Real-time dynamics of soliton diffusion

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We study the nonequilibrium dynamics of solitons in model Hamiltonians for Peierls dimerized quasi-one-dimensional conducting polymers and commensurate charge-density-wave systems. The *real-time* equation of motion for the collective coordinate of the soliton and the associated Langevin equation is found in a consistent adiabatic expansion in terms of the ratio of the optical phonon or phason frequency to the soliton mass. The equation of motion for the soliton collective coordinate allows one to obtain the frequency-dependent soliton conductivity. In lowest order we find that although the coefficient of *static* friction vanishes, there is dynamical dissipation represented by a non-Markovian dissipative kernel associated with two-phonon processes. The correlation function of the noise in the quantum Langevin equation and the dissipative kernel are related by a generalized quantum-fluctuation dissipation theorem. To lowest adiabatic order we find that the noise is Gaussian, additive, and colored. We numerically solve the equations of motion in lowest adiabatic order and compare to the Markovian approximation which is shown to fail both in the ϕ^4 and the sine-Gordon models even at high temperatures. [S0163-1829(98)05202-3]

I. INTRODUCTION AND MOTIVATION

Since the original work of Krumhansl and Schrieffer[1] on solitons as excitations in quasi-one-dimensional systems, it has been realized that solitons play a fundamental role in the transport properties of quasi-one-dimensional Peierls-dimerized conducting polymers[2–4] and commensurate charge-density-wave systems.[5–9]

An important line of experimental and theoretical study has been to determine the dissipative aspects of soliton dynamics.[3,10] Soliton diffusion may play an important role in the dynamics of photoexcitations, in the photoconductivity in conducting polymers, and in the transport phenomena associated with phase solitons in charge-density-wave systems.[5–9]

Early numerical simulations of classical model Hamiltonians revealed[11] that solitons undergo Brownian-like motion. A study of the interaction of solitons with phonon wave packets showed that wave-packet–soliton collisions induce a randomlike motion of the soliton.[12] One of the main focuses of study was the determination of the diffusion constant which was estimated in Ref. 12 for the ϕ^4 model Hamiltonian and in Ref. 13 for the continuum model of *trans*-polyacetylene.[14] In these studies the process of soliton scattering off optical[12,13] and acoustical[13] phonons was studied and input in (semi)classical estimates of the diffusion constant based on the classical fluctuation dissipation theorem. A more microscopic formulation of the calculation of the friction and diffusion coefficients of solitons based on the linear response analysis in terms of Mori's formulation was presented in Ref. 15. These authors focused on obtaining the *static* friction coefficient by evaluating the correlation functions of the soliton velocity and using Mori's formulation.

There are very few experimental data available on the dynamics of soliton diffusion. Although neutral soliton diffusion has been observed (for a thorough review see Refs. 3 and 10), the main dependence seems to be determined by soliton trapping and pinning. Thus the experimental evidence for soliton diffusion is at best inconclusive.

Recently a more microscopic approach to the study of the nonequilibrium aspects of soliton dynamics has been proposed.[16] This approach is based on the treatment of particle-reservoir models in which the soliton is taken to be the particle and the phonon fluctuations as the reservoir. The phonon degrees of freedom are ''integrated out'' in a perturbative manner, leading to a nonequilibrium effective action of the soliton.

In this article we study the nonequilibrium dynamics of the soliton following this latest approach applied to microscopic models relevant to the description of solitons. The soliton dynamics is treated via the collective coordinate method in which the coordinate representing the center of mass of the soliton becomes a quantum mechanical variable.

We use the Schwinger-Keldysh[17–25] formulation of nonequilibrium statistical mechanics to obtain the *real-time* equations of motion for this collective coordinate and the corresponding Langevin equation by tracing out the phonon degrees of freedom in a consistent adiabatic expansion in the ratio of the optical phonon (phason) frequency to the soliton mass.

This Langevin equation allows the unambiguous identification of the dissipative kernels and the noise correlation function, thus allowing us to establish a generalized fluctuation dissipation relation.

To lowest order in the adiabatic expansion we find that the dissipative kernels have memory and a Markovian approximation is unreliable. For the materials of interest, such as polyacetylene with a typical optical phonon frequency of ≈ 0.1–0.2 eV or charge-density-wave systems with a typical phason frequency $\approx 10^{-3}$ eV and bandwidths of several eV, we find that the classical limit of the generalized fluctuation dissipation theorem is not applicable.

To our knowledge none of the previous approaches to soliton dynamics focused on obtaining the real-time equations of motion, and its solutions in particularly relevant cases, nor on the quantum Langevin equation and the properties of the stochastic noise and the quantum-fluctuation dissipation relation.

In Sec. II we introduce and motivate the models to be studied and determine the range of parameters that are experimentally relevant. Section III summarizes the relevant aspects of collective coordinate quantization as applied to the problems under study. Section IV presents the nonequilibrium formulation for obtaining the equations of motion and the Langevin equation in the general case and discusses the features of the solution and the generalized quantum-fluctuation dissipation relation between the noise correlation function and the dissipative kernel. Section V studies specific model Hamiltonians—the ϕ^4 and sine-Gordon field theories—and analyzes the Markovian approximation and the validity of the classical limit. Section VI summarizes our conclusions, and poses further questions and possible future directions.

II. MODELS

Although we are primarily interested in studying nonequilibrium soliton dynamics in quasi-one-dimensional conducting polymers such as *trans*-polyacetylene and charge-density-wave systems which are electron-phonon systems, we will use microscopic model Hamiltonians that are somewhat simpler to study. In what follows we will set for convenience $\hbar = k_B = 1$. For polyacetylene in principle we should start our analysis from the continuum model of Takayama, Lin-Liu, and Maki;[14] however, as these authors showed the solitons in this continuum model are similar to those of the Hamiltonian model studied by Krumhansl and Schrieffer.[1] In particular Ogata *et al.*[15] had previously used the ϕ^4 field theory as model Hamiltonians for conducting polymers. Thus we will study the simpler microscopic model defined by the Hamiltonian[1]

$$H = \int \frac{dx}{l}\left[\frac{P^2(x)}{2m} + \frac{A}{2}u^2(x) + \frac{B}{4}u^4(x) + \frac{mc_0^2}{2}\left(\frac{du(x)}{dx}\right)^2\right]. \tag{1}$$

Clearly the quantitative details of the dissipative processes in this model will be different from those of the continuum model since this model does not incorporate electrons. However, we expect the qualitative features to be robust. Upon rescaling the length and time scales, performing a canonical transformation, and adding suitable constants, the Hamiltonian (1) obtains the form of a ϕ^4 field theory,

$$H = \int dx\left[\frac{\Pi^2}{2} + \frac{1}{2}\left(\frac{d\phi}{dx}\right)^2 + U(\phi)\right],$$

$$U(\phi) = \frac{1}{2g}(m^2 - g\phi^2)^2, \tag{2}$$

where the constants m and g are determined by the original parameters in Eq. (1). These two parameters can be related to the optical phonon frequency $\omega_o = 2m$ and the soliton mass $M = 4m^3/3g$ (see next section). As will become clear in the following sections, the equation of motion can be obtained in a systematic expansion in the adiabatic ratio m/M which is identified with the dimensionless coupling constant g/m^2 of the field theory. In this model we identify the soliton mass with the rest energy of the soliton, and using the parameters for *trans*-polyacetylene given by[2–4] $\omega_o \approx 0.12$ eV and $M \approx 0.4$ eV we find that the adiabatic ratio $m/M \approx 0.15$ is small and a perturbative expansion in this ratio may be appropriate.

In charge-density-wave systems, beginning from the Landau-Ginzburg description of the quasi-one-dimensional system,[5–9] and fixing the amplitude of the order parameter (gap) but allowing the phase to fluctuate, the dynamics is determined by the effective Hamiltonian for the phase of the order parameter (for details see Refs. 5–9),

$$H = \frac{n(\epsilon_F)}{4}\int dx\left[v_f^2\left(\frac{d\phi}{dx}\right)^2 + \frac{m_e^*}{m_e}\left(\frac{d\phi}{dt}\right)^2 + \frac{\omega_F^2 m_e^*}{\mathcal{M}^2 m_e}\cos(\mathcal{M}\phi)\right], \tag{3}$$

with m_e and m_e^* the electron mass and its effective mass, ω_F and v_F the Fermi frequency and velocity, and $\mathcal{M}$ the commensurability of the charge density wave.[5–9] Again, after suitable rescalings of time and space and a canonical transformation, the Hamiltonian can be cast as in Eq. (2) above but with the potential given by

$$U(\phi) = U(\phi) = \frac{m^4}{g}\left(1 - \cos\left[\frac{\sqrt{g}}{m}\phi\right]\right). \tag{4}$$

In this model the gap in the phason spectrum is identified with m and the soliton energy is given by $M = 8m^3/g$. For a typical material, such as $K_{0.3}M_oO_3$ the gap in the phason spectrum is $\approx 10^{-3}$ eV whereas the soliton energy is $\approx 3\times 10^{-2}$ eV.[5–9] Therefore for this type of material the adiabatic ratio $m/M \approx 0.03$ and a perturbative expansion is reliable.

We must note that for both cases the temperatures of experimental relevance correspond to $T < 3\times 10^{-2}$ eV which are of the order of (or smaller than) the typical optical phonon or phason frequencies and the nature of a classical limit must be understood carefully.

III. COLLECTIVE COORDINATE QUANTIZATION

In the previous section we have provided a rational for studying the dynamics of solitons in model field theories described by Hamiltonians of the form

$$H=\int dx\left\{\frac{\pi^2}{2}+\frac{1}{2}\left(\frac{d\phi}{dx}\right)^2+U(\phi)\right\} \tag{5}$$

after suitable rescaling of the parameters.

A static soliton is a solution of the time-independent field equation

$$-\frac{d^2\phi_s}{dx^2}+\frac{\partial U(\phi_s)}{\partial\phi}=0, \tag{6}$$

with boundary conditions such that $|x|\to\infty$, $\phi_s\to\pm\phi_\infty$, and $U(\phi_\infty)=0$.[26,27] Translational invariance implies that such a solution is of the form $\phi_s(x-x_0)$ with x_0 an arbitrary translation chosen such that $\phi_s(0)=0$; therefore x_0 is identified with the position of the soliton.

Including the time derivatives in the equations of motion one sees that after proper rescalings of time and space that led to the form of the Hamiltonian given above they are invariant under a ''Lorentz'' transformation. A soliton moving with constant velocity is given by $\phi_s[(x-x_0-vt)/(\sqrt{1-v^2})]$.[1,12,5] The energy of a static soliton is identified in these models with the soliton mass M and is given by

$$M\equiv E[\phi_s]=\int dx\left(\frac{d\phi_s}{dx}\right)^2. \tag{7}$$

Quantization around the static soliton solution implies writing

$$\hat{\phi}(x,t)=\phi_s(x-x_0)+\hat{\psi}(x-x_0;t), \tag{8}$$

where the fluctuation operator is expanded in terms of a complete set of harmonic modes around the soliton,

$$\hat{\psi}(x-x_0;t)=\sum_n^\infty q_n(t)\mathcal{U}_n(x-x_0), \tag{9}$$

where the mode functions $\mathcal{U}_n(x-x_0)$ obey

$$\left[-\frac{d^2}{dx^2}+\left.\frac{d^2U}{d\phi^2}\right|_{\phi_s}\right]\mathcal{U}_n(x-x_0)=\omega_n^2\mathcal{U}_n(x-x_0), \tag{10}$$

with the completeness relation given by

$$\sum_b \mathcal{U}_b^*(x-x_0)\mathcal{U}_b(x'-x_0)+\int dk\,\mathcal{U}_k^*(x-x_0)\mathcal{U}_k(x'-x_0) =\delta(x-x') \tag{11}$$

and the subscript b stands for summation over bound states and k for scattering states. For bound states, the eigenvectors are chosen to be real, and for scattering states, we label them as $\mathcal{U}_k(x-x_0)$ and are chosen such that $\mathcal{U}_k^*=\mathcal{U}_{-k}$, in which case the coordinate operators obey the Hermiticity condition $q_k^*(t)=q_{-k}(t)$.

These eigenvectors are normalized as

$$\int dx\mathcal{U}_p^*(x-\hat{x}_0)\mathcal{U}_q(x-\hat{x}_0)=\delta_{p,q}. \tag{12}$$

As a consequence of translational invariance, there is a mode with zero eigenvalue given by[26]

$$\mathcal{U}_0(x-x_0)=\frac{1}{\sqrt{M}}\left(\frac{d\phi_s}{dx}\right). \tag{13}$$

Depending on the particular form of the potential $U(\phi)$ there may be other bound states (as is the case with the ϕ^4 potential). There is a continuum of scattering states with frequencies $\omega_k^2=k^2+\omega_o^2$ and $\omega_o^2=d^2U(\phi)/d^2\phi|_{\phi_\infty}$. These scattering states correspond asymptotically to phase-shifted plane waves in the cases under consideration because the relevant potentials are reflectionless.[26,27] The frequencies ω_o are identified with the optical phonon frequencies in the case of the ϕ^4 model[1,12,15] and of the phason gap in the case of phase solitons in charge-density-wave systems.[5–9]

The fluctuation along the functional direction corresponding to the zero-frequency mode represents an infinitesimal translation of the soliton that costs no energy. Since this mode has no restoring force, any arbitrarily large-amplitude fluctuation along this direction is energetically allowed. Therefore fluctuations along this direction must be treated nonperturbatively. The variable x_0, i.e., the center of mass of the soliton, is elevated to the status of a quantum mechanical variable, and the fluctuations are orthogonal to the zero mode. This treatment is the basis of the collective coordinate method[28–35] which was previously used within the context of soliton dynamics by Wada and Schrieffer,[12] Maki,[13] and Ogata *et al.*[15] and within the context of polaron dynamics by Holstein and Turkevich.[34] More recently Castro Neto and Caldeira implemented the collective coordinate quantization method combined with influence functional techniques for the treatment of solitons and polarons.[16]

In collective coordinates quantization instead of the expansion (8) with (9) we expand $\phi(x,t)$ as

$$\phi(x,t)=\phi_s(x-\hat{x}_0(t))+\sum_{n\neq0}^\infty Q_n(t)\mathcal{U}_n(x-\hat{x}_0(t)). \tag{14}$$

This amounts to a change of basis in functional space, from the ''Cartesian'' coordinates $\{q_n\}$ to ''curvilinear'' coordinates $\{\hat{x}_0,Q_{n\neq0}\}$.

The next step is to express the Hamiltonian in terms of the new variables $\hat{x}_0(t)$ and $Q_n(t)$. For this we find more clear and convenient the analysis presented by Holstein and Turkevich[34] which we summarize below for the cases under consideration.

A. Kinetic and potential energies

In the Schrödinger representation the kinetic energy can be expressed as a functional derivative as

$$T=-\frac{1}{2}\int dx\frac{\delta}{\delta\phi}\frac{\delta}{\delta\phi}, \tag{15}$$

where the functional derivative is written in the new coordinates using the chain rule

$$\frac{\delta}{\delta\phi(x)}=\frac{\delta\hat{x}_0}{\delta\phi(x)}\frac{\delta}{\delta\hat{x}_0}+\sum_{m\neq 0}\frac{\delta Q_m}{\delta\phi(x)}\frac{\delta}{\delta Q_m}. \tag{16}$$

Taking the functional variation of the field ϕ, Eq. (14), we obtain

$$\begin{aligned}\delta\phi(x)&=\frac{\delta\phi(x)}{\delta\hat{x}_0}\delta\hat{x}_0+\sum_{m\neq 0}\frac{\delta\phi(x)}{\delta Q_m}\delta Q_m\\&=\left[\frac{\partial\phi_s(x-\hat{x}_0)}{\partial\hat{x}_0}+\sum_{m\neq 0}Q_m\frac{\partial\mathcal{U}_m(x-\hat{x}_0)}{\partial\hat{x}_0}\right]\delta\hat{x}_0\\&\quad+\sum_{n\neq 0}\mathcal{U}_n(x-\hat{x}_0)\,\delta Q_n.\end{aligned} \tag{17}$$

Projecting both sides of the above equation on $\mathcal{U}_0^*(x-\hat{x}_0)$ and then $\mathcal{U}_p^*(x-\hat{x}_0)$ with $p\neq 0$, using Eq. (13) and the orthonormalization condition (12), we obtain

$$\frac{\delta\hat{x}_0}{\delta\phi(x)}=-\frac{1}{\sqrt{M}}\frac{1}{[1+(1/\sqrt{M})\Sigma_{m\neq 0}Q_mS_m]}\mathcal{U}_0^*(x-\hat{x}_0), \tag{18}$$

$$\begin{aligned}\frac{\delta Q_p}{\delta\phi(x)}&=\mathcal{U}_p^*(x-\hat{x}_0)-\frac{1}{\sqrt{M}}\frac{\Sigma_{n\neq 0}G_{pn}Q_n}{[1+(1/\sqrt{M})\Sigma_{m\neq 0}Q_mS_m]}\\&\quad\times\mathcal{U}_0^*(x-\hat{x}_0),\end{aligned} \tag{19}$$

where the matrix elements G_{pm} are defined as

$$G_{pm}=\int dx\mathcal{U}_p^*(x-\hat{x}_0)\frac{\partial\mathcal{U}_m(x-\hat{x}_0)}{\partial x}, \tag{20}$$

$$S_m\equiv G_{0m}=\int dx\mathcal{U}_0(x-\hat{x}_0)\frac{\partial\mathcal{U}_m(x-\hat{x}_0)}{\partial x}. \tag{21}$$

At this stage it is straightforward to follow the procedure detailed in Ref. 34 to find the final form of the kinetic term in the Hamiltonian in the Schrödinger representation of the coordinates $\hat{x}_0, Q_{m\neq 0}$:

$$\begin{aligned}T=-\frac{1}{2}\Bigg\{&\frac{1}{D}\frac{\delta}{\delta\hat{x}_0}\frac{\delta}{\delta\hat{x}_0}+\frac{1}{\sqrt{D}}\frac{\delta}{\delta\hat{x}_0}\sum_{p,m\neq 0}\left[\frac{G_{pm}Q_m}{\sqrt{D}}\frac{\delta}{\delta Q_p}\right.\\&\left.+\frac{\delta}{\delta Q_p}\frac{G_{pm}Q_m}{\sqrt{D}}\right]+\frac{1}{\sqrt{D}}\sum_{p,q,m,n\neq 0}\frac{\delta}{\delta Q_p}\Bigg[\delta_{-p,q}\sqrt{D}\\&+\frac{G_{pm}Q_m}{\sqrt{D}}G_{qn}Q_n\Bigg]\frac{\delta}{\delta Q_q}\Bigg\},\end{aligned} \tag{22}$$

where $\sqrt{D}$ is the Jacobian associated with the change of coordinates[34,26] and is given by

$$\sqrt{D}\equiv\sqrt{M}\left[1+\frac{1}{\sqrt{M}}\sum_{m\neq 0}Q_mS_m\right]. \tag{23}$$

The total potential energy, including the elastic term $V[\phi]$ [see Eq. (5)] is given by

$$V[\phi]\equiv\int dx\left[\frac{1}{2}\left(\frac{\partial\phi}{\partial x}\right)^2+U(\phi)\right]. \tag{24}$$

Using the expansion given by Eq. (14) we find that it can be written in terms of the new coordinates as

$$V[\phi]=M+\frac{1}{2}\sum_{m\neq 0}Q_mQ_{-m}\omega_m^2+\mathcal{O}(Q^3)+\cdots. \tag{25}$$

By translational invariance the potential energy does not depend on the collective coordinate. Identifying the canonical momenta conjugate to $\hat{x}_0, Q_n$ as

$$\pi_0\equiv P=-i\frac{\delta}{\delta\hat{x}_0},\quad \pi_k=-i\frac{\delta}{\delta Q_{-k}}\quad\text{for } k\neq 0, \tag{26}$$

and using the commutation relation of $\sqrt{D}$ and $1/\sqrt{D}$ with Q_n, π_n, and P given by

$$[\pi_n,\sqrt{D}]=-iS_n\quad\text{and}\quad\left[\pi_n,\frac{1}{\sqrt{D}}\right]=-i\frac{S_n}{D}, \tag{27}$$

we find the final form of the Hamiltonian:

$$\begin{aligned}H=M+\frac{1}{2}\Bigg\{&\frac{P^2}{D}+\frac{P}{\sqrt{D}}\sum_{p,m\neq 0}\left[\frac{G_{pm}Q_m}{\sqrt{D}}\pi_{-p}+\pi_{-p}\frac{G_{pm}Q_m}{\sqrt{D}}\right]\\&+\sum_{p\neq 0}\omega_p^2Q_pQ_{-p}+\frac{1}{\sqrt{D}}\sum_{p,q,m,n\neq 0}\pi_{-p}\Bigg[\delta_{-p,q}\sqrt{D}\\&+\frac{G_{pm}Q_m}{\sqrt{D}}G_{qn}Q_n\Bigg]\pi_{-q}\Bigg\}+\mathcal{O}(Q^3)+\cdots,\end{aligned} \tag{28}$$

where Q_p are now operators. The coordinates Q_k associated with the scattering states describe optical phonon (or phason) degrees of freedom with the optical phonon (phason) frequency $\omega_o=d^2U(\phi)/d^2\phi|_{\phi_\infty}$. Since the Hamiltonian does not depend on $\hat{x}_0$, its canonical momentum P is conserved, and it is identified with the total momentum of the soliton-phonon (phason) system.[34,26] The soliton velocity, however, is not proportional to P and depends on the momentum of the phonon (phason) field.

B. Coupling to external fields

The main goal of studying the nonequilibrium dynamics of soliton is a deeper understanding of transport processes by these topological excitations. In the case of conducting polymers in which the underlying physics is described by electron-phonon interactions, the soliton excitation in the dimerized state induces a fractionally charged state associated with an electronic bound state in the middle of the electronic gap.[36] The charge density associated with the electronic bound state is proportional to the profile of the phonon zero mode given by Eq. (13), i.e., $\rho_c(x,t)=e\mathcal{C}\mathcal{U}_0(x-x_0(t))$

which is localized at the center of mass of the soliton, the constant $\mathcal{C}$ depends on the (fractional) charge localized around the soliton.[36,37]

In the case of charge density waves, the transport current is identified with the topological current $j_\mu \propto \epsilon_{\mu\nu}\partial_\nu\phi$.[5–9] Therefore in both cases the charge density is associated with the translational zero mode. Furthermore, current conservation[37] implies that the spatial current is given by $\mathcal{J}_x(x,t)=e\mathcal{C}\dot{x}_0(t)\mathcal{U}_0(x-x_0(t))$. Hence, a spatially constant external electric field couples to the translational zero mode and introduces a term in the Lagrangian of the form

$$\delta\mathcal{L}=-\int dx E(t)x\rho_c(x). \tag{29}$$

Taking $\rho_c(x)=e\mathcal{C}\mathcal{U}_0(x-\hat{x}_0)$ we find that an external spatially constant electric field induces a linear term in $\hat{x}_0$ in the Lagrangian as a consequence of the breakdown of translational invariance,

$$\delta\mathcal{L}=-\tilde{j}(t)\hat{x}_0, \quad \tilde{j}=e\mathcal{C}E(t). \tag{30}$$

This term is responsible for accelerating the soliton and changing the total momentum of the system.

The total (spatially integrated) current transported by the soliton is then given by

$$\int dx\mathcal{J}_x(x,t)=\mathcal{C}\Delta\phi\dot{x}_0(t), \tag{31}$$

with $\Delta\phi=\phi(x=\infty)-\phi(x=-\infty)$. The expression given by Eq. (31) will allow us to obtain the soliton conductivity when the equation of motion for the collective coordinate is obtained.

IV. SOLITON IN THE PHONON HEAT BATH

Our goal is to study the dynamics of a soliton in interaction with the phonons (or phasons). This is achieved by obtaining the real-time equations of motion of the collective coordinate $\hat{x}_0$ by treating the phonons (phasons) as a ''bath'' and obtaining an influence functional[38–42] by ''tracing out'' the phonon degrees of freedom. We assume that the total density matrix for the soliton-phonon system decouples at the initial time t_i, i.e.,

$$\rho(t_i)=\rho_s(t_i)\otimes\rho_R(t_i), \tag{32}$$

where $\rho_s(t_i)$ is the density matrix of the system which is taken to be that of a free particle associated with the collective coordinate of the soliton, i.e., $\rho_s(t_i)=|x_0\rangle\langle x_0|$ and $\rho_R(t_i)$ is the density matrix of the phonon bath and describes harmonic phonons (or phasons) in thermal equilibrium at a temperature T.

Since the solitons can never be separated from the phonon fluctuations, this factorization must be understood to hold in the limit in which the initial time $t_i\to-\infty$ with an adiabatic switching-on the soliton-phonon interaction. An approximate influence functional has been previously obtained in lowest order in Ref. 16, but our approach is different in the sense that we obtain the real-time nonequilibrium evolution equations for the collective coordinate as well as the quantum Langevin equation. Furthermore, whereas in Ref. 16 only processes that conserve the phonon number were considered, we account for all the two-phonon processes consistently to lowest order in the adiabatic expansion.

The time evolution is completely contained in the time-dependent density matrix

$$\rho(t)=U(t,t_i)\rho(t_i)U^{-1}(t,t_i), \tag{33}$$

with $U(t,t_i)$ the time evolution operator. Real-time nonequilibrium expectation values and correlation functions can be obtained via functional derivatives with respect to sources[24] of the generating functional[17–24]

$$Z[j^+,j^-]=\mathrm{Tr}U(\infty,-\infty;j^+)\rho_i U^{-1}(\infty,-\infty;j^-)/\mathrm{Tr}\rho(t_i), \tag{34}$$

where $j^\pm$ are sources coupled to the fields. This generating functional is readily obtained using the Schwinger-Keldysh method which involves a path integral in a complex contour in time:[17–24] a branch corresponding to the time evolution forward, a backward branch corresponding to the inverse time evolution operator, and a branch along the imaginary time axis from t_i to $t_i-i\beta$ to represent the initial thermal density matrix. We will obtain the equation of motion for the soliton collective coordinate in an expansion of the ''adiabatic'' parameter $m/M\approx\omega_0/M$; as discussed in Sec. II, this is also the weak-coupling limit of the scalar field theories under consideration.[26] As will be shown explicitly below in the particular cases studied, the matrix elements given by Eqs. (20) and (21) will provide the necessary powers of m. The lowest order in m/M is formally obtained by keeping only the $1/M$ terms in the Hamiltonian and neglecting the nonlinear $\mathcal{O}(Q^3)$ terms. Under these approximations, $1/D\simeq 1/M$ and the Hamiltonian has the form

$$H=M+\frac{1}{2M}\left(P+\sum_{m,n\neq 0}D_{mn}\pi_m Q_n\right)^2+\frac{1}{2}\sum_{m\neq 0}[\pi_m\pi_{-m}+\omega_m^2 Q_m Q_{-m}]+\tilde{j}(t)\hat{x}_0, \tag{35}$$

where we define

$$D_{mn}=G_{-mn}. \tag{36}$$

At this point it proves convenient to write the coordinates and momenta of the phonons in terms of creation and annihilation operators obeying the standard Bose commutation relations,

$$Q_k=\frac{1}{\sqrt{2\omega_k}}[a_k+a_{-k}^\dagger], \quad \pi_k=-i\sqrt{\frac{\omega_k}{2}}[a_k-a_{-k}^\dagger]. \tag{37}$$

The Hamiltonian can be expressed in terms of a and $a^\dagger$ as

$$H=\frac{1}{2M}(P+F[a^\dagger,a])^2+\sum_{k\neq 0}\omega_k(a_k^\dagger a_k+1/2)+\tilde{j}(t)\hat{x}_0+M, \tag{38}$$

where

$$F[a^\dagger,a]=\sum_{p,k\neq 0}[T^{(S)}_{pk}(a_p a_k-a^\dagger_{-p}a^\dagger_{-k})+T^{(A)}_{pk}(a^\dagger_{-p}a_k - a^\dagger_{-k}a_p)]. \quad (39)$$

We have made use of the symmetries of the operators and defined the symmetric $T^{(S)}_{pk}$ and antisymmetric $T^{(A)}_{pk}$ matrices that provide the interaction vertices as

$$T^{(S)}_{kp}=\frac{1}{4i}\left[\sqrt{\frac{\omega_k}{\omega_p}}-\sqrt{\frac{\omega_p}{\omega_k}}\right]D_{kp},$$

$$T^{(A)}_{kp}=\frac{1}{4i}\left[\sqrt{\frac{\omega_k}{\omega_p}}+\sqrt{\frac{\omega_p}{\omega_k}}\right]D_{kp}. \quad (40)$$

To use the path integral formulation we need the Lagrangian, which to the order that we are working $[\mathcal{O}(m/M)]$ and properly accounting for normal ordering, is given by

$$\mathcal{L}[\hat{\dot{x}}_0,a,a^\dagger]=\frac{M}{2}\hat{\dot{x}}_0{}^2-\hat{\dot{x}}_0F[a^\dagger,a]-\sum_{k\neq 0}\omega_k(a^\dagger_k a_k+1/2) - \tilde{j}(t)\hat{x}_0-M. \quad (41)$$

The interaction of the collective coordinate and the phonon degrees of freedom is now clear. Only time derivatives of the collective coordinate couple, a consequence of the Goldstone character of the collective coordinate. There are two processes described by the interaction: (i) creation and destruction of two phonons and (ii) scattering of phonons. Whereas the first type can contribute with the phonons in their ground state, the second can only contribute if phonon states are occupied.

Since we have preferred to work in terms of the creation and annihilation operators, it is convenient to write the path integral for the nonequilibrium generating functional in the coherent state representation.[43] Following the steps presented in Refs. 16 and 43, we find that the generating functional of nonequilibrium Green's functions is given by

$$\mathcal{Z}[j^+,j^-]=\int\mathcal{D}x^+\int\mathcal{D}x^-\int\mathcal{D}^2\gamma^+\int\mathcal{D}^2\gamma^- \times\exp\left\{i\int dt(\mathcal{L}[\dot{x}^+,\gamma^{*+},\gamma^+,j^+] - \mathcal{L}[\dot{x}^-,\gamma^-,\gamma^{*-},j^-])\right\}, \quad (42)$$

with the Lagrangian density defined on each branch given by

$$\mathcal{L}[\dot{x}^\pm,\gamma^\pm,\gamma^{*\pm},j^\pm]=\frac{M}{2}(\dot{x}^\pm)^2+\sum_{k\neq 0}\left[i\gamma^{*\pm}_k\frac{d\gamma^\pm_k}{dt} - \omega_k\gamma^{*\pm}_k\gamma^\pm_k+\gamma^\pm_k j^{*\pm}_k+\gamma^{*\pm}_k j^\pm_k\right] + x^\pm j^\pm_o-\dot{x}^\pm F[\gamma^{*\pm},\gamma^\pm]-\tilde{j}(t)x^\pm \quad (43)$$

and with proper boundary conditions on the fields that reflect the factorized initial condition with the phonons in thermal equilibrium. The signs $\pm$ in the above expressions correspond to the fields and sources on the forward $(+)$ and backward $(-)$ branches. The contribution from the branch along the imaginary time is canceled by the normalization factor. This is the nonequilibrium generalization of the coherent-state path integrals. For more details the reader is referred to the literature.[16,43] Nonequilibrium Green's functions are now obtained as functional derivatives with respect to the sources $j^\pm$. There are four types of free phonon propagators:[17–24]

$$\langle a^{\dagger+}_k(t)a^+_p(t')\rangle=\delta_{k,p}e^{-i\omega_k(t'-t)}[\theta(t'-t)+n_k], \quad (44)$$

$$\langle a^+_k(\tau)a^{\dagger+}_p(\tau')\rangle=\delta_{k,p}e^{i\omega_k(t'-t)}[\theta(t-t')+n_k],$$

$$\langle a^{\dagger(\pm)}_k(t)a^{\dagger(\pm)}_p(t')\rangle=0,$$

$$\langle a^{(\pm)}_k(t)a^{(\pm)}_p(t')\rangle=0,$$

$$\langle a^{\dagger+}_k(\tau)a^-_p(\tau')\rangle=\delta_{k,p}e^{-i\omega_k(t'-t)}[1+n_k],$$

$$\langle a^+_k(\tau)a^{\dagger-}_p(\tau')\rangle=\delta_{k,p}e^{i\omega_k(t'-t)}n_k,$$

where n_k is Bose-Einstein distribution for phonons of quantum number k and $\langle\cdots\rangle$ refer to averages in the initial density matrix. The $++$ $(--)$ propagators correspond to the time-ordered (anti-time-ordered), whereas the $\pm\mp$ are linear combinations of the advanced and retarded propagators.[24]

An important point to notice is that

$$\langle F[a^\dagger,a]\rangle=0 \quad (45)$$

in the noninteracting case, since it is proportional to $\Sigma_k D_{k,-k}=0$.

A. Soliton equation of motion

The equation of motion of the soliton can be derived by expanding $x^\pm(t)=q(t)+\xi^\pm(t)$ and requiring $\langle\xi^\pm(t)\rangle=0$ to all orders in perturbation theory. Imposing the condition $\langle\xi^+(\tau')\rangle=0$, treating the interaction term up to second order in perturbation theory, and using Eq. (45), we obtain the following equation of motion:

$$\int_{-\infty}^{\infty}dt'\langle\xi^+(t)\dot{\xi}^+(t')\rangle\left[\left\{M\dot{q}(t')+\int_{-\infty}^{t}dt''\Gamma_m(t'-t'')\times\dot{q}(t'')\right\}+\langle\xi^+(t)\xi^+(t')\rangle\tilde{j}(t')\right]=0, \quad (46)$$

where the retarded kernel is given by

$$-i\Gamma_m(t-t')\theta(t-t') =\langle F[a^{\dagger+}(t),a^+(t)]\,F[a^{\dagger+}(t'),a^+(t')]\rangle -\langle F[a^{\dagger+}(t),a^+(t)]\,F[a^{\dagger-}(t').a^-(t')]\rangle. \quad (47)$$

Alternatively this equation of motion may be obtained by computing the influence functional[38–42] in second-order perturbation theory. The resulting influence functional is quadratic in the collective coordinate, and performing the shift $x^\pm(t)=q(t)+\xi^\pm(t)$ the above equation of motion is obtained by requesting that the linear terms in $\xi^\pm$ vanish (there are two linear terms; both give the same equation of motion).

The kernel $\Gamma_m(t-t')$ is found by using Eqs. (47) and (45) and it is given by

$$\Gamma_m(t-t')=-4\sum_{p,k\neq 0}\{T^{(S)}_{pk}T^{(S)}_{-p-k}(1+2n_p)\sin[(\omega_p+\omega_k)\times(t-t')]-2T^{(A)}_{pk}T^{(A)}_{-p-k}n_p\times\sin[(\omega_p-\omega_k)(t-t')]\}. \tag{48}$$

Performing the integral over t' in Eq. (46) by parts, we obtain the final form of the equation of motion,

$$M\ddot{q}(t)+\int_{-\infty}^{t}dt'\Sigma_m(t-t')\dot{q}(t')=\tilde{j}(t), \tag{49}$$

where the nonlocal kernel is given by

$$\Sigma_m(t-t')=\frac{\partial\Gamma_m(t-t')}{\partial t}=-\frac{\partial\Gamma_m(t-t')}{\partial t'}. \tag{50}$$

Using Eq. (48) we find the final expression for the kernel Σ_m:

$$\Sigma_m(t-t')=-4\sum_{p,k\neq 0}\{T^{(S)}_{pk}T^{(S)}_{-p-k}(1+2n_p)(\omega_p+\omega_k)\times\cos[(\omega_p+\omega_k)(t-t')]-2T^{(A)}_{pk}T^{(A)}_{-p-k}n_p(\omega_p-\omega_k)\times\cos[(\omega_p-\omega_k)(t-t')]\}. \tag{51}$$

We will see in the next sections that the two kernels Σ_m and Γ_m have a very special significance: Whereas Σ_m is identified with the real-time retarded self-energy of the collective coordinate, Γ_m will provide the coefficient of *dynamical friction* in the Markovian approximation.

It is more convenient to express the equation of motion of the soliton in terms of the velocity

$$M\dot{V}(t)+\int_{-\infty}^{t}dt'\Sigma_m(t-t')V(t')=\tilde{j}(t), \tag{52}$$

with Σ_m given by Eq. (51).

The relation (51) ensures to this order in the perturbative expansion that with an adiabatic switching on the convergence factor introduced to regularize the lower limit of the integral and to provide an initial factorization of the density matrix as $t_i\to-\infty$ the total integral of the retarded self-energy kernel vanishes, i.e.,

$$\int_{-\infty}^{t}\Sigma_m(t-t')dt'=0. \tag{53}$$

Therefore, in the absence of a driving term that explicitly breaks translational invariance, i.e., for $\tilde{j}=0$, any constant velocity of the soliton is a solution of the equation of motion (52). This result is a consequence of the Galilean invariance of the effective Lagrangian.

B. General properties of the solution

Consider switching on a spatially constant electric field at $t=0$ to study the linear response of the soliton velocity. Assuming that for $t<0$ the soliton traveled with a constant velocity v_0, after switching on the electric field the soliton will accelerate, but it will also transfer energy and excite the phonon degrees of freedom and this will lead to dissipative processes. Therefore writing $V(t)=v_0+v(t)$ with $\tilde{j}(t<0)=0$ and $\tilde{j}(t>0)\neq 0$ and using the property (53) the equation of motion for the velocity change becomes

$$M\dot{v}(t)+\int_{0}^{t}dt'\Sigma_m(t-t')v(t')=\tilde{j}(t). \tag{54}$$

The solution of this equation is found by Laplace transform, in terms of $\tilde{v}(s)$, $\tilde{\Sigma}_m(s)$, and $\tilde{J}(s)$, the Laplace transforms of the velocity, self-energy kernel, and current, respectively, in terms of the Laplace variable s. We find that the solution is given by

$$\tilde{v}(s)=\frac{v_0+(\tilde{J}(s)/M)}{s+(1/M)\tilde{\Sigma}_m(s)}. \tag{55}$$

The quantity

$$G(s)=\frac{1}{s+(1/M)\tilde{\Sigma}_m(s)} \tag{56}$$

is the Laplace transform of the propagator of the velocity of the collective coordinate. We can now extract the frequency-dependent conductivity associated with the moving soliton by taking $v_0=0$ and analytically continuing $s\to i\omega+0^+$ to obtain the retarded Fourier transform. We find

$$\sigma(\omega)=\frac{\Delta\phi(e\mathcal{C})^2}{M}G(s=i\omega+0^+). \tag{57}$$

Therefore the frequency-dependent conductivity is solely determined by $G(s)$ which can be found in a consistent adiabatic expansion.

The real-time evolution is found by the inverse Laplace transform

$$v(t)=\frac{1}{2\pi i}\int_C e^{st}\tilde{v}(s)ds, \tag{58}$$

where C refers to the Bromwich contour running along the imaginary axis to the right of all the singularities of $\tilde{v}(s)$ in the complex s plane. Therefore we need to understand the analytic structure of $G(s)$ in Eq. (55) to obtain the real-time dynamics. The Laplace transform of the self-energy kernel is given by

$$\tilde{\Sigma}_m(s)=s\tilde{\Gamma}_m(s), \tag{59}$$

$$\tilde{\Gamma}_m(s)=-4\sum_{p,k\neq 0}\left\{T^{(S)}_{pk}T^{(S)}_{-p-k}(1+2n_p)\frac{(\omega_p+\omega_k)}{s^2+(\omega_p+\omega_k)^2}\right.$$

$$\left.-2T^{(A)}_{pk}T^{(A)}_{-p-k}n_p\frac{(\omega_p-\omega_k)}{s^2+(\omega_p-\omega_k)^2}\right\}, \tag{60}$$

where $\tilde{\Gamma}_m(s)$ is the Laplace transform of the kernel Γ_m given above.

The presence of a static friction coefficient will be revealed by a pole in $G(s)$ with a negative real part, since this will translate into an exponential relaxation of the velocity.

In the absence of interactions $G(s)$ has a simple pole at $s=0$. Since we obtained the expression for the kernels in perturbation theory, the position of a pole must be found in a consistent perturbative expansion by writing $s_p=(1/M)s_1+\cdots$; we find

$$s_p=\tilde{\Sigma}_m(s=0)\equiv 0. \tag{61}$$

Therefore the coefficient of *static* friction vanishes. This is a consequence of the vanishing of the integral (53). Therefore up to this order in perturbation theory the position of the pole in the s variable remains at $s=0$. This is consistent with the results of Ogata *et al.*[15] who also found that to lowest order in the adiabatic expansion the *static* friction coefficient vanishes.

From the expression (60) we also find that $G(s)$ has cuts along the imaginary s axis: (i) a two-phonon cut beginning at $s=\pm 2i\omega_o$ corresponding to the virtual processes of spontaneous and stimulated two-phonon creation and destruction and (ii) a cut with a pinch singularity beginning at $s=i0^{\pm}$ corresponding to the processes of phonon scattering. The contribution from this second cut vanishes at $T=0$. In summary, the analytic structure of $G(s)$ in the complex s plane corresponds to a pole at $s=0$ with residue

$$Z_s=\frac{1}{1+(1/M)\tilde{\Gamma}_m(0)} \tag{62}$$

and cuts along the imaginary axis beginning at $\pm 2i\omega_o$ and $\pm i\epsilon$ with $\epsilon\rightarrow 0$ to clarify that the beginning of this cut pinches the pole.

The residue Z_s has a very clear interpretation; it is the ''wave function renormalization'' and its effect can be understood in two alternative manners.

Consider the case in which $\tilde{j}=0$ in Eq. (55). Performing the inverse Laplace transform and invoking the Riemann-Lebesgue lemma, the long-time behavior will be completely dominated by the pole at $s=0$. Therefore, if the velocity of the soliton has been changed at $t=0$ by some external source, this disturbance will relax in time to an asymptotic value given by

$$v_\infty=Z_s v_0. \tag{63}$$

Alternatively, consider the case of $v_0=0$ but with an electric field switched on at $t=0$ and constant in time thereafter. Again the inverse Laplace transform at long time will be dominated by the pole, and we find that the soliton moves with constant acceleration given by

$$\dot{v}=\frac{\tilde{j}}{M_{\rm eff}} \quad \text{with} \quad M_{\rm eff}=\frac{M}{Z_s}. \tag{64}$$

Thus the wave function renormalization can also be understood as a renormalization of the soliton mass. The ratio of the asymptotic acceleration to the initial acceleration is given by Z_s. As the soliton moves, the interaction with the phonon (phason) bath ''dresses'' it, changing its effective mass, which will be seen in specific models to be *larger* than the bare mass. This result is similar to that found by Holstein and Turkevich in the polaron case within a different approach.[34]

A further understanding of the dynamics will necessarily require knowledge of the matrix elements to establish the details of the kernels. This will be studied in particular models in the next section.

C. Semiclassical Langevin equation

The classical Langevin equation is an adequate phenomenological description of Brownian motion obtained by considering the dynamics of one (or few) degrees of freedom that interact with a bath in equilibrium. It contains a term proportional to the velocity of the particle which incorporates friction and dissipation and a stochastic term which reflects the random interaction of the heat bath with the particle. These two terms are related by the classical fluctuation-dissipation relation.

At the quantum mechanical level it is also possible to obtain a ''reduced'' or coarse-grained description of the dynamics of one (or few) degrees of freedom in interaction with a bath. The coarse-graining procedure has a very precise meaning: The full time-dependent density matrix is traced over the bath degrees of freedom, yielding an effective or ''reduced'' density matrix for the degrees of freedom whose dynamics is studied.

Such a description of the nonequilibrium dynamics of a quantum mechanical particle coupled to a dissipative environment by a Langevin equation was presented by Caldeira and Leggett[39] and by Schmid.[40] Their technique is based on the influence-functional method of Feynman and Vernon[38] that naturally leads to a semiclassical Langevin equation.

In this section we follow the procedure of Refs. 39–42 generalized to our case to derive the Langevin equation for solitons in a heat bath to lowest order in the adiabatic coupling.

The main step is to perform the path integrals over the phonon degrees of freedom, thus obtaining an effective functional for the collective coordinate of the soliton. Unlike the most usually studied cases of a particle linearly coupled to an harmonic reservoir[39–42] we have here a bilinear coupling to the phonons (phasons). Therefore the influence functional cannot be obtained exactly, but it can be obtained in a consistent perturbative expansion. For this we treat the interaction term $\mathcal{L}_I[\dot{x}^{\pm},\gamma^{\pm},\gamma^{*\pm}]$ in perturbation theory up to second order in the vertex proportional to $\dot{x}^{\pm}$ (which is equivalent to lowest order in the adiabatic coupling m/M). Integrating over the phonon variables and using $\langle F[a^{\dagger},a]\rangle=0$, we obtain

$$\mathcal{Z}[j^+,j^-=0]=\int \mathcal{D}x^+\mathcal{D}x^-\exp\left(i\int_{-\infty}^{\infty}dt'(\mathcal{L}_0[\dot{x}^+]-\mathcal{L}_0[\dot{x}^-])\right)\mathcal{F}[\dot{x}^+,\dot{x}^-], \tag{65}$$

where

$$\mathcal{L}_0[\dot{x}^\pm]=\frac{1}{2}M(\dot{x}^\pm)^2-\tilde{j}x^\pm \tag{66}$$

and $\mathcal{F}[\dot{x}^+,\dot{x}^-]$ is the influence functional.[38–42] To lowest adiabatic order we find

$$\begin{aligned}\mathcal{F}[\dot{x}^+,\dot{x}^-]=\exp\Big\{-\frac{1}{2}\int dtdt'[&\dot{x}^+(t)G^{++}(t,t')\dot{x}^+(t')\\&+\dot{x}^-(t)G^{--}(t,t')\dot{x}^-(t')\\&+\dot{x}^+(t)G^{+-}(t,t')\dot{x}^-(t')\\&+\dot{x}^-(t)G^{-+}(t,t')\dot{x}^+(t')]\Big\}\end{aligned} \tag{67}$$

in terms of the real-time phonon correlation functions (see Appendix A)

$$\begin{aligned}G^{++}(t,t')&=\langle F[a^{\dagger+}(t),a^+(t)]F[a^{\dagger+}(t'),a^+(t')]\rangle,\\G^{--}(t,t')&=\langle F[a^{\dagger-}(t),a^-(t)]F[a^{\dagger-}(t'),a^-(t')]\rangle,\\G^{+-}(t,t')&=-\langle F[a^{\dagger+}(t),a^+(t)]F[a^{\dagger-}(t'),a^-(t')]\rangle,\\G^{-+}(t,t')&=-\langle F[a^{\dagger-}(t),a^-(t)]F[a^{\dagger+}(t'),a^+(t')]\rangle.\end{aligned} \tag{68}$$

At this stage it is convenient to introduce the center of mass and relative coordinates, x and R, respectively, which are defined as

$$x(t)=\frac{1}{2}[x^+(t)+x^-(t)],\quad R(t)=x^+(t)-x^-(t). \tag{69}$$

These are recognized as the coordinates used in the Wigner transform of the density matrix[39–42] in terms of which the partition function becomes

$$\mathcal{Z}[0]=\int \mathcal{D}x\mathcal{D}Re^{iS[x,R]}, \tag{70}$$

with the nonequilibrium effective action given by

$$S[x,R]=\int dtR(t)\left[-M\ddot{x}(t)-\frac{i}{2}\int dt'[K_1(t-t')\dot{x}(t')-K(t-t')R(t')]\right] \tag{71}$$

in terms of the kernels $K_1(t-t')$ and $K(t-t')$ which are given by (see Appendix B)

$$\begin{aligned}K_1(t-t')&=8i\theta(t-t')\sum_{p,k\neq 0}\{T^{(S)}_{pk}T^{(S)}_{-p-k}(1+n_p+n_k)(\omega_p+\omega_k)\cos[(\omega_p+\omega_k)(t-t')]-T^{(A)}_{pk}T^{(A)}_{-p-k}(n_p-n_k)(\omega_p-\omega_k)\cos[(\omega_p-\omega_k)(t-t')]\}\\&=-2i,\Sigma_m(t-t')\end{aligned} \tag{72}$$

and

$$\begin{aligned}K(t-t')=-2\sum_{p,k\neq 0}\{&T^{(S)}_{pk}T^{(S)}_{-p-k}(1+n_p+n_k+n_pn_k)(\omega_p+\omega_k)^2\cos[(\omega_p+\omega_k)(t-t')]\\&+2T^{(A)}_{pk}T^{(A)}_{-p-k}n_k(1+n_p)(\omega_p-\omega_k)^2\cos[(\omega_p-\omega_k)(t-t')]\}.\end{aligned} \tag{73}$$

At this stage it proves convenient to introduce the identity

$$\begin{aligned}\exp\left(-\frac{1}{2}\int dtdt'R(t)K(t-t')R(t')\right)&\\=C(t)\int\mathcal{D}\xi\exp\left(-\frac{1}{2}\int dtdt'\xi(t)K^{-1}(t-t')\xi(t')\right.&\\\left.+i\int dt\xi(t)R(t)\right),&\end{aligned} \tag{74}$$

with $C(t)$ being an inessential normalization factor, to cast the nonequilibrium effective action of the collective coordinate in terms of a stochastic noise variable with a definite probability distribution,[40–42]

$$\mathcal{Z}[0]=\int\mathcal{D}x\mathcal{D}R\mathcal{D}\xi P[\xi]\exp\left\{i\int dtR(t)\left[-M\ddot{x}(t)-\frac{i}{2}\int dt'K_1(t-t')\dot{x}(t')+\xi(t)\right]\right\}, \tag{75}$$

where the probability distribution of the stochastic noise, $P[\xi]$, is given by

$$P[\xi]=\int\mathcal{D}\xi\exp\left\{-\frac{1}{2}\int dtdt'\xi(t)K^{-1}(t-t')\xi(t')\right\}. \tag{76}$$

In this approximation we find that the noise is Gaussian, additive, and with a correlation function given by

$$\langle\xi(t)\xi(t')\rangle=K(t-t'). \tag{77}$$

The semiclassical Langevin equation is obtained by extremizing the effective action in Eq. (75) with respect to $R(t)$,[39–42]

$$M\ddot{x}(t)+\int_{-\infty}^{t}dt'\Sigma_m(t-t')\dot{x}(t')-\tilde{j}(t)=\xi(t). \tag{78}$$

Two features of the semiclassical Langevin equation deserve comment. The first is that the kernel $K_1(t-t')$, as can be seen from Eq. (72), is non-Markovian. The second is that the noise correlation function $K(t-t')$ is colored; i.e., it is not a delta function $\delta(t-t')$. The relationship between the kernels $K_1(t-t')$ and $K(t-t')$ established in Appendix B

constitutes a generalized quantum-fluctuation-dissipation relation.[39–42] Finally we recognize that taking the average of Eq. (78) with the noise probability distribution $P[\xi]$ yields the equation of motion for the expectation value of the collective coordinate [Eq. (52)].

A classical description is expected to emerge when the occupation distribution for the phonons can be approximated by their classical counterparts,[39] i.e., when $n_k \approx T/\omega_k$ (in units in which the natural constants had been set to 1). However, this classical limit requires that $T \gg m$, and with m being identified with the optical phonon or phason frequency in these models, such a classical approximation will be valid when temperatures are much larger than these frequencies. In the models under consideration the optical phonon frequencies are in the range $\omega_o \approx 0.1$ eV and the phason frequencies (in the case of charge-density-wave systems) $\omega_o \approx 10^{-3}$ eV. A more stringent criterion for the validity of the classical limit is when the temperature is larger than the bandwidth.[39] In the situations under consideration the bandwidth is typically several eV. Hence a classical description will be valid in a temperature regime that far exceeds the experimentally relevant region in the case of conducting polymers. In the case of charge-density-wave (CDW) systems the experimentally relevant temperatures are of the order of a few times ω_o. For these systems whether the fluctuation and dissipation kernels achieve a classical limit for these temperatures must be studied in detail. This will be done with particular model Hamiltonians below.

If the kernels Σ_m and K admit a Markovian limit, then a diffusion coefficient could be extracted by computing the long-time limit of the correlation function $\langle\langle [x(t) - x(0)]^2 \rangle\rangle / t$ where $\langle\langle \cdots \rangle\rangle$ stand for average over the noise distribution function. However, when the kernels do not become Markovian, such a definition is not appropriate.

This summarizes the general formulation of the description of the dynamics of the collective coordinate both at the level of the evolution equation for the expectation value as well as for the effective Langevin dynamics in terms of stochastic noise terms arising from the fluctuations in the phonon bath. We are now in condition to study specific models.

V. SPECIFIC MODELS

In the previous sections we established the general aspects of the real-time dynamics of solitons in the presence of the phonon bath, obtaining the equation of motion as well as the Langevin equation for the collective coordinate in lowest adiabatic order. Further progress in the understanding of the dynamics necessarily involves the details of particular models which determine the matrix elements $T^{(A,S)}$ and therefore the time dependence of the kernels involved. In this section we study these details for the sine-Gordon and ϕ^4 models.

A. Sine-Gordon

As discussed in Sec. II, sine-Gordon field theory provides an effective microscopic description for phase solitons in CDW systems[5–9] in the limit in which the amplitude of the lattice distortion is kept constant.

For the sine-Gordon model the potential is given by

$$U(\phi) = \frac{m^4}{g}\left(1 - \cos\left[\frac{\sqrt{g}}{m}\phi\right]\right) \tag{79}$$

and the static soliton solution is given by[27,26,33]

$$\phi_s(x) = \frac{4m}{\sqrt{g}} \arctan[e^{mx}]. \tag{80}$$

The normal modes of this theory are the solutions of the equation [see Eq. (10)]

$$\left[-\frac{d^2}{dx^2} + m^2 - \frac{2m^2}{\cosh^2(mx)}\right]\psi_n(x) = \omega_n^2 \psi_n(x). \tag{81}$$

The solutions of the above differential equation are well known[44,27,33]. There is only one bound state with zero eigenvalue, the zero mode, followed by a continuum with wave functions given by

$$\mathcal{U}_k(x) = \frac{1}{\sqrt{2\pi}\omega_k}[-ik + m\ \tanh(mx)]e^{ikx}, \tag{82}$$

with $\omega_k^2 = k^2 + m^2$. The scattering states represent the phason (harmonic fluctuations of the phase) excitations around the soliton.[5–9]

The matrix elements D_{pk} were already calculated by de Vega[33] [see Eqs. (36) and (20)] and are given by

$$D_{kp} = ip\,\delta(k+p) + \frac{i(p^2-k^2)}{4\omega_k\omega_p \sinh[(\pi/2)(p+k)/m]} \quad \text{for} \quad p \neq k, \tag{83}$$

which determine the symmetric and antisymmetric matrix elements

$$T^{(S)}_{pq} = \frac{1}{4}\left[\left(\frac{\omega_p}{\omega_q}\right)^{1/2} - \left(\frac{\omega_q}{\omega_p}\right)^{1/2}\right] \times \left\{\frac{(q^2-p^2)}{4\omega_k\omega_p \sinh[(\pi/2)(q+p)/m]}\right\},$$

$$T^{(A)}_{pq} = \frac{1}{4}\left[\left(\frac{\omega_p}{\omega_q}\right)^{1/2} + \left(\frac{\omega_q}{\omega_p}\right)^{1/2}\right]\left\{\frac{(q^2-p^2)}{4\omega_k\omega_p \sinh[(\pi/2)(q+p)/m]}\right\}. \tag{84}$$

Since in this theory there are no bound states other than the zero mode, $F[a^\dagger, a]$ is given only by the first two terms in Eq. (B6). Substituting Eq. (84) into Eqs. (48) and (51), we obtain the final form of the kernels in this case,

$$\Gamma_m(t-t') = \frac{1}{4^3}\int_{-\infty}^{\infty} \frac{dp\,dk}{\omega_p^3\omega_k^3} \frac{(p^2-k^2)^2}{\sinh^2[(\pi/2)(p+k)/m]} \times \{(1+2n_p)(\omega_p-\omega_k)^2 \sin[(\omega_p+\omega_k)(t-t')] - 2n_p(\omega_p+\omega_k)^2 \sin[(\omega_p-\omega_k)(t-t')]\}, \tag{85}$$

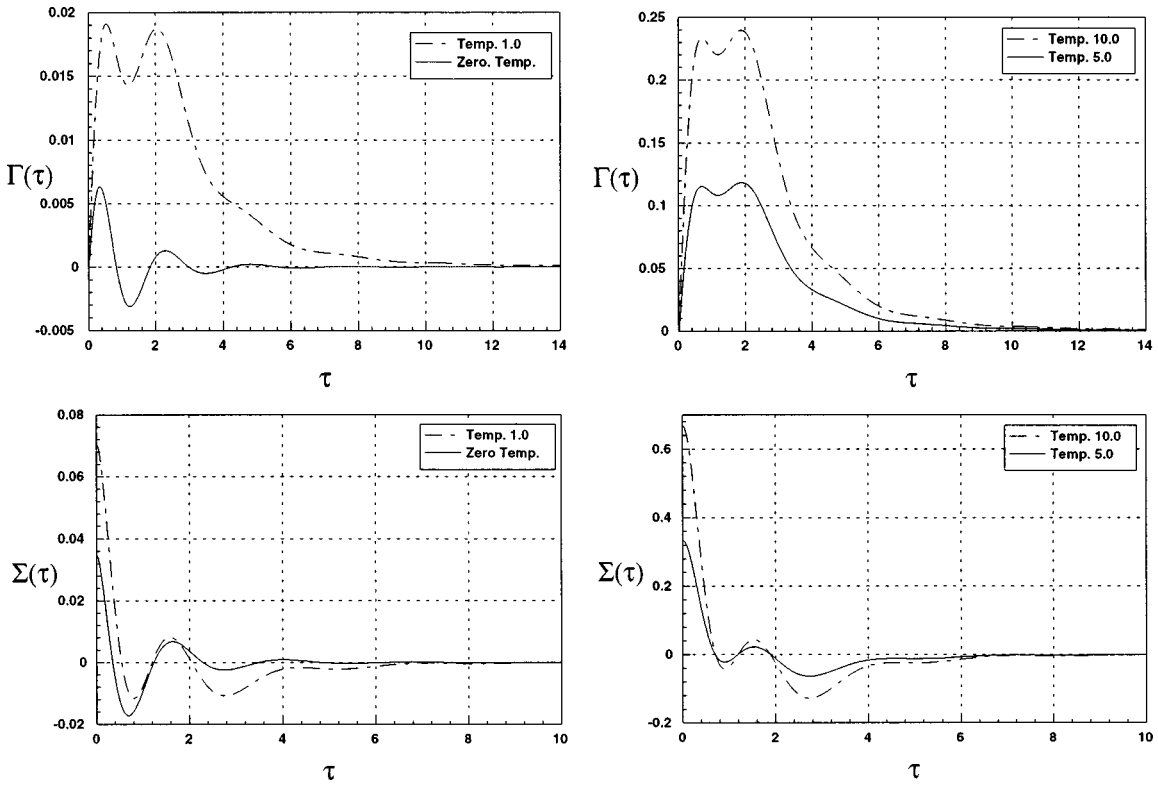

FIG. 1. The functions $\Gamma(\tau)$ and $\Sigma(\tau)$ for temperatures $\mathcal{T}=0$, 1.0, 5.0, and 10.0 for sine-Gordon theory.

$$\Sigma_m(t-t')=\frac{1}{4^3}\int_{-\infty}^{\infty}\frac{dpdk}{\omega_p^3\omega_k^3}\frac{(p^2-k^2)^3}{\sinh^2[(\pi/2)(p+k)/m]}\{(\omega_p-\omega_k)(1+n_p+n_k)\cos[(\omega_p+\omega_k)(t-t')]-(n_p-n_k)(\omega_p+\omega_k)\cos[(\omega_p-\omega_k)(t-t')]\}. \quad (86)$$

At this point it proves useful to express $\Gamma_m(t-t')$ and $\Sigma_m(t-t')$ in terms of dimensionless quantities to display at once the nature of the adiabatic expansion. To achieve this let us make the following change of variables:

$$p\to\frac{p}{m},\quad k\to\frac{k}{m},\quad \tau=mt,\quad \text{and}\quad \mathcal{T}=\frac{T}{m}. \quad (87)$$

Then $\Gamma_m(t-t')$ and $\Sigma_m(t-t')$ can be written as

$$\Gamma_m(t-t')=m^2\Gamma(\tau-\tau')\quad\text{and}\quad\Sigma_m(t-t')=m^3\Sigma(\tau-\tau'), \quad (88)$$

where

$$\Gamma(\tau)=\int_{-\infty}^{\infty}dpdk\{\Gamma_1(p,k)\sin[(w_p+w_k)(\tau)]+\Gamma_2(p,k)\sin[(w_p-w_k)(\tau)]\}, \quad (89)$$

$$\Sigma(\tau)=\int_{-\infty}^{\infty}dpdk\{\Sigma_1(p,k)\cos[(w_p+w_k)(\tau)]+\Sigma_2(p,k)\cos[(w_p-w_k)(\tau)]\}, \quad (90)$$

with

$$\Gamma_1(p,k)=\frac{1}{4^3}\frac{(1+2n_p)(p^2-k^2)^2(w_p-w_k)^2}{w_p^3w_k^3\sinh^2[(\pi/2)(p+k)]},$$

$$\Gamma_2(p,k)=-\frac{1}{32}\frac{n_p(p^2-k^2)^2(w_p+w_k)^2}{w_p^3w_k^3\sinh^2[(\pi/2)(p+k)]},$$

$$\Sigma_1(p,k)=(w_p+w_k)\Gamma_1(p,k),$$

$$\Sigma_2(p,k)=(w_p-w_k)\Gamma_2(p,k),$$

$$w_p^2=p^2+1,\quad n_p=\frac{1}{e^{w_p/\mathcal{T}}-1}. \quad (91)$$

Figure 1 shows the numerical evaluation of $\Gamma(\tau)$ and $\Sigma(\tau)$ vs τ for different values of $\mathcal{T}$. We clearly see that the self-energy kernel Σ is peaked near $\tau=0$ and localized within a time scale $\tau_s\approx m^{-1}\approx\omega_0^{-1}$ at low and intermediate temperatures. We find numerically that this time scale becomes very short, of the order of T^{-1} for $T\geqslant 10m$ which for the case of charge-density-wave systems is about the maximum temperature scale of experimental relevance. Similarly, the kernel Γ varies slowly over a large time scale $\approx(5$–$10)$ m^{-1} for large temperatures, but at small and intermediate temperatures $T\leqslant m(\omega_o)$ it oscillates within time scales comparable to the inverse phason frequency.

1. Equation of motion: (i) Exact solution

With the purpose of providing a numerical solution to the equations of motion, we now consider the case of an externally applied electric field switched on at $t=0$ and main-

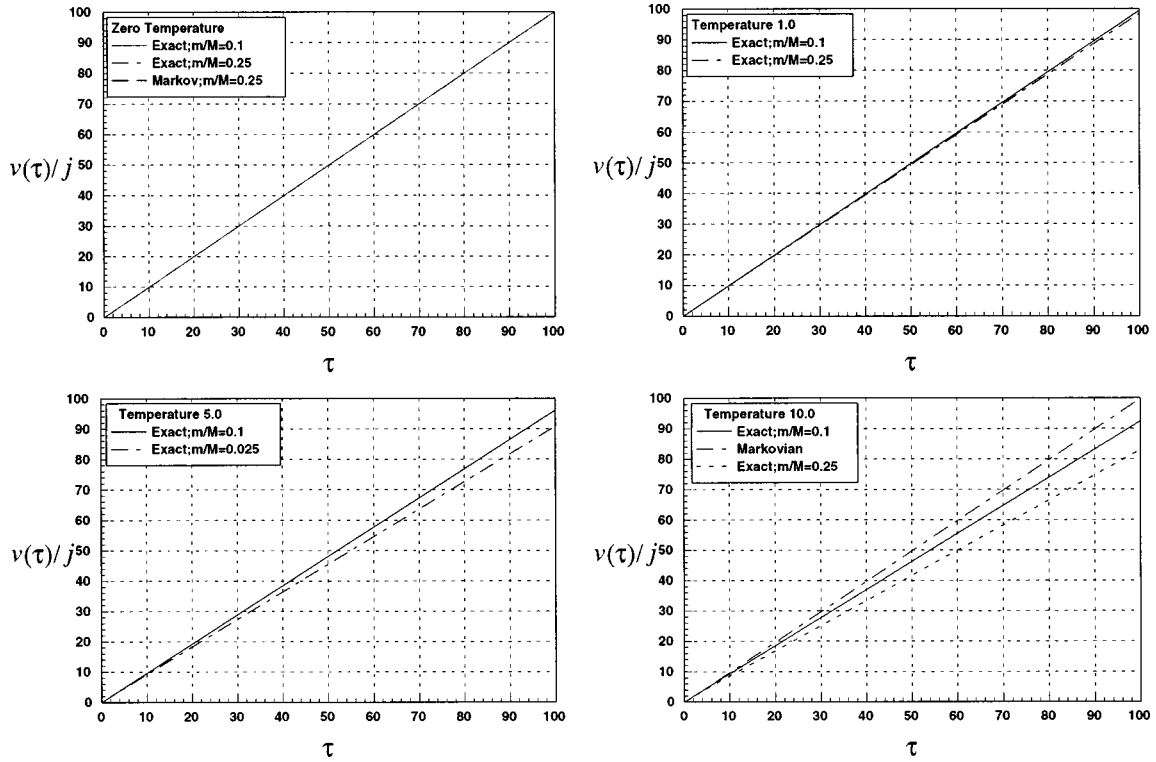

FIG. 2. Numerical evaluation of the velocity of the soliton in the presence of a constant electric field for temperatures $\mathcal{T}=$ 0, 1.0, 5.0, and 10.0 in sine-Gordon theory.

tained constant in time thereafter. In terms of dimensionless quantities the equation of motion (52) becomes in this case

$$\dot{v}(\tau)+\frac{m}{M}\int_0^\tau d\tau'\Sigma(\tau-\tau')v(\tau')=j, \tag{92}$$

where $j=\tilde{j}/(mM)$ and the overdot stands for derivative with respect to the dimensionless variable τ.

We will choose the initial condition $v_0=v(\tau=0)=0$. From the solution $v_j(\tau)$ of Eq. (92) with this initial condition, the solution to the homogeneous equation with $v_0\neq 0$ is obtained as

$$v(\tau)=v_0\frac{\dot{v}_j(\tau)}{j} \tag{93}$$

and the general solution is given by the sum of the inhomogeneous and homogeneous ones.

2. Equation of motion: (ii) The Markovian approximation

As shown in Fig. 1, the kernel $\Sigma(\tau)$ has ''memory'' on time scales a few times the inverse of the phason frequency at low and intermediate temperatures $T\leqslant m$. If the soliton velocity varies on time scales larger than the ''memory'' of the kernel, a Markovian approximation to the dynamics may be reasonable. The first step in the Markovian approximation corresponds to replacing $v(\tau')$ by $v(\tau)$ inside the integral in Eq. (92) and taking it outside the integral. A second stage of approximation would take the upper limit of the integral to ∞, thus integrating the peak of the kernel. However, we have shown above that the total integral of the kernel vanishes, and thus this second stage cannot be invoked. Recognizing that $\int_0^\tau\Sigma(\tau-\tau')d\tau'=\Gamma(\tau)$ the Markovian approximation to Eq. (92) is given by

$$\dot{v}(\tau)+\frac{m}{M}v(\tau)\Gamma(\tau)=j. \tag{94}$$

As advanced in the previous section, we now identify the kernel $\Gamma(\tau)$ as the *dynamical* friction coefficient in the Markovian approximation. The property (53) determines that $\Gamma(\tau\to\infty)=0$.

Figure 2 shows numerical solutions of Eqs. (92) and (94) for temperatures $\mathcal{T}=0$, 1.0, 5.0, and 10.0. As can be seen from the figures, the departure of the exact solution [we refer to the numerical solution of Eq. (92) as the exact solution to distinguish it from the numerical solution in the Markovian approximation, Eq. (94)] from a straight line (free case) is larger the larger the ratio m/M and the temperature $\mathcal{T}$. This is expected since larger adiabatic ratio implies a stronger coupling between soliton and bath, whereas larger the temperature implies that more phonons are excited in the bath that contribute to the scattering term and stimulated creation and absorption of excitations. At zero temperature, the soliton moves, experiencing negligible dissipative force, since to dissipate energy the soliton needs to excite two phonons in a virtual state, but there is a gap for this process, making it rather inefficient. The solution in the Markovian approximation, $v_m(\tau)$, is almost indistinguishable from the free evolution even at very large temperature and couplings. Thus we see that memory effects are extremely important even at high temperatures and a Markovian approximation will be unwarranted at least to the order in which this calculation has been performed.

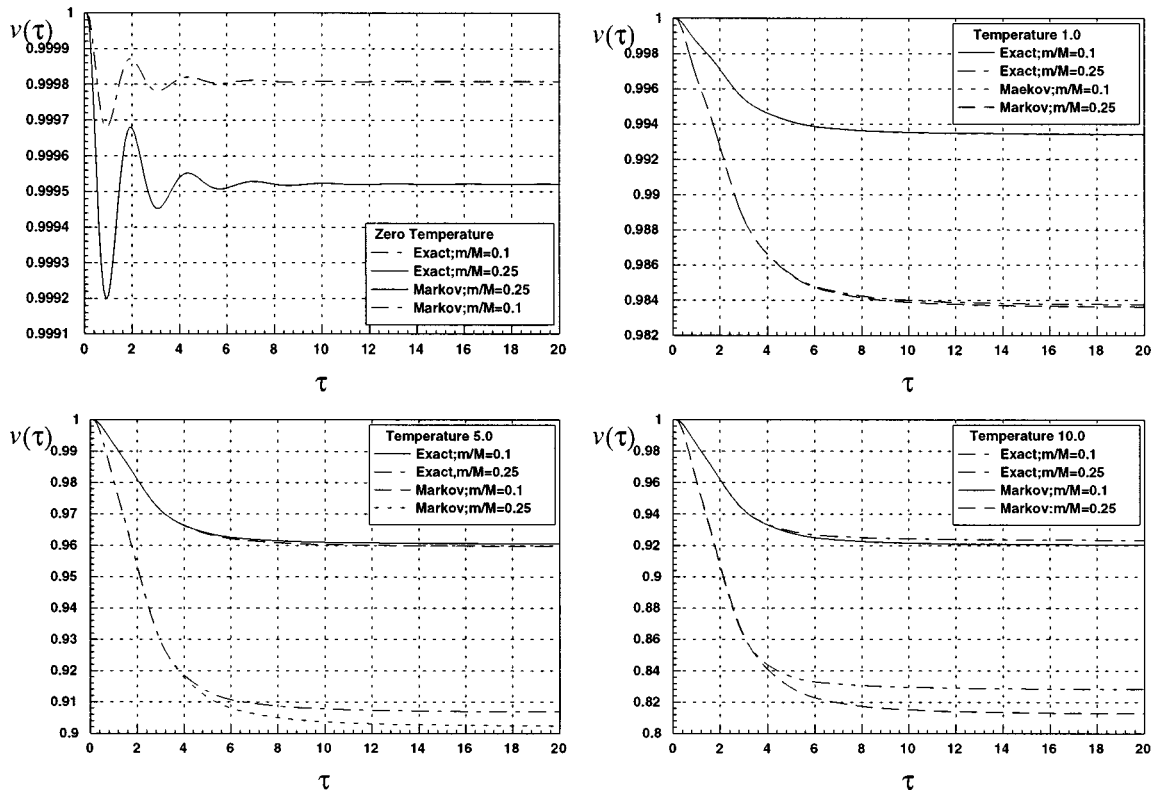

FIG. 3. Numerical evaluation of the velocity of the soliton for $j=0$ and $v_0=1$ for temperatures $\mathcal{T}=0$, 1.0, 5.0, and 10.0 in sine-Gordon theory.

3. Velocity relaxation and wave function renormalization

In order to display more clearly the dissipative effects, we now study the relaxation of the soliton velocity. For this consider that $j(t>0)=0$ but an initial velocity v_0 at $t=0$. With this initial condition and $j\equiv 0$, Eq. (92) becomes an initial value problem.

As the soliton moves in the bath, its velocity decreases because of the interaction with the fluctuations, the asymptotic final velocity is related to the initial velocity through the wave function renormalization as explained Sec. IV B above. We present the numerical solution of the homogeneous equation with initial velocity $v_0=1$ in Fig. 3, where we also present the homogeneous solution in the Markovian approximation described above. We clearly see that the initial velocity relaxes to an asymptotic value v_∞. However, the time dependence cannot be fit with an exponential.

According to the analysis of the general solution, the ratio v_∞/v_0 should be given by the wave function renormalization, i.e.,

$$Z_s=\frac{1}{1+(m/M)\tilde{\Gamma}(s=0)}=\frac{v_\infty}{v_0}. \tag{95}$$

Table I below compares the ratio v_∞/v_0 obtained from the numerical solution to the exact evolution equation, with the value of the wave function renormalization. Clearly the agreement is excellent, confirming the analysis of the asymptotic behavior of the solution in real time.

4. Kernels for the semiclassical Langevin equation

Knowledge of the matrix elements $T^{(A)}$ and $T^{(S)}$ allows us to obtain the final form of the kernels that enter in the semiclassical Langevin equation given by Eqs. (72) and (73), and Eq. (84). These kernels can be written in terms of the dimensionless quantities given by Eq. (87). Since $K_1(t-t')=-2i\Sigma_m(t-t')$, we focus on $K(t-t')$. In terms of dimensionless quantities, $K(t)=m^4\mathcal{K}(\tau)$, where

TABLE I. Numerical evaluation of Z_s and V_∞/V_0 in sine-Gordon theory for $m/M=0.1$, 0.25.

	v_∞/v_0		Z_s	
	$m/M=0.1$	$m/M=0.25$	$m/M=0.1$	$m/M=0.25$
Zero Temperature	0.999808	0.999521	0.999808	0.999521
Temperature 1.0	0.993438	0.983754	0.993438	0.983753
Temperature 5.0	0.96055	0.906885	0.96055	0.90687
Temperature 10.0	0.923458	0.828352	0.923446	0.828303

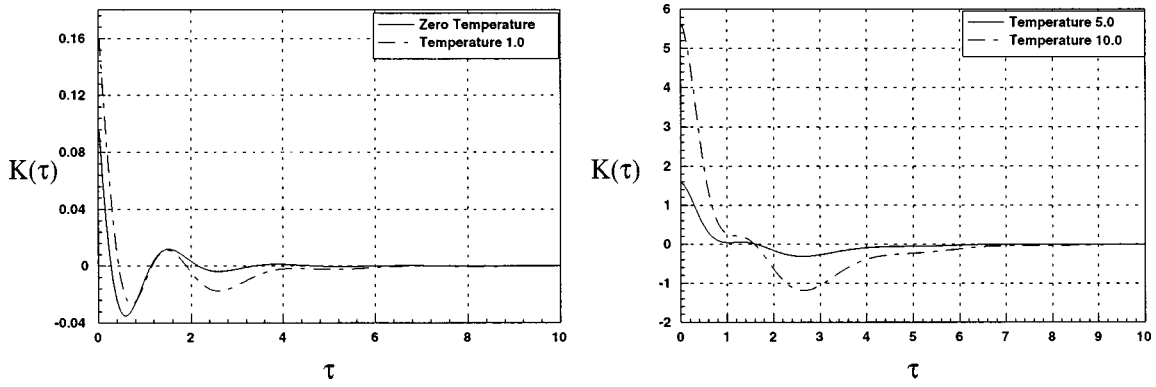

FIG. 4. The correlation function $\mathcal{K}(\tau)$ for temperatures $\mathcal{T}=0$, 1.0, 5.0, and 10.0 in the sine-Gordon theory.

$$\mathcal{K}(\tau)=\int_{-\infty}^{\infty} dpdk\{C_1(p,k)\cos[(w_p+w_k)(\tau)] + C_2(p,k)\cos[(w_p-w_k)(\tau)]\}, \tag{96}$$

with

$$C_1(p,k)=\frac{2}{4^4}\frac{(1+n_p+n_k+n_pn_k)(p^2-k^2)^4}{w_p^3w_k^3\sinh^2[(\pi/2)(p+k)]}, \tag{97}$$

$$C_2(p,k)=\frac{1}{4^3}\frac{n_k(1+n_p)(p^2-k^2)^4}{w_p^3w_k^3\sinh^2[(\pi/2)(p+k)]}. \tag{98}$$

Figure 4 shows $\mathcal{K}(\tau)$ for different temperatures $\mathcal{T}$. Notice that at large temperatures the kernel becomes strongly peaked at $\tau=0$ and one would be tempted to conclude that the classical limit corresponds to a δ function. However, the coefficients (97) and (98) are such that the total integral in τ (leading to δ functions of sums and differences of frequencies) vanishes. We then conclude that even in the high-temperature limit the noise-noise correlation function is not a δ function; i.e., the noise is ''colored,'' and the classical fluctuation-dissipation relation does not emerge and a diffusion coefficient cannot be appropriately defined.

B. ϕ^4 theory

In this model, originally studied by Krumanshl and Schrieffer,[1] the interaction is given by

$$U(g,\phi)=\frac{1}{2g}(m^2-g\phi^2)^2, \tag{99}$$

where m is a parameter with dimension of mass. The static soliton solution is given by

$$\phi_s(x-x_0)=\frac{m}{\sqrt{g}}\tanh[m(x-x_0)], \tag{100}$$

and the normal modes are the solutions to the equation [see Eq. (10)]

$$\left[-\frac{d^2}{dx^2}+4m^2-\frac{6m^2}{\cosh^2(mx)}\right]\psi_n(x)=\omega_n^2\psi_n(x). \tag{101}$$

The solution of the above differential equation is well known.[44,27] It has two bound states followed by a continuum. The normalized eigenvectors are given by

$$\mathcal{U}_0(x)=\frac{\sqrt{3m}}{2}\mathrm{sech}^2[mx]\propto\frac{d\phi_s}{dx} \quad \text{with} \quad \omega_0=0,$$

$$\mathcal{U}_b(x)=\frac{\sqrt{3m}}{2}\,\mathrm{sech}[mx]\,\tanh[mx] \quad \text{with} \quad \omega_b^2=3m^2,$$

$$\mathcal{U}_k(x)=\frac{m^2e^{ikx}}{\sqrt{2\pi(k^2+m^2)}\omega_k}\left\{3\tanh^2[mx]-3i\frac{k}{m}\tanh[mx] -1-\frac{k^2}{m^2}\right\}, \tag{102}$$

with $\omega_k^2=k^2+4m^2$. The scattering states are identified with optical phonon modes and the optical phonon frequency is identified with $\omega_o=2m$.

The bound state with zero frequency is the ''zero mode,'' whereas the bound state with $\omega_b^2=3m^2$ corresponds to an amplitude distortion[1,26] of the soliton.

The matrix elements D_{pk} are given by [see Eqs. (36) and (20)]

$$D_{bk}=\frac{\sqrt{3\pi}}{8}\frac{\mathrm{sech}[\pi k/2m]}{m^{3/2}\omega_k}\sqrt{k^2+m^2}(k^2+3m^2)$$

(from the bound state),

$$D_{pk}=ik\delta(p+k)+\frac{3i\pi(k^2-p^2)(p^2+k^2+4m^2)}{4m^4N_pN_k\sinh[(\pi/2)(p+k)/m]} \quad \text{for} \quad p\neq k, \tag{103}$$

where N_k is defined as

$$N_k = \sqrt{\frac{2\pi w_k^2(k^2+m^2)}{m^4}}. \tag{104}$$

We notice that the coupling to the continuum through the bound state given by the matrix element D_{bk} is of the same order as the coupling to the continuum-continuum transition matrix elements D_{pk}. This will have interesting consequences for the dissipational dynamics. The symmetric and antisymmetric matrix elements for the continuum states are given by

$$T_{pq}^{(S)} = \frac{3}{32}\left[\left(\frac{\omega_p}{\omega_q}\right)^{1/2} - \left(\frac{\omega_q}{\omega_p}\right)^{1/2}\right]\left\{\frac{(q^2-p^2)(p^2+q^2+4m^2)}{\sqrt{q^2+m^2}\sqrt{p^2+m^2}\,\omega_q\omega_p \sinh[(\pi/2)(q+p)/m]}\right\},$$

$$T_{pq}^{(A)} = \frac{3}{32}\left[\left(\frac{\omega_p}{\omega_q}\right)^{1/2} + \left(\frac{\omega_q}{\omega_p}\right)^{1/2}\right]\left\{\frac{(q^2-p^2)(p^2+q^2+4m^2)}{\sqrt{q^2+m^2}\sqrt{p^2+m^2}\,\omega_q\omega_p \sinh[(\pi/2)(q+p)/m]}\right\}, \tag{105}$$

whereas those involving the bound state are obtained by replacing the matrix elements D_{bk} for the D_{pk}.

Since in this model there is one bound state other than the zero mode, the interaction vertex $F[a^\dagger, a]$ is given by Eq. (B6) in Appendix B. The contributions from bound-state–continuum virtual transitions do not mix with the continuum-continuum transition to this order in the adiabatic expansion. As a consequence of this simplification the dimensionless kernels [in terms of the dimensionless variables introduced in Eq. (87)] become

$$\Gamma(\tau) = \int_{-\infty}^{\infty} dp \Big(\Gamma_1^b(p)\sin[(w_p+w_b)(\tau)] + \Gamma_2^b(p)\sin[(w_p - w_b)(\tau)] + \int_{-\infty}^{\infty} dk \{ \Gamma_1(p,k)\sin[(w_p+w_k)(\tau)] + \Gamma_2(p,k)\sin[(w_p-w_k)(\tau)]\} \Big),$$

$$\Sigma(\tau) = \int_{-\infty}^{\infty} dp \Big(\Sigma_1^b(p)\cos[(w_p+w_b)(\tau)] + \Sigma_2^b(p)\cos[(w_p - w_b)(\tau)] + \int_{-\infty}^{\infty} dk \{ \Sigma_1(p,k)\cos[(w_p+w_k)(\tau)] + \Sigma_2(p,k)\cos[(w_p-w_k)(\tau)]\} \Big), \tag{106}$$

with

$$\Gamma_1(p,k) \equiv \frac{3^2}{4^4}\frac{(1+n_p+n_k)(p^2-k^2)^2(w_p-w_k)^2(p^2+k^2+4)^2}{w_p^3 w_k^3 (p^2+1)(k^2+1)\sinh^2[(\pi/2)(p+k)]},$$

$$\Gamma_2(p,k) \equiv \frac{3^2}{4^4}\frac{(n_k-n_p)(p^2-k^2)^2(w_p+w_k)^2(p^2+k^2+4)^2}{w_p^3 w_k^3 (p^2+1)(k^2+1)\sinh^2[(\pi/2)(p+k)]},$$

$$\Gamma_1^b(p) \equiv \frac{\pi\sqrt{3}}{128}\frac{(p^4+4p^2+3)^2(w_p-w_b)(1+n_b+n_p)}{w_p^3(w_p+w_b)}\operatorname{sech}^2\left[\frac{\pi p}{2}\right],$$

$$\Gamma_2^b(p) \equiv \frac{\pi\sqrt{3}}{128}\frac{(p^4+4p^2+3)^2(w_p+w_b)(n_b-n_p)}{w_p^3(w_p-w_b)}\operatorname{sech}^2\left[\frac{\pi p}{2}\right],$$

$$\Sigma_1(p,k) \equiv (w_p+w_k)\Gamma_1(p,k),$$

$$\Sigma_2(p,k) = (w_p-w_k)\Gamma_2(p,k),$$

$$\Sigma_1^b(p) \equiv (w_p+w_b)\Gamma_1^b(p), \quad \Sigma_2^b(p) = (w_p-w_b)\Gamma_2^b(p),$$

$$w_p^2 = p^2+4, \tag{107}$$

where $\Sigma(\tau)$ and $\Gamma(\tau)$ are defined as in Eq. (88). The functions $\Sigma(\tau)$ and $\Gamma(\tau)$ were evaluated numerically at different temperatures $\mathcal{T}$, and the results are displayed in Fig. 5. The behavior of these functions differ from those in the sine-Gordon theory because of the presence of the bound state which is interpreted as an excited state of the soliton. As the soliton moves in the dissipative medium, energy is transferred between the soliton and the bound state, resulting in the Rabi-like oscillations displayed in the figure. We notice that the contribution of the bound state is of the same order of magnitude as that of the continuum.

1. Equation of motion: Exact solution vs Markovian approximation

The solution to the equation of motion and the comparison to the Markovian approximation proceeds just as in the the case of the sine-Gordon model. The equation of motion is again solved for the case of a constant electric field (after switching on at $t=0$). The exact and Markovian solutions are displayed in Fig. 6.

The new feature of the solution is the oscillations that result from virtual transitions to the bound state. We interpret these in the following manner: As the soliton moves it excites the bound state that corresponds to a soliton distortion; this excitation in turn reacts back in the dynamics of the collective coordinate in a retarded manner.

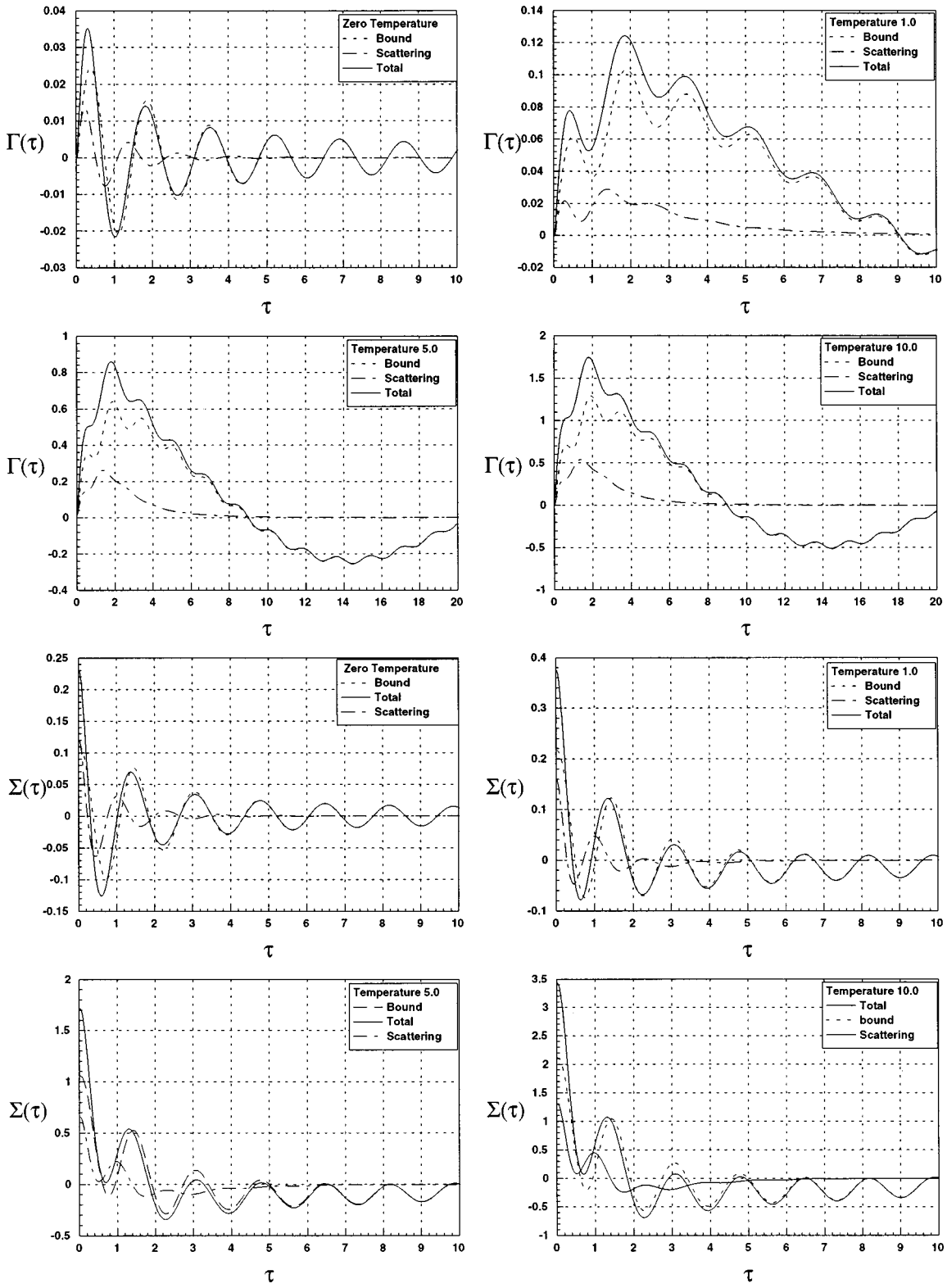

FIG. 5. The functions $\Gamma(\tau)$ and $\Sigma(\tau)$ for temperatures $\mathcal{T}=0$, 1.0, 5.0, and 10.0 in ϕ^4 theory. Contributions from bound and scattering states are displayed separately.

While the exact solution in this model is qualitatively similar to that of the sine-Gordon model, we see, however, that quantitatively they are different: There is stronger dynamical dissipation in the ϕ^4 model as compared to the sine-Gordon case, due to the strong coupling to the bound-state-continuum intermediate states. Figure 6 reveals that whereas the oscillations arising from the excitation of the bound state are not very noticeable in the exact solution, the Markovian approximation is very sensitive to these oscillations and provides a misrepresentation of the dynamics. We infer from this analysis that the memory terms are very important and cannot be neglected.

TABLE II. Numerical evaluation of Z_s and V_∞/V_0 in ϕ^4 theory for $m/M=0.1$, 0.25.

	v_∞/v_0		Z_s	
	$m/M=0.1$	$m/M=0.25$	$m/M=0.1$	$m/M=0.25$
Zero temperature	0.999225	0.998064	0.999176	0.997943
Temperature 1.0	0.961561	0.911004	0.96376	0.914072
Temperature 5.0	0.784934	0.593058	0.787734	0.597494
Temperature 10.0	0.642698	0.417231	0.646577	0.422562

2. Velocity relaxation and wave function renormalization

In this model the Laplace transform of the functions $\Gamma(\tau)$ and $\Sigma(\tau)$ are given by

$$\tilde{\Sigma}(s)=\int_{-\infty}^{\infty}dpdk\left\{\frac{\Sigma_1(p,k)s}{s^2+(w_p+w_k)^2}+\frac{\Sigma_2(p,k)s}{s^2+(w_p-w_k)^2}\right\}+\int_{-\infty}^{\infty}dp\left\{\frac{\Sigma_1^b(p)s}{s^2+(w_p+w_b)^2}+\frac{\Sigma_2^b(p)s}{s^2+(w_p-w_b)^2}\right\},$$

$$\tilde{\Sigma}(s)\equiv s\tilde{\Gamma}(s),$$

$$\tilde{\Gamma}(s)=\int_{-\infty}^{\infty}dpdk\left\{\frac{\Gamma_1(p,k)(w_p+w_k)}{s^2+(w_p+w_k)^2}+\frac{\Gamma_2(p,k)(w_p-w_k)}{s^2+(w_p-w_k)^2}\right\}+\int_{-\infty}^{\infty}dp\left\{\frac{\Gamma_1^b(p)(w_p+w_b)}{s^2+(w_p+w_b)^2}+\frac{\Gamma_2^b(p)(w_p-w_b)}{s^2+(w_p-w_b)^2}\right\},\tag{108}$$

with the quantities Σ^b and Γ^b given above. The homogeneous equations of motion given by Eq. (92) (exact) and its Markovian approximation (94) both with $j=0$ are solved with the kernels $\Sigma(\tau)$ and $\Gamma(\tau)$ given above with initial condition $v_0=1$. The asymptotic behavior of the exact solution will be compared with the prediction $v_\infty/v_0=Z_s$, with the wave function renormalization Z_s given by Eq. (95) but with the $\tilde{\Gamma}(s=0)$ appropriate to the ϕ^4 model.

Figure 7 shows the numerical solutions of Eqs. (92) and (94) with $j=0$ for temperatures $\mathcal{T}=0$, 1.0, 5.0, and 10.0 with initial condition $v_0=1$. Again the Rabi-like oscillations associated with the excitation of the bound state are apparent in the solutions. We have checked numerically that asymptotically the velocity tends to a constant value v_∞ but not exponentially. Table II shows the values of v_∞ and Z_s for these temperatures for $m/M=0.1$ and 0.25 where v_∞ was evaluated at $\tau=200$ for the exact solution with $v_0=1$. Within our numerical errors, we can see that Eq. (95) is fulfilled.

3. Kernels for the semiclassical Langevin equation

From the definition of the kernels $K_1(t-t')$ and $K(t-t')$, Eqs. (72) and (73), and Eq. (105), these kernels can be written in terms of the dimensionless quantities given by Eq. (87) as

$$\mathcal{K}_1(\tau-\tau')=-2i\Sigma(\tau-\tau'),\tag{109}$$

where $\Sigma(\tau-\tau')$ is given by Eq. (106) and $K(t)=m^4\mathcal{K}(\tau)$ with

$$\mathcal{K}(\tau)=\int_{-\infty}^{\infty}dp\Big(C_1^b(p)\cos[(w_p+w_b)(\tau)]+C_2^b(p)\cos[(w_p-w_b)(\tau)]+\int_{-\infty}^{\infty}\mathrm{d}k\{C_1(p,k)\cos[(w_p+w_k)(\tau)]+C_2(p,k)\cos[(w_p-w_k)(\tau)]\}\Big),\tag{110}$$

with the dimensionless matrix elements

$$C_1(p,k)\equiv\frac{18}{4^5}\frac{(1+n_p+n_k+n_pn_k)(p^2-k^2)^4(p^2+k^2+4)^2}{w_p^3w_k^3(p^2+1)(k^2+1)\sinh^2[(\pi/2)(p+k)]},$$

$$C_2(p,k)\equiv\frac{9}{4^4}\frac{n_k(1+n_p)(p^2-k^2)^4(p^2+k^2+4)^2}{w_p^3w_k^3(p^2+1)(k^2+1)\sinh^2[(\pi/2)(p+k)]},$$

$$C_1^b(p)\equiv\frac{\pi\sqrt{3}}{4^4}\frac{(p^4+4p^2+3)^2(p^2+1)(1+n_b+n_p+n_bn_p)}{w_p^3\cosh^2[\pi p/2]},$$

$$C_2^b(p)\equiv\frac{2\pi\sqrt{3}}{4^4}\frac{(p^4+4p^2+3)^2(p^2+1)n_p(1+n_b)}{w_p^3\cosh^2[\pi p/2]}.\tag{111}$$

Figure 8 shows $\mathcal{K}(\tau)$ vs τ for temperatures $\mathcal{T}=0,1,5,10$. Again the oscillations are a consequence of the bound-state contribution, and as in the sine-Gordon case we find that despite the fact that in the high-temperature limit the kernel becomes very localized in time, the total integral $\int_{-\infty}^{\infty}d\tau\mathcal{K}(\tau)=0$, preventing a representation of the noise-noise correlation function as a δ function in time even in the high-temperature limit, which, for example, for *trans*-polyacetylene is beyond the experimentally relevant scales. The ''color'' in the noise-noise correlation function is enhanced by the strong coupling to the continuum via the bound state which is also responsible for the strong oscillatory behavior of the real-time correlation function.

The high-temperature limit $T\gg m$ also implies a breakdown of the adiabatic (perturbative) expansion. In this limit the relevant scale in the kernels is T and the rescaling of variables in Eqs. (87) should be in terms of T rather than m. This implies that the expansion is now in terms of the ratio T/M which for high temperatures will imply strong coupling for the models under consideration when the parameters are fixed to make contact with the materials of interest. This is

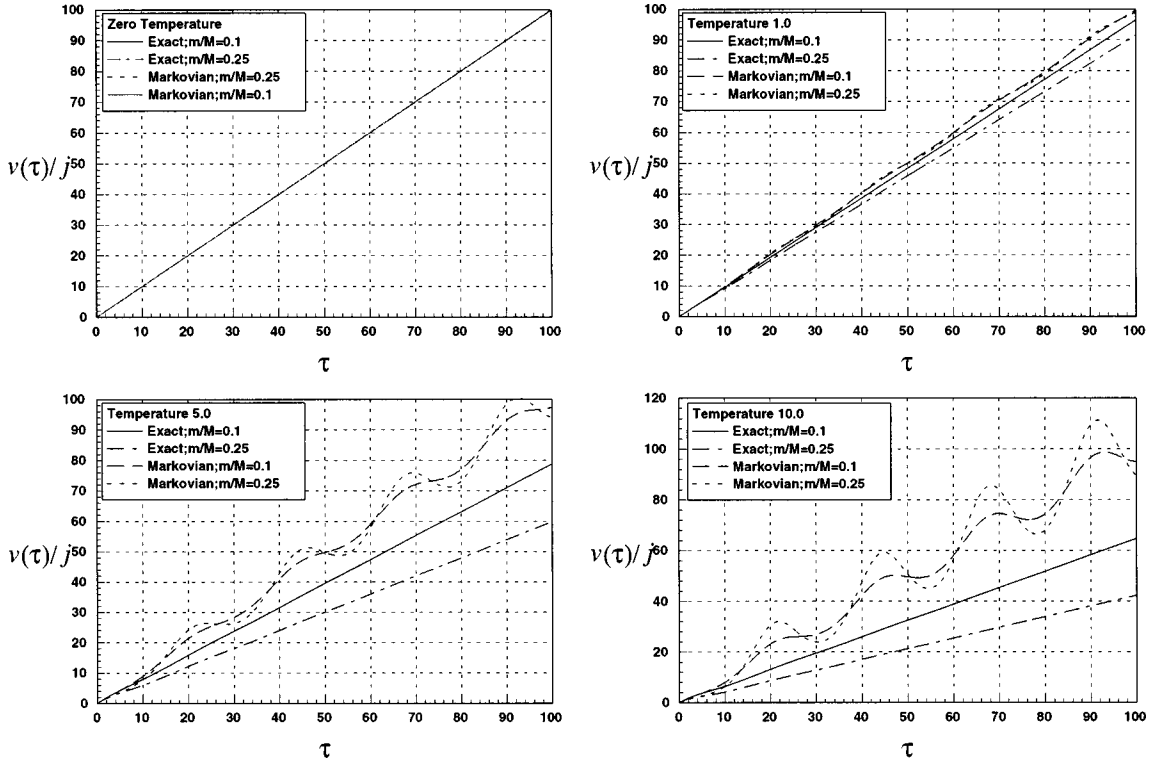

FIG. 6. Numerical evaluation of the velocity of the soliton in the presence of a constant electric field for temperatures $\mathcal{T}=0$, 1.0, 5.0, and 10.0 in ϕ^4 theory.

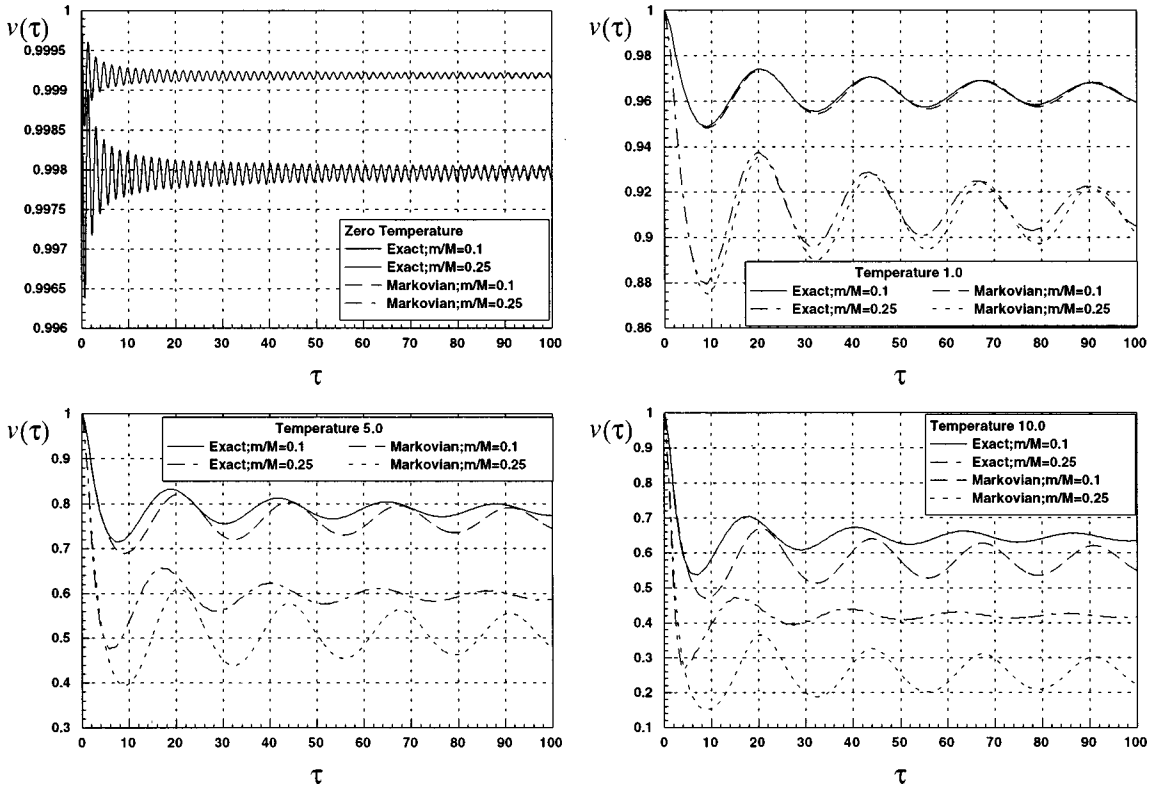

FIG. 7. Numerical evaluation of the velocity of the soliton for $j=0$ and $v_0=1$ for temperatures $\mathcal{T}=0$, 1.0, 5.0, and 10.0 in ϕ^4 theory.

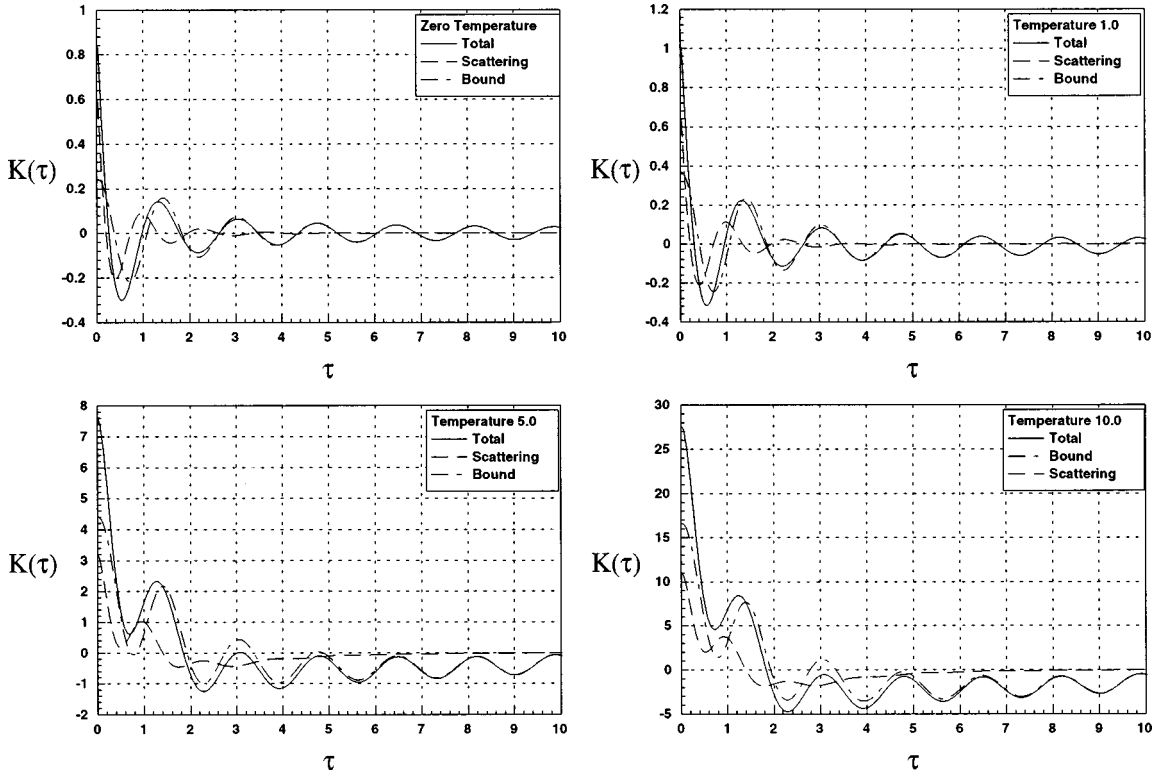

FIG. 8. The correlation function $\mathcal{K}(\tau)$ for temperatures $\mathcal{T}=0$, 1.0, 5.0, and 10.0 in the ϕ^4 theory.

common to both the ϕ^4 and sine-Gordon models, leading us to conclude that the classical limit requires a nonperturbative approach, which is clearly beyond the realm of this work.

VI. CONCLUSIONS AND FURTHER QUESTIONS

We have studied the nonequilibrium dynamics of solitons by obtaining the real-time equations of motion for the expectation value of the collective coordinate and also the quantum Langevin equation to lowest order in the adiabatic expansion. These allowed us to obtain the frequency-dependent soliton conductivity in this expansion.

The Hamiltonian for a ϕ^4 field theory was studied as a model for conducting polymers and the sine-Gordon model was used to describe the phase soliton dynamics for charge-density-wave systems. In both cases parameters were chosen to describe the experimental realizations of these systems.

To lowest order in the adiabatic coupling we found that the real-time equation of motion involves a non-Markovian self-energy kernel and that the static friction coefficient vanishes. However, there is dynamical friction which is a result of the memory effects in the self-energy and is associated with two-phonon processes. We studied the Markovian approximation and showed numerically that this approximation is unreliable in the relevant range of temperatures.

The quantum Langevin equation was obtained by computing the influence functional obtained by tracing out the phonon (or phason) degrees of freedom to the same order in the adiabatic expansion. We found that the dissipative kernel and the noise correlation function obey a generalized form of fluctuation-dissipation relation but that a Markovian limit is not available and the noise is Gaussian, additive, but colored. We have studied the high-temperature limit to establish whether the classical limit emerges, and found that to first adiabatic order and for the experimentally relevant range of temperatures, the classical limit of these kernels is not achieved. We pointed out that formally the high-temperature limit leads to a breakdown of the adiabatic expansion and requires a nonperturbative treatment.

There are several possible avenues to pursue: a higher-order calculation for example as carried out by Ogata *et al.*[15] but implemented in real time to obtain the nonequilibrium evolution of solitons and the associated quantum Langevin equation with a detailed study of the classical limit.

In the case of *trans*-polyacetylene the adiabatic ratio is not so small and a perturbative (adiabatic) expansion could be deemed suspect and certainly untrustworthy in the high-temperature regime. A possible avenue to pursue in this case would be a variational calculation with a few variational parameters; one of them would be the collective coordinate and others related to the soliton distortion. Such a treatment would also be valuable to study the situation of large soliton velocities which necessarily imply a ''Lorentz contraction'' of the soliton profile. In this case a more realistic model to study would be the continuum model of Takayama, Liu, and Maki[14] that incorporates the electronic degrees of freedom, which we expect would add quantitative changes to the dissipative contributions. Furthermore, in order to establish a close connection with experiments, the effects of impurities and other pinning potentials must be understood.

Work on some of these aspects is in progress.

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APPENDIX A: REAL-TIME PHONON CORRELATION FUNCTIONS

In this appendix, we will calculate the Green's functions which are defined in Eq. (68) in terms of the vertex given by Eq. (39).

Applying Wick's theorem and Eq. (45), it is a matter of straightforward algebra to find the following results:

$$\begin{aligned}
G^{++}(t,t') = -2\sum_{p,k\neq 0} \Big(T^{(S)}_{pk}T^{(S)}_{-p-k}\{e^{-i(\omega_p+\omega_k)(t-t')}[n_p n_k \\
+\theta(t-t')(1+n_p+n_k)] + e^{+i(\omega_p+\omega_k)(t-t')} \\
\times[n_p n_k+\theta(t'-t)(1+n_p+n_k)]\} \\
+2T^{(A)}_{pk}T^{(A)}_{-p-k}\{e^{-i(\omega_p-\omega_k)(t-t')}[n_p n_k+n_p\theta(t' \\
-t)+n_k\theta(t-t')]\}\Big),
\end{aligned}$$

$$\begin{aligned}
G^{--}(t,t') = -2\sum_{p,k\neq 0} \Big(T^{(S)}_{pk}T^{(S)}_{-p-k}\{e^{-i(\omega_p+\omega_k)(t-t')}[n_p n_k \\
+\theta(t'-t)(1+n_p+n_k)] + e^{+i(\omega_p+\omega_k)(t-t')} \\
\times[n_p n_k+\theta(t-t')(1+n_p+n_k)]\} \\
+2T^{(A)}_{pk}T^{(A)}_{-p-k}\{e^{-i(\omega_p-\omega_k)(t-t')}[n_p n_k \\
+n_k\theta(t'-t)+n_p\theta(t-t')]\}\Big),
\end{aligned}$$

$$\begin{aligned}
G^{+-}(t,t') = 2\sum_{p,k\neq 0} \Big(T^{(S)}_{pk}T^{(S)}_{-p-k}\{e^{-i(\omega_p+\omega_k)(t-t')}n_p n_k \\
+e^{+i(\omega_p+\omega_k)(t-t')}[n_p n_k+n_p+n_k+1)]\} \\
+2T^{(A)}_{pk}T^{(A)}_{-p-k}[e^{-i(\omega_p-\omega_k)(t-t')}n_p(1+n_k)]\Big),
\end{aligned}$$

$$\begin{aligned}
G^{-+}(t,t') = 2\sum_{p,k\neq 0} \{T^{(S)}_{pk}T^{(S)}_{-p-k}[e^{-i(\omega_p+\omega_k)(t-t')}(n_p n_k+n_p \\
+n_k+1)+e^{+i(\omega_p+\omega_k)(t-t')}n_p n_k] \\
+2T^{(A)}_{pk}T^{(A)}_{-p-k}[e^{-i(\omega_p-\omega_k)(t-t')}n_k(1+n_p)]\}.
\end{aligned} \tag{A1}$$

These Green's functions satisfy the following relation:

$$G^{++}+G^{--}+G^{+-}+G^{-+}=0, \tag{A2}$$

which is a consequence of unitary time evolution.[24]

Furthermore, using the antisymmetry property of the matrix elements $T^{(A)}_{pk}$ one finds that

$$G^{+-}(t,t')=[G^{-+}(t,t')]^*. \tag{A3}$$

The Green's functions $G^{++}(t,t')$ and $G^{--}(t,t')$ can be written in terms of $G^{+-}(t,t')$ and its complex conjugate; therefore we see that there is only one independent Green's function (and its complex conjugate).

APPENDIX B: CALCULATING $K_1(t-t')$ AND $K(t-t')$

Performing the coordinate transformation in Eq. (69), the influence functional becomes

$$\begin{aligned}
\mathcal{F}[\dot{x},\dot{R}] = \exp\Bigg\{-\frac{1}{2}\int dt dt' \Bigg[\frac{\dot{R}(t)\dot{R}(t')}{4}[G^{++}(t,t') \\
+G^{--}(t,t')-G^{+-}(t,t')-G^{-+}(t,t')] \\
+\Bigg(\frac{1}{2}\dot{R}(t)\dot{x}(t')[G^{++}(t,t')-G^{--}(t,t') \\
+G^{+-}(t,t')-G^{-+}(t,t')]+\frac{1}{2}\dot{x}(t)\dot{R}(t') \\
\times[G^{++}(t,t')-G^{--}(t,t')-G^{+-}(t,t') \\
+G^{-+}(t,t')]\Bigg)\Bigg]\Bigg\}.
\end{aligned} \tag{B1}$$

Integrating the linear term in $\dot{R}$ by parts once and the quadratic term twice, the influence functional can be cast in the following form:

$$\begin{aligned}
\mathcal{F}[\dot{x},\dot{R}] = \exp\Bigg\{\frac{1}{2}\int dt dt'[R(t)K_1(t-t')\dot{x}(t') \\
-R(t)K(t-t')\dot{R}(t')]\Bigg\},
\end{aligned} \tag{B2}$$

where

$$\begin{aligned}
K_1(t-t') = \frac{1}{2}\frac{\partial}{\partial t}\{[G^{++}(t,t')-G^{--}(t,t')+G^{+-}(t,t') \\
-G^{-+}(t,t')]+[G^{++}(t',t)-G^{--}(t',t) \\
-G^{+-}(t',t)+G^{-+}(t',t)]\},
\end{aligned} \tag{B3}$$

$$\begin{aligned}
K(t-t') = \frac{1}{4}\frac{\partial^2}{\partial t^2}[G^{++}(t,t')+G^{--}(t,t')-G^{+-}(t,t') \\
-G^{-+}(t,t')].
\end{aligned} \tag{B4}$$

The generalized fluctuation-dissipation relation is obtained by writing the two kernels above in terms of $G^{\pm}(t,t')$, the only independent Green's function.

Substituting the values of the Green's functions from Eq. (A1) in the above equations, one obtains the expressions for $K_1(t-t')$ and $K(t-t')$ in Eqs. (72) and (73).

In the case that there are bound states other than the zero mode, such as the case of ϕ^4, the sum in Eq. (39) runs over all bound and scattering states, i.e.,

$$F[a^\dagger,a]=\frac{1}{2i}\int dpdk\,\sqrt{\frac{\omega_p}{\omega_k}}D_{pk}[a_k a_p-a^\dagger_{-k}a^\dagger_{-p}+a^\dagger_{-k}a_p - a^\dagger_{-p}a_k]+\frac{1}{2i}\sum_b\int dk\,\sqrt{\frac{\omega_b}{\omega_k}}D_{bk}[a_k a_b-a^\dagger_{-k}a^\dagger_b + a^\dagger_{-k}a_b-a^\dagger_b a_k]+\frac{1}{2i}\sum_b\int dk\,\sqrt{\frac{\omega_k}{\omega_b}}D_{kb}[a_b a_k - a^\dagger_b a^\dagger_{-k}+a^\dagger_b a_k-a^\dagger_{-k}a_b] + \frac{1}{2i}\sum_{a,b}\sqrt{\frac{\omega_a}{\omega_b}}D_{ab}[a_b a_a-a^\dagger_b a^\dagger_a+a^\dagger_b a_a-a^\dagger_a a_b], \tag{B5}$$

where the indices a and b stand for summation over discrete bound states and p and k stand for summation over continuum scattering states. The models which we considered in this paper have at most one bound state, that is, the case in the ϕ^4 theory. In this case, the last term will not contribute since D_{bb} vanishes. Thus for only one bound state, Eq. (B5) can be written as

$$F[a^\dagger,a]=\int dpdk[T^{(S)}_{pk}(a_p a_k-a^\dagger_{-p}a^\dagger_{-k})+T^{(A)}_{pk}(a^\dagger_{-p}a_k - a^\dagger_{-k}a_p)]+\int dk[T^{(S)}_{bk}(a_k a_b-a^\dagger_{-k}a^\dagger_b) + T^{(A)}_{bk}(a^\dagger_{-k}a_b-a^\dagger_b a_k)], \tag{B6}$$

where the matrices $T^{(S)}_{pk}$ and $T^{(A)}_{pk}$ for scattering states are given by Eq. (40), and if one of the states is a bound state, then

$$T^{(S)}_{bk}=\frac{1}{2i}\left[\sqrt{\frac{\omega_b}{\omega_k}}-\sqrt{\frac{\omega_k}{\omega_b}}\right]D_{bk},$$

$$T^{(A)}_{bk}=\frac{1}{2i}\left[\sqrt{\frac{\omega_b}{\omega_k}}+\sqrt{\frac{\omega_k}{\omega_b}}\right]D_{bk}. \tag{B7}$$

In the sine-Gordon theory, the last two terms in Eq. (B6) do not contribute since in this theory there are no bound states other than the zero mode and the Green's functions are given by Eq. (A1) but with integration over p and k instead of the summation.

In the ϕ^4 case, to lowest adiabatic order the contributions from the bound and scattering states decouple. This implies that the Green's functions will have a contribution from the bound state which is given by the same expression as that of the scattering states, with $p\to b$, but multiplied by a factor of 1/2 since the bound-state wave function is chosen to be real.

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