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In and Out-of-Equilibrium *Ab Initio* Theory of Electrons and Phonons

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In this work, we lay down the *ab initio* many-body quantum theory of electrons and phonons in equilibrium as well as in steady-state or time-varying settings. Our focus is on the harmonic approximation, but the developed tools can readily incorporate anharmonic effects. We begin by showing the necessity of determining the *ab initio* Hamiltonian in a *self-consistent* manner to ensure the existence of an equilibrium state. We then identify the correct partitioning into a "noninteracting" and an "interacting" part to carry out diagrammatic expansions in terms of dressed propagators and screened interactions. The final outcome is the finite-temperature nonequilibrium extension of the Hedin equations, showcasing the emergence of the coupling between electrons and coherent phonons through the time-local Ehrenfest diagram. The Hedin equations have limited practical utility for real-time simulations of systems driven out of equilibrium by external fields. To overcome this limitation, we leverage the versatility of the diagrammatic approach to generate a closed system of differential equations for the dressed propagators and nuclear displacements. These are the Kadanoff-Baym equations for electrons and phonons. The formalism naturally merges with the theory of conserving approximations, which guarantee the satisfaction of the continuity equation and the conservation of total energy during time evolution. As an example, we show that the popular Born-Oppenheimer approximation is not conserving whereas its dynamical extension is conserving, provided that the electrons are treated in the Fan-Migdal approximation with a dynamically screened electron-phonon coupling. We also derive the formal solution of the Kadanoff-Baym equations for nonequilibrium steady states, which is useful for studies in photovoltaics and optoelectronics. Interestingly, the expansion of the phononic Green's function around the quasiphonon energies points to a correlation-induced splitting of the phonon dispersion in materials with no time-reversal invariance.

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I. INTRODUCTION

The concept of phonons as quasiparticles describing independent excitations of the nuclear lattice dates back to almost a century ago [1,2]. Nonetheless, the first rigorous theory of electrons and phonons saw the light of day in 1961 [3]. In a seminal paper, Baym showed how to map the original electron-nuclear Hamiltonian onto a low-energy or, equivalently, electron-phonon (*e-ph*) Hamiltonian and derived a set of equations for the electronic and phononic Green's functions (GF) G and D. The GF describe how electrons and phonons move in the interacting system and can be used to extract a wealth of physical information. The Baym equation for the electronic GF was rather implicit, though. In the mid-1960s, Hedin used the same technique as Baym, the so-called source-field method or field-theoretic approach, to generate a more explicit set of equations for the electronic GF at clamped nuclei [4]. The contributions by Baym and Hedin have been largely ignored by the electron-phonon community (including ourselves) in favor of semiempirical Hamiltonians. Only a few years ago, the works of Baym, Hedin, and a few others [5–7] have been rigorously merged by Giustino in a unified many-body GF framework [8], which we keep naming the *Hedin-Baym equations* (instead of "Hedin equations") after Giustino.

Despite these recent notable advances, the *formal* theory of electrons and phonons is still not complete. We stress here the word "formal," as this paper does not address specific aspects or computational strategies related to the *e-ph* interaction, for which we refer the reader to excellent textbooks [9–15] and modern comprehensive reviews [8]; rather, it establishes a mathematically rigorous apparatus for the quantum treatment of electrons and nuclei in the

so-called harmonic approximation (in this approximation, one neglects those effects that are more than quadratic in the field fluctuations; see also below).

Three pivotal issues are still waiting to be clarified and solved. The first issue has to do with the *ab initio e-ph* Hamiltonian, often replaced by semiempirical Hamiltonians or left unspecified as unnecessary for the implementation of approximate formulas for the phononic dispersions, lifetimes, etc. The *ab initio e-ph* Hamiltonian is, however, of paramount relevance. It is necessary for assessing the validity of semiempirical approaches, for improving approximations based on perturbation theory, and for making fair comparisons between different methods and between different approximations within the same method, as well as for benchmarking the harmonic approximation against other methods like, e.g., the surface hopping approach [16] or the exact-factorization scheme [17,18]. A plausible explanation for the scarce attention given to the *ab initio e-ph* Hamiltonian is that at zero *e-ph* coupling it does not contain physical phonons [12]. A clean derivation of the *e-ph* Hamiltonian can be found in Baym's work [3]. However, Baym's original expression as well as equivalent expressions designed for having a good starting point for many-body expansions [7] necessitate the knowledge of the exact equilibrium electronic density n^0. This means that the *ab initio e-ph* Hamiltonian is *unknown* unless n^0 is calculated by other means, e.g., by solving the original electron-nuclear problem. Even assuming that we could find n^0 somehow, we would still have to face a practical problem. All many-body techniques (including those based on GF) can be implemented only in some approximation, for the exchange-correlation (xc) potential in density functional theory (DFT), for the self-energy in GF theory, for the configuration state functions in the multiconfigurational Hartree-Fock method, for the intermediate states in the algebraic diagrammatic construction scheme, etc. An approximation in any of the available many-body methods generates an approximate equilibrium density n^0_{approx} which inevitably leads to an inconsistency if the *ab initio e-ph* Hamiltonian is evaluated at the exact n^0. The inconsistency lies in the fact that the forces acting on the nuclei are proportional to $n^0_{\text{approx}} - n^0$, and, therefore, they would not vanish in equilibrium. As we shall see, the *ab initio e-ph* Hamiltonian must be considered as a *functional* of the equilibrium density, which must be determined *self-consistently* to avoid inconsistencies. Such a self-consistent concept is completely general; i.e., it is not limited to GF approaches. Of course, if an exact method is used, then the self-consistent density coincides with the exact one.

The second issue is the extension of the theory at finite temperature and out of equilibrium. This is especially relevant in light of the overwhelming and steadily increasing number of time-resolved spectroscopy experiments. We mention that at zero temperature a nonequilibrium Green's function (NEGF) formulation has been put forward in terms of the nuclear-density correlation function [6,19,20]. We here present the finite-temperature and nonequilibrium generalization of the Hedin-Baym equations as formulated in Ref. [8]. The novel aspects are as follows. (i) In all internal vertices, the time arguments must be integrated over the L-shaped Konstantinov-Perel' contour in the complex plane [21–25]; see Fig. 1. This contour accounts for thermal fluctuations through the imaginary-time segment and allows for the inclusion of arbitrary time-varying fields through the forward and backward real-time segments (needed to overcome the adiabatic assumption). (ii) The electronic GF satisfies a Dyson equation with an extra time-local self-energy, whose inclusion is fundamental to recovering the Ehrenfest (mixed quantum-classical) dynamics [26–36]. In the context of material science, the Ehrenfest self-energy plays a key role in the description of polarons [31,37], and it is expected to be fundamental to detecting the phonon-induced coherent modulation of the excitonic resonances [38].

The Hedin-Baym equations have limited practical utility in nonequilibrium problems. Furthermore, the original derivation based on the source-field method allows for solving these equations only *iteratively*, starting from an approximation to the electronic polarization (or, equivalently, the so-called vertex function). The question of whether the iterative procedure converges toward the exact solution is still open. In most applications, only one iteration step is performed, since the equations resulting from the second iteration are already too complex. All these considerations bring us to the third issue, i.e., how to systematically improve the approximations possibly preserving all fundamental conservation laws. We here present a *diagrammatic* derivation of the Hedin-Baym equations based on the expansion of the electronic and phononic self-energies in terms of interacting electronic and phononic GF and the screened interaction. We highlight three essential merits of the diagrammatic derivation: (i) the possibility of including relevant scattering mechanisms through a selection of Feynman diagrams (to be converted into mathematical expressions using the Feynman rules which we provide); (ii) the possibility of using the Φ-derivable criterion [39] to generate approximations yielding a fully conserving dynamics; and (iii) the possibility of closing the Kadanoff-Baym equations (KBE) [25,40,41] by expanding the self-energies in terms of only interacting GF. The KBE are integro-differential equations for the electronic and phononic NEGF, and they are definitely more practical than the Hedin-Baym equations for investigating the real-time evolution of systems driven out of equilibrium. Furthermore, by employing the so-called generalized Kadanoff-Baym ansatz (GKBA) for fermions [42] and bosons [43], the KBE can be mapped onto a much simpler system of ordinary differential equations for a large number of self-energy approximations [43–49].

The GKBA KBE can be used to calculate time-local observables but give no access to the spectral properties of the GF.

The paper is organized as follows. In Sec. II, we derive the low-energy Hamiltonian for any system of electrons and nuclei, highlighting its dependence on the equilibrium electronic density and pointing out the necessity of a self-consistent procedure for its determination. In Sec. III, we specialize the discussion to lattice periodic systems, introduce general time-dependent external perturbations, and derive the *e-ph* Hamiltonian on the L-shaped contour. The equations of motion for the electronic and phononic field operators are derived in Sec. IV. In Sec. V, we define the many-particle electronic and phononic GF on the contour and construct the Martin-Schwinger hierarchy that these GF satisfy. In Sec. VI, we present the Wick theorem as the solution of the noninteracting Martin-Schwinger hierarchy, and in Sec. VII we provide the exact formula of the many-body expansion of the interacting GF in terms of the noninteracting ones. The many-body expansion is mapped onto a diagrammatic theory in Sec. VIII, where we also introduce the notion of self-energies and skeleton diagrams. The skeletonic expansion of the self-energies in terms of the interacting GF and screened Coulomb interaction is shown to lead to the Hedin-Baym equations in Sec. IX. The Hedin-Baym equations are applicable to systems in and out of equilibrium as well as at zero and finite temperature. To study the system evolution or the finite-temperature spectral properties, the equations of motion for the GF are more convenient than the Hedin-Baym equations. These equations of motion are derived in Sec. X. In Sec. XI, we discuss the so-called Φ-derivable approximations to the self-energies. The GF satisfying the equations of motion with Φ-derivable self-energies guarantee the fulfillment of all fundamental conservation laws. In Sec. XII, we convert the equations of motion into a coupled system of integro-differential equations for the Keldysh components of the GF; these are the KBE. We first discuss the self-consistent solution of the equilibrium problem and then derive the real-time equations of motion to study the system evolution. We also present the formal solution of the KBE in the long-time limit and for steady-state conditions. The expansion of the phononic GF around the quasiphonon energies reveals the possibility of a correlation-induced splitting of the phonon dispersion in materials with no time-reversal invariance. The presented formalism can be extended to deal with much more general Hamiltonians than the *e-ph* Hamiltonian. In Sec. XIII, we provide a summary of the main results, illustrate possible extensions, and discuss their physical relevance.

II. QUANTUM SYSTEMS OF ELECTRONS AND NUCLEI

In this section, we lay down a quantum theory of electrons and nuclei which is suited whenever the average nuclear positions remain close to the equilibrium values. Under this "near-equilibrium hypothesis," the nuclei stay away from each other and they can be treated as quantum *distinguishable* particles. In fact, we can distinguish them by means of techniques like scanning tunneling microscopy or electron diffraction [8].

Let $\hat{\psi}(\mathbf{x}=\mathbf{r}\sigma)$ be the field operators that annihilate an electron in position $\mathbf{r}$ with spin σ—hence, they satisfy the anticommutation relations $\{\hat{\psi}(\mathbf{x}),\hat{\psi}^\dagger(\mathbf{x}')\}=\delta_{\sigma\sigma'}\delta(\mathbf{r}-\mathbf{r}')\equiv\delta(\mathbf{x}-\mathbf{x}')$—and $\hat{\mathbf{R}}_i$ and $\hat{\mathbf{P}}_i$ be the position and momentum operators, respectively, of the ith nucleus, $i=1,\ldots,N_n$, satisfying the standard commutation relations $[\hat{R}_{i,\alpha},\hat{P}_{j,\beta}]=i\delta_{ij}\delta_{\alpha\beta}$, with α and β running over the three components of the vectors. The nonrelativistic Hamiltonian describing an unperturbed system of electrons interacting with N_n nuclei of charge Z_i and mass M_i reads (we use atomic units throughout the paper)

$$\hat{H}=\hat{H}_e+\hat{H}_n+\hat{H}_{e\text{-}n}, \tag{1}$$

where

$$\hat{H}_e=\int d\mathbf{x}\hat{\psi}^\dagger(\mathbf{x})\left[-\frac{\nabla^2}{2}\right]\hat{\psi}(\mathbf{x}) +\frac{1}{2}\int d\mathbf{x}d\mathbf{x}'\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')v(\mathbf{r},\mathbf{r}')\hat{\psi}(\mathbf{x}')\hat{\psi}(\mathbf{x}) \tag{2}$$

is the electronic Hamiltonian,

$$\hat{H}_n=\sum_{i=1}^{N_n}\frac{\hat{P}_i^2}{2M_i}+\frac{1}{2}\sum_{i\neq j}^{N_n}Z_iZ_jv(\hat{\mathbf{R}}_i,\hat{\mathbf{R}}_j) \tag{3}$$

is the nuclear Hamiltonian (with $\hat{P}_i^2=\hat{\mathbf{P}}_i\cdot\hat{\mathbf{P}}_i$), and

$$\hat{H}_{e\text{-}n}=-\int d\mathbf{x}\hat{n}(\mathbf{x})\sum_{j=1}^{N_n}Z_jv(\mathbf{r},\hat{\mathbf{R}}_j) \tag{4}$$

is the electron-nucleus interaction. In Eqs. (2)–(4), the integral $\int d\mathbf{x}\equiv\int d\mathbf{r}\sum_\sigma$ signifies a spatial integral and a sum over spin, $v(\mathbf{r},\mathbf{r}')=1/|\mathbf{r}-\mathbf{r}'|$ is the Coulomb interaction, and $\hat{n}(\mathbf{x})\equiv\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})$ is the density operator in $\mathbf{r}$ for particles of spin σ. For later purposes, we find it convenient to collect all nuclear position and momentum operators into the vectors $\hat{\mathbf{R}}=(\hat{\mathbf{R}}_1,\ldots,\hat{\mathbf{R}}_{N_n})$ and $\hat{\mathbf{P}}=(\hat{\mathbf{P}}_1,\ldots,\hat{\mathbf{P}}_{N_n})$. We also find it useful to define the nuclear potential energy

$$E_{n\text{-}n}(\hat{\mathbf{R}})\equiv\frac{1}{2}\sum_{i\neq j}^{N_n}Z_iZ_jv(\hat{\mathbf{R}}_i,\hat{\mathbf{R}}_j), \tag{5}$$

appearing in Eq. (3), and the electron-nuclear potential

$$V(\mathbf{r},\hat{\mathbf{R}}) \equiv -\sum_{j=1}^{N_n} Z_j v(\mathbf{r},\hat{\mathbf{R}}_j), \tag{6}$$

appearing in Eq. (4). The operators of $\hat{H}$ act on the direct-product space $\mathbb{F}\otimes\mathbb{D}_{N_n}$, where $\mathbb{F}$ is the electronic Fock space and $\mathbb{D}_{N_n}$ is the Hilbert space of the N_n distinguishable nuclei. Relativistic corrections [50] can be incorporated without any conceptual complication. In particular, the spin-orbit coupling emerges from the relativistic correction to the electron-nuclear interaction Hamiltonian in Eq. (4).

A. Expansion around thermal equilibrium

Consider the interacting system of electrons and nuclei in thermal equilibrium at a certain temperature. Under the "near-equilibrium hypothesis," we can approximate the full Hamiltonian by its second-order Taylor expansion around the equilibrium values of the nuclear positions, which we name $\mathbf{R}^0=(\mathbf{R}_1^0,\ldots,\mathbf{R}_{N_n}^0)$, and around the equilibrium value of the electronic density, which we name $n^0(\mathbf{x})$. In fact, also the electronic density must stay close to $n^0(\mathbf{x})$, for otherwise the forces acting on the nuclei would be strong enough to drive the nuclei away from $\mathbf{R}^0$. Notice that $\mathbf{R}^0$ and $n^0(\mathbf{x})$ do, in general, depend on the temperature. We also observe that the existence of an inertial reference frame for the coordinates $\mathbf{R}^0$ is supported by the macroscopic size of the system, i.e., $N_n\to\infty$. For finite systems, e.g., molecules or molecular aggregates, the choice of a suitable reference frame is more subtle; see Refs. [51–56].

We introduce the displacement (or position fluctuation) operators $\hat{\mathbf{U}}_i$ and the density fluctuation operator $\Delta\hat{n}$ according to

$$\hat{\mathbf{U}}_i=\hat{\mathbf{R}}_i-\mathbf{R}_i^0, \qquad \Delta\hat{n}(\mathbf{x})=\hat{n}(\mathbf{x})-n^0(\mathbf{x}). \tag{7}$$

In the following, we refer to these operators as the *fluctuation operators*. Formally, the near-equilibrium hypothesis is equivalent to restricting the full space $\mathbb{F}\otimes\mathbb{D}_{N_n}$ to the subspace of states giving a small average of $\hat{\mathbf{U}}_i$ and $\Delta\hat{n}$.

The expansion of the nuclear potential energy around the equilibrium nuclear positions yields to second order

$$E_{n\text{-}n}(\hat{\mathbf{R}})=E_{n\text{-}n}(\mathbf{R}^0)+\sum_{i\alpha}\left.\frac{\partial E_{n\text{-}n}(\mathbf{R})}{\partial R_{i,\alpha}}\right|_{\mathbf{R}=\mathbf{R}^0}\hat{U}_{i,\alpha} +\frac{1}{2}\sum_{i\alpha,j\beta}\left.\frac{\partial^2 E_{n\text{-}n}(\mathbf{R})}{\partial R_{i,\alpha}\partial R_{j,\beta}}\right|_{\mathbf{R}=\mathbf{R}^0}\hat{U}_{i,\alpha}\hat{U}_{j,\beta}. \tag{8}$$

In the first term, we recognize the electrostatic energy of a nuclear geometry $\mathbf{R}^0$. As this term is responsible only for an overall energy shift, we do not include it in the following discussion. Similarly, the expansion of the electron-nuclear potential yields to second order

$$V(\mathbf{r},\hat{\mathbf{R}})=V(\mathbf{r})+\sum_{i\alpha}g_{i,\alpha}(\mathbf{r})\hat{U}_{i,\alpha}+\frac{1}{2}\sum_{i\alpha,j\beta}g^{\mathrm{DW}}_{i,\alpha;j,\beta}(\mathbf{r})\hat{U}_{i,\alpha}\hat{U}_{j,\beta}, \tag{9}$$

where we define

$$V(\mathbf{r})\equiv V(\mathbf{r},\mathbf{R}^0), \tag{10a}$$

$$g_{i,\alpha}(\mathbf{r})\equiv\left.\frac{\partial V(\mathbf{r},\mathbf{R})}{\partial R_{i,\alpha}}\right|_{\mathbf{R}=\mathbf{R}^0}=Z_i\frac{\partial}{\partial r_\alpha}v(\mathbf{r},\mathbf{R}_i^0), \tag{10b}$$

$$g^{\mathrm{DW}}_{i,\alpha;j,\beta}(\mathbf{r})\equiv\left.\frac{\partial^2 V(\mathbf{r},\mathbf{R})}{\partial R_{i,\alpha}\partial R_{j,\beta}}\right|_{\mathbf{R}=\mathbf{R}^0}=-\delta_{ij}Z_i\frac{\partial^2}{\partial r_\alpha\partial r_\beta}v(\mathbf{r},\mathbf{R}_i^0). \tag{10c}$$

Inserting Eq. (9) into Eq. (4), we see that the first term gives rise to a purely electronic operator; it is the potential energy operator for electrons in the classical field generated by a nuclear geometry $\mathbf{R}^0$. The second and third terms emerge when relaxing the infinite-mass approximation for the nuclei. The third term in Eq. (9) is already quadratic in the displacements, and it can, therefore, be multiplied by the equilibrium density, i.e., $\hat{n}\to n^0$ [3]. Going beyond the quadratic (or harmonic) approximation, the replacement $\hat{n}\to n^0$ is no longer justified; in this case, the third term gives rise to the so-called Debye-Waller (DW) interaction [57].

B. The low-energy Hamiltonian

Inserting the expansion of $E_{n\text{-}n}$ and V into Eqs. (3) and (4), the total Hamiltonian becomes

$$\hat{H}=\hat{H}_{0,e}+\hat{H}_{0,ph}+\hat{H}_{e\text{-}e}+\hat{H}'. \tag{11}$$

The first two terms describe an uncoupled system of noninteracting electrons and N_n interacting nuclei in the electric field generated by a *frozen* electronic density $n^0(\mathbf{r})$:

$$\hat{H}_{0,e}=\int d\mathbf{x}\hat{\psi}^\dagger(\mathbf{x})\left[-\frac{\nabla^2}{2}+V(\mathbf{r})\right]\hat{\psi}(\mathbf{x}), \tag{12}$$

$$\hat{H}_{0,ph}=\sum_{i=1}^{N_n}\frac{\hat{P}_i^2}{2M_i}+\frac{1}{2}\sum_{i\alpha,j\beta}\hat{U}_{i,\alpha}K_{i,\alpha;j,\beta}\hat{U}_{j,\beta}, \tag{13}$$

where we define the *elastic tensor*

$$K_{i,\alpha;j,\beta}\equiv\left.\frac{\partial^2 E_{n\text{-}n}(\mathbf{R})}{\partial R_{i,\alpha}\partial R_{j,\beta}}\right|_{\mathbf{R}=\mathbf{R}^0}+\int d\mathbf{x}n^0(\mathbf{x})g^{\mathrm{DW}}_{i,\alpha;j,\beta}(\mathbf{r}), \tag{14}$$

which is real and symmetric under the exchange $(i,\alpha)\leftrightarrow(j,\beta)$. Already at this stage of the presentation,

a remark is due. The eigenvalues ω_λ^2 of the tensor $\bar{K}_{i,\alpha;j,\beta} \equiv K_{i,\alpha;j,\beta}/\sqrt{M_i M_j}$ are not physical and can even be *negative* such that $\hat{H}_{0,ph}$ does not have a proper ground state. It is, therefore, generally *not* possible to define annihilation and creation operators $\hat{b}_\lambda$ and $\hat{b}_\lambda^\dagger$ to rewrite Eq. (13) in the form $\hat{H}_{0,ph} = \sum_\lambda \omega_\lambda(\hat{b}_\lambda^\dagger \hat{b}_\lambda + \frac{1}{2})$. The *ab initio* low-energy Hamiltonian evaluated at vanishing coupling $g_{i,\alpha}$ [hence, $\hat{H}' = 0$; see Eq. (21)] does not contain physical quanta of vibrations (phonons in solids). These excitations can emerge only from a proper *nonperturbative* treatment; see Sec. XII A.

The third term in Eq. (11) is the electron-electron (e-e) interaction Hamiltonian

$$\hat{H}_{e\text{-}e} = \frac{1}{2}\int d\mathbf{x} d\mathbf{x}' \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')v(\mathbf{r},\mathbf{r}')\hat{\psi}(\mathbf{x}')\hat{\psi}(\mathbf{x}), \tag{15}$$

while the last term is the contribution linear in the nuclear displacements

$$\hat{H}' = \sum_{i\alpha}\left[\left.\frac{\partial E_{n\text{-}n}(\mathbf{R})}{\partial R_{i,\alpha}}\right|_{\mathbf{R}=\mathbf{R}^0} + \int d\mathbf{x} g_{i,\alpha}(\mathbf{r})\hat{n}(\mathbf{x})\right]\hat{U}_{i,\alpha}. \tag{16}$$

The Hamiltonian in Eq. (11) with the four contributions as in Eqs. (12), (13), (15), and (16) is identical to that in Ref. [3]. We here make a step further. Although it is not evident, the operator $\hat{H}'$ is quadratic in the fluctuation operators. To show it, we consider the Heisenberg equation of motion for the time-dependent average of the nuclear momentum operators. Let $\hat{\mathcal{U}}(t,t_0)$ be the evolution operator from some initial time t_0 to time $t > t_0$ and $\hat{\mathcal{U}}(t_0,t) = [\hat{\mathcal{U}}(t,t_0)]^\dagger$. Henceforth, any operator $\hat{O}(t)$ in the Heisenberg picture carries a subscript "H," i.e., $\hat{O}_H(t) = \hat{\mathcal{U}}(t_0,t)\hat{O}(t)\hat{\mathcal{U}}(t,t_0)$. The time-dependent average $O(t)$ of the operator $\hat{O}(t)$ is defined according to

$$O(t) = \mathrm{Tr}[\hat{\rho}\hat{O}_H(t)], \tag{17}$$

where

$$\hat{\rho} = \frac{e^{-\beta(\hat{H}-\mu\hat{N}_e)}}{\mathrm{Tr}[e^{-\beta(\hat{H}-\mu\hat{N}_e)}]} \tag{18}$$

is the thermal density matrix, with β the inverse temperature, μ the chemical potential, and $\hat{N}_e = \int d\mathbf{x}\hat{n}(\mathbf{x})$ the operator for the total number of electrons. Using $i(d/dt)\hat{O}_H(t) = [\hat{O}_H(t), \hat{H}_H(t)]$, we find

$$\frac{dP_{i,\alpha}(t)}{dt} = -\left.\frac{\partial E_{n\text{-}n}(\mathbf{R})}{\partial R_{i,\alpha}}\right|_{\mathbf{R}=\mathbf{R}^0} - \int d\mathbf{x} g_{i,\alpha}(\mathbf{r})n(\mathbf{x},t) - \sum_{j\beta} K_{i,\alpha;j,\beta}U_{j,\beta}(t), \tag{19}$$

where $n(\mathbf{x},t)$ and $U_{j,\beta}(t)$ are the time-dependent averages of the electronic density $\hat{n}(\mathbf{r})$ and nuclear displacement $\hat{U}_{j,\beta}$, respectively. In thermal equilibrium, the lhs vanishes and, by definition, we also have $n(\mathbf{x},t) = n^0(\mathbf{x})$ and $U_{j,\beta} = 0$. Therefore,

$$\left.\frac{\partial E_{n\text{-}n}(\mathbf{R})}{\partial R_{i,\alpha}}\right|_{\mathbf{R}=\mathbf{R}^0} = -\int d\mathbf{x} g_{i,\alpha}(\mathbf{r})n^0(\mathbf{x}), \tag{20}$$

according to which we can rewrite Eq. (16) as

$$\hat{H}' = \sum_{i\alpha}\int d\mathbf{x} g_{i,\alpha}(\mathbf{r})\Delta\hat{n}(\mathbf{x})\hat{U}_{i,\alpha}, \tag{21}$$

where $\Delta\hat{n}(\mathbf{r})$ is the density fluctuation operator defined in Eq. (7). In this form, $\hat{H}'$ is manifestly quadratic in the fluctuation operators.

Inserting Eq. (20) in Eq. (19), we also see that the equation of motion for the momentum operators simplifies to

$$\frac{dP_{i,\alpha}(t)}{dt} = -\int d\mathbf{x} g_{i,\alpha}(\mathbf{r})\Delta n(\mathbf{x},t) - \sum_{j\beta} K_{i,\alpha;j,\beta}U_{j,\beta}(t). \tag{22}$$

We can interpret the elastic tensor K as the *nuclear-force tensor* of a system with frozen electronic density, i.e., with $\Delta n(\mathbf{x},t) = 0$, or, alternatively, with vanishing coupling $g_{i,\alpha}$. In general, $g_{i,\alpha} \neq 0$ and out of equilibrium $\Delta n(\mathbf{x},t) \neq 0$, and the first term in Eq. (22) significantly contributes to the nuclear forces.

The Hamiltonian in Eq. (11) is the low-energy approximation of the full Hamiltonian in Eq. (1). The expansion around the equilibrium nuclear geometry and around the equilibrium density inevitably makes Eq. (11) depend on these quantities. The scalar potential V and the electron-nuclear coupling g are determined from the sole knowledge of the equilibrium positions $\mathbf{R}^0$, whereas the elastic tensor K depends on both $\mathbf{R}^0$ and n^0; see Eq. (14). Notice that the dependence of $\hat{H}$ on n^0 is through K as well as $\Delta\hat{n}$; see Eq. (21). In the following, we assume that $\mathbf{R}^0$ is known and, therefore, that V and g are given. Strategies to obtain good approximations to the equilibrium nuclear geometry are indeed available, e.g., the Born-Oppenheimer approximation; see also the discussion in Ref. [20]. Alternatively, $\mathbf{R}^0$ can be taken from x-ray crystallographic measurements. The equilibrium density n^0 must instead be determined, and the proper way of doing it is *self-consistently*. Let us expand on this point.

We write the dependence of $\hat{H}$ on n^0 explicitly: $\hat{H} = \hat{H}[n^0]$. For any given many-body treatment (whether exact or approximate), a possible self-consistent strategy to obtain n^0 is to (i) make an initial guess n_1^0 and (ii) use the chosen many-body treatment to calculate the equilibrium

density n_2^0 of $\hat{H}[n_1^0]$, then the equilibrium density n_3^0 of $\hat{H}[n_2^0]$, and so on and so forth until convergence. If the initial guess n_1^0 does already produce a good approximation to K, then a partial self-consistent scheme in which K is not updated is also conceivable. Self-consistency is, however, unavoidable to determine n^0 in $\Delta\hat{n}$. In fact, it is only at self-consistency that the equilibrium value $\Delta n = 0$, an essential requirement for the rhs of Eq. (22) to vanish and, hence, for the nuclear geometry to remain stationary. In Sec. XII A, we discuss how to implement the self-consistent strategy using NEGF. In particular, we show that n^0 can be obtained from the self-consistent solution of the Dyson equation for the Matsubara GF.

For any given equilibrium geometry $\mathbf{R}^0$, different scenarios are possible. If $\mathbf{R}^0$ is too off target, the self-consistent scheme may not converge, indicating that the nuclear geometry must be improved. If convergence is achieved, then the self-consistent equilibrium state can be either stable or unstable. In the unstable scenario, an infinitesimally small perturbation brings the nuclei away from $\mathbf{R}^0$, indicating again that the nuclear geometry must be improved. Let us finally consider the stable scenario. The nuclear geometry can, in this case, be further optimized by minimizing the total energy (at zero temperature) or the grand potential (at finite temperature) with respect to $\mathbf{R}^0$. At the minimum, the equilibrium geometry is the exact one only if an exact many-body treatment is used. Needless to say, the minimum is defined up to arbitrary overall shifts and rotations of the nuclear coordinates.

III. INTERACTING HAMILTONIAN FOR ELECTRONS AND PHONONS IN AND OUT OF EQUILIBRIUM

Independently of the method chosen to find $\mathbf{R}^0$ and of the self-consistent many-body treatment chosen to determine n^0, the low-energy Hamiltonian of a system of electrons and nuclei is given by Eq. (11). Let us discuss in detail the case of a crystal and introduce some notations.

In a crystal, we can label the position of every nucleus with the vector (of integers) $\mathbf{n}$ of the unit cell it belongs to and with the position s relative to some point of the unit cell, i.e., $\mathbf{R}^0_{i=\mathbf{n},s} = \mathbf{R}^0_{\mathbf{n}} + \mathbf{R}^0_s$. If the unit cell contains N_u nuclei, then $s = 1, \ldots, N_u$. By definition, the vector $\mathbf{R}^0_s$ for the sth nucleus is the same in all unit cells, and the mass $M_{i=\mathbf{n},s} = M_s$ and charge $Z_{i=\mathbf{n},s} = Z_s$ of the sth nucleus in cell $\mathbf{n}$ are independent of $\mathbf{n}$. The invariance of the crystal under discrete translations implies that the elastic tensor depends only on the difference between unit cell vectors, i.e.,

$$K_{\mathbf{n}s,\alpha;\mathbf{n}'s',\alpha'} = K_{s,\alpha;s',\alpha'}(\mathbf{n}-\mathbf{n}'). \tag{23}$$

The periodicity of the crystal also implies an important property for the electron-nuclear coupling g. According to the definition in Eq. (10b), we have $g_{\mathbf{n}s,\alpha}(\mathbf{r}) = Z_s(\partial/\partial r_\alpha)v(\mathbf{r}, \mathbf{R}^0_{\mathbf{n}s})$. The Coulomb interaction depends only on the relative coordinate, and, therefore, $v(\mathbf{r}, \mathbf{R}^0_{\mathbf{n}s}) = v(\mathbf{r}+\mathbf{R}^0_{\mathbf{n}'}, \mathbf{R}^0_{\mathbf{n}s}+\mathbf{R}^0_{\mathbf{n}'}) = v(\mathbf{r}+\mathbf{R}^0_{\mathbf{n}'}, \mathbf{R}^0_{\mathbf{n}+\mathbf{n}'s})$ for all vectors $\mathbf{R}^0_{\mathbf{n}'}$. This implies that

$$g_{\mathbf{n}s,\alpha}(\mathbf{r}) = g_{\mathbf{n}+\mathbf{n}'s,\alpha}(\mathbf{r}+\mathbf{R}^0_{\mathbf{n}'}). \tag{24}$$

A. Equilibrium Hamiltonian

We consider a finite piece of the crystal with N_α cells along direction $\alpha = x, y, z$ and impose the Born–von Kármán boundary conditions. The total number of cells is, therefore, $N = N_x N_y N_z$. Accordingly, the displacement and momentum operators can be expanded as

$$\hat{U}_{\mathbf{n}s,\alpha} = \frac{1}{\sqrt{M_s N}} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{n}} \sum_{\nu} e^{\nu}_{s,\alpha}(\mathbf{q}) \hat{U}_{\mathbf{q}\nu}, \tag{25a}$$

$$\hat{P}_{\mathbf{n}s,\alpha} = \sqrt{\frac{M_s}{N}} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{n}} \sum_{\nu} e^{\nu}_{s,\alpha}(\mathbf{q}) \hat{P}_{\mathbf{q}\nu}, \tag{25b}$$

respectively, where the sum over $\mathbf{q} = (q_x, q_y, q_z)$ runs over all vectors satisfying the property $q_\alpha N_\alpha = 2\pi m_\alpha$ with m_α integers and $q_\alpha \in (-\pi, \pi]$ for $\alpha = x, y, z$. In Eqs. (25), the vectors $\mathbf{e}^\nu(\mathbf{q})$ with components $e^\nu_{s,\alpha}(\mathbf{q})$ form an orthonormal basis for each $\mathbf{q}$, i.e., $\mathbf{e}^\nu(\mathbf{q})^\dagger \cdot \mathbf{e}^{\nu'}(\mathbf{q}) = \delta_{\nu\nu'}$. In three dimensions, the set of all vectors $\mathbf{e}^\nu(\mathbf{q})$ spans a $3N_u$-dimensional space for each $\mathbf{q}$. We refer to these vectors as the *normal modes*. As we see, the most convenient choice of normal modes depends on the approximation made to treat the problem. A typical choice is the eigenbasis of the Hessian of the Born-Oppenheimer energy. At this stage of the presentation, the set of normal modes is just a basis to expand the displacement and momentum operators.

The Hermiticity of the operators $\hat{U}_{\mathbf{n}s,\alpha}$ and $\hat{P}_{\mathbf{n}s,\alpha}$ imposes the following constraints on the operators $\hat{U}_{\mathbf{q}\nu}$ and $\hat{P}_{\mathbf{q}\nu}$ and on the normal modes:

$$\hat{U}_{\mathbf{q}\nu} = \hat{U}^\dagger_{-\mathbf{q}\nu}, \quad \hat{P}_{\mathbf{q}\nu} = \hat{P}^\dagger_{-\mathbf{q}\nu}, \quad \mathbf{e}^{\nu *}(-\mathbf{q}) = \mathbf{e}^\nu(\mathbf{q}). \tag{26}$$

Inserting the expansions Eqs. (25) into Eqs. (13) and (21), we obtain

$$\hat{H}_{0,ph} = \frac{1}{2}\sum_{\mathbf{q}\nu} \hat{P}^\dagger_{\mathbf{q}\nu}\hat{P}_{\mathbf{q}\nu} + \frac{1}{2}\sum_{\mathbf{q}\nu\nu'} \hat{U}^\dagger_{\mathbf{q}\nu} K_{\nu\nu'}(\mathbf{q}) \hat{U}_{\mathbf{q}\nu'}, \tag{27}$$

$$\hat{H}' = \sum_{\mathbf{q}\nu} \int d\mathbf{x}\, g_{-\mathbf{q}\nu}(\mathbf{r}) \Delta\hat{n}(\mathbf{x}) \hat{U}_{\mathbf{q}\nu}, \tag{28}$$

where

$$K_{\nu\nu'}(\mathbf{q}) \equiv \sum_{\mathbf{n}} e^{-i\mathbf{q}\cdot\mathbf{n}} \sum_{s\alpha,s'\alpha'} e^{\nu*}_{s,\alpha}(\mathbf{q}) \frac{K_{s,\alpha;s'\alpha'}(\mathbf{n})}{\sqrt{M_s M_{s'}}} e^{\nu'}_{s'\alpha'}(\mathbf{q}) = K^*_{\nu\nu'}(-\mathbf{q}) = K^*_{\nu'\nu}(\mathbf{q}) \tag{29}$$

and

$$g_{-\mathbf{q}\nu}(\mathbf{r}) \equiv \sum_{\mathbf{n}s\alpha} \frac{1}{\sqrt{M_s N}} e^{i\mathbf{q}\cdot\mathbf{n}} e^{\nu}_{s,\alpha}(\mathbf{q}) g_{\mathbf{n}s,\alpha}(\mathbf{r}) = g^*_{\mathbf{q}\nu}(\mathbf{r}). \tag{30}$$

For crystals, the Hamiltonian in Eq. (11) is known as the electron-phonon (*e-ph*) Hamiltonian.

B. Nonequilibrium Hamiltonian

We are interested in formulating a NEGF approach to deal with systems described by the *e-ph* Hamiltonian in Eq. (11) possibly driven out of equilibrium by external driving fields. Of course, the external fields must be such that the nonequilibrium density and displacements are small enough to justify the harmonic approximation. As we see, the developed formalism can accommodate many different kinds of drivings.

Without any loss of generality, we take the system in thermal equilibrium for times $t < t_0$ and then perturb it by letting

$$\left[-\frac{\nabla^2}{2} + V(\mathbf{r})\right] \to h(\boldsymbol{\nabla}, \mathbf{r}, t), \tag{31a}$$

$$K_{\nu\nu'}(\mathbf{q}) \to K_{\nu\nu'}(\mathbf{q}, t), \tag{31b}$$

$$v(\mathbf{r}, \mathbf{r}') \to v(\mathbf{r}, \mathbf{r}', t), \tag{31c}$$

$$g_{\mathbf{q}\nu}(\mathbf{r}) \to g_{\mathbf{q}\nu}(\mathbf{r}, t). \tag{31d}$$

Correspondingly, $\hat{H}_{0,e} \to \hat{H}_{0,e}(t)$, $\hat{H}_{0,ph} \to \hat{H}_{0,ph}(t)$, $\hat{H}_{e\text{-}e} \to \hat{H}_{e\text{-}e}(t)$, $\hat{H}' \to \hat{H}'(t)$, and, hence, $\hat{H} \to \hat{H}(t)$. The time dependence of the Coulomb interaction v and *e-ph* coupling g may be due to, e.g., an adiabatic switching protocol or a sudden quench of the interaction, whereas the time dependence of the one-particle Hamiltonian h and elastic tensor K may be due to laser fields, phonon drivings, etc. For simplicity, we specialize the discussion to the relevant case of external perturbations that do not break the lattice periodicity of the crystal (long-wavelength limit), albeit the developed formalism is far more general.

C. Hamiltonian on the contour

The explicit form of the evolution operators is $\hat{\mathcal{U}}(t, t_0) = T\{\exp[-i\int_{t_0}^{t} d\bar{t}\, \hat{H}(\bar{t})]\}$, with T the time-ordering operator, and $\hat{\mathcal{U}}(t_0, t) = \bar{T}\{\exp[i\int_{t_0}^{t} d\bar{t}\, \hat{H}(\bar{t})]\}$, with $\bar{T}$ the anti-time-ordering operator. Therefore, the time-dependent average in Eq. (17) can be written as [22,25]

$$O(t) = \mathrm{Tr}\left[\hat{\rho}\, \bar{T}\left\{e^{i\int_{t_0}^{t} d\bar{t}\, \hat{H}(\bar{t})}\right\} \hat{O}(t) T\left\{e^{-i\int_{t_0}^{t} d\bar{t}\, \hat{H}(\bar{t})}\right\}\right] = \frac{\mathrm{Tr}\left[\mathcal{T}\left\{e^{-i\int_{\gamma} d\bar{z}\, \hat{H}(\bar{z})} \hat{O}(z)\right\}\right]}{\mathrm{Tr}\left[\mathcal{T}\left\{e^{-i\int_{\gamma} d\bar{z}\, \hat{H}(\bar{z})}\right\}\right]}. \tag{32}$$

In the second equality, z and $\bar{z}$ are contour times running on the L-shaped oriented contour γ [21] consisting of a forward branch γ_- going from the initial time t_0 to ∞, a backward branch γ_+ going from ∞ to t_0, and a vertical track on the complex plane γ^M going from t_0 to $t_0 - i\beta$ (see Fig. 1) and $\mathcal{T}$ is the contour-ordering operator. Henceforth, we denote by $z = t_\pm$, $\bar{z} = \bar{t}_\pm$, $z' = t'_\pm$, etc. contour times on $\gamma_\pm$. For any quantity $q(z)$, be it a function or an operator, we define $q(t_\pm) = q(t)$ and $q(t_0 - i\tau) = q$ independent of $\tau \in (0, \beta)$. The only exception is $h(\boldsymbol{\nabla}, \mathbf{r}, t_0 - i\tau) = h(\boldsymbol{\nabla}, \mathbf{r}) - \mu$. Thanks to this different definition for h, we have $\hat{H}(t_\pm) = \hat{H}(t)$ and $\hat{H}(t_0 - i\tau) = \hat{H} - \mu\hat{N}_e$. Notice that the Hamiltonian $\hat{H}(z)$ depends on z through the dependence of h, K, v, and g; see Eqs. (31).

One remark about the dependence of $\hat{O}(z)$ on z. If the operator does not depend on z, we can safely write $\hat{O}(t) = \hat{O}$ in the first line in Eq. (32). However, if we do so in the second line, then it is not clear where to place the operator $\hat{O}$ after the contour ordering. The reason to keep the contour argument even for operators that do not have an explicit time dependence (like the operators $\hat{\psi}$, $\hat{U}$, and $\hat{P}$) stems from the need of specifying their position along the contour, thus rendering unambiguous the action of $\mathcal{T}$. Once the operators are ordered, we can omit the time arguments if there is no time dependence.

To shorten the equations, we gather the displacement and momentum operators into a two-dimensional vector of operators having components

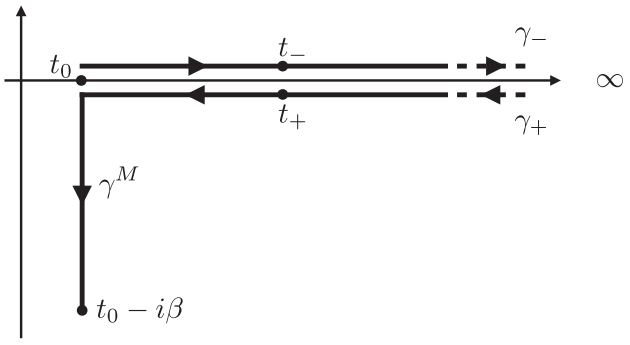


FIG. 1. L-shaped Konstantinov-Perel' contour.

$$\hat{\boldsymbol{\phi}}_{\mathbf{q}\nu} = \begin{pmatrix} \hat{\phi}^1_{\mathbf{q}\nu} \\ \hat{\phi}^2_{\mathbf{q}\nu} \end{pmatrix} = \begin{pmatrix} \hat{U}_{\mathbf{q}\nu} \\ \hat{P}_{\mathbf{q}\nu} \end{pmatrix}. \tag{33}$$

The commutation relations for the $\hat{\phi}$ operators follow from the commutation relations $[\hat{U}_{\mathbf{n}s,\alpha}, \hat{P}_{\mathbf{n}'s',\alpha'}] = i\delta_{\mathbf{n}\mathbf{n}'}\delta_{ss'}\delta_{\alpha\alpha'}$ after inserting the expansions in Eqs. (25) and using the properties in Eq. (26). We find

$$\left[\hat{\phi}^i_{\mathbf{q}\nu}, \hat{\phi}^{i'}_{-\mathbf{q}'\nu'}\right] = \left[\hat{\phi}^i_{\mathbf{q}\nu}, \hat{\phi}^{i'\dagger}_{\mathbf{q}'\nu'}\right] = \delta_{\mathbf{q},\mathbf{q}'}\alpha^{ii'}_{\nu\nu'}, \tag{34}$$

where

$$\alpha^{ii'}_{\nu\nu'} = \delta_{\nu\nu'}\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}_{ii'}. \tag{35}$$

Let us express the contour Hamiltonian $\hat{H}(z)$ [see Eqs. (11) and (31)] in terms of the $\hat{\phi}$ operators. We first write the final result and then prove its correctness. We have

$$\hat{H}(z) = \hat{H}^s_{0,e}(z) + \hat{H}^s_{0,ph}(z) + \hat{H}_{e\text{-}e}(z) + \hat{H}_{e\text{-}ph}(z), \tag{36}$$

where

$$\hat{H}^s_{0,e}(z) = \int d\mathbf{x}\hat{\psi}^\dagger(\mathbf{x})\Big[h(\boldsymbol{\nabla}, \mathbf{r}, z) + \sum_{\mathbf{q}\nu}\boldsymbol{g}^\dagger_{\mathbf{q}\nu}(\mathbf{r}, z)\cdot\boldsymbol{s}_{\mathbf{q}\nu}(z)\Big]\hat{\psi}(\mathbf{x}), \tag{37a}$$

$$\hat{H}^s_{0,ph}(z) = \frac{1}{2}\sum_{\mathbf{q}}\sum_{\nu\nu'}\hat{\boldsymbol{\phi}}^\dagger_{\mathbf{q}\nu}\mathcal{Q}_{\nu\nu'}(\mathbf{q}, z)\hat{\boldsymbol{\phi}}_{\mathbf{q}\nu'} - \sum_{\mathbf{q}\nu}\int d\mathbf{x}n^0(\mathbf{x})\boldsymbol{g}^\dagger_{\mathbf{q}\nu}(\mathbf{r}, z)\cdot\hat{\boldsymbol{\phi}}_{\mathbf{q}\nu}, \tag{37b}$$

$$\hat{H}_{e\text{-}e}(z) = \frac{1}{2}\int d\mathbf{x}d\mathbf{x}'\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')v(\mathbf{r}, \mathbf{r}', z)\hat{\psi}(\mathbf{x}')\hat{\psi}(\mathbf{x}), \tag{37c}$$

$$\hat{H}_{e\text{-}ph}(z) = \sum_{\mathbf{q}\nu}\int d\mathbf{x}\hat{n}(\mathbf{x})\boldsymbol{g}^\dagger_{\mathbf{q}\nu}(\mathbf{r}, z)\cdot[\hat{\boldsymbol{\phi}}_{\mathbf{q}\nu} - \boldsymbol{s}_{\mathbf{q}\nu}(z)], \tag{37d}$$

and

$$\mathcal{Q}_{\nu\nu'}(\mathbf{q}, z) = \begin{pmatrix} K_{\nu\nu'}(\mathbf{q}, z) & 0 \\ 0 & \delta_{\nu\nu'}, \end{pmatrix} \tag{38a}$$

$$\boldsymbol{g}_{\mathbf{q}\nu}(\mathbf{r}, z) = \begin{pmatrix} g_{\mathbf{q}\nu}(\mathbf{r}, z) \\ 0 \end{pmatrix}. \tag{38b}$$

In Eqs. (37a) and (37d), we introduce a (two-dimensional vector) shift $\boldsymbol{s}_{\mathbf{q}\nu}(z)$ with the purpose of simplifying the NEGF treatment; see below. The exact form of the shift is irrelevant for the time being, as the terms containing $\boldsymbol{s}_{\mathbf{q}\nu}(z)$ cancel out in the sum of Eq. (36); thereby, $\hat{H}(z)$ is independent of this quantity. The shifted electronic Hamiltonian $\hat{H}^s_{0,e}(z)$ evaluated at zero shift, i.e., $\boldsymbol{s}_{\mathbf{q}\nu}(z) = 0$, is the same as $\hat{H}_{0,e}(z)$; see Eqs. (12) and (31a). The first term of the shifted phononic Hamiltonian $\hat{H}^s_{0,ph}(z)$ is the same as $\hat{H}_{0,ph}(z)$ [see Eqs. (27) and (31b)], whereas the second term coincides with the contribution to $\hat{H}'$ coming from n^0 in $\Delta\hat{n}$ [see Eqs. (28) and (31d)]. The e-e interaction Hamiltonian $\hat{H}_{e\text{-}e}(z)$ has not changed; see Eqs. (11) and (31c). Finally, the e-ph interaction Hamiltonian $\hat{H}_{e\text{-}ph}(z)$ evaluated at zero shift coincides with the contribution to $\hat{H}'$ coming from $\hat{n}$ in $\Delta\hat{n}$. We conclude that Eq. (36) is identical to the contour Hamiltonian for any two-dimensional vector $\boldsymbol{s}_{\mathbf{q}\nu}(z)$.

IV. EQUATIONS OF MOTION FOR OPERATORS IN THE CONTOUR-HEISENBERG PICTURE

The *contour-Heisenberg picture* is an extremely useful concept to develop the NEGF formalism. We define the contour evolution operators according to

$$\hat{\mathcal{U}}(z, t_0) = \mathcal{T}\left\{e^{-i\int_{t_0}^z d\bar{z}\,\hat{H}(\bar{z})}\right\}, \tag{39a}$$

$$\hat{\mathcal{U}}(t_0, z) = \bar{\mathcal{T}}\left\{e^{i\int_{t_0}^z d\bar{z}\,\hat{H}(\bar{z})}\right\}, \tag{39b}$$

where $\bar{\mathcal{T}}$ is the anti-contour-ordering operator. These operators are unitary for $z = t_\pm$ and Hermitian for $z = t_0 - i\beta$. For all $z \in \gamma$, we have the property $\hat{\mathcal{U}}(t_0, z)\hat{\mathcal{U}}(z, t_0) = 1$. We define an operator in the contour-Heisenberg picture as

$$\hat{O}_H(z) \equiv \hat{\mathcal{U}}(t_0, z)\hat{O}(z)\hat{\mathcal{U}}(z, t_0). \tag{40}$$

It is straightforward to verify that $O_H(t_\pm) = O_H(t)$. The equation of motion for operators in the contour-Heisenberg picture follows directly from the definitions in Eqs. (39):

$$i\frac{d\hat{O}_H(z)}{dz} = \hat{\mathcal{U}}(t_0, z)\left([\hat{O}(z), \hat{H}(z)] + i\frac{dO(z)}{dz}\right)\hat{\mathcal{U}}(z, t_0). \tag{41}$$

As the Hamiltonian is written in terms of $\hat{\psi}(\mathbf{x})$ and $\hat{\boldsymbol{\phi}}_{\mathbf{q}\nu}$, it is clear that the equation of motion for these operators plays a crucial role in the following derivation.

A. Equations of motion

Using Eq. (41), the equation of motion for the $\hat{\phi}$ operators reads

$$\sum_{\nu'}\left[i\frac{d}{dz}\alpha_{\nu\nu'}-Q_{\nu\nu'}(\mathbf{q},z)\right]\hat{\boldsymbol{\phi}}_{\mathbf{q}\nu',H}(z)=\int d\mathbf{x}\boldsymbol{g}_{\mathbf{q}\nu}(\mathbf{r},z)[\hat{n}_H(\mathbf{x},z)-n^0(\mathbf{x})]. \tag{42}$$

To remove the inhomogeneous term with n^0, we define the 2×2 GF $D_{0,\mathbf{q}\nu\nu'}$ as the solution of

$$\sum_{\bar{\nu}}\left[i\frac{d}{dz}\alpha_{\nu\bar{\nu}}-Q_{\nu\bar{\nu}}(\mathbf{q},z)\right]D_{0,\mathbf{q}\bar{\nu}\nu'}(z,z')=\mathbb{1}\delta_{\nu\nu'}\delta(z,z') \tag{43}$$

and satisfying the periodic Kubo-Martin-Schwinger (KMS) boundary conditions along the contour γ. We use D_0 to define the shift in Eqs. (37):

$$\boldsymbol{s}_{\mathbf{q}\nu'}(z)=-\sum_{\bar{\nu}}\int d\bar{z}D_{0,\mathbf{q}\nu'\bar{\nu}}(z,\bar{z})\int d\mathbf{x}\boldsymbol{g}_{\mathbf{q}\bar{\nu}}(\mathbf{r},\bar{z})n^0(\mathbf{x}). \tag{44}$$

Then, the equation of motion for the (time-dependent) shifted displacement

$$\hat{\boldsymbol{\varphi}}_{\mathbf{q}\nu}(z)\equiv\hat{\boldsymbol{\phi}}_{\mathbf{q}\nu}-\boldsymbol{s}_{\mathbf{q}\nu}(z) \tag{45}$$

reads

$$\sum_{\nu'}\left[i\frac{d}{dz}\alpha_{\nu\nu'}-Q_{\nu\nu'}(\mathbf{q},z)\right]\hat{\boldsymbol{\varphi}}_{\mathbf{q}\nu',H}(z)=\int d\mathbf{x}\boldsymbol{g}_{\mathbf{q}\nu}(\mathbf{r},z)\hat{n}_H(\mathbf{x},z), \tag{46}$$

which is a homogeneous equation in the field operators. Notice that the shift is proportional to the identity operator and, therefore, $\boldsymbol{s}_{\mathbf{q}\nu,H}(z)=\boldsymbol{s}_{\mathbf{q}\nu}(z)$. Such proportionality also implies that the operators $\hat{\boldsymbol{\varphi}}(z)$ and $\hat{\boldsymbol{\phi}}(z')$ [these operators are not in the contour-Heisenberg picture and, in particular, $\hat{\boldsymbol{\phi}}(z')$ does not depend on z'] satisfy the same commutation relations for any z and z':

$$[\hat{\varphi}^{i}_{\mathbf{q}\nu}(z),\hat{\varphi}^{i'\dagger}_{\mathbf{q}'\nu'}(z')]=\left[\hat{\varphi}^{i}_{\mathbf{q}\nu}(z),\hat{\phi}^{i'\dagger}_{\mathbf{q}'\nu'}(z')\right]=\left[\hat{\phi}^{i}_{\mathbf{q}\nu}(z),\hat{\phi}^{i'\dagger}_{\mathbf{q}'\nu'}(z')\right]. \tag{47}$$

From the commutator $[\hat{\psi}(\mathbf{x}),\hat{H}(z)]$, we can easily derive the equation of motion for the electronic field operators:

$$\left[i\frac{d}{dz}-h^s(\boldsymbol{\nabla},\mathbf{r},z)\right]\hat{\psi}_H(\mathbf{x},z)=\int d\mathbf{x}'v(\mathbf{r},\mathbf{r}',z)\hat{n}_H(\mathbf{x}',z)\hat{\psi}_H(\mathbf{x},z)+\sum_{\mathbf{q}\nu}\hat{\psi}_H(\mathbf{x},z)\boldsymbol{g}^{\dagger}_{\mathbf{q}\nu}(\mathbf{r},z)\cdot\hat{\boldsymbol{\varphi}}_{\mathbf{q}\nu,H}(z), \tag{48}$$

where we define the shifted one-particle Hamiltonian

$$h^s(\boldsymbol{\nabla},\mathbf{r},z)\equiv h(\boldsymbol{\nabla},\mathbf{r},z)+\sum_{\mathbf{q}\nu}\boldsymbol{g}^{\dagger}_{\mathbf{q}\nu}(\mathbf{r},z)\cdot\boldsymbol{s}_{\mathbf{q}\nu}(z) \tag{49}$$

[see Eq. (37a)] and in the last term of the rhs we recognize that the density operator in Eq. (37d) multiples the shifted displacement $\hat{\boldsymbol{\varphi}}$ defined in Eq. (45).

V. GREEN'S FUNCTIONS AND MARTIN-SCHWINGER HIERARCHY

The building blocks of the NEGF formalism are the electronic and phononic GF. Let us introduce a notation which is used throughout the remainder of the paper. We denote the position, spin, and contour-time coordinates of an electronic field operator with the collective indices

$$\begin{aligned} k&=\mathbf{x}_k,z_k, & j&=\mathbf{x}_j,z_j, & &\dots\\ k'&=\mathbf{x}'_k,z'_k, & j'&=\mathbf{x}'_j,z'_j, & &\dots \end{aligned} \tag{50}$$

etc. Thus, for instance, $\hat{\psi}(1)=\hat{\psi}(\mathbf{x}_1,z_1)$ and $\hat{\psi}(2')=\hat{\psi}(\mathbf{x}'_2,z'_2)$. We recall that the electronic field operators have no explicit dependence on the contour time, i.e., $\hat{\psi}(\mathbf{x},z)=\hat{\psi}(\mathbf{x})$. Without any risk of ambiguity, we use the same notation to denote the momentum, branch, component, and contour-time coordinates of a phononic field operator:

$$\begin{aligned} k&=\mathbf{q}_k,\nu_k,i_k,z_k, & j&=\mathbf{q}_j,\nu_j,i_j,z_j, & &\dots\\ k'&=\mathbf{q}'_k,\nu'_k,i'_k,z'_k, & j'&=\mathbf{q}'_j,\nu'_j,i'_j,z'_j, & &\dots \end{aligned} \tag{51}$$

etc. Thus, for instance, $\hat{\varphi}(1)=\hat{\varphi}^{i_1}_{\mathbf{q}_1\nu_1}(z_1)$ and $\hat{\varphi}(2')=\hat{\varphi}^{i'_2}_{\mathbf{q}'_2\nu'_2}(z'_2)$. We also use the superscript star "$*$" to denote the composite index with reversed momentum, e.g., $k^*=-\mathbf{q}_k,\nu_k,i_k,z_k$. Of course, starring twice is the same as no starring, i.e., $k^{**}=k$. We then define

$$\vec{D}_0^{-1}(1,2)\equiv\left[i\frac{d}{dz_1}\alpha^{i_1i_2}_{\nu_1\nu_2}-Q^{i_1i_2}_{\nu_1\nu_2}(\mathbf{q}_1,z_1)\right]\delta_{\mathbf{q}_1\mathbf{q}_2}\delta(z_1,z_2), \tag{52a}$$

$$\vec{G}_0^{-1}(1;2)\equiv\left[i\frac{d}{dz_1}-h^s(\boldsymbol{\nabla}_1,\mathbf{r}_1,z_1)\right]\delta(\mathbf{x}_1-\mathbf{x}_2)\delta(z_1,z_2), \tag{52b}$$

$$g(1;2)\equiv\delta(z_1,z_2)g^{i_2}_{\mathbf{q}_2\nu_2}(\mathbf{r}_1,z_1), \tag{52c}$$

$$v(1;2)\equiv\delta(z_1,z_2)v(\mathbf{r}_1,\mathbf{r}_2,z_1), \tag{52d}$$

where $\delta(z_1, z_2)$ is the Dirac delta on the contour [25]. Accordingly, the equations of motion for the field operators, i.e., Eqs. (46) and (48), are shortened as

$$\int d\tilde{2}\vec{D}_0^{-1}(1,\tilde{2})\hat{\varphi}_H(\tilde{2}) = \int d\bar{2}g(\bar{2};1)\hat{\psi}_H^\dagger(\bar{2})\hat{\psi}_H(\bar{2}), \quad (53a)$$

$$\int d\bar{2}\vec{G}_0^{-1}(1;\bar{2})\hat{\psi}_H(\bar{2}) = \int d\bar{2}v(1;\bar{2})\hat{\psi}_H^\dagger(\bar{2})\hat{\psi}_H(\bar{2})\hat{\psi}_H(1) + \int d\tilde{2}g(1;\tilde{2}^*)\hat{\psi}_H(1)\hat{\varphi}_H(\tilde{2}). \quad (53b)$$

To distinguish the integration variables of the electronic operators $\hat{\psi}$ from those of the phononic operators $\hat{\varphi}$, we use a bar for the former and a tilde for the latter; thus, $\int d\bar{1} \equiv \int d\bar{\mathbf{x}}_1 d\bar{z}_1$ and $\int d\tilde{1} \equiv \sum_{\tilde{q}_1\tilde{\nu}_1\tilde{i}_1}\int d\tilde{z}_1$. Setting $v = g = 0$ in the rhs of Eqs. (53), we obtain the equations of motion of the field operators governed by the Hamiltonian

$$\hat{H}_0^s(z) \equiv \hat{H}_{0,e}^s(z) + \hat{H}_{0,ph}^s(z). \quad (54)$$

We use this observation in the next section.

A. Green's functions

The m-particle phononic and electronic GF are contour-ordered correlators of strings of phononic and electronic field operators. We define them here in full generality, as we need them to derive the Martin-Schwinger hierarchy. The hierarchy is then solved in Sec. VI for independent electrons and phonons, and the solution is used to work out the expansion of the interacting electronic and phononic GF with $m = 1$, i.e., G and D. The m-particle phononic GF is defined as

$$\tilde{D}_m(1,2,\ldots,2m) \equiv \frac{1}{i^m}\mathrm{Tr}[\hat{\rho}\mathcal{T}\{\hat{\varphi}_H(1)\hat{\varphi}_H(2)\ldots\hat{\varphi}_H(2m)\}] = \frac{1}{i^m}\frac{\mathrm{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\hat{H}(\bar{z})}\hat{\varphi}(1)\hat{\varphi}(2)\ldots\hat{\varphi}(2m)\right\}\right]}{\mathrm{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\hat{H}(\bar{z})}\right\}\right]}. \quad (55)$$

In this definition, m can also be a *half-integer*; in particular, $\tilde{D}_{1/2}(1) = \varphi(1)/i^{1/2}$. The phononic GF $\tilde{D}_m$ differs from that in Refs. [58,59], as it is defined in terms of the shifted operators $\hat{\varphi}$ instead of $\hat{\phi}$. We observe that the operators appearing in the second equality are not in the contour-Heisenberg picture [compare with Eq. (32)]. The phononic GF is totally symmetric under an arbitrary permutation of its arguments $1, 2, \ldots, 2m$. Similarly, we define the n-particle electronic GF as

$$G_n(1,\ldots,n;1',\ldots,n') = \frac{1}{i^n}\mathrm{Tr}[\hat{\rho}\mathcal{T}\{\hat{\psi}_H(1)\ldots\hat{\psi}_H(n)\hat{\psi}_H^\dagger(n')\ldots\hat{\psi}_H^\dagger(1')\}] = \frac{1}{i^n}\frac{\mathrm{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\hat{H}(\bar{z})}\hat{\psi}(1)\ldots\hat{\psi}(n)\hat{\psi}^\dagger(n')\ldots\hat{\psi}^\dagger(1')\right\}\right]}{\mathrm{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\hat{H}(\bar{z})}\right\}\right]}. \quad (56)$$

The electronic GF is totally antisymmetric under an arbitrary permutation of the arguments $1, 2, \ldots, n$ and $1', 2', \ldots, n'$.

B. Martin-Schwinger hierarchy

Taking into account that the commutation relations for the operators $\hat{\varphi}$ are identical to the commutation relations for the operators $\hat{\phi}$ [see Eq. (47)], the equations of motion for $\tilde{D}_m$ with $m = 1/2, 1, 3/2, \ldots$ read

$$\int d\tilde{1}\vec{D}_0^{-1}(k,\tilde{1})\tilde{D}_m(1,\ldots,\tilde{1},\ldots,2m) = \frac{1}{i^m}\int d\bar{1}g(\bar{1};k)\mathrm{Tr}\left[\hat{\rho}\mathcal{T}\left\{\hat{\varphi}_H(1),\ldots,\underbrace{\hat{\psi}_H^\dagger(\bar{1})\hat{\psi}_H(\bar{1})}_{k\text{th place}},\ldots,\hat{\varphi}_H(2m)\right\}\right] + \sum_{\substack{j=1\\ j\neq k}}^{2m}\delta(k,j^*)\tilde{D}_{m-1}(1,\ldots,\overset{\sqcap}{k},\ldots,\overset{\sqcap}{j},\ldots,2m), \quad (57)$$

where the variable $\tilde{1}$ in the lhs is at place k and we define $\tilde{D}_0 = 1$ and $\tilde{D}_{-1/2} = 0$. The first term in the rhs originates from the equation of motion Eq. (53a). The last term in the rhs originates from the derivative of the Heaviside step functions implicit in the contour ordering [25]. These derivatives generate quantities like $\delta(z_k, z_j)[\hat{\varphi}^{i_k}_{\mathbf{q}_k\nu_k,H}(z_k), \hat{\varphi}^{i_j}_{\mathbf{q}_j\nu_j,H}(z_j)] = \delta(z_k, z_j)\delta_{\mathbf{q}_k,-\mathbf{q}_j}\alpha^{i_k i_j}_{\nu_k\nu_j}$ [see Eq. (34)], which multiplied by α lead to $\delta(k, j^*) \equiv \delta(z_k, z_j)\delta_{\mathbf{q}_k,-\mathbf{q}_j}\delta_{\nu_k\nu_j}\delta_{i_k i_j}$.

To shorten the equations, we also introduce the symbol "⊓" above an index to indicate that the index is missing from the list. In a similar way, we can derive the equations of motion for the n-particle GF and find for $n = 1, 2, 3, \ldots$

$$\begin{aligned}
&\int d\bar{1}\vec{G}_0^{-1}(k;\bar{1})G_n(1,\ldots,\bar{1},\ldots,n;1',\ldots,n') \\
&\quad = -i\int d\bar{1}\, v(k;\bar{1})G_{n+1}(1,\ldots,n,\bar{1};1',\ldots,n',\bar{1}^+) \\
&\qquad + \frac{1}{i^n}\int d\tilde{1}g(k;\tilde{1}^*)\mathrm{Tr}\left[\hat{\rho}\mathcal{T}\left\{\hat{\psi}_H(1),\ldots,\underbrace{\hat{\psi}_H(k)\hat{\varphi}_H(\tilde{1})}_{k\text{th place}},\ldots,\hat{\psi}_H(n)\hat{\psi}_H(n'),\ldots,\hat{\psi}_H^\dagger(1')\right\}\right] \\
&\qquad + \sum_{j=1}^{n}(-)^{k+j}\delta(k;j')G_{n-1}(1,\ldots,\overset{\sqcap}{k},\ldots,n;1',\ldots,\overset{\sqcap}{j'},\ldots,n'),
\end{aligned} \tag{58}$$

where the variable $\bar{1}$ in the lhs is at place k and we define $G_0 = 1$. The first two terms in the rhs originate from the equation of motion Eq. (53b). The last term in the rhs originates from the derivative of the Heaviside step functions implicit in the contour ordering. In the electronic case, $\delta(k;j) \equiv \delta(\mathbf{x}_k - \mathbf{x}_j)\delta(z_k, z_j)$. We further notice that the last argument of the GF G_{n+1} is $\bar{1}^+$. We use the superscript "+" to indicate that the contour time is infinitesimally later than $\bar{z}_1$. This infinitesimal shift guarantees that the creation operator $\hat{\psi}^\dagger(\bar{1})$ in G_{n+1} ends up to the left of the annihilation operator $\hat{\psi}(\bar{1})$ when the operators are contour ordered.

The equation of motion for G_n with derivative with respect to the primed arguments can be worked out similarly. All equations of motion must be solved with KMS boundary conditions; i.e., $\tilde{D}_m$ must be periodic on the contour with respect to all times $z_1, \ldots, z_{2m}$ and G_n must be antiperiodic on the contour with respect to all times $z_1, \ldots, z_n, z_1', \ldots, z_n'$.

If the e-ph coupling $g = 0$, then $\tilde{D}_m$ couples only to $\tilde{D}_{m-1}$. In the electronic sector, things are different. For $g = 0$, the equations of motion reduce to the Martin-Schwinger hierarchy for a system of only electrons, and G_n couples to G_{n-1} and G_{n+1} through the Coulomb interaction v. For G_n to couple only to G_{n-1}, the Coulomb interaction has to vanish, too.

When both e-e and e-ph interactions are present, G_n couples to G_{n-1} and G_{n+1} as well as to mixed GF consisting of a mix string of $\hat{\psi}$, $\hat{\psi}^\dagger$, and $\hat{\varphi}$ operators; see the third line in the equations of motion. Likewise, $\tilde{D}_m$ couples to $\tilde{D}_{m-1}$ but also to mixed GF; see the first term in the rhs of the equations of motion. The equations of motion for the mixed GF can be derived in precisely the same way; see also Ref. [60]. We refer to the full set of equations as the Martin-Schwinger hierarchy for electron-phonon systems. In the next sections, we lay down a perturbative method to calculate all GF.

VI. WICK'S THEOREM FOR THE MANY-PARTICLE GREEN'S FUNCTIONS

The Wick theorem provides the solution of the Martin-Schwinger hierarchy with the rhs evaluated at $g = v = 0$. This is the same as solving the Martin-Schwinger hierarchy for a system of electrons and phonons governed by the Hamiltonian $\hat{H}_0^s$; see the comment above Eq. (54). As $\hat{H}_0^s$ depends on g explicitly, setting $g = v = 0$ in the rhs of Eqs. (57) and (58) is not the same as solving the Martin-Schwinger hierarchy with $\hat{H}|_{g=v=0}$ (noninteracting hierarchy). Henceforth, we name the GF governed by $\hat{H}_0^s$ as the *independent* GF, and we denote them by $D_{0,m}$ and $G_{0,n}$. We then have

$$\int d\tilde{1}\vec{D}_0^{-1}(k,\tilde{1})D_{0,m}(1,\ldots,\tilde{1},\ldots,2m) = \sum_{\substack{j=1\\ j\neq k}}^{2m}\delta(k,j^*)D_{0,m-1}(1,\ldots,\overset{\sqcap}{k},\ldots,\overset{\sqcap}{j},\ldots,2m), \tag{59a}$$

$$\int d\bar{1}\vec{G}_0^{-1}(k;\bar{1})G_{0,n}(1,\ldots,\bar{1},\ldots,n;1',\ldots,n') = \sum_{j=1}^{n}(-)^{k+j}\delta(k;j')G_{0,n-1}(1,\ldots,\overset{\sqcap}{k},\ldots,n;1',\ldots,\overset{\sqcap}{j'},\ldots,n'), \tag{59b}$$

and the like with time derivatives with respect to the primed arguments. The independent GF satisfy two independent hierarchies. Despite the similarities, the phononic and electronic hierarchies present important differences. The sum in the rhs runs over all arguments of $D_{0,m}$ in Eq. (59a), whereas it runs over only the primed arguments of $G_{0,n}$ in Eq. (59b).

Moreover, in the phononic case, m can also be a half-integer. From Eq. (59a), we see that the integer m connects with the integer $m-1$ and the half-integer m connects with the half-integer $m-1$. Therefore, we have two separate hierarchies of equations for the phononic GF.

A. Wick's theorem for phonons

The proof of Wick's theorem for $D_{0,m}$ goes along the same lines as in Ref. [59]. The phononic GF $D_{0,m}=0$ for all half-integers m. This can easily be proven by considering the average of the equation of motion Eq. (46) with $g=0$. By definition, this average is proportional to $D_{0,1/2}$, and the only solution satisfying the KMS boundary conditions is $D_{0,1/2}=0$. Consider now $m=3/2$:

$$\int d\tilde{1}\vec{D}_0^{-1}(1,\tilde{1})D_{0,3/2}(\tilde{1},2,3) = \delta(1,2^*)D_{0,1/2}(3)+\delta(1,3^*)D_{0,1/2}(2)=0 \tag{60}$$

and the like for the variables 2 and 3. We see that $D_{0,3/2}=0$ is a solution satisfying the KMS boundary conditions. By induction, $D_{0,m}=0$ for half-integers. Henceforth, we consider only integers m in the noninteracting case.

For $m=1$, we have the equation of motion for $D_{0,1}$:

$$\int d\tilde{1}\vec{D}_0^{-1}(1,\tilde{1})D_{0,1}(\tilde{1},2)=\delta(1,2^*). \tag{61}$$

Comparing with Eq. (43), we realize that

$$D_{0,1}(1,2)=\delta_{\mathbf{q}_1,-\mathbf{q}_2}D^{i_1 i_2}_{0,\mathbf{q}_1\nu_1\nu_2}(z_1,z_2). \tag{62}$$

Without any risk of ambiguity, we denote $D_{0,1}(1,2)$ simply by $D_0(1,2)$ in the remainder of the paper. For $D_{0,m}$ with $m>1$, the solution of Eq. (59a) is given by the so-called *Hafnian* [60–62]. The Hafnian can be defined recursively starting from any of the arguments in $D_{0,m}$. Choosing, for instance, the argument k, we have

$$D_{0,m}(1,\ldots,2m)=\sum_{\substack{j=1\\ j\neq k}}^{2m} D_0(k,j)D_{0,m-1}(1,\ldots,\overset{\sqcap}{k},\ldots,\overset{\sqcap}{j},\ldots,2m). \tag{63}$$

Using again Eq. (63) for $D_{0,m-1}$ and then for $D_{0,m-2}$ and so on and so forth, we obtain an expansion of $D_{0,m}$ in terms of products of m D_0's. A compact way to write this expansion is

$$D_{0,m}(1,\ldots,2m)=\frac{1}{2^m m!}\sum_P D_0(P(1),P(2))\ldots \times D_0(P(2m-1),P(2m)), \tag{64}$$

where the sum runs over all permutations of the indices $1,2,\ldots,2m$. The recursive form of Eq. (63) makes it clear that $D_{0,m}$ satisfies Eq. (59a) and the KMS boundary conditions.

B. Wick's theorem for electrons

The solution of Eq. (58) is discussed at length in Refs. [25,63]. We here write the final result for completeness. For $n=1$, Eq. (59b) yields

$$\int d\bar{1}\vec{G}_0^{-1}(1;\bar{1})G_{0,1}(\bar{1};2)=\delta(1;2), \tag{65}$$

to be solved with KMS boundary conditions. Like for the phononic case, we shorten the notation and write $G_{0,1}(1;2)=G_0^s(1;2)$. The superscript "s" reminds us that this GF depends on g through h^s. For $G_{0,n}$ with $n>1$, the solution of Eq. (58) is again defined recursively choosing either an unprimed or a primed argument:

$$\begin{aligned} &G_{0,n}(1,\ldots,n;1',\ldots,n') \\ &=\sum_{k=1}^{n}(-)^{k+j}G_0^s(k;j')G_{0,n-1}(1,\ldots,\overset{\sqcap}{k},\ldots,n;1',\ldots,\overset{\sqcap}{j'},\ldots,n') \\ &=\sum_{j=1}^{n}(-)^{k+j}G_0^s(k;j')G_{0,n-1}(1,\ldots,\overset{\sqcap}{k},\ldots,n;1',\ldots,\overset{\sqcap}{j'},\ldots,n'). \end{aligned} \tag{66}$$

Using again Eq. (66) for $G_{0,n-1}$ and then for $G_{0,n-2}$ and so on and so forth, we obtain an expansion of $G_{0,n}$ in terms of products of n G_0^s's. A compact way to write this expansion is the determinant

$$\begin{aligned} G_{0,n}(1,\ldots,n;1',\ldots,n') &= \begin{vmatrix} G_0^s(1;1') & \cdots & G_0^s(1;n') \\ \vdots & & \vdots \\ G_0^s(n;1') & \cdots & G_0^s(n;n') \end{vmatrix} \\ &=\sum_P (-)^P G_0^s(P(1);1')\ldots G_0^s(P(n);n'), \end{aligned} \tag{67}$$

where the sum runs over all permutations of the indices $1,2,\ldots,n$ and $(-)^P$ is the sign of the permutation.

The recursive form of the Wick theorem highlights the differences between the phononic and the electronic case. For $G_{0,n}$, we need to connect unprimed arguments to primed arguments in all possible ways. For $D_{0,m}$, there is no such distinction, and we need to connect all arguments in all possible ways.

VII. EXACT GREEN'S FUNCTIONS FROM WICK'S THEOREM

The interacting GF $\tilde{D}_m$ and G_n can be expanded in powers of the e-e interaction v and e-ph coupling g. In this section, we focus on the one-particle electronic GF $G \equiv G_1$, the one-particle phononic GF $\tilde{D} \equiv \tilde{D}_1$, and the half-particle phononic GF $\tilde{D}_{1/2}$. The final results are Eqs. (75), (77), and (78); the reader can directly move to these equations if not interested in their derivation. In Sec. IX, we show that the perturbative expansion leads to a closed system of equations for these quantities. Higher-order Green's functions as well as mixed Green's functions (relevant for linear response theory) can be investigated along the same lines; see Ref. [25].

The starting point is the Hamiltonian written in the form of Eq. (36), i.e., $\hat{H} = \hat{H}_0^s + \hat{H}_{e\text{-}e} + \hat{H}_{e\text{-}ph}$ with $\hat{H}_0^s$ defined in Eq. (54). Inside the contour ordering, the Hamiltonians $\hat{H}_0^s$, $\hat{H}_{e\text{-}e}$, and $\hat{H}_{e\text{-}ph}$ can be treated as commuting operators, and, hence, the exponential of their sum can be separated into the product of three exponentials. It is then natural to define the independent averages as

$$\langle \mathcal{T}\{\cdots\}\rangle_0^s \equiv \mathrm{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\hat{H}_0^s(\bar{z})}\ldots\right\}\right]. \tag{68}$$

We emphasize again that the independent averages are not the same as the noninteracting averages, i.e., the averages with $v = g = 0$, since both $\hat{H}_{0,e}^s$ and $\hat{H}_{0,ph}^s$ depend on g; see Eqs. (37a) and (37b).

A. One-particle electronic Green's function

The GF $G \equiv G_1$ is defined in Eq. (56). We have

$$G(a;b) = \frac{1}{i}\frac{\mathrm{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\hat{H}_0^s(\bar{z})}e^{-i\int_\gamma d\bar{z}\hat{H}_{e\text{-}e}(\bar{z})}e^{-i\int_\gamma d\bar{z}\hat{H}_{e\text{-}ph}(\bar{z})}\hat{\psi}(a)\hat{\psi}^\dagger(b)\right\}\right]}{\mathrm{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\hat{H}_0^s(\bar{z})}e^{-i\int_\gamma d\bar{z}\hat{H}_{e\text{-}e}(\bar{z})}e^{-i\int_\gamma d\bar{z}\hat{H}_{e\text{-}ph}(\bar{z})}\right\}\right]}, \tag{69}$$

where $a = \mathbf{x}_a, z_a$ and $b = \mathbf{x}_b, z_b$ in accordance with the notation of Eq. (50). The denominator in this equation is the interacting partition function $\mathcal{Z} = \mathrm{Tr}[e^{-\beta(\hat{H}-\mu\hat{N}_e)}]$. Expanding the exponentials containing $\hat{H}_{e\text{-}e}$ and $\hat{H}_{e\text{-}ph}$, we find

$$G(a;b) = \frac{1}{i}\frac{\sum_{k,p=0}^{\infty}\frac{(-i)^{k+p}}{k!p!}\int_\gamma dz_1\ldots dz_k d\tilde{z}_1\ldots d\tilde{z}_p\langle\mathcal{T}\{\hat{H}_{e\text{-}e}(z_1)\ldots\hat{H}_{e\text{-}e}(z_k)\hat{H}_{e\text{-}ph}(\tilde{z}_1)\ldots\hat{H}_{e\text{-}ph}(\tilde{z}_p)\hat{\psi}(a)\hat{\psi}^\dagger(b)\}\rangle_0^s}{\sum_{k,p=0}^{\infty}\frac{(-i)^{k+p}}{k!p!}\int_\gamma dz_1\ldots dz_k d\tilde{z}_1\ldots d\tilde{z}_p\langle\mathcal{T}\{\hat{H}_{e\text{-}e}(z_1)\ldots\hat{H}_{e\text{-}e}(z_k)\hat{H}_{e\text{-}ph}(\tilde{z}_1)\ldots\hat{H}_{e\text{-}ph}(\tilde{z}_p)\}\rangle_0^s}. \tag{70}$$

To facilitate the identification of the expansion terms, we use a tilde for the contour times of the e-ph interaction Hamiltonian. Let us write the integrated Hamiltonians in terms of $g(i;j)$ and $v(i;j)$; see Eqs. (52c) and (52d). We have

$$\int d\tilde{z}_j\hat{H}_{e\text{-ph}}(\tilde{z}_j) = \int d\bar{j}d\tilde{j}g(\bar{j};\tilde{j}^*)\hat{\psi}^\dagger(\bar{j}^+)\hat{\psi}(\bar{j})\hat{\varphi}(\tilde{j}), \tag{71a}$$

$$\int dz_j\hat{H}_{e\text{-}e}(z_j) = \frac{1}{2}\int djdj' v(j;j')\hat{\psi}^\dagger(j^+)\hat{\psi}^\dagger(j'^+)\hat{\psi}(j')\hat{\psi}(j). \tag{71b}$$

The infinitesimal shift in the contour times of the electronic creation operators guarantees that these operators end up to the left of the annihilation operators calculated at the same contour times after the contour reordering. Inserting Eqs. (71) into Eq. (70), we are left with the evaluation of contour-ordered strings like $\langle\mathcal{T}\{\hat{\psi}\ldots\hat{\psi}\hat{\psi}^\dagger\ldots\hat{\psi}^\dagger\hat{\varphi}\ldots\hat{\varphi}\}\rangle_0^s$ with an arbitrary number of operators. We observe that $\hat{H}_{0,e}^s$ acts on the Fock space $\mathbb{F}$ of the electrons and $\hat{H}_{0,ph}^s$ acts on the Hilbert space $\mathbb{D}_{N_n}$ of N_n distinguishable nuclei. As such, the eigenkets of $\hat{H}_0^s = \hat{H}_{0,e}^s + \hat{H}_{0,ph}^s$ factorize into tensor products of kets in $\mathbb{F}$ and kets in $\mathbb{D}_{N_n}$. Therefore, the partition function for independent electrons and phonons

$$\mathcal{Z}_0^s = \mathrm{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\hat{H}_0^s(\bar{z})}\right\}\right] = \mathrm{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\hat{H}_{0,e}^s(\bar{z})}\right\}\right]\times\mathrm{Tr}\left[\mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\hat{H}_{0,ph}^s(\bar{z})}\right\}\right] = \mathcal{Z}_{0,e}^s\mathcal{Z}_{0,ph}^s \tag{72}$$

factorizes into electron and phonon contributions. The same type of factorization allows us to simplify the independent average of any string of operators as

$$\langle \mathcal{T}\{\hat{\psi}\ldots\hat{\psi}\hat{\psi}^\dagger\ldots\hat{\psi}^\dagger\hat{\varphi}\ldots\hat{\varphi}\}\rangle_0^s = \langle \mathcal{T}\{\hat{\psi}\ldots\hat{\psi}\hat{\psi}^\dagger\ldots\hat{\psi}^\dagger\}\rangle_{0,e}^s \times \langle \mathcal{T}\{\hat{\varphi}\ldots\hat{\varphi}\}\rangle_{0,ph}^s, \tag{73}$$

where the average $\langle\cdots\rangle_{0,e}^s$ is performed with $\hat{H}_{0,e}^s$ and the average $\langle\cdots\rangle_{0,ph}^s$ is performed with $\hat{H}_{0,ph}^s$.

To the order of k in v and to the order of p in g, the numerator of the GF contains the independent average of the following string:

$$\begin{aligned}
&\Big\langle \mathcal{T}\Big\{\underbrace{\hat{\psi}^\dagger(1^+)\hat{\psi}^\dagger(1'^+)\hat{\psi}(1')\hat{\psi}(1)\ldots}_{4k\text{ operators}}\underbrace{\hat{\psi}^\dagger(\bar{1}^+)\hat{\psi}(\bar{1})\hat{\varphi}(\tilde{1})\ldots}_{3p\text{ operators}}\hat{\psi}(a)\hat{\psi}^\dagger(b)\Big\}\Big\rangle_0^s \\
&= (-)^p\Big\langle \mathcal{T}\Big\{\hat{\psi}(a)\underbrace{\hat{\psi}(1)\hat{\psi}(1')\ldots}_{2k\,\hat{\psi}}\underbrace{\hat{\psi}(\bar{1})\ldots}_{p\,\hat{\psi}}\underbrace{\ldots\hat{\psi}^\dagger(\bar{1}^+)}_{p\,\hat{\psi}^\dagger}\underbrace{\ldots\hat{\psi}^\dagger(1'^+)\hat{\psi}^\dagger(1^+)}_{2k\,\hat{\psi}^\dagger}\hat{\psi}^\dagger(b)\Big\}\Big\rangle_{0,e}^s \times \Big\langle \mathcal{T}\Big\{\underbrace{\hat{\varphi}(\tilde{1})\ldots}_{p\,\hat{\varphi}}\Big\}\Big\rangle_{0,\mathrm{ph}}^s \\
&= (-)^p \mathcal{Z}_{0,e}^s i^{2k+p+1} G_{0,2k+p+1}(a,1,1',\ldots,\bar{1},\ldots;b,1^+,1'^+,\ldots,\bar{1}^+,\ldots) \times \mathcal{Z}_{0,\mathrm{ph}}^s i^{p/2} D_{0,p/2}(\tilde{1},\ldots).
\end{aligned} \tag{74}$$

With similar manipulations, we can work out the expansion of the partition function. Taking into account that $D_{0,p/2}$ is nonvanishing only for even integers p, the expansion of the interacting GF reads

$$\begin{aligned}
G(a;b) = \frac{\mathcal{Z}_0^s}{\mathcal{Z}}\sum_{k,p=0}^{\infty}\frac{i^{k+p}}{2^k k!(2p)!}\int d1d1'\ldots dkdk' v(1;1')\ldots v(k;k')\int d\tilde{1}d\bar{1}\ldots d(\widetilde{2p})d(\overline{2p})g(\bar{1};\tilde{1}^*)\ldots g(\overline{2p};\widetilde{2p}^*) \\
\times G_{0,2k+2p+1}(a,1,1',\ldots,\bar{1},\ldots;b,1^+,1'^+,\ldots,\bar{1}^+,\ldots)D_{0,p}(\tilde{1},\ldots),
\end{aligned} \tag{75}$$

with

$$\begin{aligned}
\frac{\mathcal{Z}}{\mathcal{Z}_0^s} = \sum_{k,p=0}^{\infty}\frac{i^{k+p}}{2^k k!(2p)!}\int d1d1'\ldots dkdk' v(1;1')\ldots v(k;k')\int d\tilde{1}d\bar{1}\ldots d(\widetilde{2p})d(\overline{2p})g(\bar{1};\tilde{1}^*)\ldots g(\overline{2p};\widetilde{2p}^*) \\
\times G_{0,2k+2p}(1,1',\ldots,\bar{1},\ldots;1^+,1'^+,\ldots,\bar{1}^+,\ldots)D_{0,p}(\tilde{1},\ldots).
\end{aligned} \tag{76}$$

The zeroth-order term in the expansion of Eq. (75) ($k = p = 0$) is the GF $G_{0,1} = G_0^s$ calculated from Eq. (65), where $\vec{G}_0^{-1}$ is defined in Eq. (52b).

Using Wick's theorem for $G_{0,n}$ and $D_{0,m}$, Eqs. (75) and (76) provide an exact expansion in terms of the one-particle electronic GF G_0^s and phononic GF D_0.

B. One-particle phononic Green's function

The interacting GF $\tilde{D} \equiv \tilde{D}_1$ is defined in Eq. (55). Writing the exponential like in Eq. (69), expanding with respect to $\hat{H}_{e\text{-}e}$ and $\hat{H}_{e\text{-}ph}$, and using Eqs. (71), we find

$$\begin{aligned}
\tilde{D}(a,b) = \frac{\mathcal{Z}_0^s}{\mathcal{Z}}\sum_{k,p=0}^{\infty}\frac{i^{k+p}}{2^k k!(2p)!}\int d1d1'\ldots dkdk' v(1;1')\ldots v(k;k')\int d\tilde{1}d\bar{1}\ldots d(\widetilde{2p})d(\overline{2p})g(\bar{1};\tilde{1}^*)\ldots g(\overline{2p};\widetilde{2p}^*) \\
\times G_{0,2k+2p}(1,1',\ldots,\bar{1},\ldots;1^+,1'^+,\ldots,\bar{1}^+,\ldots)D_{0,p+1}(a,b,\tilde{1},\ldots),
\end{aligned} \tag{77}$$

where we take into account that $D_{0,m}$ vanishes for half-integers m. In Eq. (77), the arguments $a = \mathbf{q}_a, \nu_a, i_a, z_a$ and $b = \mathbf{q}_b, \nu_b, i_b, z_b$.

Using Wick's theorem for $G_{0,n}$ and $D_{0,m}$, we have an exact expansion of the interacting one-particle phononic GF in terms of G_0^s and D_0. The zeroth-order term ($k = p = 0$) is the GF D_0, since $G_{0,0} = 1$.

C. Half-particle phononic Green's function

The interacting GF $\tilde{D}_{1/2}$ is proportional to the time-dependent average of the field operator $\hat{\varphi}$, i.e., $\tilde{D}_{1/2}(a) = (1/i^{1/2})\varphi(a)$. Proceeding along the same lines as for the derivation of the expansion Eq. (77), we find

$$\begin{aligned}\varphi(a) = -\frac{\mathcal{Z}_0^s}{\mathcal{Z}}\sum_{k,p=0}^{\infty}\frac{i^{k+p+1}}{2^k k!(2p+1)!}\int d1d1'\ldots dkdk' v(1;1')\ldots v(k;k')\\ \times\int d\tilde{1}d\bar{1}\ldots d\left(\widetilde{2p+1}\right)d(\overline{2p+1})g(\bar{1};\tilde{1}^*)\ldots g\left(\overline{2p+1};\widetilde{2p+1}^*\right)\\ \times G_{0,2k+2p+1}(1,1',\ldots,\bar{1},\ldots;1^+,1'^+,\ldots,\bar{1}^+,\ldots)D_{0,p+1}(a,\tilde{1},\ldots),\end{aligned} \tag{78}$$

where we take into account that $D_{0,m}$ vanishes for half-integers m. The average φ vanishes for $g = 0$, in agreement with the equation of motion Eq. (46).

VIII. DIAGRAMMATIC THEORY

The expansions of G, $\tilde{D}$, and φ contain the GF G_0^s and D_0, the Coulomb interaction v, and the *e-ph* coupling g. Let us assign a graphical object to these quantities. We use an oriented line from 2 to 1 to represent $G_0^s(1;2)$ and a wiggly line between 1 and 2 to represent $v(1;2) = v(2;1)$. For the noninteracting phononic GF $D_0(1,2) = D_0(2,1)$, we use a spring from 1 to 2. The *e-ph* coupling $g(1;2^*)$ is instead represented by a square, half black and half white, where 1 is attached to the black vertex and 2 is attached to the white vertex. In summary,

$G_0^s(1;2) =$ 1  2

$D_0(1,2) =$ 1  2

$v(1;2) =$ 1  2 (79)

$g(1,2^*) =$ 1  2

We can now represent every term of the expansions with diagrams. The diagrams for G are either connected or products of a connected diagram and a vacuum diagram. In a connected diagram for $G(a;b)$ all internal vertices are connected to both a and b through G_0^s, D_0, v, and g. Thus, a disconnected G diagram is characterized by a subset of internal vertices that are not connected to either a or b, and, hence, they form a vacuum diagram. Similarly, the diagrams for $\varphi(a)$ fall into two main classes: those with all internal vertices connected to a and those where a subset of internal vertices is disconnected, thus forming a vacuum diagram. The diagrams for $\tilde{D}(a,b)$ can instead be grouped into three different classes: (c1) all internal vertices connected to both a and b, (c2) a subset of internal vertices connected only to a and the complementary set connected only to b, and (c3) diagrams where a subset of internal vertices is not connected to either a or b, thus forming a vacuum diagram. In all cases, the contributions containing vacuum diagrams factorize and cancel with the expansion of the partition function $\mathcal{Z}$; see Eq. (76). Furthermore, many connected diagrams are topologically equivalent, and it is, therefore, enough to consider only the topologically inequivalent diagrams. The number of topologically equivalent diagrams cancel the combinatorial factor $2^k k!(2p)!$ in Eqs. (75) and (77) and $2^k k!(2p+1)!$ in Eq. (78). The proof of these statements goes along the same lines as the proof for only electrons, and we refer to Refs. [25,60] for more details. The resulting formulas for G, $\tilde{D}$, and φ become

$$\begin{aligned}G(a;b) = \sum_{k,p=0}^{\infty} i^{k+p}\int d1d1'\ldots dkdk' v(1;1')\ldots v(k;k')\int d\tilde{1}d\bar{1}\ldots d(\widetilde{2p})d(\overline{2p})g(\bar{1};\tilde{1}^*)\ldots g(\overline{2p};\widetilde{2p}^*)\\ \times G_{0,2k+2p+1}(a,1,1',\ldots,\bar{1},\ldots;b,1^+,1'^+,\ldots,\bar{1}^+,\ldots)D_{0,p}(\tilde{1},\ldots)\Big|_{\substack{c\\ t.i.}},\end{aligned} \tag{80}$$

$$\begin{aligned}\tilde{D}(a,b) = \sum_{k,p=0}^{\infty} i^{k+p}\int d1d1'\ldots dkdk' v(1;1')\ldots v(k;k')\int d\tilde{1}d\bar{1}\ldots d(\widetilde{2p})d(\overline{2p})g(\bar{1};\tilde{1}^*)\ldots g(\overline{2p};\widetilde{2p}^*)\\ \times G_{0,2k+2p}(1,1',\ldots,\bar{1},\ldots;1^+,1'^+,\ldots,\bar{1}^+,\ldots)D_{0,p+1}(a,b,\tilde{1},\ldots)\Big|_{\substack{c\\ t.i.}},\end{aligned} \tag{81}$$

and

$$\varphi(a) = -\sum_{k,p=0}^{\infty} i^{k+p+1} \int d1d1' \ldots dkdk' v(1;1') \ldots v(k;k') \int d\tilde{1}d\bar{1} \ldots d(\widetilde{2p+1}) d(\overline{2p+1}) g(\bar{1};\tilde{1}^*) \ldots g(\overline{2p+1};\widetilde{2p+1}^*) \times G_{0,2k+2p+1}(1,1',\ldots,\bar{1},\ldots;1^+,1'^+,\ldots,\bar{1}^+,\ldots) D_{0,p+1}(a,\tilde{1},\ldots)\Big|_{t.i.}^{c}, \tag{82}$$

where the labels "c" and "$t.i.$" indicate that, when expanding $G_{0,n}$ in determinants and $D_{0,m}$ in Hafnians, only connected and topologically inequivalent diagrams are retained. In particular, the expansion Eq. (81) for $\tilde{D}$ contains all diagrams in classes (c1) and (c2).

A. Diagrammatic expansion for G

In Fig. 2, we show a few low-order Feynman diagrams for G. The Feynman rules to convert the diagrams into a mathematical expression are

(i) number all vertices and assign an interaction $v(i;j)$ to a wiggly line connecting i and j, an e-ph coupling $g(i;j^*)$ to a square with white vertex in j and black vertex i, a GF $G_0^s(i;j^+)$ to an oriented line from j to i, and a GF $D_0(i,j)$ to a spring connecting i and j;
(ii) integrate over all internal vertices and multiply by $i^{k+p}(-)^l$, where l is the number of electronic loops, k is the number of wiggly lines, and $2p$ is the number of squares.

There are diagrams (fifth and seventh diagrams in the second row in Fig. 2) that are one-G_0^s-line reducible; i.e., they can be disconnected into two pieces by cutting an internal G_0^s line. We define the irreducible self-energy Σ as the set of all one-G_0^s-line irreducible diagrams with the external (ingoing and outgoing) G_0^s line removed. Then, G can be written as a geometric series:

$$G = G_0^s + G_0^s\Sigma G_0^s + G_0^s\Sigma G_0^s\Sigma G_0^s + \cdots = G_0^s + G_0^s\Sigma G. \tag{83}$$

Each product in this formula stand for a space-spin-time convolution. The self-energy $\Sigma = \Sigma[G_0^s, D_0, v, g]$ is an infinite sum of irreducible diagrams with G_0^s lines and D_0 lines connected through v and g.

Among the self-energy diagrams, there are some with self-energy insertions, i.e., diagrams that can be disconnected into two pieces by cutting two G_0^s lines—examples are the last three diagrams in Fig. 2. We say that a diagram is G-skeletonic if it does not contain self-energy insertions. Then, the full set of Σ diagrams is obtained by dressing the G_0^s lines of the skeleton diagrams with all possible self-energy insertions. This amounts to evaluating the skeleton diagrams with the interacting GF G instead of G_0^s [25]. Denoting by $\Sigma_{1\,\mathrm{skel}}$ the sum of only G-skeleton diagrams, we can write

$$\Sigma = \Sigma[G_0^s, D_0, v, g] = \Sigma_{1\,\mathrm{skel}}[G, D_0, v, g]. \tag{84}$$

B. Diagrammatic expansion for $\tilde{D}$

Let us now consider the one-particle phononic GF $\tilde{D}$. Expanding $G_{0,n}$ and $D_{0,m}$ in Eq. (81) according to Wick's theorem and representing every term of the expansion with a diagram, we obtain the diagrammatic expansion of $\tilde{D}$. The Feynman rules for the $\tilde{D}$ diagrams are the same as for the G diagrams. In Fig. 3, we illustrate a few low-order diagrams.

We can clearly distinguish the diagrams belonging to class (c2). These are the double-tadpole diagrams (see the second, fourth, fifth, and sixth diagrams in Fig. 3).

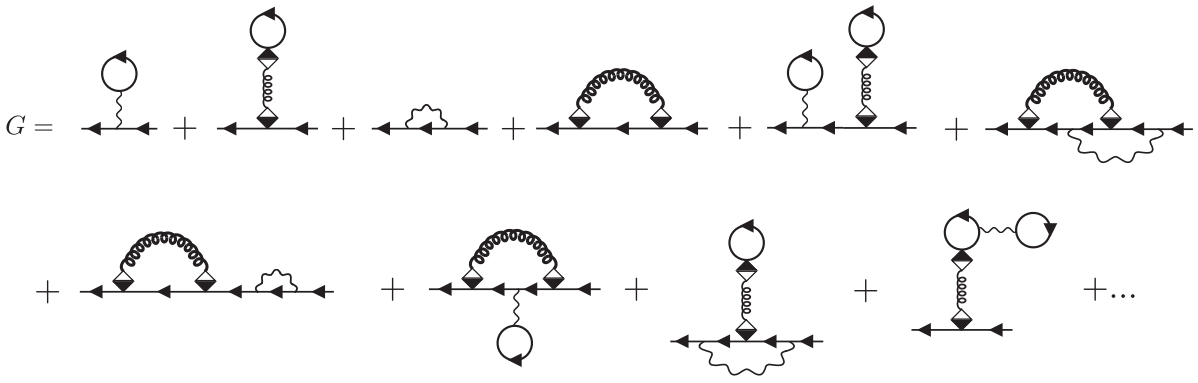


FIG. 2. Low-order diagrams in the expansion of the interacting electronic Green's function G.

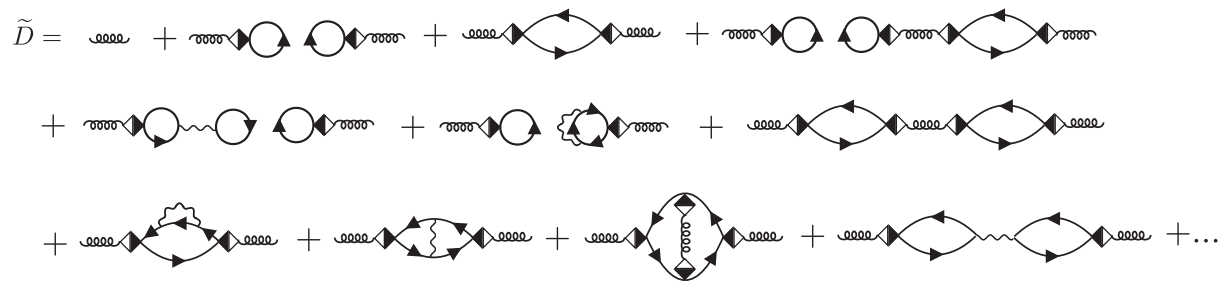


FIG. 3. Low-order diagrams in the expansion of the interacting phononic Green's function $\tilde{D}$.

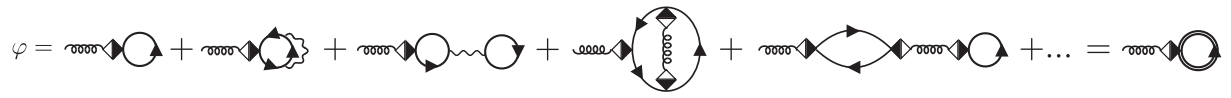


FIG. 4. Resummation of the tadpole diagrams.

The single-tadpole diagrams constitute the diagrammatic expansion of the half-particle phononic GF $\tilde{D}_{1/2} = \varphi/i^{1/2}$. In Fig. 4, we show the diagrammatic expansion of φ. The full set of diagrams can be easily summed up; see the rhs in Fig. 4, where the oriented double line denotes the interacting GF G. The Feynman rules for the φ diagrams are the same as for the G diagrams and D diagrams except that the prefactor is $i^{k+p+1}(-)^{l+1}$, where l is the number of electronic loops, k is the number of wiggly lines, and $2p+1$ is the number of squares; see Eq. (82). We, thus, have

$$\varphi(a) = -i \int d\tilde{1} d\bar{1} D_0(a,\tilde{1}) g(\bar{1};\tilde{1}^*) G(\bar{1},\bar{1}^+), \quad (85)$$

a result that could alternatively be found by direct integration of the equation of motion Eq. (46) after taking into account that the electronic density $n(1) = -iG(1;1^+)$. We can, therefore, write the expansion of $\tilde{D}$ as

$$\begin{aligned}\tilde{D}(a,b) &= \tilde{D}_{1/2}(a)\tilde{D}_{1/2}(b) \\ &\quad + [D_0 + D_0\Pi D_0 + D_0\Pi D_0\Pi D_0 + \cdots](a,b),\end{aligned} \quad (86)$$

in which the products in this formula stand for momentum-mode-component-time convolutions. The phononic self-energy $\Pi = \Pi[G_0^s, D_0, v, g]$ is the set of all diagrams that, after the removal of the ingoing and outgoing D_0 lines, cannot be cut into two pieces by cutting an internal D_0 line (one-D_0-line irreducible diagrams).

The phononic Green's function $\tilde{D}(a,b)$ does *not* fulfill a Dyson equation, but the fully connected phononic GF

$$\begin{aligned}D(a,b) &\equiv \tilde{D}(a,b) - \tilde{D}_{1/2}(a)\tilde{D}_{1/2}(b) \\ &= \tilde{D}(a,b) - \frac{1}{i}\varphi(a)\varphi(b)\end{aligned} \quad (87)$$

does. The GF $D(a,b)$ can alternatively be written in terms of the fluctuation operators $\Delta\hat{\varphi}(a) \equiv \hat{\varphi}(a) - \varphi(a) = \hat{\phi}(a) - \phi(a) = \Delta\hat{\phi}(a)$. We have

$$\begin{aligned}D(a,b) &= \frac{1}{i}\mathrm{Tr}[\hat{\rho}\mathcal{T}\{\Delta\hat{\varphi}_H(a)\Delta\hat{\varphi}_H(b)\}] \\ &= \frac{1}{i}\mathrm{Tr}[\hat{\rho}\mathcal{T}\{\Delta\hat{\phi}_H(a)\Delta\hat{\phi}_H(b)\}].\end{aligned} \quad (88)$$

The GF $D(a,b)$ fulfills a Dyson equation, since

$$\begin{aligned}D(a,b) &= [D_0 + D_0\Pi D_0 + D_0\Pi D_0\Pi D_0 + \cdots](a,b) \\ &= D_0(a,b) + (D_0\Pi D)(a,b).\end{aligned} \quad (89)$$

Like for the electronic Green's function, we can express the phononic self-energy in terms of G-skeleton diagrams. We remove all diagrams with Σ insertions inside the Π diagrams and then replace G_0^s by the full GF G, thus obtaining the functional $\Pi_{1\,\mathrm{skel}}$:

$$\Pi = \Pi[G_0^s, D_0, v, g] = \Pi_{1\,\mathrm{skel}}[G, D_0, v, g]. \quad (90)$$

The topological idea of the skeletonic expansion in G is completely general, and it can be extended to the phononic GF D and the screened Coulomb interaction W. This is done in the next section.

IX. FROM THE SKELETONIC EXPANSION IN D and W TO THE HEDIN-BAYM EQUATIONS

A. Skeletonic expansion in D

If we remove all phononic self-energy insertions inside the $\Pi_{1\,\mathrm{skel}}$ diagrams and then replace D_0 with D, we can write

$$\Pi = \Pi_{1\,\mathrm{skel}}[G, D_0, v, g] = \Pi_{2\,\mathrm{skel}}[G, D, v, g]. \quad (91)$$

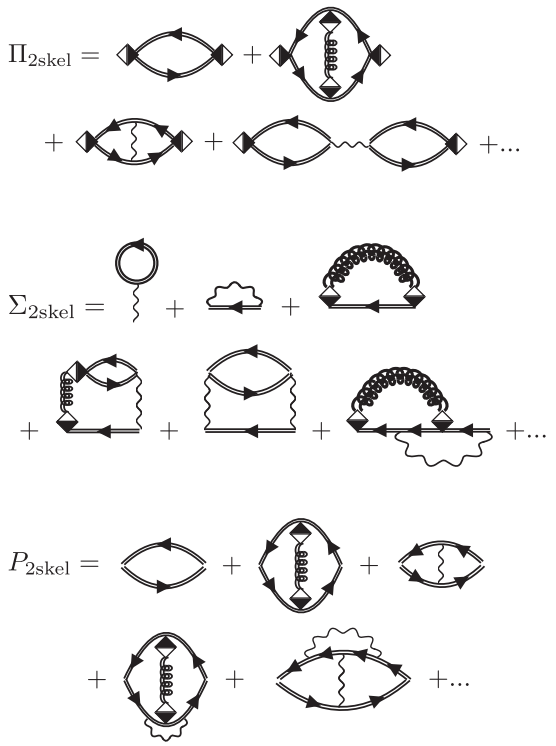


FIG. 5. Expansion of the phononic (top) and electronic (middle) self-energies and of the polarization (bottom) in G-skeleton diagrams and D-skeleton diagrams.

Here, $\Pi_{2\,\mathrm{skel}}$ contains all doubly skeletonic self-energy diagrams, i.e., all those diagrams that do not contain either Σ insertions or Π insertions. Examples of $\Pi_{2\,\mathrm{skel}}$ diagrams are shown in Fig. 5 (top), where the double spring represents D. A similar procedure can be applied to the electronic self-energy except that for Σ we must exclude the time-local diagrams. In fact, a Π insertion is here equivalent to a Σ insertion, and it would, therefore, lead to a double counting. Therefore,

$$\Sigma = \Sigma_{1\,\mathrm{skel}}[G, D_0, v, g] = \Sigma_{\mathrm{Eh}}[G, D_0, g] + \Sigma_{2\,\mathrm{skel}}[G, D, v, g], \tag{92}$$

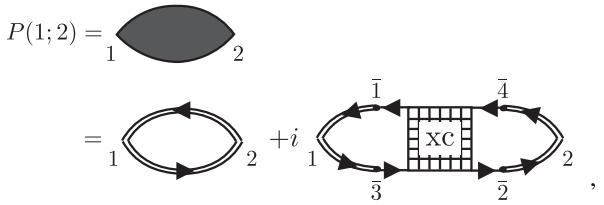
where Σ_{Eh} is the self-energy in the second diagram in Fig. 2 with $G_0^s \to G$. Using the Feynman rules,

$$\begin{aligned}\Sigma_{\mathrm{Eh}}(1;2) &= -i\delta(1;2)\int d\tilde{1}d\tilde{2}d\bar{1}g(1;\tilde{1}^*)\\ &\quad\times D_0(\tilde{1},\tilde{2})g(\bar{1};\tilde{2}^*)G(\bar{1};\bar{1}^+)\\ &= \delta(1;2)\int d\tilde{1}g(1;\tilde{1}^*)\varphi(\tilde{1}),\end{aligned} \tag{93}$$

where in the last equality we use Eq. (85). The self-energy Σ_{Eh} is known as the *Ehrenfest self-energy*. The Ehrenfest approximation consists in including the phononic feedback on the electrons through Σ_{Eh}, the electronic feedback on the phonons through the density [see Eq. (85)], and in setting $\Pi = 0$. In this approximation, the nuclei are, therefore, treated as classical particles, since they are described in terms of displacements and momenta only, i.e., the components of φ [26–36]. The importance of the Ehrenfest diagram in the description of polarons is pointed out in Refs. [31,37]. We expect that the Ehrenfest diagram is also crucial to capture the phonon-induced coherent modulation of the excitonic resonances [38]. Examples of $\Sigma_{2\,\mathrm{skel}}$ diagrams are shown in Fig. 5 (middle).

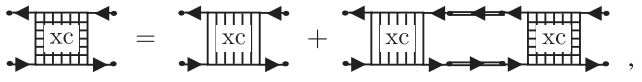
B. Skeletonic expansion in W

Like in the case of only electrons [4], we can further reduce the number of diagrams by removing all those diagrams containing a polarization insertion, which we here define as a piece that can be cut away by cutting two v lines *and at the same time* it does not break into two disjoint pieces by cutting one v line or one D line; an example is the fifth diagram in the Σ expansion in Fig. 5 (middle). The polarization diagrams are, therefore, one-v-line irreducible *and* one-D-line irreducible. To the best of our knowledge, the diagrammatic definition of the polarization P in systems of electrons and phonons is given here for the first time. In Fig. 5 (bottom), we show a few low-order diagrams for $P = P_{2\,\mathrm{skel}}[G, D, v, g]$ which are both G-skeletonic and D-skeletonic. The polarization P contains both electronic and phononic contributions. For later purposes, we also define the one-v-line irreducible, one-D-line irreducible, and two-G-lines reducible kernel $K_{\mathrm{xc}}^{(r)}$ from the polarization according to



(94)

where the dark-gray bubble represents P and the square grid represents $K_{\mathrm{xc}}^{(r)}(\bar{1},\bar{2};\bar{3},\bar{4}) = K_{\mathrm{xc}}^{(r)}(\bar{2},\bar{1};\bar{4},\bar{3})$. This is the same definition used in the case of systems of only electrons. In fact, the so-called vertex function $\Gamma = \delta - K_{\mathrm{xc}}^{(r)}GG$ relates to P through the well-known formula $P = -iGG\Gamma$ (the factor of "i" in the second diagram in Eq. (94) comes from the Feynman rules for the polarization diagrams). Following the same strategy as in Ref. [25], one can show that the kernel $K_{\mathrm{xc}}^{(r)}$ satisfies the Bethe-Salpeter equation



(95)

where the kernel $K_{\rm xc}$, represented by the square with only vertical lines, is one-v-line irreducible, one-D-line irreducible, and two-G-lines irreducible.

From the polarization diagrams, we can construct the dynamically screened interaction in the usual manner:

$W =$  (96)

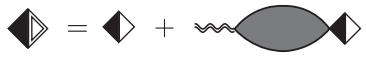
We say that a diagram is W-skeletonic if it does not contain P insertions. Then, the desired expression for Π and Σ is obtained by discarding all those diagrams which are not W-skeletonic and then replacing v with W.

C. Phononic self-energy

For the phononic self-energy, we get

$$\Pi = \Pi_{2\,\mathrm{skel}}[G, D, v, g] = \Pi_{3\,\mathrm{skel}}[G, D, W, g], \quad (97)$$

where $\Pi_{3\,\mathrm{skel}}$ is the sum of all the triply skeletonic self-energy diagrams, i.e., all those diagrams that do not contain either Σ insertions, Π insertions, or P insertions. In Fig. 6 (top), we show a few low-order diagrams of the triply skeletonic expansion for $\Pi_{3\,\mathrm{skel}}$. They are one-G-line irreducible, one-D-line irreducible, and two-W-lines irreducible; i.e., they cannot break into disjoint pieces by cutting two W lines, for otherwise they would contain a polarization insertion. We then have either diagrams connected by a single W-line or one-W-line irreducible diagrams. We can write Π in a compact form using the polarization P. We define the *dressed* (or *screened*) e-ph coupling g^d as (notice the double line in the diagrammatic representation)

$g^d =$  (98)

In terms of the dressed e-ph coupling, the phononic self-energy can be represented as

$\Pi =$  ,
$= g P g^d$, (99)

in agreement with the field-theoretic approach [8]. We see from this expression that one e-ph coupling is bare, whereas the other is dressed. As pointed out in Refs. [8,64,65], this structure has to be properly taken into account for the calculation of phonons; see also Ref. [66].

D. Electronic self-energy

For the electronic self-energy Σ, the only diagram for which we should not proceed with the replacement is the Hartree diagram [first diagram in Fig. 5 (middle)], since here every polarization insertion is equivalent to a self-energy insertion, and, hence, $v \to W$ would lead to a double counting. Therefore,

$$\begin{aligned}\Sigma &= \Sigma_{\mathrm{Eh}}[G, D_0, g] + \Sigma_{2\,\mathrm{skel}}[G, D, v, g] \\ &= \Sigma_{\mathrm{Eh}}[G, D_0, g] + \Sigma_{\mathrm{H}}[G, v] + \Sigma_{3\,\mathrm{skel}}[G, D, W, g], \quad (100)\end{aligned}$$

where Σ_{H} is the Hartree diagram. The self-energy $\Sigma_{3\,\mathrm{skel}}$ is also called the exchange-correlation (xc) self-energy.

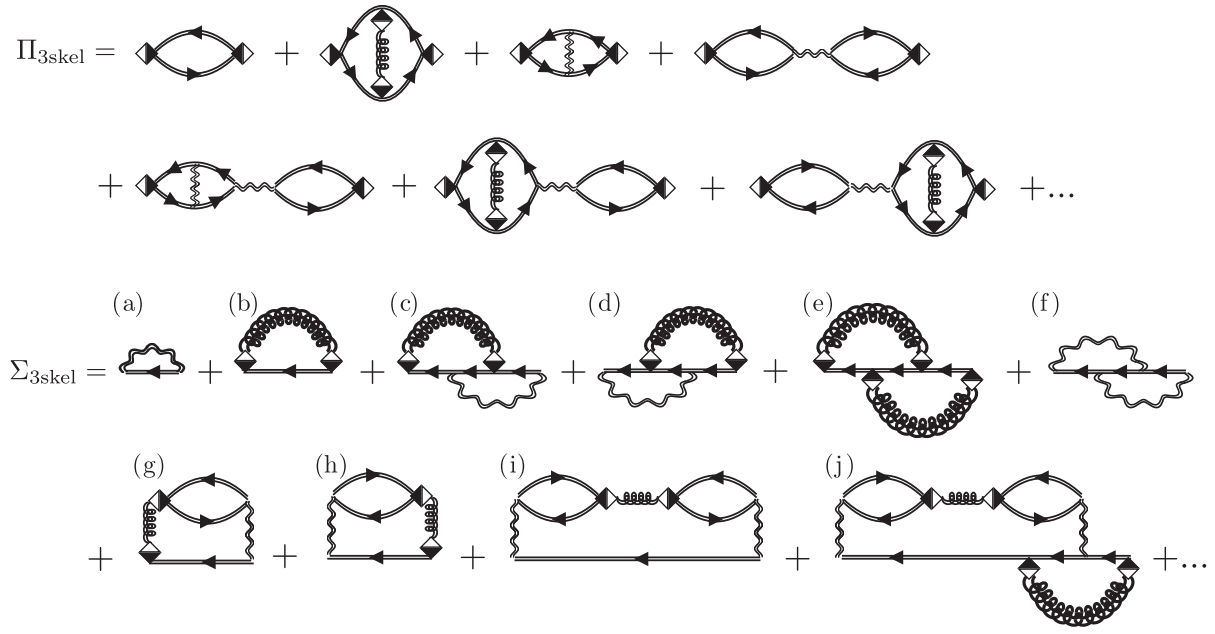


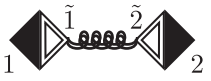
FIG. 6. Expansion of the phononic (top) and electronic (bottom) self-energy in G-skeleton diagrams, D-skeleton diagrams, and W-skeleton diagrams. To facilitate the discussion in the main text, we label the Σ diagrams.

Henceforth, we shall equivalently write $\Sigma_{3\,\mathrm{skel}}$ or Σ_{xc}. The diagrammatic expansion of the xc self-energy plays a crucial role in diagrammatic theory, since the Bethe-Salpeter kernel $K_{\mathrm{xc}}(1,2;3,4) = -\delta\Sigma_{\mathrm{xc}}(1;3)/\delta G(4;2)$; see Eq. (95). This statement can be proven along the same lines as in Ref. [25]. We illustrate in Fig. 6 (bottom) a few low-order diagrams of the triply skeletonic expansion of $\Sigma_{3\,\mathrm{skel}}$. Diagrams like the last two in the figure must be included, since by cutting the two W lines we get a piece that is neither a polarization insertion nor a Π insertion.

Like the phononic self-energy, also the electronic self-energy Σ can be written in a compact form using the polarization P or, more precisely, the kernel $K_{\mathrm{xc}}^{(r)}$. Let us consider the admissible "effective" interactions that can sprout from, e.g., the left vertex of Σ_{xc}. Keeping an eye on Fig. 6 (bottom), we realize that we can have W [see diagrams (a), (d), and (f)] and $[gDg]$ [see diagrams (b), (c), and (e)]. We can also have $WP[gDg]$ [see diagram (h)], but we cannot have WPW, since the corresponding diagram would contain a P insertion. We can further have $[gDg]PW$ [see diagram (g)], but we cannot have $[gDg]P[gDg]$, since the corresponding diagram would contain a Π insertion. We can finally have $WP[gDg]PW$ [see diagrams (i) and (j)]. All other structures are nonskeletonic: $WP[gDg]P[gDg]$ and $[gDg]PWP[gDg]$ contain a Π insertion, whereas $[gDg]PWPW$ contains a polarization insertion. We conclude that the total "effective" interaction sprouting from the left vertex is

$$\begin{aligned}\widetilde{W} &= W + gDg + WPgDg + gDgPW + WPgDgPW \\ &= W + (g + WPg)D(g + gPW) \\ &= W + g^d D g^d. \end{aligned} \tag{101}$$

To make these graphical considerations rigorous, we define the phonon-mediated e-e interaction from the dressed e-ph coupling according to

$W_{ph}(1;2) =$ 

, (102)

or in formulas

$$W_{ph}(1;2) = \int d\tilde{1}d\tilde{2}\, g^d(1;\tilde{1}^*)D(\tilde{1},\tilde{2})g^d(2;\tilde{2}^*), \tag{103}$$

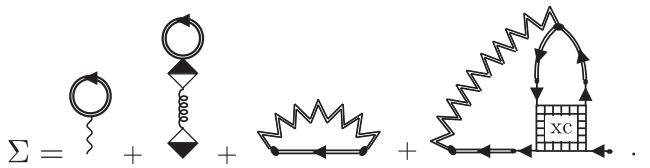
and the total screened interaction $\widetilde{W} \equiv W + W_{ph}$ according to

$\widetilde{W} =$ 
, (104)

or in formulas

$$\widetilde{W}(1;2) = W(1;2) + W_{ph}(1;2). \tag{105}$$

The total electronic self-energy can then be written as

$\Sigma =$ 

. (106)

E. Hedin-Baym equations

We summarize in Table I the fundamental equations that relate the various many-body quantities, i.e., G, D, Σ, Π, $\widetilde{W}$, W, P, g^d, and $K_{\mathrm{xc}}^{(r)}$. We here align with Ref. [8] and call the full set of equations in Table I the *Hedin-Baym equations* for electrons and phonons. The Hedin-Baym equations provide a closed system of equations for any diagrammatic approximation to the xc self-energy through the irreducible kernel $K_{\mathrm{xc}} = -\delta\Sigma_{\mathrm{xc}}/\delta G$. They are equations on the contour and can, therefore, be used to study systems in equilibrium at any temperature as well as systems driven away from equilibrium by external fields. For systems in equilibrium at zero temperature, the *adiabatic* assumption in conjunction with the assumption of a *nondegenerate ground state* allows for deforming the contour into a single branch going from $-\infty$ to $+\infty$, i.e., the real axis [25]. In this case, the contour Green's functions become the more familiar time-ordered Green's functions, and the Hedin-Baym equations reduce to those presented in Ref. [8]. We emphasize that no such shortcut is possible at finite temperature. One way to avoid the use of the L-shaped contour for equilibrium systems at finite temperature is the analytic continuation (from Matsubara to retarded to time ordered), which may, however, be rather cumbersome in the presence of singularities or branch cuts, although notable progresses have been recently made [67–69].

Like for the Hedin equations for only electrons, the Hedin-Baym equations can be iterated to obtain an expansion of Σ and Π in terms of G, W, D, and g. If we start with $K_{\mathrm{xc}}^{(r)} = 0$, and, hence,

$$P \simeq \chi^0 = -iGG, \tag{107}$$

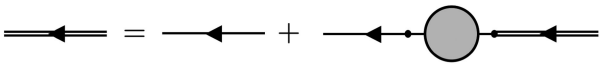
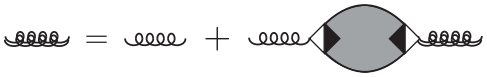
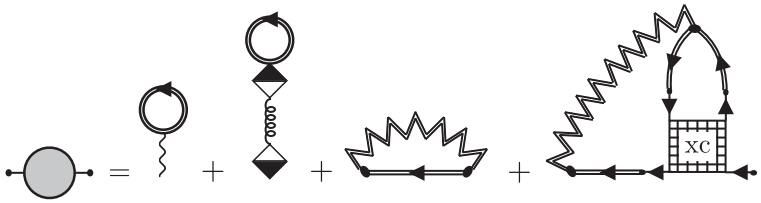
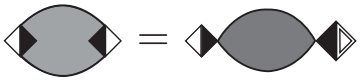
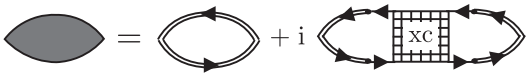
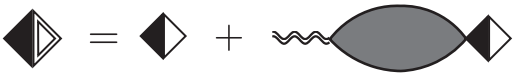
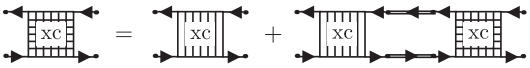
the electronic self-energy Σ is approximated by

$$\Sigma = \Sigma_{\mathrm{Eh}} + \Sigma_{\mathrm{H}} + \Sigma_{GW} + \Sigma_{\mathrm{FM}}, \tag{108}$$

where $\Sigma_{GW} = iGW$ is the well-known GW self-energy with RPA screened interaction $W = v + v\chi^0 W$ and

$$\Sigma_{\mathrm{FM}} = ig^d G D g^d \tag{109}$$

TABLE I. Mathematical expression (left column) and diagrammatic representation (right column) of the Hedin-Baym equations for systems of interacting electrons and phonons.

$G = G_0^s + G_0^s \Sigma G$	
$D = D_0 + D_0 \Pi D$	
$\Sigma = \Sigma_{\mathrm{Eh}} + \Sigma_{\mathrm{H}} + iG\widetilde{W}(\delta - GGK_{\mathrm{xc}}^{(r)})$	
$\Pi = gPg^d$	
$\widetilde{W} \equiv W + g^d D g^d$	
$W = (\delta + WP)v$	
$P = -iGG(\delta - K_{\mathrm{xc}}^{(r)} GG)$	
$g^d = (\delta + WP)g$	
$K_{\mathrm{xc}}^{(r)} = -\frac{\delta \Sigma_{\mathrm{xc}}}{\delta G}(\delta - GGK_{\mathrm{xc}}^{(r)})$	

is the so-called *Fan-Migdal self-energy* [70,71] with dressed electron-phonon coupling

$$g^d = (\delta + W\chi^0)g. \tag{110}$$

The phononic self-energy for $K_{\mathrm{xc}}^{(r)} = 0$ is simply

$$\Pi = g\chi^0 g^d = g(\chi^0 + \chi^0 W \chi^0)g. \tag{111}$$

We remark that the response function χ^0 appearing in W and Π cannot, in general, be built with a quasiparticle GF G, since both Σ_{GW} and Σ_{FM} are nonlocal in time. Although the time-local Coulomb-hole plus screened exchange version of Σ_{GW} often provides a good compromise in the trade-off between accuracy and computational cost, we are not aware of a similar time-local version of Σ_{FM}. In Sec. X, we show that the approximation in Eqs. (108) and (111) is conserving; i.e., the resulting GF satisfy all fundamental conservation laws.

Inserting an approximation for the self-energies Σ and Π into the Dyson equations $G = G_0^s + G_0^s \Sigma G$ and $D = D_0 + D_0 \Pi D$, we obtain a closed system of equations for G and D for any G_0^s and D_0. The GF D_0 depends only on the parameters of the Hamiltonian (see also Appendix A), whereas the GF G_0^s depends also on the nuclear displacements through h^s. The Hedin-Baym equations must, therefore, be coupled to Eq. (85).

The Hedin-Baym equations can alternatively be derived using the field-theoretic approach [6,8,20,65,72]. We emphasize that the field-theoretic approach prescinds from any diagrammatic notion; i.e., it does not tell us how to expand the various many-body quantities diagrammatically.

X. EQUATIONS OF MOTION FOR THE GREEN'S FUNCTIONS

An alternative route to solving the Hedin-Baym equations is the solution of the equations of motion for the GF. This second route is more convenient for systems at finite temperature or out of equilibrium. We here consider the self-energies as functionals of G and D (doubly skeletonic expansion). Using the equation of motion for D_0 [see Eq. (61)] and for G_0^s [see Eq. (65)], we can convert the Dyson equations Eqs. (83) and (89) into integro-differential equations on the contour:

$$\int d\bar{1}\vec{G}_0^{-1}(1;\bar{1})G(\bar{1};2) = \delta(1;2) + \int d\bar{1}\Sigma(1;\bar{1})G(\bar{1};2), \tag{112a}$$

$$\int d\tilde{1}\vec{D}_0^{-1}(1,\tilde{1})D(\tilde{1},2^*) = \delta(1,2) + \int d\tilde{1}\Pi(1^*,\tilde{1})D(\tilde{1},2^*). \tag{112b}$$

A. Equation of motion for G

We separate the electronic self-energy into a time-local (singular) contribution $\Sigma^\delta(1;2) \propto \delta(z_1,z_2)$ and a rest $\Sigma_c(1;2)$ which is called the *correlation self-energy*:

$$\Sigma = \Sigma^\delta + \Sigma_c. \tag{113}$$

The singular contribution is given by the sum of the Hartree-Fock (HF) self-energy $\Sigma_{HF}(1;2) = \delta(z_1,z_2)V_{HF}(\mathbf{x}_1,\mathbf{x}_2,z_1)$, with V_{HF} the spatially nonlocal HF potential, and the Ehrenfest self-energy $\Sigma_{Eh}(1;2) = \delta(1;2)\sum_{\mathbf{q}\nu} g^\dagger_{\mathbf{q}\nu}(\mathbf{r}_1,z_1)\cdot \boldsymbol{\varphi}_{\mathbf{q}\nu}(z_1)$; see Eq. (93). Then, Eq. (112a) can be rewritten as

$$\int d\bar{1}\vec{G}_{mf}^{-1}(1;\bar{1})G(\bar{1};2) = \delta(1;2) + \int d\bar{1}\Sigma_c(1;\bar{1})G(\bar{1};2), \tag{114}$$

where the mean-field operator $\vec{G}_{mf}^{-1}(1;2) \equiv \vec{G}_0^{-1}(1;2) - \Sigma^\delta(1;2)$. Taking into account the definition of $\vec{G}_0^{-1}$ in Eq. (52b) and the definition of the shifted one-particle Hamiltonian h^s in Eq. (49), one finds

$$\vec{G}_{mf}^{-1}(1;2) = \left[i\frac{d}{dz_1} - h(\boldsymbol{\nabla},\mathbf{r},z) - \sum_{\mathbf{q}\nu} g_{-\mathbf{q}\nu}(\mathbf{r},z)U_{\mathbf{q}\nu}(z)\right]\delta(1;2) - V_{HF}(\mathbf{x}_1,\mathbf{x}_2,z_1)\delta(z_1,z_2), \tag{115}$$

where we also take into account Eq. (45) and the fact that electrons are coupled to the phonons only through the displacements; see Eq. (38b).

Let us write the coordinates $\mathbf{r} = (x,y,z)$ of any point in space as the sum of the vector $\mathbf{R}^0_{\mathbf{n}}$ of the unit cell the point $\mathbf{r}$ belongs to and a displacement $\mathbf{u}$ spanning the unit cell centered at the origin, i.e., $\mathbf{r} = \mathbf{R}^0_{\mathbf{n}} + \mathbf{u}$. We introduce a generic one-electron Bloch basis, e.g., the Kohn-Sham basis, $\Psi_{\mathbf{k}\mu}(\mathbf{x} = \mathbf{r}\sigma) = e^{i\mathbf{k}\cdot\mathbf{n}}u_{\mathbf{k}\mu}(\mathbf{u}\sigma)/\sqrt{N}$, where the vector $\mathbf{k}$ takes the same values as the vector $\mathbf{q}$ defined below Eqs. (25). The wave functions $\Psi_{\mathbf{k}\mu}(\mathbf{x})$ can be thought of as the one-electron eigenfunctions in some potential, e.g., the Kohn-Sham potential, with the periodicity of our lattice; hence, the index μ can be thought of as a band index. The matrix element of any two-point correlator with the same periodicity, calculated by sandwiching with $\Psi^*_{\mathbf{k}_1\mu_1}$ and $\Psi_{\mathbf{k}_2\mu_2}$, is proportional to $\delta_{\mathbf{k}_1,\mathbf{k}_2}$; see Appendix D. If we then multiply Eq. (114) by $\Psi^*_{\mathbf{k}\mu_1}(\mathbf{x}_1)$ from the left and by $\Psi_{\mathbf{k}\mu_2}(\mathbf{x}_2)$ from the right and we integrate over $\mathbf{x}_1$ and $\mathbf{x}_2$, we find (in matrix form)

$$\left[i\frac{d}{dz_1} - h_{HF}(\mathbf{k},z_1) - \sum_\nu \tilde{g}_\nu(\mathbf{k},z_1)U_{\mathbf{0}\nu}(z_1)\right]G_{\mathbf{k}}(z_1,z_2) = \delta(z_1,z_2) + \int_\gamma d\bar{z}\Sigma_{c,\mathbf{k}}(z_1,\bar{z})G_{\mathbf{k}}(\bar{z},z_2), \tag{116}$$

where

$$h_{HF,\mu_1\mu_2}(\mathbf{k},z_1) = \int d\mathbf{x}_1 d\mathbf{x}_2 \Psi^*_{\mathbf{k}\mu_1}(\mathbf{x}_1) \times [h(\boldsymbol{\nabla}_1,\mathbf{r}_1,z_1)\delta(\mathbf{x}_1-\mathbf{x}_2) + V_{HF}(\mathbf{x}_1,\mathbf{x}_2,z_1)]\Psi_{\mathbf{k}\mu_2}(\mathbf{x}_2) \tag{117}$$

and the like for the matrix elements $G_{\mathbf{k}\mu_1\mu_2}$ and $\Sigma_{c,\mathbf{k}\mu_1\mu_2}$. The term proportional to $U_{\mathbf{0}\nu}$ in Eq. (116) originates from

$$\int d\mathbf{x}_1 \Psi^*_{\mathbf{k}\mu_1}(\mathbf{x}_1)g_{-\mathbf{q}\nu}(\mathbf{r}_1,z_1)\Psi_{\mathbf{k}\mu_2}(\mathbf{x}_1) = \delta_{\mathbf{q},\mathbf{0}}\tilde{g}_{\nu,\mu_1\mu_2}(\mathbf{k},z_1), \tag{118}$$

which implicitly defines the matrix $\tilde{g}_\nu(\mathbf{k},z_1)$. The Kronecker delta in the rhs follows from the property Eq. (24) of the e-ph coupling, which, in turn, implies [see Eq. (30)]

$$g_{-\mathbf{q}\nu}(\mathbf{r}+\mathbf{R}^0_{\mathbf{n}},z) = e^{i\mathbf{q}\cdot\mathbf{n}}g_{-\mathbf{q}\nu}(\mathbf{r},z). \tag{119}$$

Equation (116) is consistent with the fact that the only displacements activated by an external perturbation preserving the lattice periodicity are the uniform ones. Of course, this does not mean that only zero-momentum phonons are emitted or absorbed; see below.

B. Equation of motion for displacements and momenta

Writing Eq. (42) componentwise, we find

$$\frac{dP_{\mathbf{q}\nu}(z)}{dz} = -\int d\mathbf{x} g_{\mathbf{q}\nu}(\mathbf{r},z)\Delta n(\mathbf{x},z) - \sum_{\nu'} K_{\nu\nu'}(\mathbf{q},z)U_{\mathbf{q}\nu'}(z), \tag{120a}$$

$$\frac{dU_{\mathbf{q}\nu}(z)}{dz} = P_{\mathbf{q}\nu}(z), \tag{120b}$$

where $P_{\mathbf{q}\nu}$ is the average of $\hat{P}_{\mathbf{q}\nu} = \hat{\phi}^2_{\mathbf{q}\nu}$ and $U_{\mathbf{q}\nu}$ is the average of $\hat{U}_{\mathbf{q}\nu} = \hat{\phi}^1_{\mathbf{q}\nu}$. The first of these equations agrees with Eq. (22), whereas the second equation establishes that $P_{\mathbf{q}\nu}$ is the conjugate momentum of $U_{\mathbf{q}\nu}$. Alternatively, $U_{\mathbf{q}\nu}$ and $P_{\mathbf{q}\nu}$ can be calculated from $\phi^i_{\mathbf{q}\nu} = \varphi^i_{\mathbf{q}\nu} + s^i_{\mathbf{q}\nu}$ [see Eq. (45)], where $\varphi^i_{\mathbf{q}\nu}$ is given by Eq. (85). It is straightforward to find

$$U_{\mathbf{q}\nu}(z) = \sum_{\nu'} \int d\bar{\mathbf{x}} d\bar{z} D^{11}_{0,\mathbf{q}\nu\nu'}(z,\bar{z}) g_{\mathbf{q}\nu'}(\bar{\mathbf{r}}) \Delta n(\bar{\mathbf{x}},\bar{z}), \quad (121a)$$

$$P_{\mathbf{q}\nu}(z) = \sum_{\nu'} \int d\bar{\mathbf{x}} d\bar{z} D^{21}_{0,\mathbf{q}\nu\nu'}(z,\bar{z}) g_{\mathbf{q}\nu'}(\bar{\mathbf{r}}) \Delta n(\bar{\mathbf{x}},\bar{z}), \quad (121b)$$

where we take into account Eq. (62). In equilibrium, $\Delta n = 0$ and, therefore, $U_{\mathbf{q}\nu} = P_{\mathbf{q}\nu} = 0$. Under the hypothesis that the external perturbation does not break the lattice periodicity, we also have $U_{\mathbf{q}\nu}(z) = P_{\mathbf{q}\nu}(z) = 0$ for all $\mathbf{q} \neq 0$.

C. Equation of motion for *D*

We have already observed that $D_0(1,2) \propto \delta_{\mathbf{q}_1,-\mathbf{q}_2}$; see Eq. (62). Let us now investigate the mathematical structure of the phononic self-energy. Combining Eqs. (98) and (99), we can write

$$\Pi = gP(g + WPg) = g(P + PWP)g = g\chi g, \quad (122)$$

where $\chi = P + PWP = P + Pv\chi$ is the density-density response function. Spelling out the space-spin-time convolutions,

$$\begin{aligned}\Pi(1,2) &= \Pi(\mathbf{q}_1\nu_1, i_1, z_1, \mathbf{q}_2\nu_2, i_2, z_2) \\ &= \delta_{i_1,1}\delta_{i_2,1} \int d\bar{\mathbf{x}}_1 d\bar{\mathbf{x}}_2 g_{-\mathbf{q}_1\nu_1}(\bar{\mathbf{r}}_1, z_1) \chi(\bar{\mathbf{x}}_1, z_1; \bar{\mathbf{x}}_2, z_2) \\ &\quad \times g_{-\mathbf{q}_2\nu_2}(\bar{\mathbf{r}}_2, z_2). \end{aligned} \quad (123)$$

Under the hypothesis that the external perturbation does not break the lattice periodicity, χ is invariant under a simultaneous translation of its spatial coordinates by an arbitrary lattice vector $\mathbf{R}^0_{\mathbf{n}}$. Therefore,

$$\Pi(1,2) = \delta_{\mathbf{q}_1,-\mathbf{q}_2} \Pi^{i_1 i_2}_{-\mathbf{q}_1\nu_1\nu_2}(z_1, z_2). \quad (124)$$

As both $D_0(1,2)$ and $\Pi(1,2)$ are proportional to $\delta_{\mathbf{q}_1,-\mathbf{q}_2}$, the interacting phononic GF $D(1,2) = [D_0 + D_0\Pi D_0 + D_0\Pi D_0\Pi D_0 + \cdots](1,2)$ is also proportional to $\delta_{\mathbf{q}_1,-\mathbf{q}_2}$, i.e.,

$$D(1,2) = \delta_{\mathbf{q}_1,-\mathbf{q}_2} D^{i_1 i_2}_{\mathbf{q}_1\nu_1\nu_2}(z_1, z_2). \quad (125)$$

Notice that the phononic self-energy Π in the rhs in Eq. (124) is defined with a $-\mathbf{q}_1$, whereas the phononic GF D in the rhs in Eq. (125) is defined with a $+\mathbf{q}_1$. These different definitions are chosen to have a more elegant equation of motion. Indeed, if we insert these expressions into Eq. (112b), we obtain (in matrix form)

$$\begin{aligned}&\left[i\frac{d}{dz_1}\alpha - Q(\mathbf{q}, z_1)\right] D_{\mathbf{q}}(z_1, z_2) \\ &\quad = \delta(z_1, z_2) + \int_\gamma d\tilde{z} \Pi_{\mathbf{q}}(z_1, \tilde{z}) D_{\mathbf{q}}(\tilde{z}, z_2). \end{aligned} \quad (126)$$

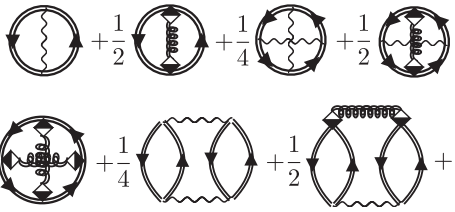
$-\Phi_{\mathrm{xc}} = \frac{1}{2}$  $+\cdots$

FIG. 7. Expansion of the Φ_{xc} functional in G-skeleton diagrams and D-skeleton diagrams.

Equations (116) and (126) and their counterparts with derivatives with respect to z_2 along with the equations of motion Eqs. (120) for the displacements and momenta form a closed system of equations for any approximate functional $\Sigma_{\mathrm{c,2\,skel}}[G, D, v, g]$ and $\Pi_{\mathrm{2\,skel}}[G, D, v, g]$.

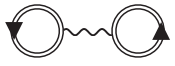
XI. CONSERVING APPROXIMATIONS

If the self-energies are Φ-derivable [39,73,74], then the GF resulting from the solution of Eqs. (116), (126), and (120) satisfy all fundamental conservation laws. To define this properly in the context of electrons and phonons, we split off the Ehrenfest-Hartree part of the self-energy like in Eq. (100). In the doubly skeletonic expansion, the remainder is the xc self-energy $\Sigma_{\mathrm{xc}}[G, D, v, g] = \Sigma_{\mathrm{3\,skel}}[G, D, W, g]$. We then construct the functional $\Phi_{\mathrm{xc}}[G, D, v, g]$ using the same rules as for a system of only electrons [25]: (i) close each skeleton diagram for Σ_{xc} with a G line, thereby producing a set of vacuum diagrams; (ii) retain only the topologically inequivalent vacuum diagrams; and (iii) multiply every diagram by the corresponding symmetry factor $1/N_{\mathrm{sym}}$, where N_{sym} is the number of equivalent G lines yielding the same self-energy diagram by their respective removal. The lowest-order diagrams of the expansion are shown in Fig. 7. The additional minus sign is due to the fact that the removal of a G line from a vacuum diagram changes the number of electronic loops by one. By construction, the Φ_{xc} functional has the property that

$$\Sigma_{\mathrm{xc}}(1;2) = \frac{\delta\Phi_{\mathrm{xc}}}{\delta G(2;1)}, \quad (127a)$$

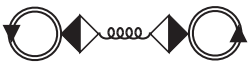
$$\Pi(1,2) = -2\frac{\delta\Phi_{\mathrm{xc}}}{\delta D(1,2)}\bigg|_S, \quad (127b)$$

where the subscript "S" refers to the symmetrized derivative $[\delta/\delta D(1,2) + \delta/\delta D(2,1)]/2$. The Hartree self-energy is obtained from the functional derivative of the Hartree functional

$-\Phi_{\mathrm{H}} = \frac{1}{2}$  , (128)

whereas the Ehrenfest self-energy is obtained from the functional derivative of the Ehrenfest functional

$$-\Phi_{\rm Eh} = \frac{1}{2}$$ (129)



Therefore, the full self-energy Σ is the functional derivative of the Φ functional defined as

$$\Phi \equiv \Phi_{\rm H}[G,v] + \Phi_{\rm Eh}[G,D_0,g] + \Phi_{\rm xc}[G,D,v,g]. \quad (130)$$

In most cases, we can deal with only approximate functionals. These are obtained by selecting an appropriate subset of Φ diagrams. We say that the self-energies are Φ-derivable whenever there exists an approximate functional Φ such that $\Sigma_{\rm xc}$ and Π can be written as in Eqs. (127). The Φ functional is invariant under gauge transformations and contour-time deformations, i.e., $z \to w(z)$ with $w(t_0) = t_0$ and $w(t_0 - i\beta) = t_0 - i\beta$, implying the fulfillment of the continuity equation and energy conservation for the GF that satisfy the equations of motion Eqs. (116) and (126) with Φ-derivable self-energies [39]. We mention here that the use of Φ-derivable self-energies evaluated at different input GF still guarantees the satisfaction of all conservation laws provided that they are convoluted with the same input GF [43]. In other words, self-consistency is *not* required for having a conserving theory.

We conclude by observing that the approximation to the self-energies discussed at the end of Sec. IX (derived by setting $K^{(r)}_{\rm xc} = 0$ in the Hedin-Baym equations) is Φ-derivable. The diagrams for $\Phi_{\rm xc}$ are those of the *GW* approximation plus a second infinite sum of ring diagrams in which one v line is replaced by (gDg); see Fig. 8.

XII. KADANOFF-BAYM EQUATIONS

Placing the arguments on different branches of the contour and using the Langreth rules [25,75], we can convert the equations of motion Eqs. (116) and (126) into a coupled system of equations for the Keldysh components of G and D. These are the *Kadanoff-Baym equations* (KBE) for systems of electrons and phonons to be solved with KMS boundary conditions. As for the case of only electrons, the equations for the Matsubara components decouple.

$$-\Phi_{\rm xc} = \frac{1}{2} + \frac{1}{4} + \frac{1}{6} + \ldots$$

$$+\frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \ldots$$

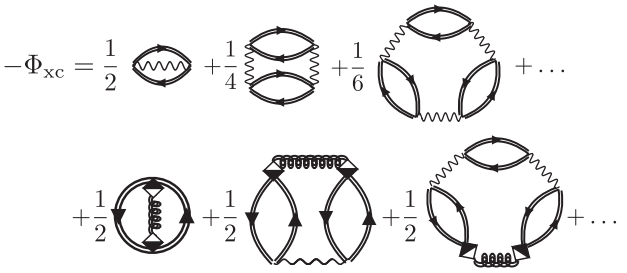


FIG. 8. Diagrams of the $\Phi_{\rm xc}$ functional leading to the self-energies Eqs. (108) and (111) through the functional derivatives in Eqs. (127).

The Matsubara GF G^M and D^M allow for calculating the initial thermal average of any one-body operator for electrons and of any quadratic operator in the displacements and momenta for the nuclei. The KBE for the GF with times on the horizontal branches [hence, the left (right) and lesser (greater) components] allow for monitoring the system evolution as well as for calculating electronic and phononic spectral functions of the system in any stationary state. As already pointed out below Eqs. (31), we can study how the system responds to different kind of external perturbations, e.g., interaction quenches, laser fields, phonon drivings, etc.

A. Self-consistent Matsubara equations

The preliminary step to solve the equations of motion for the GF consists in solving the Matsubara problem. The Matsubara self-energies do indeed depend only on the Matsubara GF [25], and, therefore, the equations for the Matsubara components are closed. The Matsubara component of any correlator $X(z_1,z_2)$ with arguments on γ is defined as $X^M(\tau_1,\tau_2) \equiv X(z_1 = t_0 - i\tau_1, z_2 = t_0 - i\tau_2)$. The KMS boundary conditions allow for expanding the Matsubara GF and self-energies according to

$$X^M(\tau_1,\tau_2) = \frac{1}{-i\beta}\sum_{m=-\infty}^{\infty} e^{-\omega_m(\tau_1-\tau_2)} X^M(\omega_m), \quad (131)$$

where the Matsubara frequencies $\omega_m = 2mi\pi/\beta$ for periodic functions like D and Π and $\omega_m = (2m+1)i\pi/\beta$ for antiperiodic functions like G and $\Sigma_{\rm c}$. Taking into account that along the vertical track $U_{\mathbf{q}\nu} = P_{\mathbf{q}\nu} = 0$ since $\Delta n = 0$ [see Eq. (121)], the equations of motion Eqs. (116) and (126) yield

$$G^M_{\mathbf{k}}(\omega_m) = \frac{1}{\omega_m - h_{\rm HF}(\mathbf{k}) - \mu - \Sigma^M_{{\rm c},\mathbf{k}}(\omega_m)}, \quad (132a)$$

$$D^M_{\mathbf{q}}(\omega_m) = \frac{1}{\omega_m \alpha - Q(\mathbf{q}) - \Pi^M_{\mathbf{q}}(\omega_m)}, \quad (132b)$$

where

$$Q(\mathbf{q}) = \begin{pmatrix} K(\mathbf{q}) & 0 \\ 0 & 1 \end{pmatrix};$$

see Eq. (38a). For any approximation to $\Sigma_{\rm c}[G,D,v,g]$ and $\Pi[G,D,v,g]$, these equations can be solved self-consistently. We recall that $K = K[n^0]$ depends on the equilibrium density

$$n^0(\mathbf{x}) = -i\sum_{\mathbf{k}\mu\mu'} \Psi_{\mathbf{k}\mu}(\mathbf{x}) G^M_{\mathbf{k}\mu\mu'}(\tau,\tau^+) \Psi^*_{\mathbf{k}\mu'}(\mathbf{x}); \quad (133)$$

see Eq. (14). Thus, the Matsubara equations are coupled even if we set $\Sigma_{\rm c} = \Pi = 0$. It is only in the partial self-consistent scheme discussed at the end of Sec. II that the

Matsubara equations with $\Sigma_c = \Pi = 0$ decouple (the elastic tensor K is not updated in this case).

1. Phononic self-energy in the clamped+static approximation

In all physical situations of relevance, setting $\Sigma_c = \Pi = 0$ is a very poor approximation. For the electronic self-energy, the *GW* approximation is a "gold standard" for obtaining accurate or at least reasonable results [76–81]. What about the phononic self-energy? Let us explore the physics of Eq. (123) when χ is calculated by summing all diagrams *without e-ph* coupling, i.e., $\chi \simeq \chi_{\text{clamp}}$. This approximation for χ corresponds to the response function of a system of only electrons interacting through the Coulomb repulsion and feeling the potential V generated by clamped nuclei in $\mathbf{R}^0$ [8]. Using the definition in Eq. (124), the Matsubara phononic self-energy in the *clamped approximation* reads

$$\Pi^{i_1 i_2,M}_{\mathbf{q}\nu_1\nu_2}(\omega_m) \simeq \delta_{i_1,1}\delta_{i_2,1}\int d\bar{\mathbf{x}}_1 d\bar{\mathbf{x}}_2 g_{\mathbf{q}\nu_1}(\bar{\mathbf{r}}_1) \times \chi^M_{\text{clamp}}(\bar{\mathbf{x}}_1,\bar{\mathbf{x}}_2;\omega_m) g_{-\mathbf{q}\nu_2}(\bar{\mathbf{r}}_2), \tag{134}$$

where we use that along the vertical track $g_{\mathbf{q}\nu}(\bar{\mathbf{r}}_1, t_0 - i\tau) = g_{\mathbf{q}\nu}(\bar{\mathbf{r}}_1)$ is independent of τ. Let us further approximate the rhs with its value at $\omega_m = 0$ [82]. This is the *static approximation,* and it is similar in spirit to the statically screened approximation of W. The response function $\chi^M(\bar{\mathbf{x}}_1,\bar{\mathbf{x}}_2;0)$ calculated at a zero frequency is identical to the retarded or advanced response function $\chi^{R/A}(\bar{\mathbf{x}}_1,\bar{\mathbf{x}}_2;0)$ also calculated at zero frequency [25]. Therefore, the phononic self-energy in the clamped + static approximation can be written as

$$\Pi^{i_1 i_2,M}_{\mathbf{q}\nu_1\nu_2}(\omega_m) \simeq \delta_{i_1,1}\delta_{i_2,1}\Pi^{\text{clamp+stat}}_{\mathbf{q}\nu_1\nu_2} \tag{135}$$

with

$$\Pi^{\text{clamp+stat}}_{\mathbf{q}\nu_1\nu_2} \equiv \int d\bar{\mathbf{x}}_1 d\bar{\mathbf{x}}_2 g_{\mathbf{q}\nu_1}(\bar{\mathbf{r}}_1)\chi^R_{\text{clamp}}(\bar{\mathbf{x}}_1,\bar{\mathbf{x}}_2;0) g_{-\mathbf{q}\nu_2}(\bar{\mathbf{r}}_2). \tag{136}$$

Inserting this approximation into Eq. (132b), we see that the effect of Π is to renormalize the (1, 1) block of Q. In other words, the interacting D in the clamped + static approximation has the same form as the noninteracting D_0 with a renormalized elastic tensor:

$$K_{\nu_1\nu_2}(\mathbf{q}) \to K^{\text{renorm}}_{\nu_1\nu_2}(\mathbf{q}) = K_{\nu_1\nu_2}(\mathbf{q}) + \Pi^{\text{clamp+stat}}_{\mathbf{q}\nu_1\nu_2}. \tag{137}$$

2. Connection with the Born-Oppenheimer approximation

If we use the BO approximation to evaluate the equilibrium nuclear positions and electronic density, then $\mathbf{R}^0 \simeq \mathbf{R}^{0,\text{BO}}$ and $n^0 \simeq n^{0,\text{BO}}$. Correspondingly, we have an approximation to the *e-ph* coupling $g \simeq g^{\text{BO}}$ and to the elastic tensor $K \simeq K^{\text{BO}}$. In the BO approximation, the renormalized elastic tensor is exactly the Hessian $\mathcal{H}$ of the BO energy calculated in $\mathbf{R}^{0,\text{BO}}$, i.e., $K^{\text{renorm}}_{\nu_1\nu_2}(\mathbf{q}) = \mathcal{H}_{\nu_1\nu_2}(\mathbf{q})$; see Ref. [8] or Appendix B. The Hessian has positive eigenvalues $\omega^2_{\mathbf{q}\nu}$, since $\mathbf{R}^{0,\text{BO}}$ is the global minimum of the BO energy. The frequencies $\omega_{\mathbf{q}\nu} \equiv \sqrt{\omega^2_{\mathbf{q}\nu}} \geq 0$ are called the *phonon frequencies,* and they provide an excellent starting point already for a clamped response function χ_{clamp} evaluated at the RPA level. Nonetheless, the importance of going beyond the static approximation (especially for metallic systems) is reported in the literature [83–85]. These considerations make it clear that, in order to extract physical phonons from the *ab initio e-ph* Hamiltonian, it is necessary to include the effects of the *e-ph* interaction at least to second order in the *e-ph* coupling.

In the basis of the normal modes of the Hessian, we have $\mathcal{H}_{\nu_1\nu_2}(\mathbf{q}) = \delta_{\nu_1\nu_2}\omega^2_{\mathbf{q}\nu_1}$. Thus, the (1, 1) block of the interacting phononic GF in the clamped + static approximation for Π is simply [see Eq. (A13)]

$$D^{11,M}_{\mathbf{q}\nu\nu'}(\omega_m) = \frac{\delta_{\nu\nu'}}{\omega_m^2 - \omega^2_{\mathbf{q}\nu}}. \tag{138}$$

As the BO phonon frequencies are all positive, we can use them to construct the phononic annihilation operators:

$$\hat{b}_{\mathbf{q}\nu} = \sqrt{\frac{\omega_{\mathbf{q}\nu}}{2}}\hat{U}_{\mathbf{q}\nu} + i\frac{\hat{P}_{\mathbf{q}\nu}}{\sqrt{2\omega_{\mathbf{q}\nu}}} \tag{139}$$

and creation operators $\hat{b}^\dagger_{\mathbf{q}\nu}$ with commutation relations $[\hat{b}_{\mathbf{q}\nu}, \hat{b}^\dagger_{\mathbf{q}'\nu'}] = \delta_{\mathbf{q},\mathbf{q}'}\delta_{\nu\nu'}$. These results have led several authors to partition the low-energy Hamiltonian in Eq. (11) in a slightly different way; see, for instance, Refs. [5,7,8,65,86]. The main difference consists in using the Hessian to define the phononic Hamiltonian

$$\begin{aligned}\hat{H}_{ph} &= \frac{1}{2}\sum_{\mathbf{q}\nu}\hat{P}^\dagger_{\mathbf{q}\nu}\hat{P}_{\mathbf{q}\nu} + \frac{1}{2}\sum_{\mathbf{q}\nu\nu'}\hat{U}^\dagger_{\mathbf{q}\nu}\mathcal{H}_{\nu\nu'}(\mathbf{q})\hat{U}_{\mathbf{q}\nu'} \\ &= \sum_{\mathbf{q}\nu}\omega_{\mathbf{q}\nu}\left(\hat{b}^\dagger_{\mathbf{q}\nu}\hat{b}_{\mathbf{q}\nu} + \frac{1}{2}\right).\end{aligned} \tag{140}$$

In such alternative partitioning, the remainder (a quadratic form in the nuclear displacements)

$$\Delta\hat{H}_{ph} \equiv \hat{H}_{0,ph} - \hat{H}_{ph} = \frac{1}{2}\sum_{\mathbf{q}\nu\nu'}\hat{U}^\dagger_{\mathbf{q}\nu}[K_{\nu\nu'}(\mathbf{q}) - \mathcal{H}_{\nu\nu'}(\mathbf{q})]\hat{U}_{\mathbf{q}\nu'} \tag{141}$$

must be treated somehow. As we show, the NEGF formalism and related diagrammatic expansions are most easily formulated with the partitioning of Eq. (36). In fact,

there is no particular convenience in rewriting the full Hamiltonian in terms of the operators $\hat{b}_{\mathbf{q}\nu}$ and $\hat{b}^\dagger_{\mathbf{q}\nu}$, since $\hat{H}_{0,ph}$ is not diagonal. There is instead a convenience in using the Hessian eigenbasis to define $\hat{U}_{\mathbf{q}\nu}$ and $\hat{P}_{\mathbf{q}\nu}$, since the interacting phononic GF in the clamped + static approximation is diagonal; see Eq. (138). In this approximation, $\hat{b}_{\mathbf{q}\nu}$ ($\hat{b}^\dagger_{\mathbf{q}\nu}$) annihilates (creates) a quantum of vibration (the phonon) characterized by a well-defined energy (the frequency $\omega_{\mathbf{q}\nu}$) and, hence, an infinitely long lifetime.

3. Conserving approximations

The clamped + static approximation is *not* a conserving approximation. Going beyond it, the concept of phonons as infinitely long-lived lattice excitations is no longer justified. Phonons become *quasiphonons* or *dressed phonons* by acquiring a finite lifetime [8]. Still, the clamped + static approximation remains an excellent starting point, often providing quantitative interpretations of Raman spectra. Accordingly, the minimal phononic self-energy which is at the same time conserving and physically sensible is $\Pi = g\chi g$ with the RPA $\chi = \chi^0 + \chi^0 v\chi$, or, equivalently, $\Pi = g\chi^0 g^d$ with $g^d = g + v\chi g = g + W\chi^0 g$ and $W = v + v\chi^0 W$. As pointed out in Sec. XI, this phononic self-energy is Φ-derivable, the xc functional being the sum of all diagrams in the second row in Fig. 8. For the theory to be conserving, the electronic self-energy must be consistently derived from the same functional Φ. Therefore, any calculation with $\Pi = g\chi g$ should be done with an electronic Fan-Migdal self-energy $\Sigma_{\rm FM} = ig^d G D g^d$. This means that χ is not the RPA response function at clamped nuclei, since the GF in $\chi^0 = -iGG$ are evaluated with the Fan-Migdal self-energy. We can add to $\Sigma_{\rm FM}$ the GW self-energy and still be conserving, since the diagrams in the first row in Fig. 8 do not contribute to Π.

B. Time-dependent evolution and steady-state solutions

With the Matsubara GF at our disposal, we can proceed with the calculation of all other Keldysh components by time propagation. The *right* component of any correlator $X(z_1, z_2)$ with arguments on γ is defined as $X^\rceil(t,\tau) \equiv X(t_\pm, t_0 - i\tau)$. The equations for the right components of G and D follow from Eqs. (116) and (126) when setting $z_1 = t_+$ or $z_1 = t_-$ and $z_2 = t_0 - i\tau$. Using the Langreth rules [25], we find

$$\left[i\frac{d}{dt} - h_{\rm HF}(\mathbf{k},t) - \sum_\nu \tilde{g}_\nu(\mathbf{k},t)U_{\mathbf{0}\nu}(t)\right] G^\rceil_{\mathbf{k}}(t,\tau) = \left[\Sigma^R_{\mathrm{c},\mathbf{k}} \cdot G^\rceil_{\mathbf{k}} + \Sigma^\rceil_{\mathrm{c},\mathbf{k}} \star G^M_{\mathbf{k}}\right](t,\tau), \tag{142a}$$

$$\left[i\frac{d}{dt}\alpha - Q(\mathbf{q},t)\right] D^\rceil_{\mathbf{q}}(t,\tau) = \left[\Pi^R_{\mathbf{q}} \cdot D^\rceil_{\mathbf{q}} + \Pi^\rceil_{\mathbf{q}} \star D^M_{\mathbf{q}}\right](t,\tau). \tag{142b}$$

Henceforth, we use the shorthand notation "$\cdot$" for time convolutions between t_0 and ∞ and "$\star$" for convolutions between 0 and β [24,25]. Similarly, the equations for the left component, defined for any correlator as $X^\lceil(\tau,t) \equiv X(t_0 - i\tau, t_\pm)$, follow when setting $z_1 = t_0 - i\tau$ and $z_2 = t_-$ or t_+ in the counterparts of the equations of motion Eqs. (116) and (126) with derivative with respect to z_2. We find

$$G^\lceil_{\mathbf{k}}(\tau,t)\left[-i\frac{\overleftarrow{d}}{dt} - h_{\rm HF}(\mathbf{k},t) - \sum_\nu \tilde{g}_\nu(\mathbf{k},t)U_{\mathbf{0}\nu}(t)\right] = \left[G^\lceil_{\mathbf{k}} \cdot \Sigma^A_{\mathrm{c},\mathbf{k}} + G^M_{\mathbf{k}} \star \Sigma^\lceil_{\mathrm{c},\mathbf{k}}\right](\tau,t), \tag{143a}$$

$$D^\lceil_{\mathbf{q}}(\tau,t)\left[-i\frac{\overleftarrow{d}}{dt}\alpha - Q(\mathbf{q},t)\right] = \left[D^\lceil_{\mathbf{q}} \cdot \Pi^A_{\mathbf{q}} + D^M_{\mathbf{q}} \star \Pi^\lceil_{\mathbf{q}}\right](\tau,t), \tag{143b}$$

where the left arrow over the derivative indicates that the derivative acts on the quantity to its left. At fixed τ, these equations are first order integro-differential equations in t which must be solved with initial conditions

$$G^\rceil_{\mathbf{k}}(t_0,\tau) = G^M_{\mathbf{k}}(0,\tau), \quad G^\lceil_{\mathbf{k}}(\tau,t_0) = G^M_{\mathbf{k}}(\tau,0), \tag{144a}$$

$$D^\rceil_{\mathbf{q}}(t_0,\tau) = D^M_{\mathbf{q}}(0,\tau), \quad D^\lceil_{\mathbf{q}}(\tau,t_0) = D^M_{\mathbf{q}}(\tau,0). \tag{144b}$$

The dependence on time in $h_{\rm HF}(\mathbf{k},t)$ and $Q(\mathbf{q},t)$ may be due to some external laser field and/or phonon driving.

The retarded and advanced as well as the left and right components of the self-energies depend not only on the left and right GF but also on the lesser and greater GF. For any correlator, the lesser component is defined as $X^<(t,t') \equiv X(t_-, t'_+)$, whereas the greater component is defined as $X^>(t,t') \equiv X(t_+, t'_-)$. The retarded and advanced components are not independent quantities, since $X^{R/A}(t,t') = \delta(t-t')X^\delta(t) \pm \theta(\pm t \mp t')[X^>(t,t') - X^<(t,t')]$, where X^δ is the weight of a possible singular part of the correlator $X(z_1,z_2)$ [for, e.g., G and D we have $G^\delta = D^\delta = 0$, while for the electronic self-energy Σ we have that Σ^δ is the sum of the HF and Ehrenfest diagrams; see Eq. (113)]. To close the set of equations, we need the equations of motion for $G^\lessgtr_{\mathbf{k}}$ and $D^\lessgtr_{\mathbf{q}}$. These are obtained by setting $z_1 = t_{1\pm}$ and $z_2 = t_{2\mp}$ in Eqs. (116) and (126) and in their counterparts with derivative with respect to z_2. We find

$$\left[i\frac{d}{dt_1} - h_{\rm HF}(\mathbf{k},t_1) - \sum_\nu \tilde{g}_\nu(\mathbf{k},t_1)U_{\mathbf{0}\nu}(t_1)\right] G^\lessgtr_{\mathbf{k}}(t_1,t_2) = \left[\Sigma^R_{\mathrm{c},\mathbf{k}} \cdot G^\lessgtr_{\mathbf{k}} + \Sigma^\lessgtr_{\mathrm{c},\mathbf{k}} \cdot G^A_{\mathbf{k}} + \Sigma^\rceil_{\mathrm{c},\mathbf{k}} \star G^\lceil_{\mathbf{k}}\right](t_1,t_2), \tag{145a}$$

$$\left[i\frac{d}{dt_1}\alpha - Q(\mathbf{q},t_1)\right] D^\lessgtr_{\mathbf{q}}(t_1,t_2) = \left[\Pi^R_{\mathbf{q}} \cdot D^\lessgtr_{\mathbf{q}} + \Pi^\lessgtr_{\mathbf{q}} \cdot D^A_{\mathbf{q}} + \Pi^\rceil_{\mathbf{q}} \star D^\lceil_{\mathbf{q}}\right](t_1,t_2), \tag{145b}$$

$$G^{\lessgtr}_{\mathbf{k}}(t_1,t_2)\left[-i\frac{\overleftarrow{d}}{dt_2}-h_{\mathrm{HF}}(\mathbf{k},t_2)-\sum_{\nu}\tilde{g}_{\nu}(\mathbf{k},t_2)U_{\mathbf{0}\nu}(t_2)\right]$$
$$=\left[G^{\lessgtr}_{\mathbf{k}}\cdot\Sigma^{A}_{\mathrm{c},\mathbf{k}}+G^{R}_{\mathbf{k}}\cdot\Sigma^{\lessgtr}_{\mathrm{c},\mathbf{k}}+G^{\rceil}_{\mathbf{k}}\star\Sigma^{\lceil}_{\mathrm{c},\mathbf{k}}\right](t_1,t_2), \quad (145c)$$

$$D^{\lessgtr}_{\mathbf{q}}(t_1,t_2)\left[-i\frac{\overleftarrow{d}}{dt_2}\alpha-Q(\mathbf{q},t_2)\right]$$
$$=\left[D^{\lessgtr}_{\mathbf{q}}\cdot\Pi^{A}_{\mathbf{q}}+D^{R}_{\mathbf{q}}\cdot\Pi^{\lessgtr}_{\mathbf{q}}+D^{\rceil}_{\mathbf{q}}\star\Pi^{\lceil}_{\mathbf{q}}\right](t_1,t_2), \quad (145d)$$

which must be solved with initial conditions

$$G^{<}_{\mathbf{k}}(t_0,t_0)=G^{M}_{\mathbf{k}}(0,0^+),\;\; G^{>}_{\mathbf{k}}(t_0,t_0)=G^{M}_{\mathbf{k}}(0^+,0), \quad (146a)$$

$$D^{<}_{\mathbf{q}}(t_0,t_0)=D^{M}_{\mathbf{q}}(0,0^+),\;\; D^{>}_{\mathbf{q}}(t_0,t_0)=D^{M}_{\mathbf{q}}(0^+,0). \quad (146b)$$

Finally, we need the equation of motion for the displacement and momentum at $\mathbf{q}=0$, since $U_{\mathbf{0}\nu}(t)$ appears explicitly in the equations for the electronic GF. These are given by Eqs. (120) when setting $z=t_{\pm}$ and read

$$\frac{dP_{\mathbf{0}\nu}(t)}{dt}=-\int d\mathbf{x}\, g_{\mathbf{0}\nu}(\mathbf{r},t)\Delta n(\mathbf{x},t)-\sum_{\nu'}K_{\nu\nu'}(\mathbf{0},t)U_{\mathbf{0}\nu'}(t), \quad (147a)$$

$$\frac{dU_{\mathbf{0}\nu}(t)}{dt}=P_{\mathbf{0}\nu}(t), \quad (147b)$$

where [compare with Eq. (133)]

$$\Delta n(\mathbf{x},t)=-i\sum_{\mathbf{k}\mu\mu'}\Psi_{\mathbf{k}\mu}(\mathbf{x})G^{<}_{\mathbf{k}\mu\mu'}(t,t)\Psi^{*}_{\mathbf{k}\mu'}(\mathbf{x})-n^{0}(\mathbf{x}). \quad (148)$$

From these equations, we see that the equilibrium density n^0 appearing in the full Hamiltonian $\hat{H}$ *must be* the same as the self-consistent density in Eq. (133), for otherwise the rhs of the equation of motion for $P_{\mathbf{0}\nu}$ does not vanish at $U_{\mathbf{0}\nu}=0$.

The set of equations Eqs. (142), (143), and (145) are the KBE for systems of electrons and phonons. The KBE, together with the initial conditions for the Keldysh components of $G_{\mathbf{k}}$ and $D_{\mathbf{q}}$, completely determine the electronic and phononic GF with one and two real times once a choice for the self-energies is made. These equations have been so far solved only in relatively simple model systems [58,60,87,88]. Under certain approximations (generalized Kadanoff-Baym ansatz [42,43], diagonal density matrices, and Markov approximation), the KBE can be shown to reduce to the well-known Boltzmann equations.

In the clamped + static approximation for $\Pi_{\mathbf{q}}$, the KBE for $D_{\mathbf{q}}$ simplify considerably, since $\Pi^{\lessgtr}_{\mathbf{q}}=\Pi^{\rceil}_{\mathbf{q}}=\Pi^{\lceil}_{\mathbf{q}}=0$ and $\Pi^{i_1i_2,R/A}_{\mathbf{q}\nu_1\nu_2}(t_1,t_2)=\delta_{i_1,1}\delta_{i_2,1}\delta(t_1-t_2)\Pi^{\mathrm{clamp+stat}}_{\mathbf{q}\nu_1\nu_2}$; see Eq. (136). We recall that in this approximation the resulting GF are not conserving, since $\Pi^{\mathrm{clamp+stat}}$ is not the functional derivative of any Φ functional. In particular, the total energy of the unperturbed system is not constant in time.

1. Steady-state solution

The KBE for the lesser and greater GF can be formally solved. This is done in Refs. [24,25] for G, where it is also shown that $\lim_{t,t'\to\infty}G^{\lessgtr}_{\mathbf{k}}(t,t')=[G^{R}_{\mathbf{k}}\cdot\Sigma^{\lessgtr}_{\mathrm{c},\mathbf{k}}\cdot G^{A}_{\mathbf{k}}](t,t')$ provided that $\Sigma_{\mathrm{c},\mathbf{k}}$ vanishes when the separation between its time arguments go to infinity. Following the same mathematical steps, one can show a similar relation for the phononic GF

$$\lim_{t,t'\to\infty}D^{\lessgtr}_{\mathbf{q}}(t,t')=[D^{R}_{\mathbf{q}}\cdot\Pi^{\lessgtr}_{\mathbf{q}}\cdot D^{A}_{\mathbf{q}}](t,t'), \quad (149)$$

which is valid provided that $\Pi_{\mathbf{q}}$ vanishes when the separation between its time arguments go to infinity. Further assuming that in the long-time limit the system attains a steady state, we can Fourier transform with respect to the time difference and find

$$D^{\lessgtr}_{\mathbf{q}}(\omega)=D^{R}_{\mathbf{q}}(\omega)\Pi^{\lessgtr}_{\mathbf{q}}(\omega)D^{A}_{\mathbf{q}}(\omega),$$

where

$$D^{R/A}_{\mathbf{q}}(\omega)=\frac{1}{(\omega\pm i\eta)\alpha-Q(\mathbf{q})-\Pi^{R/A}_{\mathbf{q}}(\omega)} \quad (150)$$

and $Q(\mathbf{q})=\lim_{t\to\infty}Q(\mathbf{q},t)$. In most physical situations, $Q(\mathbf{q},t)=Q(\mathbf{q})$ is independent of time. By construction [see Eq. (88) and Appendix C], $D^{R}_{\mathbf{q}}(\omega)=[D^{A}_{\mathbf{q}}(\omega)]^{\dagger}$ and, hence, $\Pi^{R}_{\mathbf{q}}(\omega)=[\Pi^{A}_{\mathbf{q}}(\omega)]^{\dagger}$. We can then uniquely write the retarded and advanced phononic self-energy as

$$\Pi^{R/A}_{\mathbf{q}}(\omega)=\Lambda_{ph,\mathbf{q}}(\omega)\mp\frac{i}{2}\Gamma_{ph,\mathbf{q}}(\omega), \quad (151)$$

where $\Lambda_{ph,\mathbf{q}}$ and $\Gamma_{ph,\mathbf{q}}$ are self-adjoint matrices. Accordingly, the phononic spectral function of the system at the steady state reads

$$A_{ph,\mathbf{q}}(\omega)\equiv i[D^{R}_{\mathbf{q}}(\omega)-D^{A}_{\mathbf{q}}(\omega)]=i[D^{>}_{\mathbf{q}}(\omega)-D^{<}_{\mathbf{q}}(\omega)]$$
$$=D^{R}_{\mathbf{q}}(\omega)[\Gamma_{ph,\mathbf{q}}(\omega)+2\eta\alpha]D^{A}_{\mathbf{q}}(\omega). \quad (152)$$

The phononic self-energy has only one nonvanishing block, which is the block (1, 1). If $\Gamma^{11}_{ph,\mathbf{q}}(\omega)\neq 0$, we can discard the positive infinitesimal η in Eq. (152) and find for the block (1, 1) of the spectral function

$$A^{11}_{ph,\mathbf{q}}(\omega)=D^{11,R}_{\mathbf{q}}(\omega)\Gamma^{11}_{ph,\mathbf{q}}(\omega)D^{11,A}_{\mathbf{q}}(\omega), \quad (153)$$

with

$$D^{11,R/A}_{\mathbf{q}}(\omega) = \frac{1}{(\omega \pm i\eta)^2 - K(\mathbf{q}) - \Pi^{11,R/A}_{\mathbf{q}}(\omega)}. \quad (154)$$

We observe that the retarded and advanced phononic GF differs from its more conventional form in that it is not multiplied by the BO frequency $\omega_{\mathbf{q}\nu}$; see, e.g., Refs. [8,65]. This is simply due to a different definition of the correlator where $\sqrt{\omega_{\mathbf{q}\nu}}\hat{U}_{\mathbf{q}\nu}$ is used in place of $\hat{U}_{\mathbf{q}\nu}$. We prefer to stick to our original definition, as it does not contain any notion of the BO approximation. The phononic GF in Eq. (154) is written in an arbitrary basis of normal modes; it reduces to the BO diagonal form in the basis of the BO normal modes if $\Pi^{11,R/A}_{\mathbf{q}}(\omega) \to \Pi^{\text{clam+stat}}_{\mathbf{q}}$.

Among the possible steady states, we have thermal equilibrium. In this case, we can obtain all Keldysh components from the spectral function. Indeed, the fluctuation-dissipation theorem implies that

$$D^{<}_{\mathbf{q}}(\omega) = -if(\omega)A_{ph,\mathbf{q}}(\omega), \quad (155a)$$

$$D^{>}_{\mathbf{q}}(\omega) = -i\bar{f}(\omega)A_{ph,\mathbf{q}}(\omega), \quad (155b)$$

where $f(\omega) = 1/(e^{\beta\omega} - 1)$ is the Bose function and $\bar{f}(\omega) = e^{\beta\omega}f(\omega)$. Taking into account that $\bar{f}(\omega) - f(\omega) = 1$, we also have

$$D^{R/A}_{\mathbf{q}}(\omega) = i\int \frac{d\omega'}{2\pi}\frac{D^{>}_{\mathbf{q}}(\omega') - D^{<}_{\mathbf{q}}(\omega')}{\omega - \omega' \pm i\eta} = \int \frac{d\omega'}{2\pi}\frac{A_{ph,\mathbf{q}}(\omega')}{\omega - \omega' \pm i\eta}. \quad (156)$$

2. Quasiphonons and lifetimes

From Eq. (154), we also see that any frequency-dependent phononic self-energy gives rise to a finite lifetime (Λ_{ph} and Γ_{ph} are related by a Hilbert transformation) in the same way as any approximation beyond HF for the electronic self-energy gives rise to a finite lifetime for the electrons.

We can estimate the frequency renormalization and the phononic lifetime assuming that the correction to the clamped + static Born-Oppenheimer approximation is small. Working in the basis of the normal modes of the BO Hessian, we approximate [8]

$$\Pi^{11,R/A}_{\mathbf{q}\nu\nu'}(\omega) \simeq \Pi^{\text{clam+stat}}_{\mathbf{q}\nu\nu'} + \delta_{\nu\nu'}\left(\Lambda^{\text{dyn}}_{\mathbf{q}\nu}(\omega) \mp \frac{i}{2}\Gamma^{\text{dyn}}_{\mathbf{q}\nu}(\omega)\right), \quad (157)$$

where $\Lambda^{\text{dyn}}_{\mathbf{q}\nu}(\omega)$ and $\Gamma^{\text{dyn}}_{\mathbf{q}\nu}(\omega)$ are real functions. Bearing in mind that $[K(\mathbf{q}) + \Pi^{\text{clam+stat}}_{\mathbf{q}}]_{\nu\nu'} = \delta_{\nu\nu'}\omega^2_{\mathbf{q}\nu}$ (see Sec. XII A), we see that the block (1,1) of the retarded and advanced phononic GF is diagonal in the chosen basis. To lowest order in $\Lambda^{\text{dyn}}_{\mathbf{q}\nu}$ and $\Gamma^{\text{dyn}}_{\mathbf{q}\nu}$, Eq. (154) yields

$$D^{11,R/A}_{\mathbf{q}\nu\nu}(\omega) = \frac{1}{\left(\omega \pm i\frac{\Gamma^{\text{dyn}}_{\mathbf{q}\nu}(\omega)}{4\omega}\right)^2 - \left(\omega_{\mathbf{q}\nu} + \frac{\Lambda^{\text{dyn}}_{\mathbf{q}\nu}(\omega)}{2\omega_{\mathbf{q}\nu}}\right)^2} = \frac{1}{2\left(\omega_{\mathbf{q}\nu} + \frac{\Lambda^{\text{dyn}}_{\mathbf{q}\nu}(\omega)}{2\omega_{\mathbf{q}\nu}}\right)}\left[\frac{1}{\omega - \omega_{\mathbf{q}\nu} - \frac{\Lambda^{\text{dyn}}_{\mathbf{q}\nu}(\omega)}{2\omega_{\mathbf{q}\nu}} \pm i\frac{\Gamma^{\text{dyn}}_{\mathbf{q}\nu}(\omega)}{4\omega}} - \frac{1}{\omega + \omega_{\mathbf{q}\nu} + \frac{\Lambda^{\text{dyn}}_{\mathbf{q}\nu}(\omega)}{2\omega_{\mathbf{q}\nu}} \pm i\frac{\Gamma^{\text{dyn}}_{\mathbf{q}\nu}(\omega)}{4\omega}}\right]. \quad (158)$$

Let us define the quasiphonon frequencies $\Omega^{\pm}_{\mathbf{q}\nu}$ as the solution of $\Omega^{\pm}_{\mathbf{q}\nu} = \pm\{\omega_{\mathbf{q}\nu} + [\Lambda^{\text{dyn}}_{\mathbf{q}\nu}(\Omega^{\pm}_{\mathbf{q}\nu})/2\omega_{\mathbf{q}\nu}]\}$. To first order in $\omega - \Omega^{\pm}_{\mathbf{q}\nu}$, we can then write

$$\omega \mp \left(\omega_{\mathbf{q}\nu} + \frac{\Lambda^{\text{dyn}}_{\mathbf{q}\nu}(\omega)}{2\omega_{\mathbf{q}\nu}}\right) \simeq \frac{\omega - \Omega^{\pm}_{\mathbf{q}\nu}}{Z^{\pm}_{ph,\mathbf{q}\nu}}, \quad (159)$$

where

$$Z^{\pm}_{ph,\mathbf{q}\nu} \equiv \frac{1}{\left(1 \mp \frac{1}{2\omega_{\mathbf{q}\nu}}\frac{\partial\Lambda^{\text{dyn}}_{\mathbf{q}\nu}}{\partial\omega}\right)_{\omega=\Omega^{\pm}_{\mathbf{q}\nu}}}. \quad (160)$$

The *quasiphonon weight* $Z^{\pm}_{ph,\mathbf{q}\nu}$ gives the probability that a lattice vibration with momentum $\mathbf{q}$ along the normal mode ν excites a phonon with quantum numbers $\mathbf{q}\nu$. The remaining spectral weight $(1 - Z^{\pm}_{ph,\mathbf{q}\nu})$ is absorbed by collective phononic excitations arising from correlation effects.

If the function $\Gamma^{\text{dyn}}_{\mathbf{q}\nu}(\omega)/\omega$ is small for $\omega \simeq \Omega^{\pm}_{\mathbf{q}\nu}$ and slowly varying in ω, then we can approximate it with its value in $\Omega^{\pm}_{\mathbf{q}\nu}$ for $\omega \simeq \Omega^{\pm}_{\mathbf{q}\nu}$ and rewrite Eq. (158) as

$$D^{11,R/A}_{\mathbf{q}\nu\nu}(\omega) = \frac{1}{2\lambda^{+}_{\mathbf{q}\nu}}\frac{Z^{+}_{ph,\mathbf{q}\nu}}{\omega - \Omega^{+}_{\mathbf{q}\nu} \pm i/(2\tau^{+}_{ph,\mathbf{q}\nu})} - \frac{1}{2\lambda^{-}_{\mathbf{q}\nu}}\frac{Z^{-}_{ph,\mathbf{q}\nu}}{\omega - \Omega^{-}_{\mathbf{q}\nu} \pm i/(2\tau^{-}_{ph,\mathbf{q}\nu})}, \quad (161)$$

where $\lambda^{\pm}_{\mathbf{q}\nu} = \omega_{\mathbf{q}\nu} + [\Lambda^{\mathrm{dyn}}_{\mathbf{q}\nu}(\Omega^{\pm}_{\mathbf{q}\nu})/2\omega_{\mathbf{q}\nu}]$ and

$$\tau^{\pm}_{ph,\mathbf{q}\nu} \equiv Z^{\pm}_{ph,\mathbf{q}\nu} \frac{\Gamma^{\mathrm{dyn}}_{\mathbf{q}\nu}(\Omega^{\pm}_{\mathbf{q}\nu})}{2\Omega^{\pm}_{\mathbf{q}\nu}} \tag{162}$$

is the *phononic lifetime*. This formula agrees with the expression in Refs. [8,10,57] for $Z^{\pm}_{ph,\mathbf{q}\nu} = 1$. We observe that, in general, $\Omega^{+}_{\mathbf{q}\nu} \neq -\Omega^{-}_{\mathbf{q}\nu}$, and, therefore, the energy lost from the emission of a phonon $\mathbf{q}\nu$ is not the same as the energy gained by the absorption of the same phonon. Energy is, however, conserved, since the same analysis carried for $[D^{11,R/A}_{-\mathbf{q}}(\omega)]_{\nu\nu}$ leads to

$$[D^{11,R/A}_{-\mathbf{q}}(\omega)]_{\nu\nu} = \frac{1}{2\lambda^{-}_{\mathbf{q}\nu}} \frac{Z^{-}_{ph,\mathbf{q}\nu}}{\omega + \Omega^{-}_{\mathbf{q}\nu} \pm i/(2\tau^{-}_{ph,\mathbf{q}\nu})} - \frac{1}{2\lambda^{+}_{\mathbf{q}\nu}} \frac{Z^{+}_{ph,\mathbf{q}\nu}}{\omega + \Omega^{+}_{\mathbf{q}\nu} \pm i/(2\tau^{+}_{ph,\mathbf{q}\nu})}, \tag{163}$$

where we use the property $\omega_{\mathbf{q}\nu} = \omega_{-\mathbf{q}\nu}$ and the properties $\Lambda^{\mathrm{dyn}}_{\mathbf{q}\nu}(\omega) = \Lambda^{\mathrm{dyn}}_{-\mathbf{q}\nu}(-\omega)$ and $\Gamma^{\mathrm{dyn}}_{\mathbf{q}\nu}(\omega) = -\Gamma^{\mathrm{dyn}}_{-\mathbf{q}\nu}(-\omega)$; see Appendix C for the derivation of the symmetry properties of the phononic GF and self-energy. In crystals with time-reversal symmetry, we also have $\Lambda^{\mathrm{dyn}}_{\mathbf{q}\nu}(\omega) = \Lambda^{\mathrm{dyn}}_{-\mathbf{q}\nu}(\omega)$, and, therefore, $\Lambda^{\mathrm{dyn}}_{\mathbf{q}\nu}(\omega) = \Lambda^{\mathrm{dyn}}_{\mathbf{q}\nu}(-\omega)$. In this case, $\Omega^{+}_{\mathbf{q}\nu} = -\Omega^{-}_{\mathbf{q}\nu}$ and no correlation-induced splitting occurs.

XIII. SUMMARY AND OUTLOOK

In this work, we develop the many-body theory of the electron-phonon problem. The first step is to clarify the dependence of the *ab initio e-ph* Hamiltonian on the equilibrium electronic density. Only through a self-consistent procedure is it possible to determine the *e-ph* Hamiltonian and, hence, to make fair comparisons between different many-body methods as well as between different approximations within the same method. The analysis also highlights an issue affecting those semiempirical approaches that include the *e-ph* effects through the addition of a term of the form $\sum_{\lambda} \omega_{\lambda} \hat{b}^{\dagger}_{\lambda} \hat{b}_{\lambda} + \sum_{\lambda,k} [g_{\lambda,k} \hat{O}^{k}_{e} \hat{b}^{\dagger}_{\lambda} + \mathrm{H.c.}]$, with $\hat{O}^{k}_{e}$ purely electronic operators, to the electronic Hamiltonian at clamped nuclei. Beside being devoid of a theoretical foundation, the phonon frequencies ω_{λ} may get significantly renormalized by the phononic self-energy, possibly becoming complex.

We identify in Eq. (36) the most suitable partitioning of the *ab initio e-ph* Hamiltonian and in Eq. (55) the most suitable phononic GF for the NEGF formulation. After mapping the cumbersome many-body expansion onto a diagrammatic theory, we delve into the diagrammatic content of the self-energies until reaching a closed form in terms of skeleton diagrams. We in this way provide the diagrammatic derivation of the Hedin-Baym equations for in and out-of-equilibrium systems at any temperature. The main differences with respect to case of equilibrium at zero temperature [8] is the domain of the time integration for the internal vertices and the appearance of the Ehrenfest self-energy. The merits of the diagrammatic approach are that (i) it provides a systematic way for improving many-body approximations through a proper selection of physically insightful Feynman diagrams, (ii) it naturally combines with the Φ-derivable theory to generate fully conserving GF, and (iii) it is versatile in the resummation of different diagrammatic series. The last point is especially relevant for the skeletonic expansion in terms of only G and D, which is crucial for closing the KBE. In fact, the Hedin-Baym equations are of scarce practical use to study the time-dependent evolution of the *e-ph* system. On the contrary, the KBE, being integro-differential equations, are better suited for real-time simulations. Considering the fast pace of progress in time-resolved experiments, we foresee a growing interest in this direction. The interest is also fueled by the possibility of solving the KBE using a time-linear scheme for a large number of self-energy approximations [43–49], thus making NEGF competitive with the fastest quantum methods currently available.

The NEGF formalism presented in this work is applicable to Hamiltonians that are far more general than the *e-ph* Hamiltonian. In fact, it lays the foundations to any fermion-boson field theory. One straightforward extension is to make the one-electron Hamiltonian nonlocal in space and nondiagonal in spin, i.e., $H^{s}_{0,e}(z) = \int d\mathbf{x} d\mathbf{x}' \hat{\psi}^{\dagger}(\mathbf{x}) h(\mathbf{x},\mathbf{x}',z) \hat{\psi}^{\dagger}(\mathbf{x}')$, and to consider a spin-dependent *e-e* interaction $v(\mathbf{x},\mathbf{x}')$. This allows for including the coupling with vector potentials as well as relativistic corrections like the spin-orbit interaction and, hence, to deal with magnetic systems and noncollinear spins [89]. It also makes possible to use pseudopotentials, thus eliminating the core degrees of freedom. Another extension consists in considering an *e-ph* interaction Hamiltonian like $\hat{H}_{e\text{-}ph} = \sum_{\mathbf{q}\nu,i} \int d\mathbf{x} d\mathbf{x}' g^{i}_{-\mathbf{q}\nu}(\mathbf{x},\mathbf{x}') \hat{\psi}^{\dagger}(\mathbf{x}) \hat{\psi}(\mathbf{x}') \hat{\phi}^{i}_{\mathbf{q}\nu}$. In fact, the only property required by our derivation is $g^{i}_{-\mathbf{q}\nu}(\mathbf{x},\mathbf{x}') = g^{i*}_{\mathbf{q}\nu}(\mathbf{x}',\mathbf{x})$, which is clearly satisfied by the *e-ph* coupling; see Eq. (30). The spatial nonlocality of g allows for coupling bosonic particles like photons to nonlocal electronic operators like the current, thereby providing a quantum treatment of the light-matter interaction. We can also study exotic couplings between electrons and the bosonic momentum, since we do not need to assume that $g^{i}_{-\mathbf{q}\nu} = 0$ for $i = 2$. A further extension concerns $H^{s}_{0,ph}$, as the only properties required by our derivation are $Q(\mathbf{q}) = Q^{\dagger}(\mathbf{q}) = Q^{*}(-\mathbf{q})$. Thus, the formalism can deal with Hamiltonians containing terms proportional to $\hat{P}^{\dagger}_{\mathbf{q}\nu} \hat{U}_{\mathbf{q}\nu}$ and $\hat{U}^{\dagger}_{\mathbf{q}\nu} \hat{P}_{\mathbf{q}\nu}$. If the bosonic particles are photons, these terms arise in the effective Hamiltonian for squeezed light [90]. We finally observe that all these

extensions widen the class of external drivings to those that break the crystal periodicity.

Coming back to the *e-ph* Hamiltonian, the theory presented in this work indicates the route for the treatment of anharmonic effects [91,92]. To third order in the fluctuation operators, we must add to the Hamiltonian in Eq. (36) the Debye-Waller interaction, which is proportional to $\hat{U}^2\Delta\hat{n}$, and the next-to-quadratic term in the expansion of $E_{n\text{-}n}$, which is proportional to $\hat{U}^3$. These two extra pieces in the Hamiltonian can be treated in precisely the same manner as we treat $\hat{H}_{e\text{-}e}$ and $\hat{H}_{e\text{-}ph}$ in Sec. VII. The diagrammatic theory is enriched by two more couplings, the Debye-Waller one connecting two G lines to two D lines and the one stemming from the cubic displacement connecting three D lines. The systematic analysis of the resulting diagrammatic expansion is a topic for future research. Another topic for future research is the generalization of the NEGF formalism for superconductors. Starting as always from the Hamiltonian Eq. (36), we here outline the steps for this achievement: (i) add to $\hat{H}$ an infinitesimally small term breaking the $U(1)$ gauge symmetry, e.g., $\int d\mathbf{x}d\mathbf{x}'\Delta(\mathbf{x},\mathbf{x}')\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')+\text{H.c.}$; (ii) derive the noninteracting Martin-Schwinger hierarchy for the many-particle GF containing n annihilation operators and m creation operators with $n \neq m$; (iii) establish the Wick theorem as the solution of the generalized noninteracting Martin-Schwinger hierarchy; and (iv) expand the GF with $n+m=1$ (this is the so-called Nambu GF) as outlined in Sec. VII.

We conclude with our perspective on the combination of the NEGF formalism with DFT, which we intentionally leave aside in this work as it is not necessary in developing the theory. Zero-temperature [93,94] or finite-temperature [95] DFT as well as density functional perturbation theory (DFPT) [96–100] provide an invaluable capacity to obtain the *ab initio* parameters of the Hamiltonian [101–107]. Through DFT and DFPT, one can minimize the total energy with respect to the nuclear positions and find an approximation for $\mathbf{R}^0$ and, hence, for the electronic potential V and coupling g through Eqs. (10a) and (10b). In the partial self-consistent scheme for the determination of the *e-ph* Hamiltonian (see the end of Sec. II), the equilibrium DFT density can also be used to calculate the elastic tensor K. However, the DFT density cannot be used in the term containing $\Delta\hat{n}$ [see Eq. (21) and following discussion], for otherwise the nuclei would start drifting away from $\mathbf{R}^0$. DFPT can also be used to approximate the dressed *e-ph* coupling, necessary for the calculation of the phononic self-energy and phonon-induced *e-e* interaction; see Table I. In fact, $g^d=(\delta+WP)g=(\delta+v\chi)g$. However, DFPT provides g^d in the clamped + static approximation which we have already observed to be nonconserving. One may think to restore the conserving properties by resorting to time-dependent (TD) DFT [108–111], which gives us access to the full frequency dependence of the clamped response function. This is unfortunately not so. The problem lies in the fact that from the TDDFT expression $\chi=\chi_0+\chi_0(v+f_{\text{xc}})\chi$, with f_{xc} the xc kernel, it is not obvious to trace the Φ-functional fulfilling $\chi=-2\delta\Phi_{\text{xc}}/\delta v$ [25]. One possibility would be to construct the kernel from the conserving linearized Sham-Schlüter equation [112] as discussed in Ref. [113]. However, the linearized Sham-Schlüter equation is itself an approximate equation; hence, the resulting theory will never be exact. We finally remark that if one is interested only in spectral properties, then the use of nonconserving approximations is much less critical. In this case, the fundamental requirement is to use positive-semidefinite (PSD) self-energies [114,115]. PSD approximations can be evaluated with the dressed DFPT *e-ph* coupling by simply paying attention to the double-counting problem.

We hope that our contribution to the *e-ph* problem will stimulate further research at a fundamental level, help in the development of accurate approximation schemes, and have implications in the implementation of computer programs to face the challenges posed by new materials and time-resolved experiments.

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APPENDIX A: NONINTERACTING GREEN'S FUNCTIONS

The GF G_0^s and D_0 are the building blocks of the diagrammatic expansions. In Refs. [24,25], we derive the explicit form of $G_0^s(z,z')$ with arguments $z,z'\in\gamma$ and then extract all its Keldysh components. In this appendix, we proceed along the lines outlined in Ref. [58] and derive the explicit form of $D_0(z,z')$ with arguments on the contour γ. We further extract all Keldysh components of $D_0(z,z')$ by choosing z and z' on the different branches of γ.

The phononic GF D_0 satisfies Eq. (43). *Mutatis mutandis*, we can derive the equation of motion with derivative with respect to z' (in matrix form):

$$D_{0,\mathbf{q}}(z,z')\left[-i\frac{\overleftarrow{d}}{dz'}\alpha-Q(\mathbf{q},z')\right]=\mathbb{1}\delta(z,z'), \tag{A1}$$

where $\mathbb{1}^{ii'}_{\nu,\nu'}=\delta_{\nu\nu'}\delta_{ii'}$. According to the definition in Eq. (33) and the result in Eq. (88), the matrix elements of D_0 are correlators between fluctuation operators of displacements and momenta. Taking into account Eq. (62), we have, for instance,

$$D^{11}_{0,\mathbf{q}\nu\nu'}(z,z')=\frac{1}{i}\frac{1}{\mathcal{Z}^s_{0,ph}}\langle\mathcal{T}\{\Delta\hat{U}_{\mathbf{q}\nu}(z)\Delta\hat{U}_{-\mathbf{q}\nu'}(z')\}\rangle^s_{0,ph}, \tag{A2}$$

where the independent average $\langle\cdots\rangle^{s}_{0,ph}$ is defined below Eq. (73). We define the nonunitary matrices $W_{L\mathbf{q}}$ and $W_{R\mathbf{q}}$ as the solution of

$$i\frac{d}{dz}W_{L\mathbf{q}}(z) = Q(\mathbf{q},z)\alpha W_{L\mathbf{q}}(z), \tag{A3a}$$

$$-i\frac{d}{dz}W_{R\mathbf{q}}(z) = W_{R\mathbf{q}}(z)Q(\mathbf{q},z)\alpha, \tag{A3b}$$

with boundary conditions $W_{L\mathbf{q}}(t_{0-}) = W_{R\mathbf{q}}(t_{0-}) = \mathbb{1}$. The explicit expression for these matrices is given in terms of the contour-ordering and anti-contour-ordering operators

$$W_{L\mathbf{q}}(z) = \mathcal{T}\left\{e^{-i\int_{t_{0-}}^{z} d\bar{z}Q(\mathbf{q},\bar{z})\alpha}\right\}, \tag{A4a}$$

$$W_{R\mathbf{q}}(z) = \bar{\mathcal{T}}\left\{e^{i\int_{t_{0-}}^{z} d\bar{z}Q(\mathbf{q},\bar{z})\alpha}\right\}, \tag{A4b}$$

from which it follows that $W_{L\mathbf{q}}(z)W_{R\mathbf{q}}(z) = W_{R\mathbf{q}}(z)W_{L\mathbf{q}}(z) = \mathbb{1}$. We look for solutions of the form

$$D_{0,\mathbf{q}}(z,z') = -i\alpha W_{L\mathbf{q}}(z)F_{\mathbf{q}}(z,z')W_{R\mathbf{q}}(z'). \tag{A5}$$

Inserting this expression into Eqs. (43) and (A1), we obtain a couple of equations for the unknown matrix function $F_{\mathbf{q}}$:

$$\frac{d}{dz}F_{\mathbf{q}}(z,z') = -\frac{d}{dz'}F_{\mathbf{q}}(z,z') = \mathbb{1}\delta(z,z'), \tag{A6}$$

which is solved by $F_{\mathbf{q}}(z,z') = \theta(z,z')F^{>}_{\mathbf{q}} + \theta(z',z)F^{<}_{\mathbf{q}}$, with

$$F^{>}_{\mathbf{q}} - F^{<}_{\mathbf{q}} = \mathbb{1}. \tag{A7}$$

Imposing the KMS relations $D_{0,\mathbf{q}}(t_{0-},z') = D_{0,\mathbf{q}}(t_0 - i\beta,z')$, we find

$$F^{<}_{\mathbf{q}} = W_{L\mathbf{q}}(t_0 - i\beta)F^{>}_{\mathbf{q}} = e^{-\beta Q(\mathbf{q})\alpha}F^{>}_{\mathbf{q}}, \tag{A8}$$

where $Q(\mathbf{q}) = Q(\mathbf{q}, t_0 - i\tau)$ is independent of τ. Equations (A7) and (A8) can be solved for $F^{<}_{\mathbf{q}}$ and $F^{>}_{\mathbf{q}}$, and the final expression for the phononic GF reads

$$\begin{aligned} D_{0,\mathbf{q}}(z,z') = -i\alpha W_{L\mathbf{q}}(z)[&\theta(z,z')\bar{f}(Q(\mathbf{q})\alpha) \\ &+ \theta(z',z)f(Q(\mathbf{q})\alpha)]W_{R\mathbf{q}}(z'), \end{aligned} \tag{A9}$$

where $f(\omega) = 1/(e^{\beta\omega} - 1)$ is the Bose function and $\bar{f}(\omega) = e^{\beta\omega}f(\omega)$. Having the GF on the contour, we can now extract all its Keldysh components.

1. Matsubara component

The Matsubara component $D^{M}_{0,\mathbf{q}}(\tau,\tau')$ is obtained by setting $z = t_0 - i\tau$ and $z' = t_0 - i\tau'$ in Eq. (A9). Alternatively, we can set $z = t_0 - i\tau$ and $z' = t_0 - i\tau'$ in one of the equations of motion and then solve for $D^{M}_{0,\mathbf{q}}$. Choosing the equation of motion Eq. (43), we have

$$\left[-\frac{d}{d\tau}\alpha - Q(\mathbf{q})\right]D^{M}_{0,\mathbf{q}}(\tau,\tau') = \mathbb{1}i\delta(\tau,\tau'). \tag{A10}$$

Expanding the Matsubara GF and the Dirac-delta function in bosonic Matsubara frequencies [see Eq. (131)], we find an algebraic equation for the coefficients of the expansion:

$$[\omega_m\alpha - Q(\mathbf{q})]D^{M}_{0,\mathbf{q}}(\omega_m) = \mathbb{1}. \tag{A11}$$

Taking into account the explicit form of the matrices α and $Q(\mathbf{q})$, Eq. (A11) is converted into a set of algebraic equations for the four blocks of the matrix $D^{M}_{0,\mathbf{q}}$:

$$\begin{aligned} &\begin{pmatrix} -K(\mathbf{q}) & i\omega_m\mathbb{1} \\ -i\omega_m\mathbb{1} & -\mathbb{1} \end{pmatrix} \begin{pmatrix} D^{11,M}_{0,\mathbf{q}}(\omega_m) & D^{12,M}_{0,\mathbf{q}}(\omega_m) \\ D^{21,M}_{0,\mathbf{q}}(\omega_m) & D^{22,M}_{0,\mathbf{q}}(\omega_m) \end{pmatrix} \\ &\quad = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix}. \end{aligned} \tag{A12}$$

In this formula, each of the entries of the 2×2 matrices is itself a matrix with indices ν,ν'. The (1,1) block corresponding to the displacement-displacement correlator in Eq. (A2) reads

$$D^{11,M}_{0,\mathbf{q}}(\omega_m) = \frac{1}{\omega_m^2 - K(\mathbf{q})}. \tag{A13}$$

If we choose to work in the basis of the normal modes of K, then $K_{\nu\nu'}(\mathbf{q}) = \delta_{\nu\nu'}\omega^2_{0\mathbf{q}\nu}$ and the displacement-displacement correlator simplifies to

$$D^{11,M}_{0,\mathbf{q}\nu\nu'}(\omega_m) = \frac{\delta_{\nu\nu'}}{\omega_m^2 - \omega^2_{0\mathbf{q}\nu}}. \tag{A14}$$

As already emphasized in Sec. II, the eigenvalues $\omega^2_{0\mathbf{q}\nu}$ are not physical and can even be negative. Therefore, there is no particular convenience to work in the basis of the normal modes of K.

2. Lesser and greater components

The lesser (greater) component is obtained by setting $z = t_-$ ($z = t_+$) and $z' = t'_+$ ($z' = t'_-$) in Eq. (A9). For times on the horizontal branches of the contour, the matrices $W_{L\mathbf{q}}$

and $W_{R\mathbf{q}}$ are independent of the branch, i.e., $W_{L\mathbf{q}}(t_\pm) = W_{L\mathbf{q}}(t)$ and $W_{R\mathbf{q}}(t_\pm) = W_{R\mathbf{q}}(t)$ with

$$W_{L\mathbf{q}}(t) = T\left\{e^{-i\int_{t_0}^{t} d\bar{t} Q(\mathbf{q},\bar{t})\alpha}\right\}, \tag{A15a}$$

$$W_{R\mathbf{q}}(t) = \bar{T}\left\{e^{i\int_{t_0}^{t} d\bar{t} Q(\mathbf{q},\bar{t})\alpha}\right\}, \tag{A15b}$$

and T and $\bar{T}$ the time-ordering and anti-time-ordering operators, respectively. We then have

$$D^{<}_{0,\mathbf{q}}(t,t') = -i\alpha W_{L\mathbf{q}}(t) f(Q(\mathbf{q})\alpha) W_{R\mathbf{q}}(t'), \tag{A16a}$$

$$D^{>}_{0,\mathbf{q}}(t,t') = -i\alpha W_{L\mathbf{q}}(t) \bar{f}(Q(\mathbf{q})\alpha) W_{R\mathbf{q}}(t'). \tag{A16b}$$

The greater component is obtained from the lesser component by replacing $f \to \bar{f}$. In the following, we then consider only $D^{<}_{0,\mathbf{q}}$.

Let us discuss the special, yet most common, case of $Q(\mathbf{q},t) = Q(\mathbf{q})$ independent of time (no phonon driving). Then $W_{L\mathbf{q}}(t) = \exp[-iQ(\mathbf{q})\alpha(t-t_0)]$ and $W_{R\mathbf{q}}(t) = \exp[iQ(\mathbf{q})\alpha(t-t_0)]$ commute with the Bose function, and the lesser component simplifies to

$$D^{<}_{0,\mathbf{q}}(t,t') = -i\alpha f(Q(\mathbf{q})\alpha) e^{-iQ(\mathbf{q})\alpha(t-t')}. \tag{A17}$$

As this function depends only on the time difference, it can be Fourier transformed with respect to $t-t'$. In frequency space, the lesser GF reads

$$\begin{aligned} D^{<}_{0,\mathbf{q}}(\omega) &= -2\pi\alpha f(Q(\mathbf{q})\alpha)\delta(\omega - Q(\mathbf{q})\alpha) \\ &= -2\pi\alpha f(\omega)\delta(\omega - Q(\mathbf{q})\alpha). \end{aligned} \tag{A18}$$

We can easily work out the four blocks of $D^{<}_{0,\mathbf{q}}(\omega)$ using the Cauchy relation

$$\begin{aligned} &-2\pi\delta(\omega - Q(\mathbf{q})\alpha) \\ &= \left[\frac{1}{\omega - Q(\mathbf{q})\alpha + i\eta} - \frac{1}{\omega - Q(\mathbf{q})\alpha - i\eta}\right] \\ &= \alpha\left[\frac{1}{(\omega + i\eta)\alpha - Q(\mathbf{q})} - \frac{1}{(\omega - i\eta)\alpha - Q(\mathbf{q})}\right]. \end{aligned} \tag{A19}$$

In the last equality, we use that $\alpha^{-1} = \alpha$ and, hence, $\alpha A^{-1} = \alpha^{-1}A^{-1} = (A\alpha)^{-1}$ for any matrix A. The fraction with $(\omega \pm i\eta)$ is the same as $D^{M}_{0,\mathbf{q}}(\omega_m)$ calculated in $\omega_m = \omega \pm i\eta$; compare with Eq. (A11). Therefore, the (1, 1) block of $D^{<}_{0,\mathbf{q}}(\omega)$ can be read off from Eq. (A13):

$$D^{11,<}_{0,\mathbf{q}}(\omega) = f(\omega)\left[\frac{1}{(\omega + i\eta)^2 - K(\mathbf{q})} - \frac{1}{(\omega - i\eta)^2 - K(\mathbf{q})}\right]. \tag{A20}$$

Using the same strategy, one can work out the explicit form of the remaining three blocks. The greater component has the same form as the lesser component with $f(\omega) \to \bar{f}(\omega)$.

3. Retarded and advanced components

The retarded and advanced components can be calculated from the lesser and greater components. We have

$$\begin{aligned} D^{R}_{0,\mathbf{q}}(t,t') &= \theta(t-t')[D^{>}_{0,\mathbf{q}}(t,t') - D^{<}_{0,\mathbf{q}}(t,t')] \\ &= -i\theta(t-t')\alpha W_{L\mathbf{q}}(t) W_{R\mathbf{q}}(t'), \end{aligned} \tag{A21}$$

and similarly

$$D^{A}_{0,\mathbf{q}}(t,t') = i\theta(t'-t)\alpha W_{L\mathbf{q}}(t) W_{R\mathbf{q}}(t'), \tag{A22}$$

from which it follows that we can write the lesser and greater components in Eq. (A16) as

$$D^{\lessgtr}_{0,\mathbf{q}}(t,t') = D^{R}_{0,\mathbf{q}}(t,t_0)\alpha D^{\lessgtr}_{0,\mathbf{q}}(t_0,t_0)\alpha D^{A}_{0,\mathbf{q}}(t_0,t'). \tag{A23}$$

This result is at the basis of the recently proposed generalized Kadanoff-Baym ansatz for bosons [43]. In fact, Eq. (A23) can equivalently be written as

$$D^{\lessgtr}_{0,\mathbf{q}}(t,t') = iD^{R}_{0,\mathbf{q}}(t,t')\alpha D^{\lessgtr}_{0,\mathbf{q}}(t',t') - iD^{\lessgtr}_{0,\mathbf{q}}(t,t)\alpha D^{A}_{0,\mathbf{q}}(t,t'). \tag{A24}$$

In the special case $Q(\mathbf{q},t) = Q(\mathbf{q})$, the retarded and advanced components depend only on the time difference, and they can be Fourier transformed. In Fourier space, we have

$$D^{R/A}_{0,\mathbf{q}}(\omega) = \frac{1}{(\omega \pm i\eta)\alpha - Q(\mathbf{q})} = D^{M}_{0,\mathbf{q}}(\omega \pm i\eta). \tag{A25}$$

The (1, 1) block can be read off from Eq. (A13):

$$D^{11,R/A}_{0,\mathbf{q}}(\omega) = \frac{1}{(\omega \pm i\eta)^2 - K(\mathbf{q})}.$$

We close the appendix by observing that from Eqs. (A18) and (A25) follows the fluctuation-dissipation theorem

$$D^{<}_{0,\mathbf{q}}(\omega) = f(\omega)[D^{R}_{0,\mathbf{q}}(\omega) - D^{A}_{0,\mathbf{q}}(\omega)]$$

and the like for the greater component.

APPENDIX B: BORN-OPPENHEIMER APPROXIMATION

The BO Hamiltonian is given by Eq. (1) in the limit of infinite nuclear masses, and it is, therefore, independent of the nuclear momenta:

$$\hat{H}^{\mathrm{BO}}(\hat{\mathbf{R}}) \equiv \lim_{\{M_i\}\to\infty} \hat{H}\,. \tag{B1}$$

The BO Hamiltonian commutes with all the nuclear position operators $\hat{\mathbf{R}}_i$. Therefore, the eigenkets of $\hat{H}^{\mathrm{BO}}(\hat{\mathbf{R}})$ have the form $|\Psi(\mathbf{R})\rangle|\mathbf{R}_1\ldots\mathbf{R}_{N_n}\rangle$, where the electronic ket $|\Psi(\mathbf{R})\rangle \in \mathbb{F}$ is an eigenket of $\hat{H}^{\mathrm{BO}}(\mathbf{R})$ and $|\mathbf{R}_1\ldots\mathbf{R}_{N_n}\rangle \in \mathbb{D}_{N_n}$ is a ket describing N_n distinguishable nuclei in positions $\mathbf{R} = (\mathbf{R}_1, \ldots, \mathbf{R}_{N_n})$.

Let $|\Psi^{\mathrm{BO}}(\mathbf{R})\rangle$ be the ground state of $\hat{H}^{\mathrm{BO}}(\mathbf{R})$ with ground-state energy $E^{\mathrm{BO}}(\mathbf{R})$. An approximation for the equilibrium positions of the nuclei and for the equilibrium electronic density is found by minimizing $E^{\mathrm{BO}}(\mathbf{R})$ over all $\mathbf{R}$. Using the Hellmann-Feynman theorem,

$$\begin{aligned}\frac{\partial E^{\mathrm{BO}}(\mathbf{R})}{\partial R_{i,\alpha}} &= \langle\Psi^{\mathrm{BO}}(\mathbf{R})|\frac{\partial \hat{H}^{\mathrm{BO}}(\mathbf{R})}{\partial R_{i,\alpha}}|\Psi^{\mathrm{BO}}(\mathbf{R})\rangle \\ &= \int d\mathbf{x} n^{\mathrm{BO}}(\mathbf{x},\mathbf{R})\frac{\partial V(\mathbf{r},\mathbf{R})}{\partial R_{i,\alpha}} + \frac{\partial E_{n\text{-}n}(\mathbf{R})}{\partial R_{i,\alpha}},\end{aligned} \tag{B2}$$

where we define the BO density

$$n^{\mathrm{BO}}(\mathbf{x},\mathbf{R}) \equiv \langle\Psi^{\mathrm{BO}}(\mathbf{R})|\hat{n}(\mathbf{x})|\langle\Psi^{\mathrm{BO}}(\mathbf{R})\rangle. \tag{B3}$$

Let $\mathbf{R}^{0,\mathrm{BO}}$ be the solution of $\partial E^{\mathrm{BO}}(\mathbf{R})/\partial R_{i,\alpha} = 0$ for all i and α. The BO approximation consists in approximating $\mathbf{R}^0 \simeq \mathbf{R}^{0,\mathrm{BO}}$ and $n^0(\mathbf{x}) \simeq n^{0,\mathrm{BO}}(\mathbf{x}) \equiv n^{\mathrm{BO}}(\mathbf{x},\mathbf{R}^{0,\mathrm{BO}})$. The approximated nuclear positions and density can then be used to obtain an approximation for $V \simeq V^{\mathrm{BO}}$, $g \simeq g^{\mathrm{BO}}$, and $K \simeq K^{\mathrm{BO}}$.

1. On the stability of the BO approximation

As already pointed out in Sec. II, the equilibrium density n^0 enters the low-energy Hamiltonian through *K as well as* $\Delta\hat{n}$. The replacement $n^0 \simeq n^{0,\mathrm{BO}}$ in $\Delta\hat{n}$ leads to an inconsistency. In fact, any exact or even approximate treatment of the low-energy Hamiltonian Eq. (11) gives a ground-state density n^0 which is, in general, different from $n^{0,\mathrm{BO}}$. In equilibrium, we then have $\Delta n = n^0 - n^{0,\mathrm{BO}} \neq 0$, and the nuclei move away from $\{\mathbf{R}\} = \{\mathbf{R}^{0,\mathrm{BO}}\}$ in accordance with the equation of motion Eq. (22). The minimal effort to get rid of the inconsistency consists in treating n^0 in $\Delta\hat{n}$ self-consistently while keeping V, g, and K fixed at the BO values. Whether this partial self-consistent scheme leads to a stable dynamics when the system is perturbed by weak external fields remains to be checked case by case.

2. Elastic tensor and Hessian of the BO energy

The elastic tensor K^{BO} can alternatively be obtained from the Hessian $\mathcal{H}$ of $E^{\mathrm{BO}}(\mathbf{R})$ and the density-density response function *at clamped nuclei*. Taking into account the definitions in Eq. (10), a second differentiation of Eq. (B2) yields [86]

$$\begin{aligned}\mathcal{H}_{i,\alpha;j,\beta} &\equiv \left.\frac{\partial^2 E^{\mathrm{BO}}(\mathbf{R})}{\partial R_{i,\alpha}\partial R_{j,\beta}}\right|_{\mathbf{R}=\mathbf{R}^{0,\mathrm{BO}}} \\ &= \int d\mathbf{x}\left.\frac{\partial n^{\mathrm{BO}}(\mathbf{x},\mathbf{R})}{\partial R_{j,\beta}}\right|_{\mathbf{R}=\mathbf{R}^{0,\mathrm{BO}}} g^{\mathrm{BO}}_{i,\alpha}(\mathbf{r}) \\ &\quad + \int d\mathbf{x} n^{0,\mathrm{BO}}(\mathbf{x}) g^{\mathrm{DW,BO}}_{i,\alpha;j,\beta}(\mathbf{r}) + \left.\frac{\partial^2 E_{n\text{-}n}(\mathbf{R})}{\partial R_{i,\alpha}\partial R_{j,\beta}}\right|_{\mathbf{R}=\mathbf{R}^{0,\mathrm{BO}}}.\end{aligned} \tag{B4}$$

The first term on the rhs can be rewritten in a more symmetric form using linear response theory. Let us imagine to manually move the infinitely heavy nuclei from $\mathbf{R}^{0,\mathrm{BO}}$ to $\mathbf{R}^{0,\mathrm{BO}} + \delta\mathbf{R}$. We indicate with $\delta\mathbf{R}(t)$ the extremely slow time-dependent function with the property that $\delta\mathbf{R}(t) = 0$ for $t = -\infty$ and $\delta\mathbf{R}(t) = \delta\mathbf{R}$ for $t = \infty$. This nuclear rearrangement induces a change in the electronic density. For the extremely slow (adiabatic) change considered here, the time-dependent electronic density $n(\mathbf{x},t)$ is identical to the ground-state electronic density $n^{\mathrm{BO}}[\mathbf{x},\mathbf{R}(t)]$ corresponding to a nuclear geometry $\mathbf{R}(t) = \mathbf{R}^{0,\mathrm{BO}} + \delta\mathbf{R}(t)$ (instantaneous relaxation). We have

$$\begin{aligned}\delta n^{\mathrm{BO}}(\mathbf{x},t) &= \int d\mathbf{x}' dt' \chi^R_{\mathrm{clamp}}(\mathbf{x},t;\mathbf{x}',t')\delta V(\mathbf{r}',\mathbf{R}(t')) \\ &= \int d\mathbf{x}' dt' \chi^R_{\mathrm{clamp}}(\mathbf{x},t;\mathbf{x}',t')\sum_{j\beta} g^{\mathrm{BO}}_{j,\beta}(\mathbf{r}')\delta R_{j,\beta}(t'),\end{aligned} \tag{B5}$$

where χ^R_{clamp} is the equilibrium density-density response function of the electronic system with clamped nuclei in $\mathbf{R}^{0,\mathrm{BO}}$. For a response function with the property that $\chi^R_{\mathrm{clamp}}(\mathbf{x},t;\mathbf{x}',t') \to 0$ for $|t-t'| \to \infty$, we can replace $\delta R_{j,\beta}(t') \to \delta R_{j,\beta}(t)$ (adiabatic change). Performing the integral over t' and taking the limit $t \to \infty$, we get

$$\delta n^{\mathrm{BO}}(\mathbf{x}) = \int d\mathbf{x}' \chi^R_{\mathrm{clamp}}(\mathbf{x},\mathbf{x}';0)\sum_{j\beta} g^{\mathrm{BO}}_{j,\beta}(\mathbf{r}')\delta R_{j,\beta}, \tag{B6}$$

where $\chi^R_{\mathrm{clamp}}(\mathbf{x},\mathbf{x}';0)$ is the Fourier transform of the response function calculated at zero frequency. Using Eq. (B6) to evaluate the derivative of the ground-state density in Eq. (B4) and comparing with Eq. (14), we conclude that

$$\mathcal{H}_{i,\alpha;j,\beta} = K^{\mathrm{BO}}_{i,\alpha;j,\beta} + \int d\mathbf{x} d\mathbf{x}' g^{\mathrm{BO}}_{i,\alpha}(\mathbf{r})\chi^R_{\mathrm{clamp}}(\mathbf{x},\mathbf{x}';0)g^{\mathrm{BO}}_{j,\beta}(\mathbf{r}'). \tag{B7}$$

The elastic tensor in the BO approximation coincides with the Hessian of the BO energy only if the electron-nuclear coupling g^{BO} vanishes.

In crystals, the relation in Eq. (B7) reads

$$\mathcal{H}_{s,\alpha;s',\beta}(\mathbf{n}-\mathbf{n}') = K^{\mathrm{BO}}_{s,\alpha;s',\beta}(\mathbf{n}-\mathbf{n}') + \int d\mathbf{x}d\mathbf{x}' g^{\mathrm{BO}}_{\mathbf{n}s,\alpha}(\mathbf{r})\chi^{R}_{\mathrm{clamp}}(\mathbf{x},\mathbf{x}';0)g^{\mathrm{BO}}_{\mathbf{n}'s',\beta}(\mathbf{r}'). \tag{B8}$$

The Hessian tensor satisfies the same properties as the elastic tensor. Let then $\omega^2_{\mathbf{q}\nu}$ and $\mathbf{e}^{\nu}(\mathbf{q})$ be the eigenvalues and normal modes of $\mathcal{H}(\mathbf{q})$, which is defined in terms of $\mathcal{H}(\mathbf{n})$ like in Eq. (29). The eigenvalues $\omega^2_{\mathbf{q}\nu}$ are by construction non-negative, since the Hessian of a function calculated in the global minimum is positive semidefinite. Multiplying Eq. (B8) by $e^{\nu*}_{s,\alpha}(\mathbf{q})e^{-i\mathbf{q}\cdot(\mathbf{n}-\mathbf{n}')}e^{\nu'}_{s'\beta}(\mathbf{q})/\sqrt{M_s M_{s'}}$ and summing over $\mathbf{n}s,\alpha$ and $\mathbf{n}'s',\beta$, we obtain

$$\delta_{\nu\nu'}\omega^2_{\mathbf{q}\nu} = K^{\mathrm{BO}}_{\nu\nu'}(\mathbf{q}) + \int d\mathbf{x}d\mathbf{x}' g^{\mathrm{BO}}_{\mathbf{q}\nu}(\mathbf{r})\chi^{R}_{\mathrm{clamp}}(\mathbf{x},\mathbf{x}';0)g^{\mathrm{BO}}_{-\mathbf{q}\nu'}(\mathbf{r}'), \tag{B9}$$

to be compared with Eqs. (136) and (137).

APPENDIX C: SYMMETRY PROPERTIES OF THE PHONONIC GREEN'S FUNCTION AND SELF-ENERGY

From the definition in Eq. (88) and the property in Eq. (125), we have

$$D^{ii'}_{\mathbf{q}\nu\nu'}(z,z') = \frac{1}{i}\mathrm{Tr}[\rho\mathcal{T}\{\Delta\hat{\phi}^{i}_{\mathbf{q}\nu,H}(z)\Delta\hat{\phi}^{i'}_{-\mathbf{q}\nu',H}(z')\}]. \tag{C1}$$

It is then straightforward to derive

$$D^{ii',<}_{\mathbf{q}\nu\nu'}(t,t') = D^{i'i,>}_{-\mathbf{q}\nu'\nu}(t',t), \tag{C2a}$$

$$D^{ii',\gtrless}_{\mathbf{q}\nu\nu'}(t,t') = -[D^{i'i,\gtrless}_{\mathbf{q}\nu'\nu}(t',t)]^*. \tag{C2b}$$

The phononic Green's function satisfies also another important property if the Hamiltonian is invariant under time reversal. Let $\hat{\Theta}$ be the antiunitary time-reversal operator. Time-reversal symmetry implies that we can choose the many-body eigenstates $|\Psi_A\rangle$ of $\hat{H}$ such that $|\Psi_A\rangle = \hat{\Theta}|\Psi_A\rangle$, and, therefore, we have the property [116]

$$\langle\Psi_A|\hat{O}|\Psi_B\rangle = \langle\Psi_B|\hat{\Theta}\hat{O}^{\dagger}\hat{\Theta}^{-1}|\Psi_A\rangle \tag{C3}$$

for any operator $\hat{O}$. Under a time-reversal transformation, the displacement operators are even, whereas the momentum operators are odd; i.e., $\hat{\Theta}\hat{U}_{\mathbf{n}s,\alpha}\hat{\Theta}^{-1} = \hat{U}_{\mathbf{n}s,\alpha}$ and $\hat{\Theta}\hat{P}_{\mathbf{n}s,\alpha}\hat{\Theta}^{-1} = -\hat{P}_{\mathbf{n}s,\alpha}$. Expanding these operators like in Eqs. (25), we immediately find

$$\hat{\Theta}\hat{U}_{\mathbf{q}\nu}\hat{\Theta}^{-1} = \hat{U}_{-\mathbf{q}\nu} = \hat{U}^{\dagger}_{\mathbf{q}\nu}, \tag{C4a}$$

$$\hat{\Theta}\hat{P}_{\mathbf{q}\nu}\hat{\Theta}^{-1} = -\hat{P}_{-\mathbf{q}\nu} = -\hat{P}^{\dagger}_{\mathbf{q}\nu}, \tag{C4b}$$

where we take into account that $\hat{\Theta}c = c^*\hat{\Theta}$ for any complex number c and we use the property Eq. (26) of the normal modes. From Eq. (C3), we then infer that

$$\langle\Psi_A|\hat{U}_{\mathbf{q}\nu}|\Psi_B\rangle = \langle\Psi_B|\hat{U}_{\mathbf{q}\nu}|\Psi_A\rangle, \tag{C5a}$$

$$\langle\Psi_A|\hat{P}_{\mathbf{q}\nu}|\Psi_B\rangle = -\langle\Psi_B|\hat{P}_{\mathbf{q}\nu}|\Psi_A\rangle. \tag{C5b}$$

Let E_A be the eigenenergy of $|\Psi_A\rangle$. If the system is in equilibrium, then $|\Psi_A\rangle$ is also an eigenket of the density matrix $\hat{\rho}$, and we denote by ρ_A its eigenvalue. Consider the (1, 1) block of the greater GF in Eq. (C1). We have

$$D^{11,>}_{\mathbf{q}\nu\nu'}(t,t') = \frac{1}{i}\sum_{A,B}\rho_A e^{i(E_A-E_B)(t-t')}\langle\Psi_A|\hat{U}_{\mathbf{q}\nu}|\Psi_B\rangle\langle\Psi_B|\hat{U}_{-\mathbf{q}\nu'}|\Psi_A\rangle = D^{11,>}_{-\mathbf{q}\nu'\nu}(t,t'), \tag{C6}$$

where in the second equality we use Eq. (C5). We can analogously derive the relations for all other blocks and for the lesser GF. The final result is

$$D^{ii',\gtrless}_{\mathbf{q}\nu\nu'}(t,t') = (-)^{i+i'}D^{i'i,\gtrless}_{-\mathbf{q}\nu'\nu}(t,t'). \tag{C7}$$

To highlight the mathematical structure of the derived relations, we denote by D^T the transpose matrix of D, i.e., $[D^T]^{ii'}_{\nu\nu'} \equiv D^{i'i}_{\nu'\nu}$, and $D^{\dagger} = [D^T]^*$. Then, Eqs. (C2) and (C7) take the following compact form:

$$D^{<}_{\mathbf{q}}(t,t') = [D^{>}_{-\mathbf{q}}(t',t)]^T, \tag{C8a}$$

$$D^{\gtrless}_{\mathbf{q}}(t,t') = -[D^{\gtrless}_{\mathbf{q}}(t',t)]^{\dagger}, \tag{C8b}$$

$$D^{\gtrless}_{\mathbf{q}}(t,t') = \sigma_z[D^{\gtrless}_{-\mathbf{q}}(t,t')]^T\sigma_z \quad [\hat{\Theta}\text{ invariance}], \tag{C8c}$$

where

$$[\sigma_z]^{ii'}_{\nu\nu'} = \delta_{\nu\nu'}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}_{ii'}.$$

In frequency space, the first two relations in Eqs. (C8) read

$$D^{<}_{\mathbf{q}}(\omega) = [D^{>}_{-\mathbf{q}}(-\omega)]^T, \qquad D^{\gtrless}_{\mathbf{q}}(\omega) = -[D^{\gtrless}_{\mathbf{q}}(\omega)]^{\dagger}, \tag{C9}$$

which imply

$$D^R_{\mathbf{q}}(\omega) = [D^A_{-\mathbf{q}}(-\omega)]^T, \qquad D^R_{\mathbf{q}}(\omega) = [D^A_{\mathbf{q}}(\omega)]^\dagger, \tag{C10}$$

which, in turn, lead to the following properties of the phononic self-energy through Eq. (150) [take into account that $\alpha^T = -\alpha$ and $Q^T(-\mathbf{q}) = Q(\mathbf{q})$]:

$$\Pi^R_{\mathbf{q}}(\omega) = [\Pi^A_{-\mathbf{q}}(-\omega)]^T, \qquad \Pi^R_{\mathbf{q}}(\omega) = [\Pi^A_{\mathbf{q}}(\omega)]^\dagger. \tag{C11}$$

Writing the retarded and advanced phononic self-energy like in Eq. (151), we can deduce the following properties of Λ_{ph} and Γ_{ph}:

$$\Lambda_{ph,\mathbf{q}}(\omega) = [\Lambda_{ph,-\mathbf{q}}(-\omega)]^T, \qquad \Lambda_{ph,\mathbf{q}}(\omega) = [\Lambda_{ph,\mathbf{q}}(\omega)]^\dagger, \tag{C12a}$$

$$\Gamma_{ph,\mathbf{q}}(\omega) = -[\Gamma_{ph,-\mathbf{q}}(-\omega)]^T, \qquad \Gamma_{ph,\mathbf{q}}(\omega) = [\Gamma_{ph,\mathbf{q}}(\omega)]^\dagger. \tag{C12b}$$

For systems with time-reversal symmetry, we have also the properties [see Eq. (C8c)]

$$D^{\lessgtr}_{\mathbf{q}}(\omega) = \sigma_z[D^{\lessgtr}_{-\mathbf{q}}(\omega)]^T\sigma_z, \tag{C13}$$

which implies

$$D^{R/A}_{\mathbf{q}}(\omega) = \sigma_z[D^{R/A}_{-\mathbf{q}}(\omega)]^T\sigma_z, \tag{C14}$$

and, therefore,

$$\Pi^{R/A}_{\mathbf{q}}(\omega) = \sigma_z[\Pi^{R/A}_{-\mathbf{q}}(\omega)]^T\sigma_z, \tag{C15}$$

or, equivalently,

$$\Lambda_{ph,\mathbf{q}}(\omega) = \sigma_z[\Lambda_{ph,-\mathbf{q}}(\omega)]^T\sigma_z, \tag{C16a}$$

$$\Gamma_{ph,\mathbf{q}}(\omega) = \sigma_z[\Gamma_{ph,-\mathbf{q}}(\omega)]^T\sigma_z. \tag{C16b}$$

APPENDIX D: FORMULATION IN THE ELECTRONIC BLOCH BASIS

In this appendix, we work out the fundamental equations in the electronic Bloch basis

$$\Psi_{\mathbf{k}\mu}(\mathbf{x}) = \langle \mathbf{x}|\mathbf{k}\mu\rangle = \frac{1}{\sqrt{N}} e^{i\mathbf{k}\cdot\mathbf{n}} u_{\mathbf{k}\mu}(\mathbf{u}\sigma). \tag{D1}$$

The Bloch kets are orthonormal; i.e., $\langle \mathbf{k}\mu|\mathbf{k}'\mu'\rangle = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\mu\mu'}$. This implies that the periodic functions $u_{\mathbf{k}\mu}(\mathbf{u}\sigma)$ are orthonormal in the volume V_u of the unit cell, since

$$\begin{aligned}\langle \mathbf{k}\mu|\mathbf{k}'\mu'\rangle &= \int d\mathbf{x}\Psi^*_{\mathbf{k}\mu}(\mathbf{x})\Psi_{\mathbf{k}'\mu'}(\mathbf{x}) \\ &= \sum_{\mathbf{n}\sigma}\int_{V_u} d\mathbf{u}\,\frac{1}{N} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{n}} u^*_{\mathbf{k}\mu}(\mathbf{u}\sigma)u_{\mathbf{k}'\mu'}(\mathbf{u}\sigma) \\ &= \delta_{\mathbf{k},\mathbf{k}'}\sum_{\sigma}\int_{V_u} d\mathbf{u}\, u^*_{\mathbf{k}\mu}(\mathbf{u}\sigma)u_{\mathbf{k}\mu'}(\mathbf{u}\sigma).\end{aligned} \tag{D2}$$

We expand the fermionic operators according to

$$\hat{\psi}(\mathbf{x}) = \sum_{\mathbf{k}\mu}\Psi_{\mathbf{k}\mu}(\mathbf{x})\hat{d}_{\mathbf{k}\mu} \Rightarrow \hat{d}_{\mathbf{k}\mu} = \int d\mathbf{x}\Psi^*_{\mathbf{k}\mu}(\mathbf{x})\hat{\psi}(\mathbf{x}). \tag{D3}$$

The fermionic anticommutation rules $\{\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')\} = \delta(\mathbf{x}-\mathbf{x}')$ imply that $\{\hat{d}_{\mathbf{k}\mu}, \hat{d}^\dagger_{\mathbf{k}'\mu'}\} = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\mu\mu'}$. Inserting the expansion of Eq. (D3) into Eq. (37), we see that we are called to calculate the integral of $h(\boldsymbol{\nabla}, \mathbf{r})$ and $\boldsymbol{g}^\dagger_{\mathbf{q}\nu}(\mathbf{r})$ multiplied by two Bloch wave functions [we omit the dependence on z for brevity]. Taking into account that $h(\boldsymbol{\nabla}, \mathbf{r}) = h(\boldsymbol{\nabla}, \mathbf{r}+\mathbf{R}^0_{\mathbf{n}})$, we have

$$\begin{aligned}&\int d\mathbf{x}\Psi^*_{\mathbf{k}\mu}(\mathbf{x})h(\boldsymbol{\nabla}, \mathbf{r})\Psi_{\mathbf{k}'\mu'}(\mathbf{x}) \\ &= \sum_{\mathbf{n}\sigma}\frac{1}{N} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{n}}\int_{V_u} d\mathbf{u}\, u^*_{\mathbf{k}\mu}(\mathbf{u}\sigma)h(\boldsymbol{\nabla}, \mathbf{u})u_{\mathbf{k}'\mu'}(\mathbf{u}\sigma) \\ &= \delta_{\mathbf{k},\mathbf{k}'}h_{\mu\mu'}(\mathbf{k}),\end{aligned} \tag{D4}$$

which implicitly defines the matrix $h(\mathbf{k})$. Similarly, using the property in Eq. (119), we find

$$\begin{aligned}&\int d\mathbf{x}\Psi^*_{\mathbf{k}\mu}(\mathbf{x})\boldsymbol{g}^\dagger_{\mathbf{q}\nu}(\mathbf{r})\Psi_{\mathbf{k}'\mu'}(\mathbf{x}) \\ &= \sum_{\mathbf{n}\sigma}\frac{1}{N} e^{-i(\mathbf{k}-\mathbf{k}'-\mathbf{q})\cdot\mathbf{n}}\int_{V_u} d\mathbf{u}\; u^*_{\mathbf{k}\mu}(\mathbf{u}\sigma)\boldsymbol{g}^\dagger_{\mathbf{q}\nu}(\mathbf{u})u_{\mathbf{k}'\mu'}(\mathbf{u}\sigma) \\ &= \delta_{\mathbf{k}-\mathbf{q},\mathbf{k}'}\tilde{\boldsymbol{g}}^\dagger_{\mathbf{q}\nu,\mu\mu'}(\mathbf{k}),\end{aligned} \tag{D5}$$

which implicitly defines the vector of matrices $\tilde{\boldsymbol{g}}^\dagger_{\mathbf{q}\nu}(\mathbf{k})$. Notice that for $\mathbf{q} = 0$ this matrix is precisely the one defined in Eq. (118). Let us make contact with an alternative popular expression for the *e-ph* coupling. Using the definition in Eq. (30), the result in Eq. (D5) can be written as

$$\begin{aligned}\tilde{g}_{-\mathbf{q}\nu,\mu\mu'}(\mathbf{k}) &= \langle \mathbf{k}\mu|g_{-\mathbf{q}\nu}(\hat{\mathbf{r}})|\mathbf{k}-\mathbf{q}\mu'\rangle \\ &= \sum_{\mathbf{n}s\alpha}\frac{1}{\sqrt{M_s N}} e^{i\mathbf{q}\cdot\mathbf{n}} e^{\nu}_{s,\alpha}(\mathbf{q})\langle \mathbf{k}\mu|g_{\mathbf{n}s,\alpha}(\hat{\mathbf{r}})|\mathbf{k}-\mathbf{q}\mu'\rangle.\end{aligned} \tag{D6}$$

The electron-nuclear potential $V(\mathbf{r},\mathbf{R}) = V(\mathbf{r},\mathbf{R}^0+\mathbf{U})$ can be thought of as a function of either $\mathbf{U}_{\mathbf{n}s\alpha}$ or $U_{\mathbf{q}\nu}$ through Eq. (25). If we calculate

$$\left.\frac{\partial V(\hat{\mathbf{r}},\mathbf{R})}{\partial U_{\mathbf{q}\nu}}\right|_{\mathbf{U}=0} = \sum_{\mathbf{n}s\alpha}\left.\frac{\partial V(\hat{\mathbf{r}},\mathbf{R})}{\partial U_{\mathbf{n}s,\alpha}}\right|_{\mathbf{U}=0}\times\frac{\partial U_{\mathbf{n}s,\alpha}}{\partial U_{\mathbf{q}\nu}} = \sum_{\mathbf{n}s\alpha} g_{\mathbf{n}s,\alpha}(\hat{\mathbf{r}})\times\frac{1}{\sqrt{M_s N}}e^{i\mathbf{q}\cdot\mathbf{n}}e^{\nu}_{s,\alpha}(\mathbf{q}), \tag{D7}$$

we find the linear combination appearing in Eq. (D6). We conclude that

$$\tilde{g}_{-\mathbf{q}\nu,\mu\mu'}(\mathbf{k}) = \langle\mathbf{k}\mu|\left.\frac{\partial V(\hat{\mathbf{r}},\mathbf{R})}{\partial U_{\mathbf{q}\nu}}\right|_{\mathbf{U}=0}|\mathbf{k}-\mathbf{q}\mu'\rangle. \tag{D8}$$

In terms of the matrices $h(\mathbf{k})$ and $\tilde{\boldsymbol{g}}_{\mathbf{q}\nu}(\mathbf{k})$, the Hamiltonian in Eq. (37) reads

$$\hat{H}^s_{0,e} = \sum_{\mathbf{k}\mu\mu'}\sum_{\mathbf{q}\nu}\left[\delta_{\mathbf{q},\mathbf{0}}h_{\mu\mu'}(\mathbf{k}) + \tilde{\boldsymbol{g}}^{\dagger}_{\mathbf{q}\nu,\mu\mu'}(\mathbf{k})\cdot\boldsymbol{s}_{\mathbf{q}\nu}\right]\hat{d}^{\dagger}_{\mathbf{k}\mu}\hat{d}_{\mathbf{k}-\mathbf{q}\mu'}. \tag{D9}$$

Analogously, we can rewrite the Hamiltonians $\hat{H}^s_{0,ph}$ in Eq. (37b) and $\hat{H}_{e\text{-}ph}$ in Eq. (37d) according to

$$\hat{H}^s_{0,ph} = \frac{1}{2}\sum_{\mathbf{q}}\sum_{\nu\nu'}\hat{\boldsymbol{\phi}}^{\dagger}_{\mathbf{q}\nu}\,Q_{\nu\nu'}(\mathbf{q})\hat{\boldsymbol{\phi}}_{\mathbf{q}\nu'} - \sum_{\mathbf{k}\mu\mu'}\sum_{\mathbf{q}\nu}\langle\hat{d}^{\dagger}_{\mathbf{k}\mu}\hat{d}_{\mathbf{k}-\mathbf{q}\mu'}\rangle_0\,\tilde{\boldsymbol{g}}^{\dagger}_{\mathbf{q}\nu,\mu\mu'}(\mathbf{k})\cdot\hat{\boldsymbol{\phi}}_{\mathbf{q}\nu}, \tag{D10}$$

$$\hat{H}_{e\text{-}ph} = \sum_{\mathbf{k}\mu\mu'}\sum_{\mathbf{q}\nu}\hat{d}^{\dagger}_{\mathbf{k}\mu}\hat{d}_{\mathbf{k}-\mathbf{q}\mu'}\tilde{\boldsymbol{g}}^{\dagger}_{\mathbf{q}\nu,\mu\mu'}(\mathbf{k})\cdot(\hat{\boldsymbol{\phi}}_{\mathbf{q}\nu}-\boldsymbol{s}_{\mathbf{q}\nu}), \tag{D11}$$

where $\langle\cdots\rangle_0$ indicates the equilibrium average.

It is common to define (i) the scaling-free displacements and momenta with the physical dimensions of a length and momentum, respectively,

$$\hat{\bar{U}}_{\mathbf{q}\nu} \equiv \frac{\hat{U}_{\mathbf{q}\nu}}{\sqrt{NM}} = \frac{1}{\sqrt{NM\omega_{\mathbf{q}\nu}}}\frac{\hat{b}_{\mathbf{q}\nu}+\hat{b}^{\dagger}_{-\mathbf{q}\nu}}{\sqrt{2}}, \tag{D12a}$$

$$\hat{\bar{P}}_{\mathbf{q}\nu} \equiv \sqrt{\frac{M}{N}}\hat{P}_{\mathbf{q}\nu} = \sqrt{\frac{M\omega_{\mathbf{q}\nu}}{N}}\frac{\hat{b}_{\mathbf{q}\nu}-\hat{b}^{\dagger}_{-\mathbf{q}\nu}}{\sqrt{2}i} \tag{D12b}$$

where $\omega_{\mathbf{q}\nu}$ are the BO phonon frequencies and $M=\sum_s M_s$ is the total mass of the unit cell [see also Eq. (139)], and (ii) the scaling-free $e\text{-}ph$ coupling with the physical dimensions of an energy

$$\tilde{g}^{*}_{\nu,\mu\mu'}(\mathbf{k},\mathbf{q}) = \sqrt{\frac{1}{M\omega_{\mathbf{q}\nu}}}\langle\mathbf{k}\mu|\left.\frac{\partial V(\hat{\mathbf{r}},\mathbf{R})}{\partial\bar{U}_{\mathbf{q}\nu}}\right|_{\mathbf{U}=0}|\mathbf{k}-\mathbf{q}\mu'\rangle = \sqrt{\frac{N}{\omega_{\mathbf{q}\nu}}}\tilde{g}^{*}_{\mathbf{q}\nu,\mu\mu'}(\mathbf{k}). \tag{D13}$$

In terms of these quantities,

$$\tilde{g}^{*}_{\mathbf{q}\nu,\mu\mu'}(\mathbf{k})U_{\mathbf{q}\nu} = \sqrt{M\omega_{\mathbf{q}\nu}}\tilde{g}^{*}_{\nu,\mu\mu'}(\mathbf{k},\mathbf{q})\bar{U}_{\mathbf{q}\nu}. \tag{D14}$$

Let us now rewrite the equation of motion for the Green's function in terms of scaling-free quantities. In Eq. (116), the quantities $h_{\mathrm{HF}}(\mathbf{k})$, $G_{\mathbf{k}}$, and $\Sigma_{\mathrm{c},\mathbf{k}}$ do not scale with N. Taking into account Eq. (D14), we find

$$\left[i\frac{d}{dz_1}-h_{\mathrm{HF}}(\mathbf{k})-\sum_{\nu}\sqrt{M\omega_{\mathbf{0}\nu}}\,\tilde{g}_{\nu}(\mathbf{k},\mathbf{0})\bar{U}_{\mathbf{0}\nu}\right]G_{\mathbf{k}}(z_1,z_2) = \delta(z_1,z_2)+\int_{\gamma}d\bar{z}\Sigma_{\mathrm{c},\mathbf{k}}(z_1,\bar{z})G_{\mathbf{k}}(\bar{z},z_2). \tag{D15}$$

Notice that if the external perturbation preserves the lattice periodicity, then $U_{\mathbf{q}\nu}=\delta_{\mathbf{q},\mathbf{0}}U_{\mathbf{0}\nu}$ and, therefore, $U_{\mathbf{n}s,\alpha}=U_{s,\alpha}$ is independent of $\mathbf{n}$. From the inverse of Eq. (25), i.e.,

$$\hat{U}_{\mathbf{q}\nu} = \sum_{\mathbf{n}s\alpha}\sqrt{\frac{M_s}{N}}e^{-i\mathbf{q}\cdot\mathbf{n}}\mathbf{e}^{\nu}_{s,\alpha}(\mathbf{q})\hat{U}_{\mathbf{n}s,\alpha}, \tag{D16}$$

we then find

$$\bar{U}_{\mathbf{0}\nu} = \sum_{s\alpha}\sqrt{\frac{M_s}{M}}\mathbf{e}^{\nu}_{s,\alpha}(\mathbf{0})U_{s,\alpha}, \tag{D17}$$

which does not scale with N.

In the equation of motion Eq. (126) for the phononic Green's function, the quantities $Q(\mathbf{q})$, $D_{\mathbf{q}}$, and $\Pi_{\mathbf{q}}$ do not scale with N, so this equation is already written in terms of scaling-free quantities only. We are left with the equation of motion for the displacements and momenta; see Eqs. (120). Taking into account Eq. (D5), we find

$$\frac{dP_{\mathbf{q}\nu}}{dz} = -\sum_{\mathbf{k}\mu\mu'}\tilde{g}_{\mathbf{q}\nu,\mu\mu'}(\mathbf{k})\Delta\langle\hat{d}^{\dagger}_{\mathbf{k}\mu}\hat{d}_{\mathbf{k}+\mathbf{q}\mu'}\rangle - \sum_{\nu'}K_{\nu\nu'}(\mathbf{q})U_{\mathbf{q}\nu'}. \tag{D18}$$

Using the definitions in Eqs. (D12) and (D13), we can rewrite the equation of motion for $\bar{P}_{\mathbf{q}\nu}$ in $\mathbf{q} = 0$ as

$$\frac{d\bar{P}_{\mathbf{0}\nu}}{dz} = -\sum_{\mathbf{k}\mu\mu'} \sqrt{M\omega_{\mathbf{q}\nu}}\, \tilde{g}_{\nu,\mu\mu'}(\mathbf{k},\mathbf{0}) \frac{\Delta\langle \hat{d}^{\dagger}_{\mathbf{k}\mu} \hat{d}_{\mathbf{k}\mu'} \rangle}{N} - M\sum_{\nu'} K_{\nu\nu'}(\mathbf{0})\bar{U}_{\mathbf{0}\nu'}, \tag{D19}$$

to be coupled with

$$\frac{d\bar{U}_{\mathbf{0}\nu}}{dz} = \frac{\bar{P}_{\mathbf{0}\nu}}{M}. \tag{D20}$$

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Correction: Equations (119), (D5), (D6), (D8), (D9), (D10), (D11), and (D13) contained errors and have been fixed.