\mathcal{D}_0)^{-1}\frac{\partial\mathcal{D}(x,T,\beta)}{\partial x_b}\bigg|_{x^0}\right]\right] .$$

$$\Gamma'_{ab}(J^*,J)=\sum_{\alpha,\alpha'} J_\alpha^*\langle\alpha|\Gamma'_{ab}|\alpha'\rangle J_{\alpha'} ,$$

and

$$S_a^{(1)}(x^0,J^*,J)=\sum_{\alpha,\alpha'} J_\alpha^*\langle\alpha|S_a^{(1)}|\alpha'\rangle J_{\alpha'} ,$$

with

$$\mathcal{D}_0=\mathcal{D}(x^0,T,\beta) ,$$

$$\Gamma'_{ab}=(I+\mathcal{D}_0)^{-1}\left[\frac{\partial\mathcal{D}(x,T,\beta)}{\partial x_a}\bigg|_{x^0}(I+\mathcal{D}_0)^{-1}\frac{\partial\mathcal{D}(x,T,\beta)}{\partial x_b}\bigg|_{x^0}\right.$$
$$\left.+\frac{\partial\mathcal{D}(x,T,\beta)}{\partial x_b}\bigg|_{x^0}(I+\mathcal{D}_0)^{-1}\frac{\partial\mathcal{D}(x,T,\beta)}{\partial x_a}\bigg|_{x^0}-\frac{\partial^2\mathcal{D}(x,T,\beta)}{\partial x_a\partial x_b}\bigg|_{x^0}\right](I+\mathcal{D}_0)^{-1} ,$$

$$S_a^{(1)}=(I+\mathcal{D}_0)^{-1}\frac{\partial\mathcal{D}(x,T,\beta)}{\partial x_a}\bigg|_{x^0}(I+\mathcal{D}_0)^{-1} .$$

The structure of (43) is identical to the SPA result for the generating function of the system in thermal equilibrium.[1] Here, however, the matrix $\mathcal{D}(x^0,T,\beta)$ depends on a complex time (t,τ) according to the time path given in Fig. 1, rather than being confined to a path from $(0,0)\rightarrow(0,\beta)$ along the imaginary-time axis.

Ensemble averages for any electronic observable can now be calculated within the SPA, using

$$\langle b_\alpha^\dagger b_{\alpha'}\rangle_T\approx\langle b_\alpha^\dagger b_{\alpha'}\rangle_T^{\rm SPA}$$
$$=\sum_{l=1}^N\langle\phi_l^0(T,0)|\alpha\rangle\langle\alpha'|\phi_l^0(T,0)\rangle f_{\rm FD}(\lambda_l^0)-\tfrac{1}{2}{\rm Tr}[(I-V\Gamma^0)^{-1}\langle\alpha'|V\Gamma'|\alpha\rangle] , \tag{44}$$

which contains the zero-order result from before and a RPA correction term. Correlation terms for n-particle expecta-

tion values are rather complicated but can readily be evaluated from the generating function. For instance, the statistical average of a generic two-particle operator is approximated by

$$\langle b^{\dagger}_{\alpha_1} b^{\dagger}_{\alpha_2} b_{\alpha_2'} b_{\alpha_1'} \rangle_T \approx \Big\{ \langle b^{\dagger}_{\alpha_1} b_{\alpha_1'} \rangle_T^{\mathrm{SPA}} \langle b^{\dagger}_{\alpha_2} b_{\alpha_2'} \rangle_T^{\mathrm{SPA}} + \tfrac{1}{2}\mathrm{Tr}[(I - V\Gamma^0)^{-1} \langle \alpha_1' | V\Gamma' | \alpha_1 \rangle (I - V\Gamma^0)^{-1} \langle \alpha_2' | V\Gamma' | \alpha_2 \rangle] + \sum_{a,b} \langle \alpha_1' | S_a^{(1)} | \alpha_1 \rangle [(I - V\Gamma^0)^{-1} V]_{ab} \langle \alpha_2' | S_b^{(1)} | \alpha_2 \rangle \Big\} - \left[\alpha_1 \leftrightarrow \alpha_2 \right] ,$$

where the terms within the second pair of large brackets are identical to the terms within the first large parentheses, albeit with the unprimed indices α_1 and α_2 interchanged. Higher-order correction terms can be obtained in a systematic way by including higher-order terms in $\bar{x}$ according to (40). This leads to loop corrections to the SPA result. For any practical purpose, however, the complexity of these expressions makes such an expansion rather academic in nature and, therefore, will not be discussed here.

It should be stressed that, while these results can also be obtained via diagrammatic techniques, we feel that this approach is much more direct and simple. First, the quartic term in (19) has a simple interpretation and suitable regrouping can be performed depending on the physical situation. From then on, the various levels of approximations can be obtained by evaluating (40). There is no need to explicitly select and count all diagrams which contribute to a certain order of correction. Moreover, the mathematical apparatus, consisting essentially of calculating Gaussian integrals, is rather simple. Approximate statistical averages can be performed directly via (11). Finally, the equations of motion (37) have a simple physical interpretation and are numerically tractable, as will be shown below at a simple example.

V. APPLICATION TO TWO-LEVEL SYSTEMS

In this section, our results are applied to a two-level system which is coupled to phonons. Two-level models are well known to be applicable to a variety of physical systems.[20] Quantum beats, characteristic for these systems, have been observed for various systems. Most recently, they have been observed in asymmetric semiconductor double wells.[21] An external electric field was used to achieve resonance between the two lowest confined levels in the wells. Monitoring the transmission probability for light at the exciton energy of the wider well, evidence for charge oscillations between the two wells could be found. In an earlier experiment, LO-phonon-enhanced tunneling was observed in double wells for which the level spacing was tuned to be equal to the LO-phonon energy.[22]

Our motivation here is primarily to investigate the role of the phonon terms which arise in the mean-field equations (35) and (37). Several theoretical studies have dealt with the inclusion of dissipation into two-level models ("spin-boson models"). Some have treated dissipation on pure phenomenological grounds,[21,23] others have followed earlier work by Feynman and Vernon,[24] and Caldeira and Leggett,[25] and used Feynman-path integral techniques to find a microscopic interpretation of dissipation.[26] Here we show that the phonon-induced mean fields, as derived above from our microscopic considerations of coupled electron-phonon systems, provide an approximate, but nonphenomenological damping of the electron system. Contrary to previous work, we do not introduce classical variables to approximately treat the system, but maintain a fully quantum-mechanical description. We consider a situation as sketched in Fig. 2. A double well, originally in thermal equilibrium, is exposed to an external bias $U(t)$ which lowers the right well relative to the left. We investigate the time evolution of the system under the influence of the bias. In particular, we address the question of whether and/or how the system approaches a new equilibrium when the coupling to phonons is accounted for via (36) and (38).

For a two-level system characterized by the states $|L\rangle$ and $|R\rangle$, the mean-field Hamiltonian in (37) takes the form of a 2×2 matrix

$$\mathcal{H}(t) = \begin{pmatrix} \varepsilon_L & V \\ V & \varepsilon_R - U(t) \end{pmatrix} + \begin{pmatrix} \bar{x}(t,0) & x(t,0) \\ x(t,0) & \bar{x}(t,0) \end{pmatrix} .$$

The first matrix characterizes the two-level system plus bias and the second matrix accounts for the electron-phonon interaction. Here, we assume that the left and right level couple to the lattice with equal strength. Moreover, we do not account for the Coulomb interaction. For convenience, we set $\hbar = 1$. We separately consider acoustical and optical (LO) phonons.

A. Acoustical phonons

It is well known that dissipative effects can be obtained if the phonons have a continuous energy spectrum which is characterized by some cutoff frequency Ω.[25] Acousti-

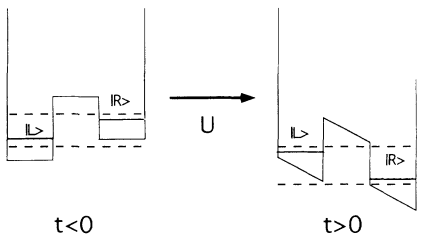

FIG. 2. Schematic representation of the two-level system considered here. The solid lines indicate the levels associated with the individual wells, the dashed line indicates the position of the eigenvalues of the two-level system.

cal phonons provide such a situation. We define

$$\sum_q \frac{M_{\alpha\gamma}^{(q)} M_{\alpha'\gamma'}^{(q)}}{\omega_q} = \mathcal{M}_{\alpha\gamma}\mathcal{M}_{\alpha'\gamma'}\Omega \ .$$

Here, we use two independent real matrix elements, $\overline{\mathcal{M}}=\mathcal{M}_{LL}=\mathcal{M}_{RR}$ and $\mathcal{M}=\mathcal{M}_{LR}=\mathcal{M}_{RL}$, to characterize the coupling to acoustical-phonon modes. More realistic electron-phonon couplings are presently under investigation.

In thermal equilibrium, the system has two eigenstates $|1^0\rangle$ and $|2^0\rangle$ with occupation probability f_1 and f_2, respectively, which can be used to express the matrix elements

$$x_{\rm acc}(0,0) = -2\mathcal{M}\Omega[\overline{\mathcal{M}}(f_1+f_2) + 2\mathcal{M}\,{\rm Re}(f_1\langle L|1^0\rangle\langle 1^0|R\rangle + f_2\langle L|2^0\rangle\langle 2^0|R\rangle)] \quad (45)$$

and

$$\bar{x}_{\rm acc}(0,0) = (\overline{\mathcal{M}}/\mathcal{M})x_{\rm acc}(0,0) \ .$$

For the time evolution,

$$x_{\rm acc}(t,0) = \mathcal{M}\int_0^t dt' f_{\rm acc}(t-t')\{\overline{\mathcal{M}}(f_1+f_2)+2\mathcal{M}\,{\rm Re}[f_1\langle L|1^0(t')\rangle\langle 1^0(t')|R\rangle + f_2\langle L|2^0(t')\rangle\langle 2^0(t')|R\rangle]\} \ . \quad (46)$$

Again, $\bar{x}_{\rm acc}(t,0)=(\overline{\mathcal{M}}/\mathcal{M})x_{\rm acc}(t,0)$. Here,

$$f_{\rm acc}(t-t') = \frac{2}{(t-t')^2}\{\Omega(t-t')\cos[\Omega(t-t')] - \sin[\Omega(t-t')]\}$$

correlates events at time t to events which occurred at time $t'<t$. $f_{\rm acc}(t)$ is given in Fig. 3 for $\Omega=20$.

For our calculation, we choose $\varepsilon_L=0$, $\varepsilon_R=10$, $V=-1$, $\beta=1.2$, and $\Omega=20$. If we use meV as the energy unit, these numbers are quite typical for semiconductor quantum wells. The chemical potential is chosen to lie in the center between the eigenvalues of the two-level system. In all our calculations we set $\overline{\mathcal{M}}=0$. We give results for an applied bias $U(t)=U_0\Theta(t)$, where $U_0=20$. We denote the eigenstates of the biased two-level system (in thermal equilibrium) $|1^U\rangle$ and $|2^U\rangle$. The coupling $\mathcal{M}$ is varied between zero and 0.2. The corresponding eigenvalues λ_i^0 and occupation probabilities f_i of the unbiased two-level system are listed in Table I. It shows that the electron-phonon interaction introduces just a minor renormalization in the present calculations.

In Fig. 4, we plot the probability $\|\langle 1^U|1^0(t)\rangle\|^2$ for $\mathcal{M}=0$ (dotted line), $\mathcal{M}=0.05$ (dashed line), $\mathcal{M}=0.1$ (dot-dashed line), and $\mathcal{M}=0.2$ (solid line). While this probability must be constant for $\mathcal{M}=0$, we see that increasing $\mathcal{M}$ leads to a more and more rapid transition of the original ground-state wave function $|1^0\rangle$ into the new one, $|1^U\rangle$. A corresponding transition is obtained for the second state, $|2\rangle$. If the applied bias U is turned off again (not shown here), the system is found to return to its original ground state. Note that for the present choice of parameters, the probability plotted in Fig. 4 is roughly equal to the probability for finding the system in the right well.

In Fig. 5, we show the probability for finding the sys-

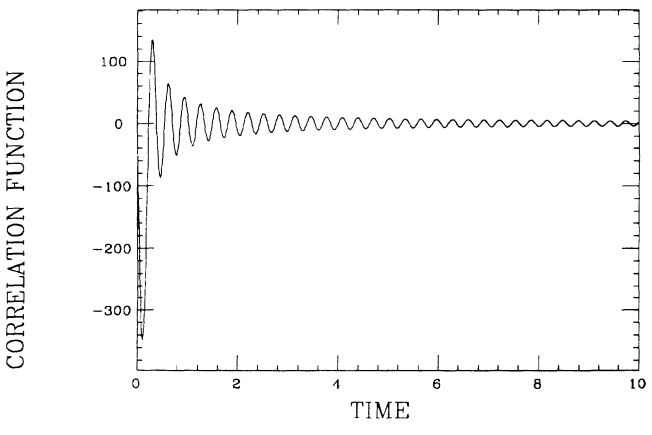

FIG. 3. The function time-correlation function $f_{\rm acc}(t)$ for $\Omega=20$.

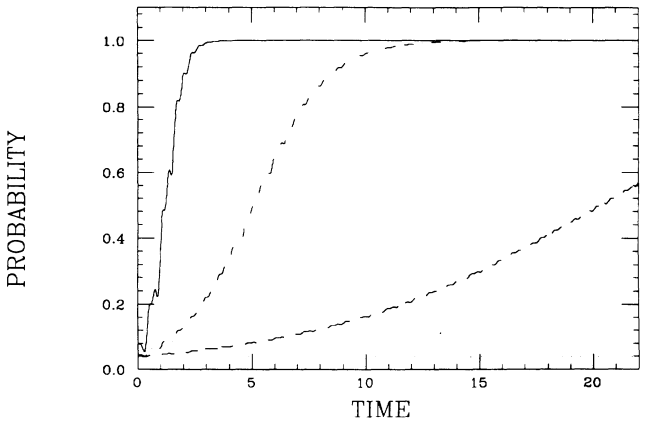

FIG. 4. The probability $\|\langle 1^U|1^0(t)\|^2$ for acoustic-phonon coupling. Dotted, dashed, dot-dashed, and solid lines for coupling strength $\mathcal{M}=0$, 0.05, 0.1, and 0.2, respectively.

TABLE I. Eigenvalues λ_i^0, occupation probabilities f_i, and the off-diagonal phonon-matrix element $x_{\rm acc}(0,0)$ of the two-level system at zero bias U as a function of coupling strength $\mathcal{M}$.

$\mathcal{M}$	λ_1^0	λ_2^0	f_1	f_2	$x_{\rm acc}(0,0)$
0	−0.1	10.1	0.998	2.2×10^{-3}	0
0.05	−0.10	10.10	0.998	2.2×10^{-3}	−1.02
0.10	−0.12	10.12	0.998	2.2×10^{-3}	−1.08
0.20	−0.20	10.20	0.998	2.0×10^{-3}	−1.44

tem in the original ground state, $\|\langle 1^0|1^0(t)\rangle\|^2$, i.e., roughly the probability for finding the system in the left well. For $U_0=20$, the system is off resonance and rapid periodic oscillations of rather small amplitude occur for $\mathcal{M}=0$. When the two-level system is put into contact with the phonons, however, the situation changes dramatically. The oscillations become nonperiodic and some increase in amplitude is observed. Increase of the coupling strength leads to an increasingly rapid transition of the probability to a small and constant value, i.e., rather than being periodic in time, the probability for finding an electron in the left well has become rather small.

Finally, the corresponding off-diagonal phonon matrix element $x_{\rm acc}(t,0)$ is plotted in Fig. 6. We see that $x_{\rm acc}(t,0)$ provides a coupling which undergoes oscillations which eventually die out. The latter originate from the correlation function (Fig. 3) and the fluctuations in the occupation amplitudes for the left and right well in Eq. (46).

Two comments should be made. First, in order to achieve relaxation of the system into the new ground state via $x_{\rm acc}(t,0)$, we find that the cutoff frequency must roughly fulfill $\Omega \geq \Omega_0$, where

$$\Omega_0=\sqrt{V^2+\tfrac{1}{4}(\varepsilon_L+U_0-\varepsilon_R)^2}$$

is the oscillation frequency of the two-level system when it is not coupled to the phonons. This can be seen from the form of $x_{\rm acc}(t,0)$ which, essentially, is a convolution of two oscillatory functions. If the frequencies that characterize these two functions are rather different from each other, the time integral will be very small and undamped oscillations prevail. From a physical standpoint, the condition on the cutoff frequency is rather clear. In order for the phonons to effectively couple to the two levels, phonons of proper energy must be available to ensure energy-conserving transitions. Note, that our original Hamiltonian operator in (1) permits only one-phonon processes.

Second, our calculations have confirmed that, given a suitable electron-phonon coupling, the old eigenfunctions evolve into the new ones. Within the lowest order of approximation, the expectation value of an observable A evolves according to

$$\sum_{i=1,2} f_i\langle i^0|A|i^0\rangle \rightarrow \sum_{i=1,2} f_i\langle i^U|A|i^U\rangle \ .$$

Note that the occupation probabilities f_i, themselves, do not evolve in time. As mentioned above, this is because the time evolution of the system is treated via the Von Neumann equation. A bath is needed to initially prepare the system in thermal equilibrium (characterized by a temperature and a chemical potential). However, the Von Neumann equation neglects the presence of this bath during the evolution of the system under the external field. The present formulation is, therefore, only meaningful if we have processes which occur on several different time scales.[27] In particular, energy and particle exchange with the bath must be slow compared to interaction processes which are accounted for explicitly by

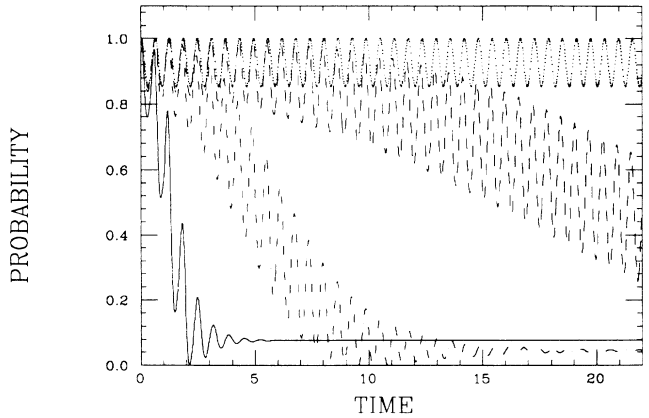

FIG. 5. The probability $\|\langle 1^U|1^0(t)\|^2$ for acoustic-phonon coupling. Dotted, dashed, dot-dashed, and solid lines for coupling strength $\mathcal{M}=0$, 0.05, 0.1, and 0.2, respectively.

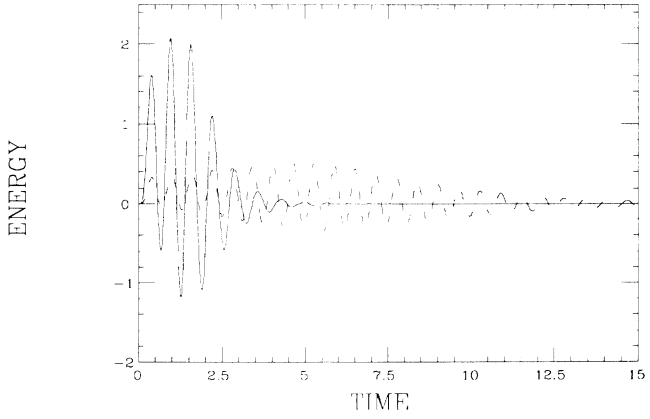

FIG. 6. The matrix element $x_{\rm acc}(t,0)$. Dotted, dashed, dot-dashed, and solid lines for coupling strength $\mathcal{M}=0$, 0.05, 0.1, and 0.2, respectively.

H in (1). Such a situation is, however, rather common in nature. For instance in polar semiconductors, electron-electron and electron–LO-phonon interaction processes are usually much faster than LO phonon decay processes and electron–acoustical-phonon interaction processes. The latter, in turn, are faster than the thermalization of acoustic phonons. Thus, the choice of H, i.e., the "system," must be based upon the physical situation. Equivalently, one may try to directly modify the Von Neumann equation.[27,28] Note, however, that the introduction of a small non-Hermitian term into the Von Neumann equation, as suggested in Ref. 29, does not resolve the problem of constant-occupation probabilities. The simplest way to account for the bath during the time evolution of the system is to relax the occupation probabilities f_i to their new equilibrium value via a phenomenological time constant which is large compared to the time constant with which the wave functions relax. In the extreme case where no hierarchy in time scales exists, one has to start from an isolated system and a microcanonical ensemble and include all interactions explicitly. This may be feasible only for simple model systems.[19]

B. Optical phonons

In this part, we briefly demonstrate how optical phonons are conceived within the mean-field approximation developed above. For simplicity, we neglect any dispersion in the LO-phonon spectrum and set

$$\sum_q \frac{M_{\alpha\gamma}^{(q)} M_{\alpha'\gamma'}^{(q)}}{\omega_q} = \frac{\mathcal{M}_{\alpha\gamma}^{\mathrm{LO}} \mathcal{M}_{\alpha'\gamma'}^{\mathrm{LO}}}{\omega_{\mathrm{LO}}} .$$

where $\omega_{\mathrm{LO}}=35$ is the LO phonon energy. Again, we set the diagonal coupling $\overline{\mathcal{M}}_{\mathrm{LO}}=0$. With this definition, we obtain

$$x_{\mathrm{LO}}(0,0) = -\frac{2\mathcal{M}_{\mathrm{LO}}}{\omega_{\mathrm{LO}}} [\overline{\mathcal{M}}_{\mathrm{LO}}(f_1+f_2) + 2\mathcal{M}_{\mathrm{LO}}\mathrm{Re}(f_1\langle L|1^0\rangle\langle 1^0|R\rangle + f_2\langle L|2^0\rangle\langle 2^0|R\rangle)]$$

and

$$\bar{x}_{\mathrm{LO}}(0,0) = (\overline{\mathcal{M}}_{\mathrm{LO}}/\mathcal{M}_{\mathrm{LO}}) x_{\mathrm{LO}}(0,0) .$$

Furthermore,

$$x_{\mathrm{LO}}(t,0) = \mathcal{M}_{\mathrm{LO}} \int_0^t dt' f_{\mathrm{LO}}(t-t') \{\overline{\mathcal{M}}_{\mathrm{LO}}(f_1+f_2) + 2\mathcal{M}_{\mathrm{LO}}\mathrm{Re}[f_1\langle L|1^0(t')\rangle\langle 1^0(t')|R\rangle + f_2\langle L|2^0(t')\rangle\langle 2^0(t')|R\rangle]\}$$

and

$$\bar{x}_{\mathrm{LO}}(t,0) = (\overline{\mathcal{M}}_{\mathrm{LO}}/\mathcal{M}_{\mathrm{LO}}) x_{\mathrm{LO}}(t,0) .$$

Here, $f_{\mathrm{LO}}(t) = -2\sin(\omega_{\mathrm{LO}} t)$. To demonstrate the effect of the LO phonon term, we consider the double well from above, but replace the acoustic phonons with LO phonons. In the present calculation, we set $\overline{\mathcal{M}}_{\mathrm{LO}}=0$ and $\mathcal{M}_{\mathrm{LO}}=3$. The renormalized eigenvalues of the two-level system are $\lambda_1^0=-0.12$ and $\lambda_2^0=10.12$ with phonon coupling and -0.10 and 10.10, respectively, without LO phonon coupling. Thus, phonon renormalization effects are minimal; nevertheless, the time evolution is strongly influenced by the coupling to the phonons, as will be shown below.

We calculate the probability for finding the system in the new ground-state wave function by solving the nonlinear mean-field equations (37) for the two-level system. The result is shown in Fig. 7 for $U_0=45$ (resonance, solid line) and $U_0=25$ (off-resonance, dashed line). As expected, at resonance (solid line) the system oscillates at a rather low frequency but large amplitude. Absorption and emission of optical phonons permit energy-conserving transitions between the two levels. In the absence of the electron-phonon interaction, the probability is constant at 1.6×10^{-2} (dotted line). Off-resonance (dashed curve)

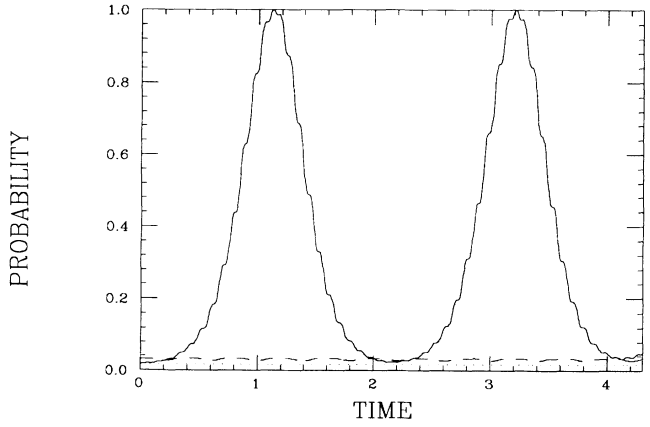

FIG. 7. The probability $\|\langle 1^U|1^0(t)\rangle\|^2$ for LO-phonon coupling. $U_0=45$ with phonon coupling (solid line); $U_0=45$ without phonon coupling (dotted line); $U_0=25$ with phonon coupling (dashed line).

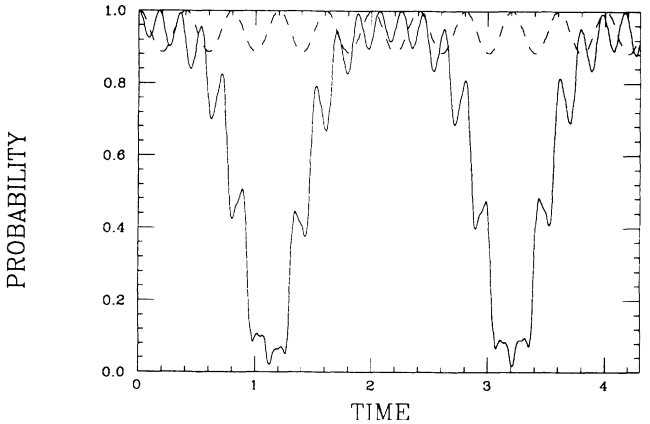

FIG. 8. The probability $\|\langle 1^0|1^0(t)\rangle\|^2$ for LO-phonon coupling. $U_0=45$ with phonon coupling (solid line); $U_0=45$ with phonon coupling (dashed line).

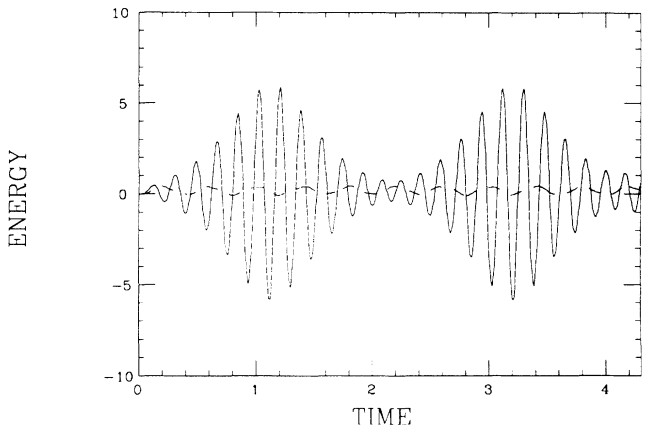

FIG. 9. The matrix element $x_{LO}(t,0)$. $U_0=45$ with phonon coupling (solid line); $U_0=25$ with phonon coupling (dashed line).

transitions are suppressed and the amplitude of the oscillation is so small that it can barely be resolved in the figure. Complimentarily, the probability for finding the system in the original ground-state wave function is given in Fig. 8. The details of the oscillations in Figs. 7 and 8, in particular the high-frequency structure, depend on the choice of the parameters. The self-consistently calculated off-diagonal electron-phonon matrix element $x_{LO}(t,0)$ is given in Fig. 9. It oscillates periodically with the amplitude modulated at the frequency of the oscillation of the system.

In summary, we have shown that the mean-field approximation can account for phonon emission and absorption processes. This all is, of course, in qualitative agreement with recent experimental results on semiconductor double wells.[21,22] In order to be able to make a quantitative comparison with recent experiments,[21,22] one certainly needs a much more refined model that accounts for details such as the electronic structure of the double well, the electron-electron interaction, a realistic carrier-phonon coupling, and more.

VI. SUMMARY AND CONCLUSIONS

In this paper, we have shown that functional-integral techniques are a convenient tool to develop an approximate treatment of the time evolution of a certain class of coupled electron-phonon systems in the presence of an arbitrarily strong external field. It has been shown that the treatment of such systems in thermal equilibrium, performed by us previously, can be generalized to general nonequilibrium situations. This approach is most direct and simple. A generating function for the statistical ensemble average of electron observables can be chosen and functional-integral techniques used to find a representation in the form of a multidimensional integral over an auxiliary field. This exact expression can be obtained for any coupled fermion-boson system which, next to the free-particle Hamiltonian operators, is characterized by a two-fermion interaction and a fermion-boson interaction which is linear in the boson creation and annihilation operators and bilinear in the fermion annihilation and creation operators. We have considered the standard situation where, up to time $T=0$, the system is in thermal equilibrium with a bath. For time $T>0$, an external perturbation in the form of a time-dependent one-electron potential is applied. During the time evolution the coupling to the bath has been neglected.

The functional-integral representation of the generating function has been used to derive a systematic approximation scheme for ensemble averages for the coupled electron-phonon system. We have shown that, within the lowest order of approximation, the time evolution of the coupled electron-phonon system is that of a free-particle system which evolves according to a generalized Schrödinger equation that contains self-consistently determined one-particle potentials. In the present approach, the effective potential is of Hartree type for the electron-electron interaction, and of a non-Markovian form for the electron-phonon interaction. Physical constraints, which are observed by the exact solution, allow the selection of the proper mean-field solutions on which to base the approximation scheme. Unlike in Feynman-path integral formulations of transport, even the lowest-order approximation gives a fully quantum-mechanical description of the system and can account for quantum-confinement effects.

Solving the mean-field equations for the coupled electron-phonon system is slightly more complicated than an ordinary time-dependent Hartree calculation for coupled electron systems, as was shown for the comparatively simple case of an electronic two-level system. Moreover, the eigenvalue and eigenfunctions from these mean-field equations may be used to express all higher-order correction terms. In particular, the stationary-phase approximation has been shown to give the random-phase approximation for ensemble averages of electron observables. This functional-integral approach also provides a *convenient* way to systematically find higher-order corrections.[12] Moreover, the approximation scheme developed in this work is complimentary to the weak-coupling and/or weak-perturbation treatment to which coupled electron-phonon systems have frequently been subjected.

A first application of this approach concerned itself with electronic two-level systems, such as a double well, with coupling to phonons. It has shown that the phonon-induced mean fields can qualitatively account for phonon emission and absorption processes. In particular for acoustical-phonon modes, it was shown that these mean fields provide dissipation terms which make the effective one-electron Schrödinger equation irreversible in time. These terms were obtained from a microscopic theory. In the presence of an external field and a suitable phonon system, they were shown to drive the system into a new equilibrium state. A variety of numerical applications of this approach to other quantum-confined electronic systems can be foreseen in the near future.

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APPENDIX: SELECTION OF PHYSICAL MEAN FIELDS

In this Appendix, the selection of the mean field x^0, Eq. (33), will be outlined in more detail.

For

$$\mathcal{D}(x^0,T,\beta)=\lim_{M\to\infty}\left[\prod_{s=1}^{3M} e^{-\epsilon_s \mathcal{A}_s(x^0)}\right]$$

to be Hermitian,

$$\mathcal{A}_s^\dagger(x^0)=\mathcal{A}_{3M-s+1}(x^0)$$

must be fulfilled. According to the expression of $\mathcal{A}$ in Eq. (24), this requires $(x_s^0)^\dagger=x_{3M-s+1}^0$, where

$$x_{\alpha\gamma s}^0=-\sum_{l=1}^{N}\sum_{\alpha',\gamma'}\sum_{s'=1}^{3M}\epsilon_{s'}\frac{V_{\alpha\gamma s,\alpha'\gamma' s'}\langle w_{ls'}^0|\alpha'\rangle\langle\gamma'|v_{ls'}^0\rangle}{1+e^{-\beta(\lambda_l^0-\mu)}} . \tag{A1}$$

It is easy to show that x^0 permits the choice of a Hermitian $\mathcal{D}(x^0,T,\beta)$ because, if $\mathcal{D}(x^0,T,\beta)$ is Hermitian, its eigenvalues $\{e^{-\beta(\lambda_l^0-\mu)}\}$ are real and left and right eigenkets of $\mathcal{D}(x^0,T,\beta)$ are identical. It follows from

$$\langle w_{ls}|=\langle w_{l,3M}|d_{3M}\cdots d_{s+1}$$

that

$$|w_{l,3M-s+1}^0\rangle=|v_{ls}^0\rangle . \tag{A2}$$

Using this identity and the symmetry properties of V in (20), $(x_s^0)^\dagger=x_{3M-s+1}^0$ can be shown.

The condition that $\mathrm{Tr}\{\rho(T)\}$ is time independent is met by setting

$$x_{\alpha\gamma}^0(t,\beta)=x_{\alpha\gamma}^0(t,0) . \tag{A3}$$

The consistency of this assumption can again be verified by observing that, with (A3) fulfilled, the two time-dependent Hartree equations (29) and (31) are identical and thus, due to the boundary conditions

$$|v_l^0(T,\beta)\rangle=e^{-\beta(\lambda_l^0-\mu)}|v_l^0(T,0)\rangle ,$$
$$|v_l^0(t,\beta)\rangle=e^{-\beta(\lambda_l^0-\mu)}|v_l^0(t,0)\rangle, \quad \text{for } t\in[0,T] . \tag{A4}$$

The structure of V, Eq. (20), and (A4) leads to (A3).

With these conditions imposed, resorting again to the continuum notation, and using the states $\{|\phi_l^0(t,\tau)\rangle\}$ which we introduced in Sec. III, x^0 takes the form

$$x_{\alpha\gamma}^0(0,\tau)=-\sum_{l=1}^{N}\sum_{\alpha',\gamma'}\int_0^\beta d\tau' V_{\alpha\gamma,\alpha'\gamma'}(\tau,\tau')\langle\phi_l^0(0,\beta-\tau')|\alpha'\rangle\langle\gamma'|\phi_l^0(0,\tau')\rangle f_{\mathrm{FD}}(\lambda_l^0) , \tag{A5}$$

for the imaginary-time path, and

$$\begin{aligned}x_{\alpha\gamma}^0(t,0)=\sum_{l=1}^{N}\sum_{\alpha',\gamma'} f_{\mathrm{FD}}(\lambda_l^0)\Bigg[&v_{\alpha\gamma,\alpha'\gamma'}\langle\phi_l^0(t,0)|\alpha'\rangle\langle\gamma'|\phi_l^0(t,0)\rangle\\ &-\frac{i}{\hbar}\sum_q\int_0^t dt'\left(M_{\gamma\alpha}^{(q)*}M_{\alpha'\gamma'}^{(q)}e^{-i\hbar^{-1}(t-t')\omega_q}-M_{\gamma'\alpha'}^{(q)*}M_{\alpha\gamma}^{(q)}e^{-i\hbar^{-1}(t'-t)\omega_q}\right)\\ &\times\langle\phi_l^0(t',0)|\alpha'\rangle\langle\gamma'|\phi_l^0(t',0)\rangle\\ &-\sum_q\frac{M_{\gamma\alpha}^{(q)*}M_{\alpha'\gamma'}^{(q)}e^{-it\hbar^{-1}\omega_q}+M_{\gamma'\alpha'}^{(q)*}M_{\alpha\gamma}^{(q)}e^{it\hbar^{-1}\omega_q}}{\omega_q}\\ &\times\langle\phi_l^0(0,0)|\alpha'\rangle\langle\gamma'|\phi_l^0(0,0)\rangle\Bigg]\end{aligned} \tag{A6}$$

for the real-time path. The boundary conditions for the integral along the imaginary-time path, Fig. 1, are

$$|\phi_l^0(0,0)\rangle=|\phi_l^0(0,\beta)\rangle$$

and the normalization is $\|\phi_l^0(0,0)\|=1$ for $l=1,2,\ldots,N$.

Finally, one needs to ensure that ensemble averages do not evolve in time in the absence of an external perturbation. This is ensured by selecting the time-independent solutions to Eq. (30), i.e., by setting

$$|v_l^0(0,\tau)\rangle=e^{-\tau(\lambda_l^0-\mu)}|v_l^0(0,0)\rangle \tag{A7}$$

for the imaginary-time path. This gives $x^0(0,\tau)$ the final form

$$x_{\alpha\gamma}^0(0,\tau)=\sum_{l=1}^{N}\sum_{\alpha',\gamma'}\left[v_{\alpha\alpha'\gamma\gamma'}-\sum_q\frac{M_{\gamma\alpha}^{(q)*}M_{\alpha'\gamma'}^{(q)}+M_{\gamma'\alpha'}^{(q)*}M_{\alpha\gamma}^{(q)}}{\omega_q}\right]\langle\phi_l^0(0,0)|\alpha'\rangle\langle\gamma'|\phi_l^0(0,0)\rangle f_{\mathrm{FD}}(\lambda_l^0) , \tag{A8}$$

Without an external perturbation,

$$\langle \phi_l^0(t',0)|\alpha'\rangle\langle\gamma'|\phi_l^0(t',0)\rangle = \langle \phi_l^0(0,0)|\alpha'\rangle\langle\gamma'|\phi_l^0(0,0)\rangle$$

and the time integral in (A6) can be performed to give $x^0(t,0)=x^0(0,0)$.

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