Functional approach to the electronic and bosonic dynamics of many-body systems perturbed with an arbitrary strong electron-boson interaction

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We present a formal derivation of the many-body perturbation theory for a system of electrons and bosons subject to a nonlinear electron-boson coupling. The interaction is treated at an arbitrary high order of bosons scattered. The considered Hamiltonian includes the well-known linear coupling as a special limit. This is the case, for example, of the Holstein and Fröhlich Hamiltonians. Indeed, whereas linear coupling has been extensively studied, the scattering processes of electrons with multiple bosonic quasiparticles are largely unexplored. We focus here on a self-consistent theory in terms of dressed propagators and generalize the Hedin's equations using the Schwinger technique of functional derivatives. The method leads to an exact derivation of the electronic and bosonic self-energies, expressed in terms of a new family of vertex functions, high-order correlators, and bosonic and electronic mean-field potentials. In the electronic case we prove that the mean-field potential is the nth-order extension of the well-known Debye-Waller potential. We also introduce a bosonic mean-field potential entirely dictated by nonlinear electron-boson effects. The present scheme, treating electrons and bosons on an equal footing, demonstrates the full symmetry of the problem. The vertex functions are shown to have purely electronic and bosonic character as well as a mixed electron-boson one. These four vertex functions are shown to satisfy a generalized Bethe-Salpeter equation. Multibosons response functions are also studied and explicit expressions for the two and the three bosons case are given.

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I. INTRODUCTION

Electron-boson (e-b) Hamiltonians are ubiquitous in particle, condensed matter physics and optics: the fundamental electron-electron interaction is mediated by photons, which are bosonic particles; lattice vibrations (phonons) play a fundamental role in superconductivity [1]; and collective excitations in many-electron systems (plasmons) as well as bound electron-hole states (excitons) have a bosonic nature. Many examples of such a duality can also be found in strongly correlated systems [2]. The interaction between electrons and bosons is typically treated *linearly* in electronic density and bosonic displacement [3]. The proportionality constant may have different expressions depending on the microscopic details of the system.

However, there are cases where nonlinear coupling is comparable in strength or even dominates the first-order electron-boson interaction.

a. Electron-phonon coupling in quantum dots. Very often the quadratic and linear effects are inseparable, and the former can arise in, e.g., perturbative elimination of the off-diagonal electron-phonon coupling in quantum dots. For instance, quadratic coupling of carriers in quantum dots to acoustic phonons modifies the polarization decay and leads to exponential dephasing [4]. Linear coupling alone generates acoustic satellites in the spectrum, but causes no Lorentzian broadening [5,6].

b. Flexural phonons. The balance between the first- and the second-order effects can be influenced by the symmetry. If a system possesses a mirror plane, the coupling to the oscillations normal to this plane cannot be linear. This fact was noticed by Mariani and von Oppen [7] who demonstrated that *flexural phonons* couple *quadratically* to the electron density. On the other hand, if the mirror symmetry is broken by the presence of a substrate or by the gating, the coupling becomes linear again [8].

c. Holstein and Fröhlich models. The interplay between the effects induced by different orders of the e-b interaction can have important consequences in the Holstein model [9]. This uses a simplified form of the Fröhlich Hamiltonian, where carriers couple to a branch of dispersionless optical phonons through a momentum-independent coupling. In this case even small positive nonlinear interaction reduces the effective coupling between the electrons and the lattice, suppressing charge-density-wave correlations, and hardening the effective phonon frequency [10,11]. These findings prompted further theoretical investigations of the Holstein model with even more complicated double-well electron-phonon interaction [12,13] using a generalization of the momentum average approximation [14], and of general form of interaction using the determinant quantum Monte Carlo approach [15]. Closely connected to these studies are recent experiments emphasizing the role of nonlinear lattice dynamics as a mean for control [16],

and as a basis for enhanced superconductivity in MgB_2 [17] and some cuprates [18]. They point toward large ionic displacement which is a prerequisite for the nonlinear electron-phonon coupling.

d. Finite temperature effects. Another prominent example is the renormalization of electronic structures due to zero or finite temperature phonons. As demonstrated by Heine, Allen, and Cardona (HAC) [19,20] the linear and quadratic couplings (in atomic displacement) are of the same order in the electron-ion interaction potential. Moreover, they need to be considered on an equal footing in order for the system to respect the system translational invariance. The effect of the second-order correction is quite large in carbon materials and can lead to a substantial band gap modification [21–23].

e. Anharmonic effects. Some recent works have also demonstrated that, potentially, even simple systems like diamond [24,25] or palladium [26] show remarkable nonlinear effects. However, at the moment, these anharmonic effects can be treated only by using an adiabatic approach based on finite displacements of the atoms. This approach ignores dynamic effects that, however, have been shown to be relevant in the linear coupling case [22] and, therefore, cannot be neglected, *a priori* in the case of nonlinear coupling.

f. Existing theoretical approaches. Nonlinear electron-boson models have been treated theoretically by essentially stretching methods developed for pure electronic case or linear coupling scenario: quantum Monte Carlo [11], the average momentum approximation [14], and the cumulant expansion [4]. Since only electronic spectrum was of interest, they rely on diagrammatic methods, without systematically exploring the *renormalization of phononic properties* due to electrons. However, as has been shown in the linear case using perturbative expansions of both electron and phonon propagators, electrons typically overscreen bare phonon frequencies leading to the conclusion that renormalized phonon frequencies must be fitted to experiments [27]. Thus, Marini *et al.* [28] have recently extended many-body perturbation theory (MBPT) for electron-phonon interaction including quadratic terms and using density functional theory [29] as a starting point. This is a remarkable achievement since even *ab initio* determination of a momentum-dependent electron-phonon linear coupling function is a nontrivial task [30]. The Born-Oppenheimer approximation is commonly used as a starting point. However, the seminal works of Abedi *et al.* [31] and Requist *et al.* [32] on the exact factorization of the fermionic and bosonic wave function show that alternative paths beyond the Born-Oppenheimer approximation are possible.

g. Diagrammatic perturbation theory. Nonexistence of the Wick theorem for bosons [33], which is a consequence of the fact that averages of the normal product of bosonic operators are nonzero, makes it difficult to develop a diagrammatic perturbation theory [34]. To circumvent this difficulty, systems above the Bose-condensation temperature are implicitly assumed [35]. Method of functional derivatives is a complementary method [36]. In contrast to diagrammatic constructions based on the series expansions of the evolution operator on a contour, it yields functional relations between the dressed propagators. They do not rely on the Wick theorem. In the seminal works of Hedin [37] and van Leeuwen [27], the Schwinger technique of functional derivatives is used to derive the linear electron-boson coupling and no Debye-Waller (DW) potential is found. This is in stringent disagreement with the HAC theory where this potential naturally appears. On the other hand, any diagrammatic approach predicts the existence of the DW potential, as, for example, in Ref. [28]. It is therefore desirable to formulate *self-consistent* (sc) MBPT for the electron-boson system with nonlinear coupling, i.e., in terms of the *dressed* propagators, in a functional derivative approach.

h. Out-of-equilibrium scenarios. Our further motivation for this work is experimental feasibility to generate *coherent* phonons [38,39] and plasmons [40–42]. For such scenarios the notion of transient spectral properties is of special interest [43–45]. A powerful method to deal with time-dependent processes is the nonequilibrium Green's function (NEGF) approach [46]. The method relies on solving the Kadanoff-Baym equations (KBE) of motion for the Green's functions (GFs) on the Keldysh time contour [47–51]. To the best of our knowledge, for systems with nonlinear coupling such theory is not available.

Our paper is organized as follows: In Sec. II we introduce the Hamiltonian and its properties. Given the Hamiltonian in Sec. III, we derive the corresponding equation of motion for the bosonic and electronic operators. The equation of motion are analyzed in terms of functional derivatives in Sec. III B. The Green's functions are introduced in Sec. IV.

We first discuss the electronic case whose self-energy is derived *exactly* to all orders in the electron-boson interaction in Sec. V. We derive the form of a generalized Debye-Waller potential in Sec. V A which, in turns, defines the remaining nonlocal and time-dependent mass operator, Sec. V B.

The bosonic subsystem is, then, split in single-boson and multiboson case in analogy with the electronic case. In Sec. VI we introduce the bosonic self-energy that we split *exactly* in a mass operator, Sec. VI C, and a mean-field potential, Sec. VI A. The exact bosonic mass operator is rewritten in terms of four generalized vertex functions whose coupled equation of motion is derived in Sec. VI D.

The presented exact formulation is illustrated by the derivations of the lowest order approximations for the electronic (Sec. VII A) and bosonic (Sec. VII B) self-energies.

The last part of the work is devoted to the electronic and bosonic response functions (Sec. VIII). We derive a Bethe-Salpeter-like equation for the electronic response in Sec. VIII A. In Sec. VIII B we discuss the bosonic case by showing how to reduce the general bosonic dynamics to diagonal number conserving response functions. Then, the cases of two and three bosons are studied, respectively, in Secs. VIII B 2 and VIII B 3.

Finally, in Appendix A we motivate our treatment of electron-electron correlation, and in Appendix B we formally connect the formalism to the electron-phonon problem. In Appendix E we finally list some key mathematical quantities and approximations used throughout the whole paper. Logical flow of the whole work is depicted in Fig. 1.

II. NOTATION AND HAMILTONIAN

We start from the generic form of the total Hamiltonian of the system that we assume to be composed by fermions and

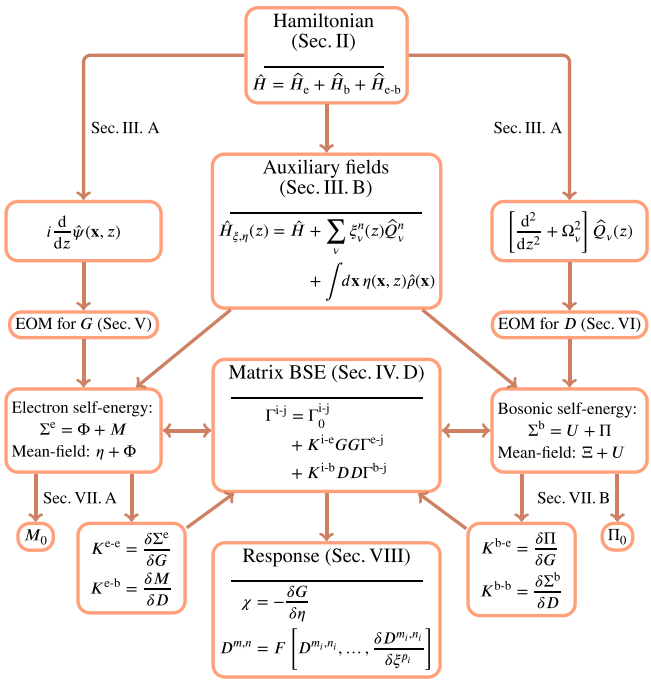

FIG. 1. Logical structure of the work.

bosons with a nonlinear interaction

$$\widehat{H} = \widehat{H}_e + \widehat{H}_b + \widehat{H}_{e\text{-}b}. \tag{1}$$

The unperturbed part of $\widehat{H}$ is $\widehat{H}_e + \widehat{H}_b$ and can be rewritten in terms of corresponding energies ($\mathcal{E}_i$ is the energy of the electronic state i, Ω_ν is the energy of the bosonic mode ν) and eigenstates obeying fermionic, bosonic statistics, respectively:

$$\widehat{H}_e = \sum_i \mathcal{E}_i \hat{c}^\dagger_i \hat{c}_i, \tag{2a}$$

$$\widehat{H}_b = \frac{1}{2}\sum_\nu \Omega_\nu\left(\widehat{P}^2_\nu + \widehat{Q}^2_\nu\right). \tag{2b}$$

In general, the partitioning of a physical Hamiltonian in the form of Eq. (1) is a highly nontrivial problem [31,32]. In the present context we are interested in the nonlinear e-b coupling and, to keep the formulation simple, we assume that such a partition does exist and that the electronic correlation can be approximatively described with a mean-field potential that renormalizes the free electrons and bosons. This is a common practice, for example, in the DFT approach to electrons and phonons. The DFT mean-field potential is defined in Appendix A.

In Eq. (2b) we have introduced the operators for the bosonic coordinates $\widehat{Q}_\nu$ and momenta $\widehat{P}_\nu$. The fermions are described by the corresponding creation ($\hat{c}^\dagger_i$) and annihilation ($\hat{c}_i$) operators. These are used to expand the electronic field operator $\hat{\psi}(\mathbf{x}) = \sum_i \phi_i(\mathbf{x})\hat{c}_i$, with $\phi_i(\mathbf{x})$ eigenfunctions of the electronic Hamiltonian in the first quantization [denoted as $h_e(\mathbf{x})$].

$\mathcal{E}_i$ and Ω_ν are the independent electrons and bosons energies. They are assumed to incorporate the mean-field potentials embodied in $\widehat{H}_e + \widehat{H}_b$. $\hat{Q}_\nu$ and $\hat{P}_\nu$ are expressed in the standard way in terms of the creation ($\hat{b}^\dagger_\nu$) and annihilation ($\hat{b}_\nu$) operators:

$$\widehat{Q}_\nu = \frac{1}{\sqrt{2}}(\hat{b}^\dagger_\nu + \hat{b}_\nu), \tag{3a}$$

$$\widehat{P}_\nu = \frac{i}{\sqrt{2}}(\hat{b}^\dagger_\nu - \hat{b}_\nu). \tag{3b}$$

The electron-boson interaction is taken to have the general form

$$\widehat{H}_{e\text{-}b} = \sum_{n,\underline{\nu}} \int d\mathbf{x}\,\hat{\psi}^\dagger(\mathbf{x})V^n_{\underline{\nu}}(\mathbf{x})\hat{\psi}(\mathbf{x})\widehat{Q}^n_{\underline{\nu}}, \tag{4}$$

with

$$\widehat{Q}^n_{\underline{\nu}} = \prod_{i=1}^n \widehat{Q}_{\nu_i}, \tag{5a}$$

$$V^n_{\underline{\nu}}(\mathbf{x}) = \frac{1}{n!}\left(\prod_{i=1}^n \partial_{\nu_i}\right)_{\text{eq}} V_{e\text{-}b}(\mathbf{x}). \tag{5b}$$

Here $V_{e\text{-}b}(\mathbf{x})$ is a generic potential that dictates the electron-boson interaction. The connection to the electron-phonon problem is given in Appendix B. Equation (5b) makes it clear that $V^n_{\underline{\nu}}(\mathbf{x})$ is a *symmetric tensor* with respect to indices $\underline{\nu}$. The differentiation is performed with respect to the bosonic coordinates evaluated at the equilibrium point. The physical form of the potential depends on the specific problem. Therefore, the equilibrium coordinates are specific to the kind of physics the bosons are describing. In the case of phonons, $(\prod_{i=1}^n \partial_{\nu_i})_{\text{eq}}$ is evaluated at the equilibrium atomic configuration, as defined in Appendix B.

Averaging the total Hamiltonian, Eq. (1), with respect to electronic coordinates leads to the effective *anharmonic* bosonic Hamiltonian. Solving such a model leads to, among other effects, the prediction of the temperature dependence of the averaged displacement. While an interesting and well-discussed problem on its own, we will not consider this effect here assuming that for each given temperature a Hamiltonian of the type defined by Eq. (1) can be derived such that

$$\langle\widehat{Q}_\nu\rangle = 0. \tag{6}$$

In contrast, as will be shown using our diagrammatic approach, other correlators of the position operator will be modified by electron-boson interaction in a nontrivial way.

Equation (5) highlights an important and crucial aspect of the notation. The symbol $\underline{\nu}$ represents a generic vector of bosonic indices of dimension n, which is indicated as a superscript and should not be confused with power. Therefore we consider the most general case where the nth-order e-b interaction is a nonlocal function of n bosonic coordinates.

For convenience we also introduce the electronic operator

$$\hat{\gamma}^n_{\underline{\nu}} \equiv \int d\mathbf{x}\,\hat{\psi}^\dagger(\mathbf{x})V^n_{\underline{\nu}}(\mathbf{x})\hat{\psi}(\mathbf{x}), \tag{7}$$

such that $\widehat{H}_{e\text{-}b}$ can be written as

$$\widehat{H}_{e\text{-}b} = \sum_{n,\underline{\nu}} \hat{\gamma}^n_{\underline{\nu}}\widehat{Q}^n_{\underline{\nu}}. \tag{8}$$

Having introduced the general electron-boson Hamiltonian (1) and specified its ingredients, our goal now is to obtain a self-consistent set of equations that relate well-defined objects such as electron and boson propagators. To this end, we generalize the Schwinger's method of functional derivatives [52], which allows us to express more complicated correlators that appear in their equations of motion (the Martin-Schwinger hierarchy) in terms of functional derivatives.

III. THE EQUATION OF MOTION FOR THE ELECTRONIC AND BOSONIC OPERATORS

A. Time-dependence

For our purpose we define operators in the Heisenberg picture (indicated here by the H subscript) with time arguments running on the Keldysh contour ($z \in \mathcal{C}$):

$$\widehat{\mathcal{O}}_H(z) \equiv \widehat{\mathcal{U}}(z_0, z)\widehat{\mathcal{O}}\,\widehat{\mathcal{U}}(z, z_0), \tag{9}$$

where z_0 is arbitrary initial time and $\hat{\mathcal{U}}(z, z_0)$ is the time-evolution operator from the initial time z_0 to z. In this picture, the operators are explicitly time-dependent, whereas wave functions are not. This allows us to make a connection with the many-body perturbation theory, which relies on the time evolution on the contour and on the Wick theorem. In what follows, the picture in which operators are given is not explicitly indicated when it can be inferred from the corresponding arguments.

The electronic, bosonic operators satisfy standard anticommutation (denoted with $+$), commutation (denoted with $-$) rules, respectively:

$$[\hat{\psi}(\mathbf{x}_1), \hat{\psi}^\dagger(\mathbf{x}_2)]_+ = \delta(\mathbf{x}_1 - \mathbf{x}_2), \tag{10a}$$

$$[\widehat{Q}_\mu\,, \widehat{P}_\nu]_- = i\delta_{\mu\nu}. \tag{10b}$$

We now introduce a short-hand notation $(\mathbf{x}_i, z_i) \equiv i$ so that $\hat{\psi}(1) \equiv \hat{\psi}(\mathbf{x}_1, z_1)$. The Heisenberg equations of motion (EOM) for $\hat{\psi}$, $\widehat{Q}$, and $\widehat{P}$ follow by applying Eqs. (10) to evaluate commutators with the full Hamiltonian $\widehat{H}$:

$$i\frac{d}{dz_1}\hat{\psi}(1) = \left[h_{\rm e}(1) + \sum_{n,\,\underline{\nu}} V^n_{\underline{\nu}}(\mathbf{x}_1)\widehat{Q}^n_{\underline{\nu}}(z_1)\right]\hat{\psi}(1), \tag{11a}$$

$$\frac{d}{dz_1}\widehat{Q}_\nu(z_1) = \Omega_\nu \widehat{P}_\nu(z_1), \tag{11b}$$

$$\frac{d}{dz_1}\widehat{P}_\nu(z_1) = -\Omega_\nu \widehat{Q}_\nu(z_1) - \sum_{m,\,\underline{\mu}} m\,\hat{\gamma}^m_{\underline{\mu}\oplus\nu}(z_1)\widehat{Q}^{m-1}_{\underline{\mu}}(z_1). \tag{11c}$$

In Eq. (11c) the combinatorial prefactor m follows from the fact that $\hat{\gamma}^m$ also is a symmetric tensor of rank m. This equation is formally demonstrated in Appendix C.

In Eq. (11c) we have introduced a general definition for a multidimensional operator whose index is a composition of two subgroups of indexes. In the case of $\hat{\gamma}^m_{\underline{\mu}\oplus\nu}$, the vector of indices $\underline{\mu}$ has $m-1$ components, and $(\underline{\mu}\oplus\nu) = (\mu_1, \ldots, \mu_{m-1}, \nu)$ is correctly m dimensional. By combining the last two of Eqs. (11) we obtain a second-order differential equation for the displacement operator [53] with a source term

$$\left[\frac{d^2}{dz_1^2} + \Omega_\nu^2\right]\widehat{Q}_\nu(z_1) = -\Omega_\nu \sum_{m,\,\underline{\mu}} m\,\hat{\gamma}^m_{\underline{\mu}\oplus\nu}(z_1)\widehat{Q}^{m-1}_{\underline{\mu}}(z_1). \tag{12}$$

More complicated operators appearing on the right-hand side of Eqs. (11) and (12) can be expressed using the method of functional derivatives.

B. Functional derivatives

In order to introduce the functional derivatives approach we couple the Hamiltonian to *time-dependent auxiliary fields* $\xi^n_{\underline{\nu}}(z)$ and $\eta(\mathbf{x}, z)$,

$$\hat{H}_{\xi,\eta}(z) = \hat{H} + \sum_{n,\,\underline{\nu}} \xi^n_{\underline{\nu}}(z)\widehat{Q}^n_{\underline{\nu}}(z) + \int d\mathbf{x}\,\eta(\mathbf{x}, z)\hat{\rho}(\mathbf{x}, z), \tag{13}$$

where a superscript in $\xi^n_{\underline{\nu}}(z)$ indicates that $\underline{\nu}$ is an n-dimensional vector of indices. We introduced the electron density operator $\hat{\rho}(1) = \hat{\psi}^\dagger(1)\hat{\psi}(1)$.

Consider now the time evolution in the presence of these external fields. The corresponding time-evolution operator is denoted as $\widehat{\mathcal{U}}_{\xi,\eta}(z_0, z)$. Now in the definition of the average operator

$$\langle\hat{\mathcal{O}}_{\xi,\eta}(z)\rangle_{\xi,\eta} = \frac{\mathrm{Tr}\{\mathcal{T}\exp\left[-i\int_{\mathcal{C}} d\bar{z}\,\widehat{H}_{\xi,\eta}(\bar{z})\right]\hat{\mathcal{O}}_{\xi,\eta}(z)\}}{\mathrm{Tr}\{\mathcal{T}\exp\left[-i\int_{\mathcal{C}} d\bar{z}\,\widehat{H}_{\xi,\eta}(\bar{z})\right]\}}, \tag{14}$$

the ξ and η functions occur twice signaling that both the operator $\hat{\mathcal{O}}$ in the Heisenberg picture $\hat{\mathcal{O}}_{\xi,\eta}(z) = \widehat{\mathcal{U}}_{\xi,\eta}(z_0, z)\hat{\mathcal{O}}\widehat{\mathcal{U}}_{\xi,\eta}(z, z_0)$ and the density matrix are defined with respect to the perturbed Hamiltonian. Starting from this form various functional derivatives can be computed. We write $\langle\cdots\rangle$ for $\langle\cdots\rangle_{\xi,\eta}$ where it does not lead to ambiguities.

Let us consider the case of a generic, contour-ordered product of operators $\prod_i \hat{\mathcal{O}}^{(i)}(z_i)$. Constituent operators depend, in general, on different times z_i and are distinguished by the subscript (i). By the formal differentiation, one can prove that

$$\begin{aligned} i\,\frac{\delta}{\delta\xi^n_{\underline{\mu}}(\bar{z})}\left\langle\mathcal{T}\left\{\prod_i \hat{\mathcal{O}}^{(i)}_{\xi,\eta}(z_i)\right\}\right\rangle\Bigg|_{\xi^n_{\underline{\mu}}=0,\,\eta=0} \\ = \left\langle\mathcal{T}\left\{\prod_i \hat{\mathcal{O}}^{(i)}(z_i)\,\widehat{Q}^n_{\underline{\mu}}(\bar{z})\right\}\right\rangle \\ - \left\langle\mathcal{T}\left\{\prod_i \hat{\mathcal{O}}^{(i)}(z_i)\right\}\right\rangle\langle\widehat{Q}^n_{\underline{\mu}}(\bar{z})\rangle, \end{aligned} \tag{15}$$

where $\mathcal{T}$ denotes the contour-ordering operator. The second term in Eq. (15) stems from the variation of denominator, i.e., it assures correct normalization. In general, this identity can contain side by side electronic and bosonic operators and also operators with equal time arguments. For the latter, the standard definition of $\mathcal{T}$ needs to be amended with a rule that equal-time operators do not change their relative order upon contour ordering. For mixed operators, only the permutations of the electronic ones induce a sign change [46].

A similar expression holds for the derivative with respect to η:

$$i\frac{\delta}{\delta\eta(1)}\left\langle\mathcal{T}\left\{\prod_i \hat{\mathcal{O}}^{(i)}_{\xi,\eta}(z_i)\right\}\right\rangle\Bigg|_{\xi^n_{\underline{\mu}}=0,\,\eta=0}$$
$$=\left\langle\mathcal{T}\left\{\prod_i \hat{\mathcal{O}}^{(i)}(z_i)\,\rho(1)\right\}\right\rangle-\left\langle\mathcal{T}\left\{\prod_i \hat{\mathcal{O}}^{(i)}(z_i)\right\}\right\rangle\langle\rho(1)\rangle. \tag{16}$$

Here and in the following we always assume that the limit of zero auxiliary fields is taken after variations. In practice, however, this means that during derivations all Green's functions are formally dependent on the auxiliary fields. This will be evident from the form of the electronic and bosonic Dyson equations with mean fields that include the auxiliary fields.

IV. GREEN'S FUNCTION AND DIAGRAMMATIC NOTATION

We use the standard definitions of the electronic Green's function (GF) on the Keldysh contour:

$$G(1,2)=-i\langle\mathcal{T}\{\hat{\psi}(1)\hat{\psi}^\dagger(2)\}\rangle, \tag{17}$$

where $\langle\cdots\rangle$ is the trace evaluated with the exact density matrix.

The bosonic propagators on the Keldysh contour extend the definition of the electronic case

$$D^{m,n}_{\underline{\mu},\underline{\nu}}(z_1,z_2)=-i\left\langle\mathcal{T}\left\{\Delta\widehat{Q}^m_{\underline{\mu}}(z_1)\Delta\widehat{Q}^n_{\underline{\nu}}(z_2)\right\}\right\rangle, \tag{18}$$

where $\Delta\hat{\mathcal{O}}\equiv\hat{\mathcal{O}}-\langle\hat{\mathcal{O}}\rangle$ is the fluctuation operator. In the case $m=n=1$ the standard bosonic propagator is recovered:

$$D_{\mu,\nu}(z_1,z_2)=D^{1,1}_{\mu,\nu}(z_1,z_2). \tag{19}$$

Thanks to Eq. (14), we can rewrite $D^{m,n}$ as

$$iD^{m,n}_{\underline{\mu},\underline{\nu}}(z_1,z_2)=\left\langle\mathcal{T}\widehat{Q}^m_{\underline{\mu}}(z_1)\widehat{Q}^n_{\underline{\nu}}(z_2)\right\rangle-\left\langle\widehat{Q}^m_{\underline{\mu}}(z_1)\right\rangle\left\langle\widehat{Q}^n_{\underline{\nu}}(z_2)\right\rangle$$
$$=i\frac{\delta\left\langle\widehat{Q}^m_{\underline{\mu}}(z_1)\right\rangle}{\delta\xi^n_{\underline{\nu}}(z_2)}. \tag{20}$$

This equation can be further generalized to

$$D^{m,n}_{\underline{\mu},\underline{\nu}}(z_1,z_2)=i\frac{\delta}{\delta\xi^k_{\underline{\kappa}}(z_1)}D^{m-k,n}_{\underline{\lambda},\underline{\nu}}(z_1,z_2)$$
$$+\left\langle\widehat{Q}^k_{\underline{\kappa}}(z_1)\right\rangle D^{m-k,n}_{\underline{\lambda},\underline{\nu}}(z_1,z_2)$$
$$+\left\langle\widehat{Q}^{m-k}_{\underline{\lambda}}(z_1)\right\rangle D^{k,n}_{\underline{\kappa},\underline{\nu}}(z_1,z_2), \tag{21}$$

for $k<m$ and $\underline{\mu}=\underline{\kappa}\oplus\underline{\lambda}$. Equation (21) is proved in Appendix D. The last two terms represent a contraction of symmetric tensors of ranks $m-k$ and k yielding a symmetric tensor of rank m (with respect to the first argument). We will make extensive use of these differential forms of $D^{m,n}$ as well as of the representations in terms of Feynman diagrams. We introduce *ad hoc* graphical objects to easily represent the multifold aspects of the nonlinear e-b interaction; in Fig. 2 all ingredients of the diagrammatic representation are shown.

In general, the selection of k bosonic operators out of m that appear on the right-hand side (r.h.s.) of Eq. (21) can be performed in $\binom{m}{k}$ ways. These correspond to all the possible

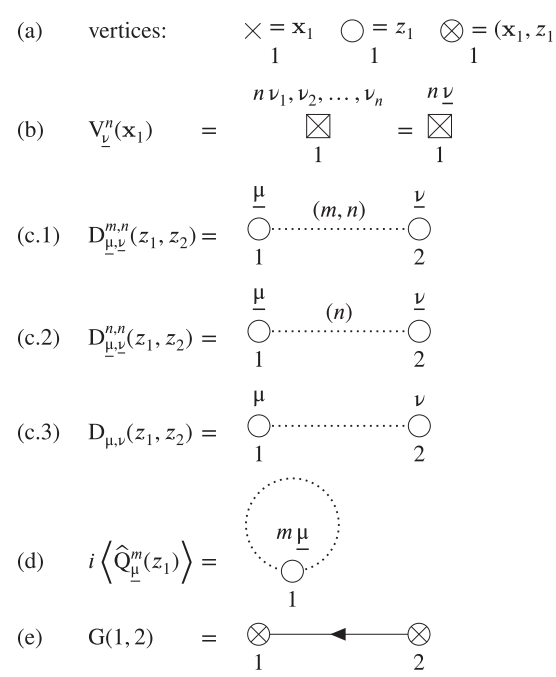

FIG. 2. Definition of the diagrammatic elements used in this work. (a) ◯ and × represent a generic time and position point, respectively. These two symbols can be combined to indicate a time and position vertex $\oplus_1$ equivalent to $1=(\mathbf{x}_1,z_1)$. (b) Finally a box around a spatial point represents the scattering integral $V^n_{\underline{\nu}}(\mathbf{x})$ with two fermionic and n bosonic dangling lines. (c) Bosonic propagators can be represented in three different forms depending on their order. (d) Expectation value of the bosonic coordinates expressed in terms of a bosonic propagator. (e) Electronic Green's function.

choices of k elements out of m. However Eq. (21) is *exact* for any choice of the $\underline{\kappa}$ elements. Therefore no combinatorial prefactor is needed whenever Eq. (21) is used.

By using Eq. (6) we can write

$$\left\langle\widehat{Q}^m_{\underline{\mu}\oplus\nu}(z_1)\right\rangle=iD^{m-1,1}_{\underline{\mu},\nu}(z_1,z_1^+). \tag{22}$$

We use here $z_1^+=z_1+0^+$. It is important to note here that in the limit $\xi^n_{\underline{\mu}}=0$, $\eta=0$ we have that $\langle\widehat{Q}^m_{\underline{\mu}\oplus\nu}(z_1)\rangle$ is constant because of the time-translation invariance. However, during the derivation the time dependence is induced by the auxiliary fields.

The EOM for bosonic displacement operators (12) leads us to consider a specific case of $D^{m-1,1}$, which can be reduced to simpler propagators by the application of Eq. (21) with $k=m-2$:

$$D^{m-1,1}_{\underline{\mu},\nu}(z_1,z_2)=i\frac{\delta}{\delta\xi^{m-2}_{\underline{\kappa}}(z_1)}D_{\lambda,\nu}(z_1,z_2)$$
$$+\left\langle\widehat{Q}^{m-2}_{\underline{\kappa}}(z_1)\right\rangle D_{\lambda,\nu}(z_1,z_2), \tag{23}$$

where we used the fact that $\langle\widehat{Q}_\lambda\rangle$ is zero in the limit of vanishing auxiliary fields and $\underline{\mu}=\underline{\kappa}\oplus\lambda$.

V. ELECTRON DYNAMICS

The EOM for G is obtained with the help of EOMs for the constituent operators and using the relation

$\frac{d}{dz_1}\theta(z_1 - z_2) = \delta(z_1 - z_2)$. Thus we have

$$\left[i\frac{\partial}{\partial z_1} - h_{\rm e}(1) - \eta(1)\right]G(1,2) = \delta(1,2) - i\sum_{n,\underline{\nu}} V^n_{\underline{\nu}}(\mathbf{x}_1)\left\langle \mathcal{T}\left\{\hat{\psi}(1)\widehat{Q}^n_{\underline{\nu}}(z_1)\hat{\psi}^\dagger(2)\right\}\right\rangle. \quad (24)$$

Using Eq. (15), the correlator on the r.h.s. of Eq. (24) can be expressed as the functional derivative

$$-i\left\langle \mathcal{T}\hat{\psi}(1)\widehat{Q}^n_{\underline{\nu}}(z_1)\hat{\psi}^\dagger(2)\right\rangle = \left[i\frac{\delta}{\delta\xi^n_{\underline{\nu}}(z_1)} + \left\langle \widehat{Q}^n_{\underline{\nu}}(z_1)\right\rangle\right]G(1,2). \quad (25)$$

Our goal is to rewrite Eq. (24) in the form of a Dyson equation, which involves a dressed mean-field potential Φ and correlated mass operator M:

$$\left[i\frac{\partial}{\partial z_1} - h_{\rm e}(1) - \eta(1) - \Phi(1)\right]G(1,2) = \delta(1,2) + \int d3\, M(1,3)G(3,2). \quad (26)$$

The potential Φ follows from the second term on the r.h.s. of Eq. (25),

$$\Phi(1) = \sum_{n,\underline{\nu}} V^n_{\underline{\nu}}(\mathbf{x}_1)\left\langle \widehat{Q}^n_{\underline{\nu}}(z_1)\right\rangle. \quad (27)$$

The mass operator is implicitly written as

$$\int d3\, M(1,3)G(3,2) = i\sum_{n,\underline{\nu}} V^n_{\underline{\nu}}(\mathbf{x}_1)\frac{\delta}{\delta\xi^n_{\underline{\nu}}(z_1)}G(1,2). \quad (28)$$

The potential Φ and the mass operator M can be conveniently combined in the electronic self-energy operator $\Sigma^{\rm e}$:

$$\Sigma^{\rm e}(1,2) = \Phi(1)\delta(1,2) + M(1,2). \quad (29)$$

A. The *n*th-order Debye-Waller potential

In order to rewrite Φ in terms of the bosonic Green's function, we apply Eq. (22) to Eq. (27). It follows that we can introduce a nth-order bosonic mean field $\Phi^n_{\rm DW}(1)$ defined as

$$\Phi^n_{DW}(1) = i\sum_{\underline{\nu}} V^n_{\underline{\nu}}(\mathbf{x}_1)D^{n-1,1}_{\underline{\mu},\nu_n}(z_1, z_1^+), \quad (30)$$

with $\underline{\nu} = \underline{\mu} \oplus \nu_n$. $\Phi^n_{\rm DW}$ is showed in diagrammatic form in Fig. 3(a) in the general case.

Equation (30) provides a generalization of the Debye-Waller (DW) potential to arbitrary orders. The expression of this potential is well known in the electron-phonon case only when $n = 2$, and it has been derived only by using a diagrammatic approach. In the present case, it naturally appears as the mean-field electronic potential induced by the nonlinear electron-boson interaction:

$$\Phi^2_{\rm DW}(1) = i\sum_{\nu_1,\nu_2} V^2_{\nu_1,\nu_2}(\mathbf{x}_1)D_{\nu_1,\nu_2}(z_1, z_1^+). \quad (31)$$

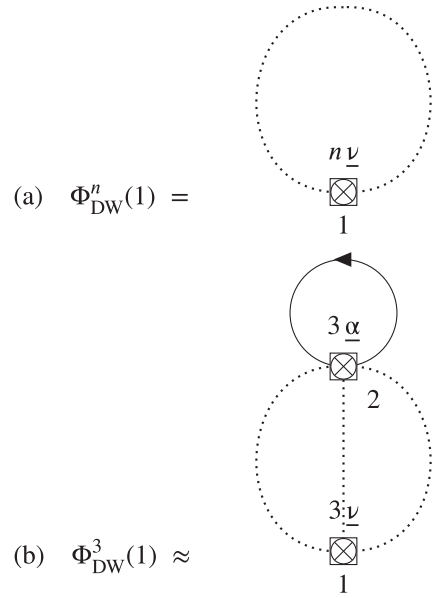

FIG. 3. (a) Diagrammatic form of the nth-order DW potential. (b) Perturbative expansions in term of *bare* bosonic propagators (they are denoted as dashed lines) lead to complicated diagrams. The inclusion of nonlinear e-b interaction leads to nonvanishing odd-order terms that are zero in the linear interaction case.

The DW potential has a long history in the electron-phonon context. Early developments are nicely summarized in the HAC approach. They present a very simple perturbation theory derivation that also emphasizes a close connection with self-energy originating from the first-order coupling (due to translational invariance).

The present approach extends its definition to arbitrary orders and, also, highlights its physical origin. The Schwinger's variational derivative technique has the merit of showing that the mean-field potential is due to the dressing of the η potential induced by the nth-order fictitious interaction ξ^n. Physically this corresponds to the dressing of the electronic potential induced by strongly anharmonic effects.

This also clarifies why the DW potential is not present in any previous treatment [27,54] of the electron-phonon interaction performed using the Schwinger's variational derivative technique. The reason is that in these works the e-b interaction is treated at the first order only.

In conventional theories involving linear electron-boson interactions the $\langle \widehat{Q}^n_{\underline{\mu}}(z_1)\rangle$ averages are, in general, connected to the boson mean displacement ($n = 1$) and the population ($n = 2$). As a consequence, it is zero for any odd value of n. The presence of higher-order e-b interactions deeply modifies this simple scenario. $\langle \widehat{Q}^n_{\underline{\mu}}(z_1)\rangle$ is a nth-order bosonic tadpole whose dynamics includes nontrivial contributions, like the one showed in Fig. 3(b). These tadpoles are, in general, nonzero.

B. The mass operator

The mass operator requires additional manipulations. We integrate by parts

$$M(1,2) = i\sum_{n,\underline{\nu}} V^n_{\underline{\nu}}(\mathbf{x}_1)\int d3\left[\frac{\delta}{\delta\xi^n_{\underline{\nu}}(z_1)}G(1,3)\right]G^{-1}(3,2)$$
$$= -i\sum_{n,\underline{\nu}} V^n_{\underline{\nu}}(\mathbf{x}_1)\int d3\, G(1,3)\frac{\delta}{\delta\xi^n_{\underline{\nu}}(z_1)}G^{-1}(3,2). \tag{32}$$

This equation is exact. Now the problem is how to evaluate this variational derivative. By noticing that

$$\left[i\frac{\partial}{\partial z_1} - h_{\mathrm{e}}(1) - \eta(1) - \Phi(1)\right]\delta(1,2)$$
$$= G^{-1}(1,2) + M(1,2), \tag{33}$$

we have that

$$-\frac{\delta}{\delta\xi^n_{\underline{\nu}}(z_1)}G^{-1}(3,2) = \frac{\delta\Phi(2)}{\delta\xi^n_{\underline{\nu}}(z_1)}\delta(2,3) + \frac{\delta M(3,2)}{\delta\xi^n_{\underline{\nu}}(z_1)}$$
$$= \frac{\delta\Phi(2)}{\delta\xi^n_{\underline{\nu}}(z_1)}\delta(2,3) - \int d4567\,\frac{\delta_t M(3,2)}{\delta_t G(4,5)}$$
$$\times G(4,6)\frac{\delta G^{-1}(6,7)}{\delta\xi^n_{\underline{\nu}}(z_1)}G(7,5). \tag{34}$$

In Eq. (34) we have introduced the δ_t symbol to make clear that we are using a *total* derivative. In this way the derivation of the electronic self-energy and vertex function closely follows the well-established procedure introduced in the case of the linear e-b coupling [27]. In the next section we will further discuss this subtle but important aspect.

We can now define a vertex function that extends to the e-b case the known electronic vertex function. In order to do so we start by expanding the first term appearing on the r.h.s. of Eq. (34) using Eq. (20):

$$\frac{\delta\Phi(2)}{\delta\xi^n_{\underline{\nu}}(z_1)} = \sum_{m,\underline{\mu}} V^m_{\underline{\mu}}(\mathbf{x}_2)\frac{\delta\langle Q^m_{\underline{\mu}}(z_2)\rangle}{\delta\xi^n_{\underline{\nu}}(z_1)}$$
$$= \sum_{m,\underline{\mu}} V^m_{\underline{\mu}}(\mathbf{x}_2)D^{m,n}_{\underline{\mu},\underline{\nu}}(z_2,z_1). \tag{35}$$

It is natural to define the electron-boson vertex function $\Gamma^{\text{e-b},m}_{\underline{\mu}}(1,2;z)$ [55] as

$$-\frac{\delta}{\delta\xi^n_{\underline{\nu}}(z_1)}G^{-1}(3,2)$$
$$\equiv \Gamma^{\text{e-b},n}_{\underline{\nu}}(3,2;z_1)$$
$$= -\sum_{m,\underline{\mu}}\int dz_4\,\frac{\delta G^{-1}(3,2)}{\delta\langle Q^m_{\underline{\mu}}(z_4)\rangle}\frac{\delta\langle Q^m_{\underline{\mu}}(z_4)\rangle}{\delta\xi^n_{\underline{\nu}}(z_1)}$$
$$= \sum_{m,\underline{\mu}}\int dz_4\,\overline{\Gamma}^{\text{e-b},m}_{\underline{\mu}}(3,2;z_4)D^{m,n}_{\underline{\mu},\underline{\nu}}(z_4,z_1). \tag{36}$$

Here we have also introduced an alternative form of the e-b vertex function:

$$\overline{\Gamma}^{\text{e-b},n}_{\underline{\mu}}(1,2;z_3) \equiv -\frac{\delta G^{-1}(1,2)}{\delta\langle Q^n_{\underline{\mu}}(z_3)\rangle}. \tag{37}$$

From Eqs. (35) and (37) it follows that $\overline{\Gamma}^{\text{e-b}}$ satisfies the following integrodifferential equation:

$$\overline{\Gamma}^{\text{e-b},n}_{\underline{\nu}}(1,2;z_3) = \overline{\Gamma}^{\text{e-b},n}_{\underline{\nu}}(1,2;z_3)\big|_0 + \int d4567\,\frac{\delta_t M(1,2)}{\delta_t G(4,5)}$$
$$\times G(4,6)\overline{\Gamma}^{\text{e-b},n}_{\underline{\nu}}(6,7;z_3)G(7,5), \tag{38}$$

with

$$\overline{\Gamma}^{\text{e-b},n}_{\underline{\nu}}(1,2;z_3)\big|_0 = \frac{\delta\Phi(1)}{\delta\langle Q^n_{\underline{\nu}}(z_3)\rangle}\delta(1-2)$$
$$= \delta(1-2)\delta(z_1-z_3)V^n_{\underline{\nu}}(\mathbf{x}_1). \tag{39}$$

In Eq. (38) appears M [defined in Eq. (29)] instead of Σ^{e} as η does not depend on ξ and the lowest-order derivative comes through Φ. This, in practice, means that in the independent particle approximation (IPA) ($\Sigma^{\mathrm{e}} = 0$) the mixed e-b vertex is zero, as it should be.

By analogy with the electronic case, it can be regarded as the Bethe-Salpeter equation for the vertex function. It was discussed in the linear electron-phonon coupling by van Leeuwen [27]. Equation (38) also defines the electron-electron kernel

$$K^{\text{e-e}}(1,5;2,4) \equiv \frac{\delta_t\Sigma^{\mathrm{e}}(1,2)}{\delta_t G(4,5)} \tag{40}$$

that will also appear in Sec. VIII A in the case of the equation of motion for the electronic response function. Note that in this section we have already introduced a specific notation for the vertex and for the kernel. Indeed, in both cases we have that the vertex/kernel is defined as the functional derivative of electronic/bosonic observable (the inverse GF for the vertex and the self-energy for the kernel) with respect to an electronic/bosonic potential (for the vertex) or GF (for the kernel). In the present case $K^{\text{e-e}}$ is purely electronic, while in $\Gamma^{\text{e-b}}$ the field ξ is bosonic. In the following sections we will introduce other vertexes and associated kernels and demonstrate that they are connected via matrix generalization of the Bethe-Salpeter equation.

The full mass operator can be finally written as

$$M(1,2) = i\sum_{n,\underline{\nu}}\sum_{m,\underline{\mu}}\int d3\int dz_4\, V^n_{\underline{\nu}}(\mathbf{x}_1)G(1,3)$$
$$\times\,\overline{\Gamma}^{\text{e-b},m}_{\underline{\mu}}(3,2;z_4)D^{m,n}_{\underline{\mu},\underline{\nu}}(z_4,z_1). \tag{41}$$

By comparing the expression for the electron self-energy with the expression in a pure electronic case one observes that $\sum_{m,\underline{\mu}}\sum_{n,\underline{\nu}} V^m_{\underline{\mu}}(3)D^{mn}_{\underline{\mu}\underline{\nu}}(z_3,z_1)V^n_{\underline{\nu}}(1)$ plays the role of the screened Coulomb interaction.

Equation (41) is not the most convenient representation of the electron self-energy because there is no simple way of computing the kernel $K^{\text{e-e}}(1,5;2,4)$ even though the diagrammatic form of Σ^{e} is known. As can be seen from the exact formula,

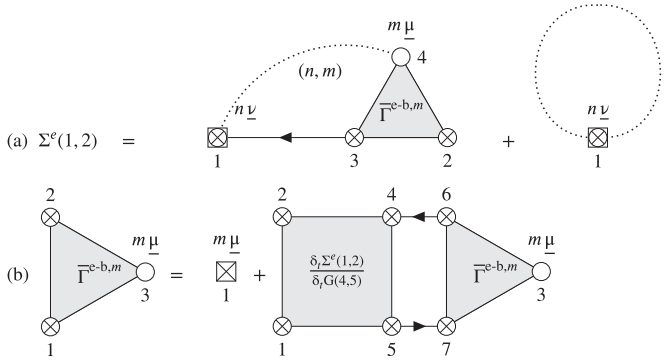

FIG. 4. Diagrammatic form of the self-energy operator (a) and of the vertex function (b) for arbitrary orders of the electron-boson interaction and arbitrary number of bosons involved in the scattering. In order to close this set of equations, expressions for the bosonic propagator $D^{m,n}$ (Secs. VI C and VIII) and the vertex function $\overline{\Gamma}^{e\text{-}b,n}$ (Sec. VI D) are additionally needed. The lowest order approximation for the electron self-energy is described in Sec. VII.

Eq. (41), and its diagrammatic representation in Fig. 4(a), the self-energy contains the bosonic propagator D, and, therefore, the variation $\frac{\delta\Sigma^e(1,2)}{\delta D(4,5)}$ is implicitly included in the $\frac{\delta_t\Sigma^e(1,2)}{\delta_t G(4,5)}$. This is the main difference from the pure electronic case, where the screened interaction *explicitly* depends on the electron Green's function. Thus, although Eq. (41) is exact, it is not practical. A better approach is to consider from the beginning the electronic self-energy to be a functional of both propagators, i.e., $\Sigma^e = \Sigma^e[G, D]$, which requires the introduction of other vertex functions. This procedure will be implemented below in combination with the bosonic self-energy.

VI. SINGLE-BOSON DYNAMICS

Starting from the equation of motion (12) for $\widehat{Q}_\mu$ we derive the equation of motion for the bosonic propagator $D_{\mu,\nu}$ in a similar way to the electronic case:

$$
\begin{aligned}
&-\frac{1}{\Omega_\mu}\left[\frac{\partial^2}{\partial z_1^2}+\Omega_\mu^2\right]D_{\mu,\nu}(z_1,z_2)\\
&\quad=\delta_{\mu\nu}\delta(z_1-z_2)\\
&\qquad-i\sum_{\underline{\zeta},n} n\Bigg[\int d\mathbf{x}_1\, V^n_{\underline{\zeta}\oplus\mu}(\mathbf{x}_1)\underbrace{\left\langle\mathcal{T}\Delta\left[\hat{\rho}(1)\,\hat{Q}^{n-1}_{\underline{\zeta}}(z_1)\right]\hat{Q}_\nu(z_2)\right\rangle}_{J_V^{(n)}}\\
&\qquad+\xi^n_{\underline{\zeta}\oplus\mu}(z_1)\underbrace{\left\langle\mathcal{T}\Delta\,\hat{Q}^{n-1}_{\underline{\zeta}}(z_1)\hat{Q}_\nu(z_2)\right\rangle}_{J_\xi^{(n)}}\Bigg],
\end{aligned}
\tag{42}
$$

The last term is driven by the auxiliary fields $\xi^n_{\underline{\zeta}}$. According to the rules specified above, the limit of zero $\xi^n_{\underline{\zeta}}$ is to be taken at the end of derivations.

In Eq. (42) we have schematically represented with $J_V^{(n)}$ and $J_\xi^{(n)}$, respectively, the term induced by the scattering potential and by the auxiliary field. The goal of this section is to rewrite

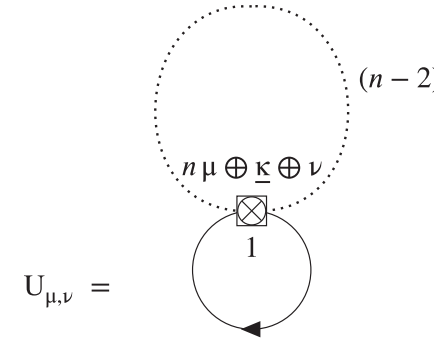

FIG. 5. The nth-order bosonic mean-field potential is one of the constituents of the total bosonic self-energy.

exactly

$$
\begin{aligned}
&-i\sum_{\underline{\zeta},n} n\left[\int d\mathbf{x}_1\, V^n_{\underline{\zeta}\oplus\mu}(\mathbf{x}_1)J_V^{(n)}+\xi^n_{\underline{\zeta}\oplus\mu}(z_1)J_\xi^{(n)}\right]\\
&\quad=\sum_\alpha\int dz_3\{\Pi_{\mu,\alpha}(z_1,z_3)\\
&\qquad+[U_{\mu,\alpha}(z_1)+\Xi_{\mu,\alpha}(z_1)]\delta(z_1-z_3)\}D_{\alpha,\nu}(z_3,z_2).
\end{aligned}
\tag{43}
$$

In Eq. (43) we have introduced the generalized bosonic mass operator Π and the mean-field potentials U and Ξ. Ξ is driven by the fictitious external field and vanishes when $\xi\to 0$. Π, U, and Ξ sum in the total bosonic self-energy Σ^b that, consistently with Eq. (29), is defined as

$$
\Sigma^b_{\mu,\nu}(z_1,z_2)=\Pi_{\mu,\nu}(z_1,z_2)+U_{\mu,\nu}(z_1)\delta(z_1-z_2). \tag{44}
$$

In order to find the explicit expression for Π, U, and Ξ, we start by observing that Eq. (42) includes linear ($n=1$) and higher-order ($n>1$) terms. In the $n=1$ case, $\langle\hat{Q}\rangle=0$, and we can use the chain rule to write

$$
\begin{aligned}
J_V^{(1)}&=\langle\mathcal{T}\hat{\rho}(1)\hat{Q}_\nu(z_2)\rangle\\
&=i\frac{\delta\langle\hat{\rho}(1)\rangle}{\delta\xi^1_\nu(z_2)}\\
&=-\int d34\, G(1,3)\frac{\delta G^{-1}(3,4)}{\delta\xi^1_\nu(z_2)}G(4,1).
\end{aligned}
\tag{45}
$$

We can now use the definition of the electronic vertex, Eq. (36), and rewrite $J_V^{(1)}$ in terms of the mass operator Π^1:

$$
\begin{aligned}
\Pi^1_{\mu,\alpha}(z_1,z_2)=\int d34\int d\mathbf{x}_1\, V^1_\mu(\mathbf{x}_1)\\
\times G(1,3)G(4,1)\overline{\Gamma}^{e\text{-}b,1}_\alpha(3,4;z_2)
\end{aligned}
\tag{46}
$$

that is diagrammatically represented in Fig. 6(a). This contribution to the bosonic mass operator does not require further manipulations and is an explicit function of the single-boson correlator D. $\Pi^{(1)}$ represents the generalization to the case of nonlinear e-b coupling of the first-order e-b mass operator well known and widely used in the literature [56,57] to calculate, for example, phonon linewidths [58].

We now move to the $n>1$ case. We observe that, thanks to Eq. (6),

$$
\left\langle\mathcal{T}\Delta\,\hat{Q}^{n-1}_{\underline{\zeta}}(z_1)\hat{Q}_\nu(z_2)\right\rangle=i\,D^{n-1,1}_{\underline{\zeta},\nu}(z_1,z_2), \tag{47}
$$

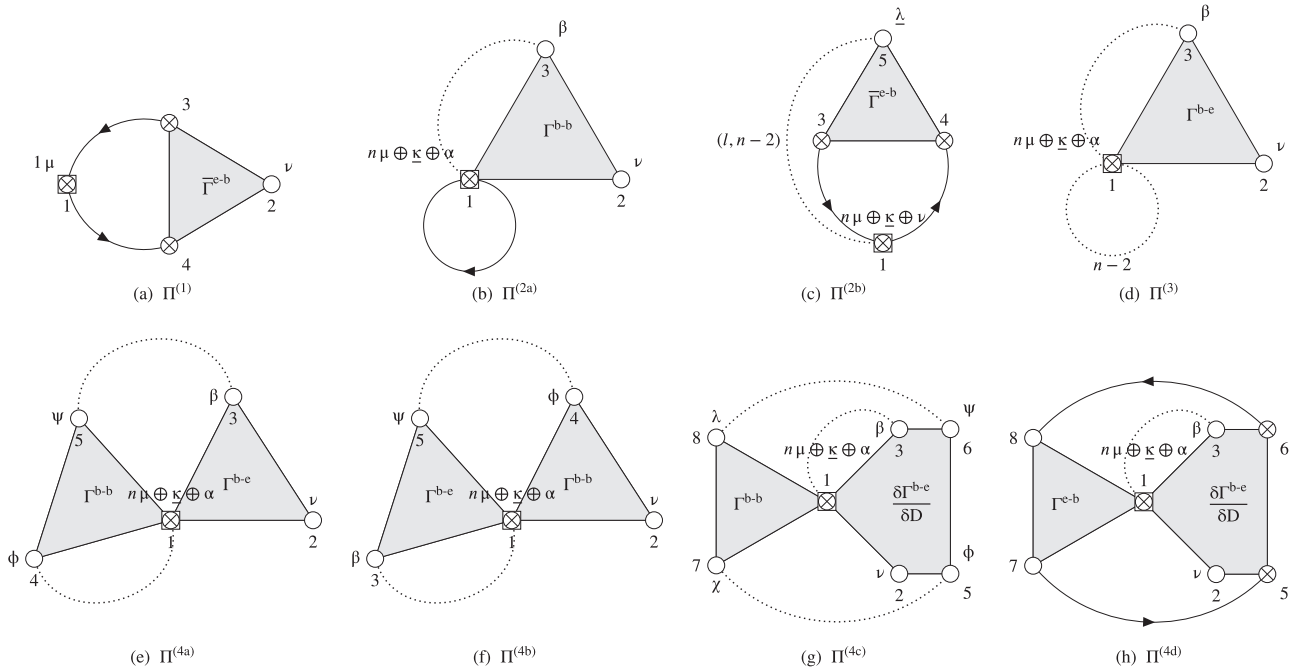

FIG. 6. A total of eight diagrams constituting the exact bosonic mass operator $\Pi_{\mu,\nu}(z_1, z_2)$.

and, by using Eq. (23) with $m = n$ and $k = n - 2$, we can express $J_{\xi}^{(n>1)}$ as

$$J_{\xi}^{(n>1)} = \sum_{\underline{\zeta}} n\, \xi^{n}_{\underline{\zeta}\oplus\mu}(z_1) D^{n-1,1}_{\underline{\zeta},\nu}(z_1, z_2) = \sum_{\underline{\kappa},\alpha} n\, \xi^{n}_{\mu\oplus\underline{\kappa}\oplus\alpha}(z_1)\left(\langle \widehat{Q}^{n-2}_{\underline{\kappa}}(z_1)\rangle + i\frac{\delta}{\delta\xi^{n-2}_{\underline{\kappa}}(z_1)}\right) D_{\alpha,\nu}(z_1, z_2), \tag{48}$$

with $\underline{\zeta} = \underline{\kappa} \oplus \alpha$.

The $J_{V}^{(n>1)}$ correlator can be evaluated by using Eq. (16):

$$J_{V}^{(n>1)} = \left(\langle \widehat{Q}^{n-2}_{\underline{\kappa}}(z_1)\rangle + i\frac{\delta}{\delta\xi^{n-2}_{\underline{\kappa}}(z_1)}\right)\left(\langle\hat{\rho}(1)\rangle + i\frac{\delta}{\delta\eta(1)}\right) D_{\alpha,\nu}(z_1, z_2). \tag{49}$$

In Eq. (49) the $\delta\eta$ derivative is made acting before the $\delta\xi$ one. In this way the limit of zero external field can be safely taken and the last term of Eq. (23) vanishes. It is, indeed, important to remind that $\langle \widehat{Q}_{\alpha}(z_1)\rangle = 0$ only when $\xi = 0$.

If we now collect Eqs. (48) and (49) and plug them into Eq. (42) we can recast the EOM for D in the form

$$-\frac{1}{\Omega_\mu}\left[\frac{\partial^2}{\partial z_1^2} + \Omega_\mu^2\right] D_{\mu,\nu}(z_1, z_2) = \delta_{\mu\nu}\delta(z_1 - z_2) + \sum_{n>1,\,\underline{\kappa},\alpha} n \underbrace{\left[\langle \hat{\gamma}^{n}_{\mu\oplus\underline{\kappa}\oplus\alpha}(z_1)\rangle + \xi^{n}_{\mu\oplus\underline{\kappa}\oplus\alpha}(z_1)\right]\langle \widehat{Q}^{n-2}_{\underline{\kappa}}(z_1)\rangle D_{\alpha,\nu}(z_1, z_2)}_{U+\Xi}$$

$$+ \sum_{\alpha}\int dz_3\, \Pi^{(1)}_{\mu,\alpha}(z_1, z_3) D_{\alpha,\nu}(z_3, z_2) + \sum_{n>1,\,\underline{\kappa},\alpha} n \int d\mathbf{x}_1\, V^{n}_{\mu\oplus\underline{\kappa}\oplus\alpha}(\mathbf{x}_1)\Bigg[\underbrace{i\frac{\delta[\rho(1) D_{\alpha,\nu}(z_1, z_2)]}{\delta\xi^{n-2}_{\underline{\kappa}}(z_1)}}_{\Pi^{(2)}}$$

$$+ \underbrace{i\langle \widehat{Q}^{n-2}_{\underline{\kappa}}(z_1)\rangle\frac{\delta D_{\alpha,\nu}(z_1, z_2)}{\delta\eta(1)}}_{\Pi^{(3)}} - \underbrace{\frac{\delta^2 D_{\alpha,\nu}(z_1, z_2)}{\delta\eta(1)\delta\xi^{n-2}_{\underline{\kappa}}(z_1)}}_{\Pi^{(4)}}\Bigg]. \tag{50}$$

Equation (50) represents a key result of this work. We have already schematically identified the different terms that compose the EOM for D. The $J_{\xi}^{(n)}$ term reduces, when $\xi^n \to 0$ only to the U potential, while the $J_{V}^{(n)}$ term reduces to the sum of three mass operators. In the following we study them in detail in order to recast Eq. (50) in the form of a Dyson equation for D.

A. Mean-field potentials

The first contribution to the EOM for D is through the mean-field potentials U and Ξ. These potentials are due to the first term on the r.h.s. of Eq. (48) and to the $\langle \widehat{Q}^{n-2}_{\underline{\kappa}}(z_1)\rangle D_{\alpha,\nu}(z_1,z_2)$ term in Eq. (50). The sum of these two terms can be rewritten as the action of two local potentials on the bosonic propagator:

$$\sum_{\alpha}[U_{\mu,\alpha}(z_1)+\Xi_{\mu,\alpha}(z_1)]D_{\alpha,\nu}(z_1,z_2), \tag{51}$$

with

$$U_{\mu,\alpha}(z_1)=\sum_{n\geqslant 2,\,\underline{\kappa}} n\langle \hat{\gamma}^{n}_{\mu\oplus\underline{\kappa}\oplus\alpha}(z_1)\rangle\langle \widehat{Q}^{n-2}_{\underline{\kappa}}(z_1)\rangle, \tag{52a}$$

$$\Xi_{\mu,\alpha}(z_1)=\sum_{n\geqslant 2,\,\underline{\kappa}} n\xi^{n}_{\mu\oplus\underline{\kappa}\oplus\alpha}(z_1)\langle \widehat{Q}^{n-2}_{\underline{\kappa}}(z_1)\rangle. \tag{52b}$$

We remind the reader that $\xi^{n}_{\mu\oplus\underline{\kappa}\oplus\alpha}$ and $\hat{\gamma}^{n}_{\mu\oplus\underline{\kappa}\oplus\alpha}$ are symmetric tensors of rank n, and $\underline{\kappa}$ is an $n-2$ dimensional vector. Equation (52a) is represented diagrammatically in Fig. 5 in the limit of vanishing auxiliary fields.

B. The pure bosonic vertex function $\Gamma^{\text{b-b}}$

A key ingredient of Eq. (50) is the first-order derivative $\frac{\delta D(z_1,z_2)}{\delta\xi^{n}(z_1)}$. This term shows some remarkable properties that we study here in detail. We start from the term

$$\frac{\delta D_{\alpha,\nu}(z_1,z_2)}{\delta\xi^{n-2}_{\underline{\kappa}}(z_1)}=\sum_{\beta,\gamma}\int dz_3dz_4\, D_{\alpha,\beta}(z_1,z_3)\Gamma^{\text{b-b},n-2}_{\beta,\gamma;\underline{\kappa}}(z_3,z_4;z_1)D_{\gamma,\nu}(z_4,z_2). \tag{53}$$

Equation (53) introduces a further vertex with an entire bosonic character:

$$\Gamma^{\text{b-b},n}_{\beta,\gamma;\underline{\kappa}}(z_1,z_2;z_3)\equiv-\frac{\delta D^{-1}_{\beta,\gamma}(z_1,z_2)}{\delta\xi^{n}_{\underline{\kappa}}(z_3)}. \tag{54}$$

The lowest-order contribution to this vertex function is from the variational derivative of the driving field entering the mean-field potential, Eq. (52a):

$$\Gamma^{\text{b-b},n}_{\beta,\gamma;\underline{\lambda}}(z_1,z_2;z_3)\big|_0=\sum_{m\geqslant 2,\,\underline{\kappa}} m\frac{\delta\big[\xi^{m}_{\mu\oplus\underline{\kappa}\oplus\alpha}(z_1)\langle \widehat{Q}^{m-2}_{\underline{\kappa}}(z_1)\rangle\big]}{\delta\xi^{n}_{\underline{\lambda}}(z_3)}\delta(z_1-z_2). \tag{55}$$

In the limit $\xi\to 0$ only the derivative of $\xi^{m}_{\mu\oplus\underline{\kappa}\oplus\alpha}(z_1)$ gives a nonzero contribution. As written previously the ξ function is totally symmetric. In practice this means that, if we call $\underline{I}$ the n-dimensional vector containing a generic permutation of the $\underline{\lambda}$ indexes, we have that $\xi^{n}_{\underline{\lambda}}=\xi^{n}_{\lambda_{I_1},\ldots,\lambda_{I_n}}$. It follows that

$$\frac{\delta\xi^{m}_{\mu\oplus\underline{\kappa}\oplus\alpha}(z_1)}{\delta\xi^{n}_{\underline{\lambda}}(z_3)}=\delta(z_1-z_3)\delta_{nm}\frac{n}{n!}\sum_{I=1}^{n!}\delta_{\kappa_1,\lambda_{I_2}}\cdots\delta_{\kappa_1,\lambda_{I_{n-1}}}\delta_{\mu,\lambda_{I_1}}\delta_{\alpha,\lambda_{I_n}}. \tag{56}$$

Equation (56) gives, in practice, only $n(n-1)$ terms as all $\binom{n}{n-2}$ permutations of $\lambda_{I_2}\cdots\lambda_{I_{n-1}}$ inside the $\langle \widehat{Q}^{m-2}_{\lambda_{I_2}\cdots\lambda_{I_{n-1}}}(z_1)\rangle$ gives the same contribution. The final form of $\Gamma^{\text{b-b},n}|_0$ is, therefore

$$\Gamma^{\text{b-b},n}_{\beta,\gamma;\underline{\lambda}}(z_1,z_2;z_3)\big|_0\equiv\Gamma^{\text{b-b},n}_{\beta,\gamma;\underline{\lambda}}(z_1)\big|_0\delta(z_1-z_2)\delta(z_1-z_3)=\frac{1}{(n-1)!}\sum_{I=1}^{n!}\langle \widehat{Q}^{n-2}_{\lambda_{I_2}\cdots\lambda_{I_{n-1}}}(z_1)\rangle\delta_{\mu,\lambda_{I_1}}\delta_{\alpha,\lambda_{I_n}}\delta(z_1-z_2)\delta(z_1-z_3). \tag{57}$$

Note the contracted single-time form of $\Gamma^{\text{b-b},n}|_0$ introduced in Eq. (57). It will be used in the zeroth-order approximations for Σ^{b}, cf. Eq. (44).

C. Nonlinear self-energies

The first term we analyze is $\Pi^{(2)}$. With the help of Eq. (53) it follows that

$$\Pi^{(2a)}_{\mu,\nu}(z_1,z_2)=i\sum_{n\geqslant 2,\,\underline{\kappa},\alpha} n\langle \hat{\gamma}^{n}_{\mu\oplus\underline{\kappa}\oplus\alpha}(z_1)\rangle\sum_{\beta}\int dz_3\, D_{\alpha,\beta}(z_1,z_3)\Gamma^{\text{b-b},n-2}_{\beta,\nu;\underline{\kappa}}(z_3,z_2;z_1). \tag{58}$$

By expressing the electron density in terms of the equal times Green's function as $\rho(1) = -iG(1,1^+)$, we compute the variation $\frac{\delta\langle\hat{\rho}(1)\rangle}{\delta\xi^{n-2}_{\underline{\kappa}}(z_1)}$. It yields

$$\Pi^{(2b)}_{\mu,\nu}(z_1) = \sum_{n\geqslant 2,\,\underline{\kappa},\underline{\lambda},l} n \int d\mathbf{x}_1\, V^n_{\mu\oplus\underline{\kappa}\oplus\nu}(\mathbf{x}_1) \int d34\, G(1,3) \int dz_5\, \overline{\Gamma}^{\text{e-b},l}_{\underline{\lambda}}(3,4;z_5) D^{l,n-2}_{\underline{\lambda},\underline{\kappa}}(z_5,z_1) G(4,1^+). \tag{59}$$

This mass operator is *local* and can be seen as a correlated correction to U. There is no analogous contribution to the mean-field potential in pure electronic systems, and to the best of our knowledge, it was not discussed in the context of e-b interactions.

Next we consider the $\langle\widehat{Q}^{n-2}_{\underline{\kappa}}\rangle\frac{\delta D}{\delta\eta}$ variation

$$\Pi^{(3)}_{\mu,\nu}(z_1,z_2) = i \sum_{n\geqslant 2,\,\underline{\kappa},\alpha} n \int d\mathbf{x}_1\, V^n_{\mu\oplus\underline{\kappa}\oplus\alpha}(\mathbf{x}_1)\langle\widehat{Q}^{n-2}_{\underline{\kappa}}(z_1)\rangle \sum_{\beta}\int dz_3\, D_{\alpha,\beta}(z_1,z_3)\Gamma^{\text{b-e}}_{\beta,\nu}(z_3,z_2;1) \tag{60}$$

[Fig. 6(d)], where we used the chain rule of differentiation and introduced a new vertex function with two bosonic and one fermionic coordinates:

$$\Gamma^{\text{b-e}}_{\beta,\gamma}(z_1,z_2;3) \equiv -\frac{\delta D^{-1}_{\beta,\gamma}(z_1,z_2)}{\delta\eta(3)} = -\int d4\,\frac{\delta D^{-1}_{\beta,\gamma}(z_1,z_2)}{\delta\langle\hat{\rho}(4)\rangle}\frac{\delta\langle\hat{\rho}(4)\rangle}{\delta\eta(3)} \equiv \int d4\,\overline{\Gamma}^{\text{b-e}}_{\beta,\gamma}(z_1,z_2;4)\chi(4,3). \tag{61}$$

Notice that similarly to the other mixed vertex, Eq. (36), we pulled out the common part of the functional derivative from the definition. The common part is given by the electron density response function

$$\chi(1,2) = \frac{\delta\langle\hat{\rho}(1)\rangle}{\delta\eta(2)} = -i\frac{\delta G\left(1,1^+\right)}{\delta\eta(2)}. \tag{62}$$

Other terms as well as contributions to the vertex function $\Gamma^{\text{b-e}}_{\beta,\gamma}(z_1,z_2;3)$ from the bosonic self-energy will be considered in the next section.

Our next contribution results from the application of double differential operators $\frac{\delta^2}{\delta\xi^{n-2}_{\underline{\kappa}}(z_1)\delta\eta(1)}$ and consists of three terms

$$\Pi^{(4a)}_{\mu,\nu}(z_1,z_2) = -\sum_{n\geqslant 2,\,\underline{\kappa},\alpha} n \int d\mathbf{x}_1\, V^n_{\mu\oplus\underline{\kappa}\oplus\alpha}(\mathbf{x}_1) \sum_{\beta,\phi,\psi}\int dz_3 dz_4 dz_5\, D_{\alpha,\phi}(z_1,z_4)\Gamma^{\text{b-b},n-2}_{\phi,\psi;\underline{\kappa}}(z_4,z_5;z_1) D_{\psi,\beta}(z_5,z_3)\Gamma^{\text{b-e}}_{\beta,\nu}(z_3,z_2;1), \tag{63a}$$

$$\Pi^{(4b)}_{\mu,\nu}(z_1,z_2) = -\sum_{n\geqslant 2,\,\underline{\kappa},\alpha} n \int d\mathbf{x}_1\, V^n_{\mu\oplus\underline{\kappa}\oplus\alpha}(\mathbf{x}_1) \sum_{\beta,\phi,\psi}\int dz_3 dz_4 dz_5\, D_{\alpha,\beta}(z_1,z_3)\Gamma^{\text{b-e}}_{\beta,\phi}(z_3,z_4;1) D_{\phi,\psi}(z_4,z_5)\Gamma^{\text{b-b},n-2}_{\psi,\nu;\underline{\kappa}}(z_5,z_2;z_1), \tag{63b}$$

$$\Pi^{(4c)}_{\mu,\nu}(z_1,z_2) + \Pi^{(4d)}_{\mu,\nu}(z_1,z_2) = -\sum_{n\geqslant 2,\,\underline{\kappa},\alpha} n \int d\mathbf{x}_1\, V^n_{\mu\oplus\underline{\kappa}\oplus\alpha}(\mathbf{x}_1) \sum_{\beta}\int dz_3\, D_{\alpha,\beta}(z_1,z_3)\frac{\delta\Gamma^{\text{b-e}}_{\beta,\nu}(z_3,z_2;1)}{\delta\xi^{n-2}_{\underline{\kappa}}(z_1)}. \tag{63c}$$

Note that Eq. (63c) produces two terms, $\Pi^{(4c)}$ and $\Pi^{(4d)}$, as it will be demonstrated in the next section.

D. Vertex functions

In the preceding sections we derived the equation of motion of the bosonic propagator $D_{\mu,\nu}$, Eq. (50). Its important ingredients are the mean-field potentials $U_{\mu,\nu}$ and $\Xi_{\mu,\nu}$, Eqs. (52a) and (52) and the bosonic mass operator Π consisting of eight terms $\Pi^{(1)}$, $\Pi^{(2a)}$, $\Pi^{(2b)}$, $\Pi^{(3)}$, $\Pi^{(4a)}$, $\Pi^{(4b)}$, $\Pi^{(4c)}$, and $\Pi^{(4d)}$. They, in turn, explicitly depend on three vertex functions: $\Gamma^{\text{e-b}}$, $\Gamma^{\text{b-e}}$, and $\Gamma^{\text{b-b}}$. $\Gamma^{\text{e-e}}$ appears implicitly through the response function χ, in Eq. (61). The vertex functions contain one, two, or three external bosonic indices. In order to close the functional equations, we still need to express these vertex functions in terms of already defined correlators.

In order to do so, let us rewrite the vertex function as components of a *Jacobian matrix*:

$$\mathbf{\Gamma}(1,2;3) \equiv -\begin{bmatrix} \frac{\delta G^{-1}(1,2)}{\delta\eta(3)} & \frac{\delta G^{-1}(1,2)}{\delta\xi^n_{\underline{\kappa}}(z_3)} \\ \frac{\delta D^{-1}_{\mu,\nu}(z_1,z_2)}{\delta\eta(3)} & \frac{\delta D^{-1}_{\mu,\nu}(z_1,z_2)}{\delta\xi^n_{\underline{\kappa}}(z_3)} \end{bmatrix} = \begin{bmatrix} \Gamma^{\text{e-e}}(1,2;3) & \Gamma^{\text{e-b},n}_{\underline{\kappa}}(1,2;z_3) \\ \Gamma^{\text{b-e}}_{\mu,\nu}(z_1,z_2;3) & \Gamma^{\text{b-b},n}_{\mu,\nu;\underline{\kappa}}(z_1,z_2;z_3) \end{bmatrix} \tag{64}$$

and

$$\mathbf{K}(1,5;2,4) \equiv \begin{bmatrix} \frac{\delta\Sigma^{\text{e}}(1,2)}{\delta G(4,5)} & \frac{\delta M(1,2)}{\delta D_{\phi,\psi}(z_4,z_5)} \\ \frac{\delta\Pi_{\mu,\nu}(z_1,z_2)}{\delta G(4,5)} & \frac{\delta\Sigma^{\text{b}}_{\mu,\nu}(z_1,z_2)}{\delta D_{\phi,\psi}(z_4,z_5)} \end{bmatrix} = \begin{bmatrix} K^{\text{e-e}}(1,5;2,4) & K^{\text{e-b}}(1,z_5;2,z_4) \\ K^{\text{b-e}}(z_1,5;z_2,4) & K^{\text{b-b}}(z_1,z_5;z_2,z_4) \end{bmatrix}. \tag{65}$$

Here $\mathbf{\Gamma}$ is built of the vertex functions, and $\mathbf{K}$ is the matrix of kernels.

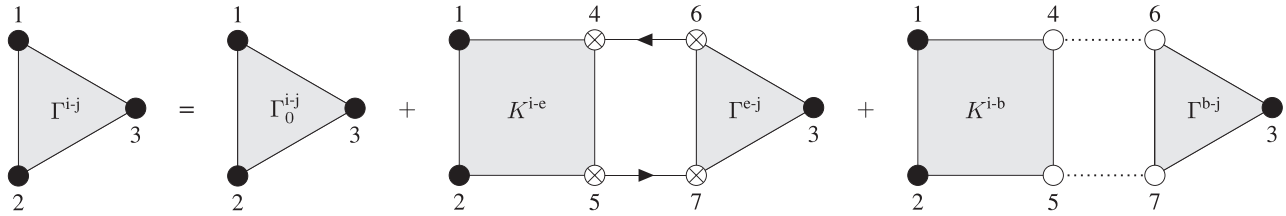

FIG. 7. Diagrammatic form of the generalized Bethe-Salpeter equation. Black dots denote generic electron or boson indexes, $i,\ j = (\mathrm{e},\ \mathrm{b})$.

The definitions introduced with Eqs. (64) and (65) make clear that the electronic and bosonic degrees of freedom are totally symmetric and treated on equal footing. Indeed the rows and columns of the two matrices can be labeled with the kind of input/output legs of the vertex/kernel $\left[\begin{smallmatrix}\text{e-e} & \text{e-b}\\ \text{b-e} & \text{b-b}\end{smallmatrix}\right]$.

For a given diagrammatic expression of the electronic and bosonic self-energies, the corresponding *partial* variations can be easily computed. Finally, we introduce the free term given by the derivatives of the mean-field electronic and bosonic potentials:

$$\mathbf{\Gamma}_0(1,2;3) \equiv \begin{bmatrix} \Gamma_0^{\text{e-e}}(1,2;3) & \Gamma_0^{\text{e-b}}(1,2;z_3) \\ \Gamma_0^{\text{b-e}}(z_1,z_2;3) & \Gamma_0^{\text{b-b}}(z_1,z_2;z_3) \end{bmatrix} \equiv \begin{bmatrix} \frac{\delta\eta(1)}{\delta\eta(3)}\delta(1-2) & \frac{\delta\Phi(1)}{\delta\xi^n_{\underline{\kappa}}(z_3)}\delta(1-2) \\ \frac{\delta U_{\mu,\nu}(z_1)}{\delta\eta(3)}\delta(z_1-z_2) & \frac{\delta\Xi_{\mu,\nu}(z_1)}{\delta\xi^n_{\underline{\kappa}}(z_3)}\delta(z_1-z_2) \end{bmatrix}, \tag{66}$$

with

$$\Gamma_0^{\text{e-e}}(1,2;3) = \delta(1-2)\delta(1-3), \tag{67a}$$

$$\Gamma_0^{\text{e-b}}(1,2;z_3) = \Gamma_{\underline{\kappa}}^{\text{e-b},n}(1,2;z_3)\big|_0 = \sum_{m,\,\underline{\mu}} V^m_{\underline{\mu}}(\mathbf{x}_1) D^{m,n}_{\underline{\mu},\underline{\kappa}}(z_1,z_3)\delta(1-2), \tag{67b}$$

$$\Gamma_0^{\text{b-e}}(z_1,z_2;3) = \Gamma^{\text{b-e}}_{\mu,\nu}(z_1,z_2;3)\big|_0 = \sum_{m,\,\underline{\lambda}} m\big\langle \hat{Q}^{m-2}_{\underline{\lambda}}(z_1)\big\rangle \int d\mathbf{x}_1\, V^m_{\mu\oplus\underline{\lambda}\oplus\nu}(\mathbf{x}_1)\chi(1,3)\delta(z_1-z_2), \tag{67c}$$

$$\Gamma_0^{\text{b-b}}(z_1,z_2;z_3) = \Gamma^{\text{b-b},n}_{\mu,\nu;\underline{\kappa}}(z_1,z_2;z_3)\big|_0 = \frac{1}{(n-1)!}\sum_{I=1}^{n!}\big\langle \widehat{Q}^{n-2}_{\kappa_{I_2}\ldots\kappa_{I_{n-1}}}(z_1)\big\rangle \delta_{\mu,\kappa_{I_1}}\delta_{\nu,\kappa_{I_n}}\delta(z_1-z_2)\delta(z_1-z_3). \tag{67d}$$

These four quantities are related by a system of linear equations:

$$\Gamma^{\text{i-j}}(1,2;3) = \Gamma_0^{\text{i-j}}(1,2,3) + K^{\text{i-e}}(1,5;2,4)G(4,6)G(7,5)\Gamma^{\text{e-j}}(6,7;3) + K^{\text{i-b}}(1,5;z_2,z_4)D_{\psi,\xi}(z_4,z_6)D_{\phi,\eta}(z_7,z_5)\Gamma^{\text{b-j}}_{\xi,\phi}(z_6,z_7;3), \tag{68}$$

where the summation and the integration over the repeated arguments is assumed, and the generic indexes are $i,\ j = (\mathrm{e},\mathrm{b})$. This is the sought *generalized Bethe-Salpeter equation* (GBSE) for the vertex functions (Figs. 7 and 8).

Now we are in the position to evaluate Eq. (63c), which, in fact, contains the variation $\frac{\delta\mathbf{\Gamma}^{\text{b-e}}}{\delta\xi^n}$. Since $\mathbf{\Gamma}$ is a solution of the complicated equation, its explicit form is not known. Therefore we use again the chain rule:

$$\begin{aligned}\frac{\delta\Gamma^{\text{b-e}}_{\beta,\gamma}(z_3,z_2;1)}{\delta\xi^n_{\underline{\kappa}}(z_4)} &= \sum_{\phi,\psi}\int dz_5 dz_6 \frac{\delta\Gamma^{\text{b-e}}_{\beta,\gamma}(z_3,z_2;1)}{\delta D_{\phi,\psi}(z_5,z_6)}\frac{\delta D_{\phi,\psi}(z_5,z_6)}{\delta\xi^n_{\underline{\kappa}}(z_4)} + \int d56\,\frac{\delta\Gamma^{\text{b-e}}_{\beta,\gamma}(z_3,z_2;1)}{\delta G(5,6)}\frac{\delta G(5,6)}{\delta\xi^n_{\underline{\kappa}}(z_4)} \\ &= \sum_{\phi,\psi}\int dz_5 dz_6 \frac{\delta\Gamma^{\text{b-e}}_{\beta,\gamma}(z_3,z_2;1)}{\delta D_{\phi,\psi}(z_5,z_6)}\sum_{\chi,\lambda}\int dz_7 dz_8\, D_{\phi,\chi}(z_5,z_7)\Gamma^{\text{b-b},n}_{\chi,\lambda;\underline{\kappa}}(z_7,z_8;z_4)D_{\lambda,\psi}(z_8,z_6) \\ &\quad + \int d5678\,\frac{\delta\Gamma^{\text{b-e}}_{\beta,\gamma}(z_3,z_2;1)}{\delta G(5,6)}G(5,7)\Gamma^{\text{e-b},n}_{\underline{\kappa}}(7,8;z_4)G(8,6).\end{aligned} \tag{69}$$

With this ingredient, the theory of interacting fermions and bosons is formally complete: the self-energies are expressed in terms of propagators and vertex functions. Note that we do not have yet determining equations for higher-order bosonic propagators and for the electron density response functions. For the former, one would have to study the equation of motion for $\widehat{Q}^n_{\underline{\nu}}$, which is rather complicated. Therefore, in Sec. VIII we use again the method of functional derivatives

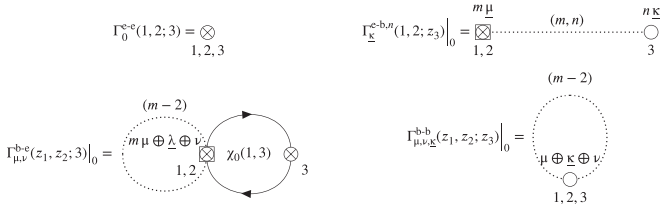

FIG. 8. Diagrammatic representation of the lowest-order vertex functions, Eq. (67).

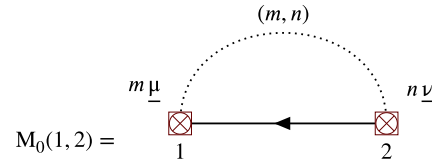

FIG. 10. The lowest-order fermionic self-energy.

to recast χ and $D^{m,n}_{\underline{\mu},\underline{\nu}}$ in terms of the simplest propagators G and D.

The vertex functions are related by the generalized Bethe-Salpeter equation which retains a surprisingly simple structure pertinent to the pure electronic case. The relation between bare and dressed vertex functions is a nontrivial point in the theory of electron-phonon interactions (see Sec. V A of Giustino [1]). In the case of linear electron-phonon interactions the vertex is renormalized solely due to the electron-electron interactions (e.g., Fig. 2 of Leeuwen [27]). In the nonlinear case considered here, the four vertex functions inevitably arise from a single electron-boson vertex, $V^n_{\underline{\nu}}(\mathbf{x})$. At a marked difference with these simpler theories, there are now four ways to renormalize the bare vertex. In Sec. VII we consider what form the electron and the boson propagators take when the lowest-order approximations [Eqs. (67)] are adopted for the vertex functions.

VII. LOWEST-ORDER APPROXIMATIONS FOR THE BOSONIC AND ELECTRONIC SELF-ENERGIES

The solution of the Dyson equations for fermions and bosons are considerably more involved than in the case of linear electron-boson coupling. The equations have two levels of internal consistency that we schematically represent in Fig. 9.

Let us take the electronic case as an example. The Dyson equation is itself nonlinear. For a given approximation for M the Dyson equation must be solved and the new G plugged in M

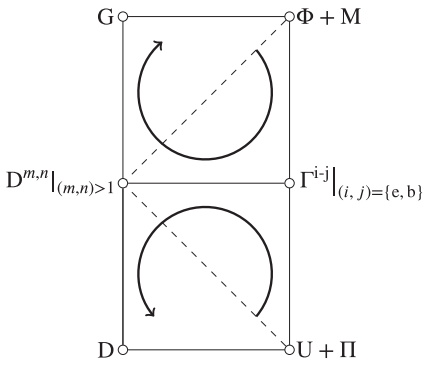

FIG. 9. Schematic representation of the self-consistent cycle involving the different components of the generalized Hedin's equations. The dashed lines correspond to the generalized GW approximation where the vertex functions Γ are taken to their lowest-order approximation and $D^{m,n} \approx D^{m,n}|_0$.

for a new solution. This process must be continued up to when self-consistency is reached. Besides this internal consistency the mass operator depends on the vertex function $\overline{\Gamma}^{\text{e-b}}$ and on the multiboson propagators $D^{n,m}$. The usual approach to cut this self-consistent loop is based on approximating the vertexes to their lowest order and to take the independent boson approximation (IBA) for $D^{n,m}$. A similar procedure can be applied in the bosonic case.

It is interesting to note that, at variance with the purely electronic case, the zeroth-order bosonic vertex functions are still dependent on $D^{n,m}$ through the $\langle \widehat{Q}^n_{\underline{\nu}} \rangle$ terms appearing in Eqs. (67c) and (67d). This dependence is resolved in the self-consistent loop of Fig. 9 by simply looking at the $\langle \widehat{Q}^n_{\underline{\nu}} \rangle$ as contractions of the bosonic response function. Therefore, for the zeroth-order vertexes will use the IBA $\langle \widehat{Q}^n_{\underline{\nu}} \rangle \approx D^{n-1,1}_{(\nu_1 \ldots \nu_{n-1}),\nu_n}(z, z^+)|_0$.

A. Electrons: The generalized Fan approximation

By using the zeroth-order $\overline{\Gamma}^{\text{b-e}}$ vertex function, Eq. (39) in the mass operator expression, Eq. (41), allows us to introduce a generalization of the Fan approximation [1,20]. Indeed we get $M(1,2) \approx M_0(1,2)$ with

$$M_0(1,2) = i \sum_{n,\underline{\nu}} \sum_{m\,\underline{\mu}} V^n_{\underline{\nu}}(\mathbf{x}_1) V^m_{\underline{\mu}}(\mathbf{x}_2) G(1,2) D^{m,n}_{\underline{\mu},\underline{\nu}}(z_2, z_1)\big|_0. \tag{70}$$

Equation (70) represents the generalization of the usual Fan approximation which is known only in the linear coupling case (corresponding to $m = n = 1$). Its diagrammatic form is shown in Fig. 10.

In Eq. (70) $D^{n,m}|_0$ is the zeroth-order approximation for the bosonic propagator which can be recast as a functional of non-interacting bosonic propagators, as described in Sec. VIII B 1 for some specific cases.

B. Bosons: A generalized polarization self-energy

As sketched in Fig. 9, the lowest-order approximation for the bosonic self-energy is obtained by using the zeroth-order generalized vertex functions, Eq. (67), and the IBA ($D^{n,m} \approx D^{n,m}|_0$) and IPA ($\chi \approx \chi_0$) for for bosons and electrons, respectively.

These approximation must be used in Eqs. (46), (52), (58)–(60), and (63). Equations (63b) and (63c) need not be considered because they contain variations of other vertex functions.

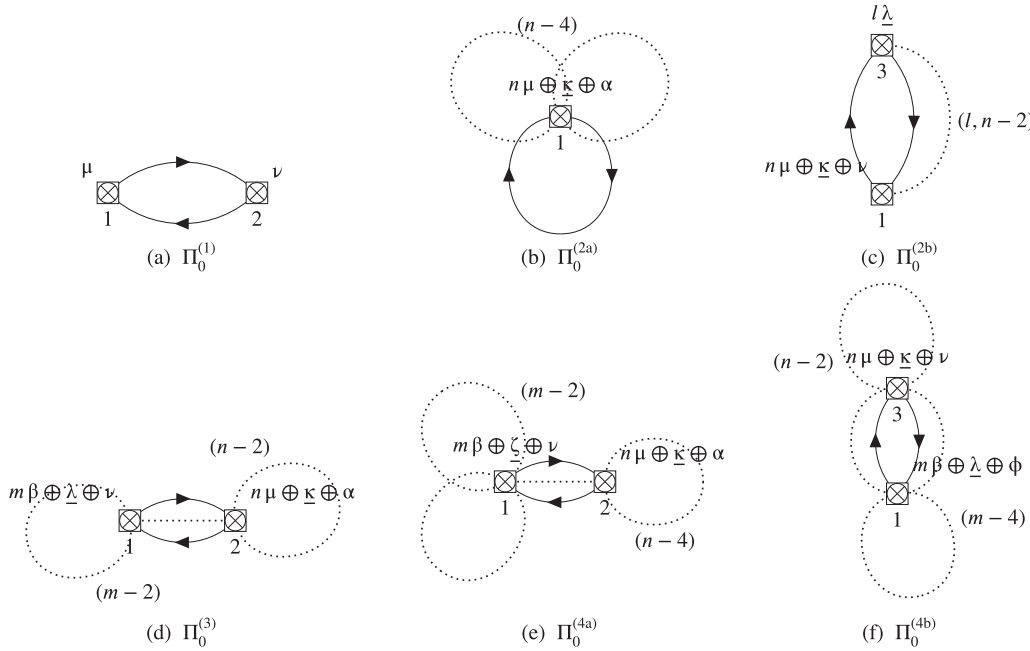

FIG. 11. Lowest-order approximation for the bosonic mass operators $\Pi_{\mu,\nu}(z_1, z_2)|_0$.

In total we obtain six terms:

$$\Pi^{(1)}_{\mu,\nu}(z_1,z_2)\big|_0 = \int d\mathbf{x}_1\, d\mathbf{x}_2\, V^1_\mu(\mathbf{x}_1) G(1,2) G(2,1) V^1_\nu(\mathbf{x}_2), \tag{71a}$$

$$\Pi^{(2a)}_{\mu,\nu}(z_1)\big|_0 = \sum_{n\geqslant 2,\,\underline{\kappa},\alpha} n\big\langle \hat{Y}^n_{\mu\oplus\underline{\kappa}\oplus\alpha}(z_1)\big\rangle \sum_\beta D_{\alpha,\beta}(z_1,z_1)\Gamma^{\text{b-b},n-2}_{\beta,\nu;\underline{\kappa}}(z_1)\big|_0, \tag{71b}$$

$$\Pi^{(2b)}_{\mu,\nu}(z_1)\big|_0 = \sum_{n,\,\underline{\kappa}} n \int d\mathbf{x}_1\, V^n_{\mu\oplus\underline{\kappa}\oplus\nu}(\mathbf{x}_1) \sum_{l,\,\underline{\lambda}} \int d3\, G(1,3) V^l_{\underline{\lambda}}(\mathbf{x}_3) D^{l,n-2}_{\underline{\lambda},\underline{\kappa}}(z_3,z_1)\big|_0 G(3,1^+), \tag{71c}$$

$$\Pi^{(3)}_{\mu,\nu}(z_1,z_2)\big|_0 = i \sum_{\substack{n,m,\,\underline{\kappa}\\ \alpha,\beta,\underline{\lambda}}} (nm) \int d\mathbf{x}_1\, V^n_{\mu\oplus\underline{\kappa}\oplus\alpha}(\mathbf{x}_1)\big\langle \widehat{Q}^{n-2}_{\underline{\kappa}}\big\rangle \int d\mathbf{x}_2\, D_{\alpha,\beta}(z_1,z_2) V^m_{\beta\oplus\underline{\lambda}\oplus\nu}(\mathbf{x}_2)\big\langle \widehat{Q}^{m-2}_{\underline{\lambda}}\big\rangle \chi_0(2,1), \tag{71d}$$

$$\begin{aligned}\Pi^{(4a)}_{\mu,\nu}(z_1,z_2)\big|_0 = &-\sum_{n,\underline{\kappa},\alpha} n \int d\mathbf{x}_1\, V^n_{\mu\oplus\underline{\kappa}\oplus\alpha}(\mathbf{x}_1) \sum_{\beta,\phi,\psi} \int dz_3 D_{\alpha,\phi}(z_1,z_1)\Gamma^{\text{b-b},n-2}_{\phi,\psi;\underline{\kappa}}(z_1)\big|_0 D_{\psi,\beta}(z_1,z_3)\\ &\times \sum_{m,\,\underline{\zeta},\beta} m \int d\mathbf{x}_2\, V^m_{\beta\oplus\underline{\zeta}\oplus\nu}(\mathbf{x}_2)\big\langle \widehat{Q}^{m-2}_{\underline{\zeta}}\big\rangle D_{\psi,\beta}(z_1,z_2)\chi_0(2,1),\end{aligned} \tag{71e}$$

$$\begin{aligned}\Pi^{(4b)}_{\mu,\nu}(z_1)\big|_0 = &-\sum_{n,\underline{\kappa},\beta,\phi,\psi,\alpha} n \int d\mathbf{x}_1\, V^n_{\mu\oplus\underline{\kappa}\oplus\alpha}(\mathbf{x}_1)\Gamma^{\text{b-b},n-2}_{\psi,\nu;\underline{\kappa}}(z_1)\big|_0\\ &\times \sum_{m,\,\underline{\lambda}} m \int d\mathbf{x}_3 dz_3\, V^m_{\beta\oplus\underline{\lambda}\oplus\phi}(\mathbf{x}_3)\big\langle \widehat{Q}^{m-2}_{\underline{\lambda}}\big\rangle D_{\alpha,\beta}(z_1,z_3) D_{\phi,\psi}(z_3,z_1)\chi_0(3,1).\end{aligned} \tag{71f}$$

These equations are depicted diagrammatically in Fig. 11.

VIII. RESPONSE FUNCTIONS

The electronic and bosonic self-energies are written, also, in terms of the response functions $\chi(1,2)$ and $D^{m,n}_{\underline{\mu},\underline{\nu}}(z_1,z_2)$ with $n>1$ or $m>1$. These response functions are more involved to calculate compared to the single-body case. Indeed, in the purely electronic case, the single electronic GF satisfies the Dyson equation, while the two-bodies GF solves a more complicated Bethe-Salpeter equation [59]. This is the contracted form of the equation of motion for the electronic vertex.

However, when the electronic and bosonic degrees of freedom are considered on equal footing as in Sec. VI D, the four vertex functions are mutually connected via a matrix integrodifferential, Eq. (68)—the generalized Bethe-Salpeter equation.

In the following sections our goal is investigate the form which take the electronic and the bosonic response functions as a consequence of the GBSE. In addition, thanks to the power of the Schwinger technique of functional derivatives, we will rewrite the equation of motion for the response function in terms of single fermion and single boson self-energies.

We have two aspects that complicate enormously the goal of this section: (i) the electronic and bosonic response functions are mutually dependent and (ii) the D may contain an arbitrary pair of incoming and outgoing bosonic lines (n, m).

A. Electronic response

The electronic response, Eq. (62), can be rewritten in terms of the purely electronic vertex $\Gamma^{\text{e-e}}$ by means of the usual chain rule and connecting ρ to the trace of G:

$$\chi(1,2) = i\int d34\, G(1,3)\frac{\delta G^{-1}(3,4)}{\delta\eta(2)}G(4,1^+)$$
$$= i\int d34\, G(1,3)G(4,1^+)\Gamma^{\text{e-e}}(3,4;2). \quad (72)$$

From Eq. (68) we do know that the equation of motion for $\Gamma^{\text{e-e}}$ corresponds to the e-e channel of GBSE. In practice this means that, at variance with the purely electronic case, *it is not possible to write the equation of motion for the response function solely in terms of* χ. Indeed, χ will depend, in general, on $D^{n,m}$ and, also, on the two mixed generalized response functions obtained by contracting $\Gamma^{\text{b-e}}$ and $\Gamma^{\text{e-b}}$ with bosonic and fermionic operators.

An alternative path, which we follow here, is to find an explicit form of $\Gamma^{\text{e-e}}$ and use Eq. (72) to obtain χ. From Eq. (68) we know that

$$\Gamma^{\text{e-e}}(3,4;2) = \Gamma_0^{\text{e-e}}(3,4,2) + \int d5678\, K^{\text{e-e}}(3,6;4,5)$$
$$\times G(5,7)G(8,6)\Gamma^{\text{e-e}}(7,8;2)$$
$$+ \sum_{\psi\xi\phi\eta}\int d56\int dz_7 z_8\, K^{\text{e-b}}_{\psi,\phi}(3,z_6;4,z_5)$$
$$\times D_{\phi,\xi}(z_5,z_7)D_{\eta,\psi}(z_8,z_6)\Gamma^{\text{b-e}}_{\xi,\eta}(z_7,z_8;2). \quad (73)$$

The first two terms in Eq. (73) represent a generalization of the usual Bethe-Salpeter equation, widely used in the context of optical absorption [59], to the case of an arbitrary number of bosons that mediate the electron-hole interaction. The second term, instead, is new and represents a boson-mediated electron-hole propagation. The electron-hole pair annihilates producing a number of bosons, which are subsequently scattered giving rise to a particle-hole pair.

In order to visualize this important modifications we consider the case where M is approximated with the generalized Fan form, Eq. (70), to evaluate $K^{\text{e-e}}$ and $K^{\text{e-b}}$:

$$K^{\text{e-e}}(3,5;4,6) \approx K_0^{\text{e-e}}(3,4)\delta(3,5)\delta(4,6)$$
$$= i\sum_{nm}\sum_{\underline{\mu}\underline{\nu}} V^n_{\underline{\nu}}(\mathbf{x}_3)V^m_{\underline{\mu}}(\mathbf{x}_4)D^{m,n}_{\underline{\mu},\underline{\nu}}(z_4,z_3)\big|_0 \quad (74)$$

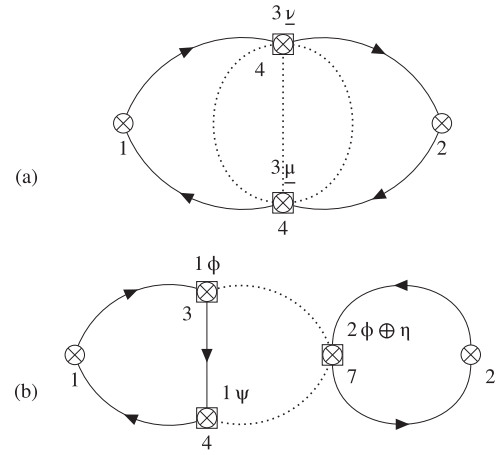

FIG. 12. First-order contributions to the electronic response function. (a) The contribution from $K_0^{\text{e-e}}$ when $n = 2$, while (b) is the contribution from $K_0^{\text{e-b}}$ when $n = 1$. Both terms are calculated with M approximated with the generalized Fan approximation, Eq. (70). Already at this simple order of perturbation theory (a) shows the simultaneous electron-hole interaction mediated by three bosons. (b), instead, is totally new and shows how the electron-hole dynamics is temporarily transformed in a two bosons dynamics already in the linear coupling.

and

$$K^{\text{e-b}}_{\phi,\psi}(3,z_5;4,z_6)$$
$$\approx K^{\text{e-b}}_{\phi,\psi}(z_3;z_4)\big|_0\delta(z_3-z_6)\delta(z_4-z_5)$$
$$= iG(3,4)\sum_{nm}\sum_{\underline{\kappa}\,\underline{\lambda}}\int d\mathbf{x}_3\mathbf{x}_4 V^n_{\underline{\kappa}\oplus\phi}(\mathbf{x}_3)V^m_{\underline{\lambda}\oplus\psi}(\mathbf{x}_4)$$
$$\times D^{m-1,n-1}_{\underline{\lambda},\underline{\kappa}}(z_4,z_3)\big|_0. \quad (75)$$

We can now use Feynman diagrams to make the different contributions to χ more transparent. Let us consider the specific case where we use $\Gamma^{\text{e-e}}(6,7;3) \approx \Gamma_0^{\text{e-e}}(6,7;3)$ and $\Gamma^{\text{b-e}}(z_6,z_7;3) \approx \Gamma^{\text{b-e}}(z_6,z_7;3)|_0$ in the r.h.s. of Eq. (73). If we plug Eqs. (74), (75) in Eq. (73) and the resulting $\Gamma^{\text{e-e}}$ in Eq. (72), a closed form expression for χ follows.

In Fig. 12 we consider two interesting cases of Eq. (73): (a) the contribution from the first integral and $K^{\text{e-e}}$ evaluated with $n = m = 3$ and (b) the contribution from the second integral when $n = m = 1$ in $K^{\text{e-b}}$ and $n = 2$ in $\Gamma^{\text{b-e}}$.

B. Bosonic response

We start from Eq. (21), applied to $D^{n+\Delta n,n}$. Thanks to this equation it is possible, for a given n, to reduce the evaluation of $D^{n+\Delta n,n}$ to the one of $D^{n,n}$, $D^{\Delta n,n}$, and the functional derivative of $D^{n,n}$. If we assume $\Delta n \leqslant n$ (the derivation can be easily extended to the case $\Delta n > n$) Eq. (21) lowers the order of $n + \Delta n$. If we further apply the same procedure to $D^{\Delta n,n} = D^{n,\Delta n} = D^{\Delta n+(n-\Delta n),\Delta n}$ the initial problem of evaluating $D^{n+m,n}$ can be cast in an expression which includes only diagonal response function, of the form $D^{m,m}$ with m an arbitrary integer $m \leqslant n$.

Let us take as an example the $D^{5,2}(z_1, z_2)$ case. From Eq. (21) it follows that

$$D^{5,2}_{\underline{\mu},\underline{\nu}}(z_1,z_2) = i\frac{\delta}{\delta\xi^3_{\underline{\kappa}}(z_1)}D^{2,2}_{\underline{\lambda},\underline{\nu}}(z_1,z_2) + \langle\widehat{Q}^3_{\underline{\kappa}}(z_1)\rangle D^{2,2}_{\underline{\lambda},\underline{\nu}}(z_1,z_2) + \langle\widehat{Q}^2_{\underline{\lambda}}(z_1)\rangle D^{3,2}_{\underline{\kappa},\underline{\nu}}(z_1,z_2), \tag{76}$$

with $\underline{\mu} = \underline{\kappa} \oplus \underline{\lambda}$. We can now apply again Eq. (21) on $D^{3,2}_{\underline{\kappa},\underline{\nu}}(z_1, z_2)$. It follows that

$$D^{3,2}_{\underline{\kappa},\underline{\nu}}(z_1,z_2) = i\frac{\delta}{\delta\xi^1_{\underline{\beta}}(z_1)}D^{2,2}_{\underline{\alpha},\underline{\nu}}(z_1,z_2) + \langle\widehat{Q}^2_{\underline{\alpha}}(z_1)\rangle D^{1,2}_{\underline{\beta},\underline{\nu}}(z_1,z_2), \tag{77}$$

with $\underline{\kappa} = \beta \oplus \underline{\alpha}$. A last application of Eq. (21) finally gives

$$D^{1,2}_{\beta,\underline{\nu}}(z_1,z_2) = D^{2,1}_{\underline{\nu},\beta}(z_2,z_1) = i\frac{\delta}{\delta\xi^1_{\nu_2}(z_2)}D_{\nu_1,\beta}(z_2,z_1). \tag{78}$$

We have finally reduced $D^{5,2}$ to an explicit functional of only diagonal response functions and their derivatives $D^{5,2} = F[D, D^{2,2}, \frac{\delta D}{\delta\xi^1}, \frac{\delta D^{2,2}}{\delta\xi^1}, \frac{\delta D^{2,2}}{\delta\xi^3}]$. From this simple example it follows that it is enough to study diagonal bosonic response functions and their functional derivatives in order to calculate any nondiagonal response functions.

In the following we discuss the IBA and give as an example the case of $D^{2,2}$ and $D^{3,3}$.

1. The independent bosons approximation

The limit of independent bosons is instructive to understand the actual number of diagrams that can be expected at any level of the perturbative expansion. In order to evaluate this number in the IBA we observe that

$$D^{m,n}_{\underline{\mu},\underline{\nu}}(z_1,z_2)\big|_0 = -i\langle\mathcal{T}\{\Delta\widehat{Q}_{\mu_1}(z_1)\cdots\Delta\widehat{Q}_{\mu_m}(z_1) \times \Delta\widehat{Q}_{\nu_1}(z_2)\cdots\Delta\widehat{Q}_{\nu_n}(z_2)\}\rangle_0, \tag{79}$$

with $\langle\cdots\rangle_0$ the thermal average corresponding to the free-bosons Hamiltonian. $D^{m,n}_{\underline{\mu},\underline{\nu}}|_0$ reduces to the sum of all possible contractions of two bosonic operators. From simple combinatorics arguments we know that the number of possible ordered pairs of two operators out of a product of $n \geqslant 2$ is given by the number of the so-called chord diagrams [60]

$$N_n = \begin{cases}(n-1)!! & \text{even } n,\\ 0 & \text{odd } n.\end{cases} \tag{80}$$

By doing simple diagrammatic expansion we see, indeed, that $D^{2,2}_{\underline{\mu},\underline{\nu}}(z_1,z_2)|_0$ produces a total of $N_4 = 3$ terms. One of them is disconnected and corresponds to the complete contractions of the two terms $\langle\Delta\widehat{Q}_{\mu_1}(z_1)\Delta\widehat{Q}_{\mu_2}(z_1)\rangle_0$ and $\langle\Delta\widehat{Q}_{\nu_1}(z_2)\Delta\widehat{Q}_{\nu_2}(z_2)\rangle_0$.

In the $D^{3,3}_{\underline{\mu},\underline{\nu}}(z_1,z_2)|_0$ case, instead, all contractions are connected because there is always at least one contraction with different time arguments. This means that we have in total $N_6 = 15$ terms. The explicit form of $D^{3,3}_{\underline{\mu},\underline{\nu}}(z_1,z_2)|_0$ will be given in Sec. VIII B 3.

We can therefore generally state that $D^{n,m}_{\underline{\mu},\underline{\nu}}(z_1,z_2)|_0$ is composed of $N_{n+m} - N_n N_m$ connected diagrams.

This simple combinatorics discussion allows us to derive some general rule on the strength of the nth order of the perturbative expansion. As it is clear from the derivation done in the precedent sections at any order of the perturbative expansion, a $D^{m,n}_{\underline{\mu},\underline{\nu}}$ appears multiplied by $V^n_{\underline{\nu}}V^m_{\underline{\mu}}$. These potentials include a $1/(n!m!)$ prefactor.

Overall we can deduce that the (n, m) order in the bosonic propagator will be weighted with a $N_{n+m}/(n!m!)$ prefactor. When n increases this term decays fast enough to make the overall expansion controllable.

2. The two-bosons case

The case of $D^{2,2}$ can be easily worked out following an approach similar to what has been used in Sec. VIII A. From Eq. (35) we know that

$$D^{2,2}_{\underline{\mu},\underline{\nu}}(z_1,z_2) = \frac{\delta\langle\widehat{Q}^2_{\underline{\mu}}(z_1)\rangle}{\delta\xi^2_{\underline{\nu}}(z_2)}. \tag{81}$$

At the same time we can rewrite the $\langle\widehat{Q}^2_{\underline{\mu}}(z_1)\rangle$ in terms of the single-body GF, using Eq. (20):

$$\langle\widehat{Q}^2_{\underline{\mu}}(z_1)\rangle = iD_{\mu_1\mu_2}(z_1,z_1^+). \tag{82}$$

By applying the chain rule we get

$$D^{2,2}_{\underline{\mu},\underline{\nu}}(z_1,z_2) = \frac{\delta\langle\widehat{Q}^2_{\underline{\mu}}(z_1)\rangle}{\delta\xi^2_{\underline{\nu}}(z_2)} = i\frac{\delta D_{\mu_1,\mu_2}(z_1,z_1^+)}{\delta\xi^2_{\underline{\nu}}(z_2)}. \tag{83}$$

We can now follow the procedure for the electronic case and connect $D^{2,2}$ to the $\Gamma^{\text{b-b}}$ vertex:

$$i\frac{\delta D_{\mu_1,\mu_2}(z_1,z_1)}{\delta\xi^2_{\underline{\nu}}(z_2)} = i\sum_{\underline{\alpha}}\int dz_3dz_4 D_{\mu_1\alpha_1}(z_1,z_3) \times \Gamma^{\text{b-b},2}_{\alpha_1,\alpha_2;\underline{\nu}}(z_3,z_4;z_2)D_{\alpha_2,\mu_2}(z_4,z_1). \tag{84}$$

Equation (84) is represented diagrammatically in Fig. 13(a).

Equation (68) provides the equation of motion for $\Gamma^{\text{b-b},2}_{\alpha_1,\alpha_2}$ that, in a similar way to Eq. (73), is written in terms of the pure bosonic (b-b) and the mixed boson-electron (b-e) vertex functions. This equation involves the kernels $K^{\text{b-b}}$ and $K^{\text{b-e}}$. We can now follow the same path of the purely electronic case and use the lowest-order bosonic self-energy, Eq. (71), to derive the corresponding expression for the b-b and b-e kernels and, consequently, of $\Gamma^{\text{b-b},2}$. Two representative diagrams contributing to $D^{2,2}$ are shown in Figs. 13(b) and 13(c).

The IBA for $D^{2,2}$ can be easily evaluated by using the zeroth-order expression for $\Gamma^{\text{b-b},2}$. From Eq. (57) we know that when $n = 2$ we have only $n!/(n-1)! = 2$ terms,

$$\Gamma^{\text{b-b},2}_{\alpha_1,\alpha_2;\underline{\nu}}(z_1,z_2;z_3)\big|_0 = \delta(z_1-z_2)\delta(z_1-z_3)\big[\delta_{\alpha_1,\nu_1}\delta_{\alpha_2,\nu_2} + \delta_{\alpha_1,\nu_2}\delta_{\alpha_2,\nu_1}\big], \tag{85}$$

which gives

$$D^{2,2}_{\underline{\mu},\underline{\nu}}(z_1,z_2)\big|_0 = i\big[D_{\mu_1,\nu_1}(z_1,z_2)D_{\nu_2,\mu_2}(z_2,z_1) + D_{\mu_1,\nu_2}(z_1,z_2)D_{\nu_2,\mu_1}(z_2,z_1)\big]. \tag{86}$$

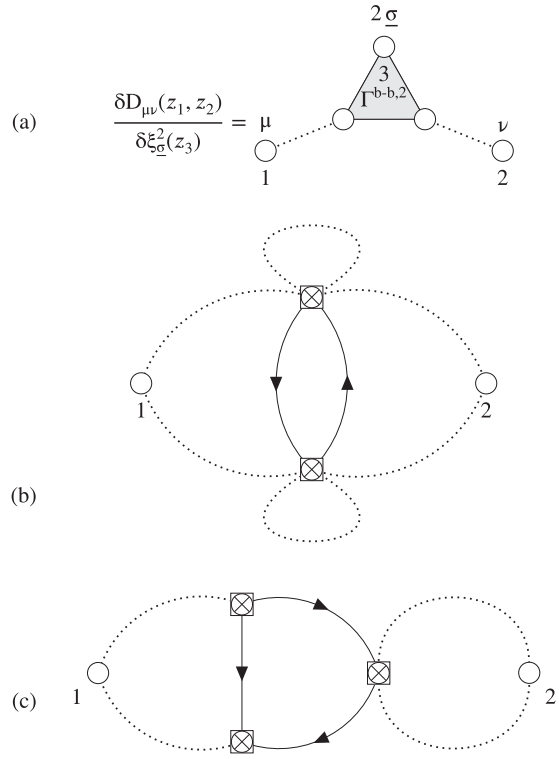

FIG. 13. (a) Diagrammatic representation of the first-order functional derivative of D, Eq. (83). (b) and (c) Two terms contributing to $D^{2,2}$ which show the connection between the single-boson self-energy and the bosonic response function. Indeed diagram (b) comes from the scattering term in $K^{\text{b-b}}$ due to $\frac{\delta\Pi^{(3)}|_0}{\delta D}$. Similarly diagram (c) is induced by the contribution of $\frac{\delta\Pi^{(1)}|_0}{\delta G}$ to $K^{\text{b-e}}$. Both terms are treated, in (b) and (c), at the first order in the generalized Bethe-Salpeter equation, Eq. (68).

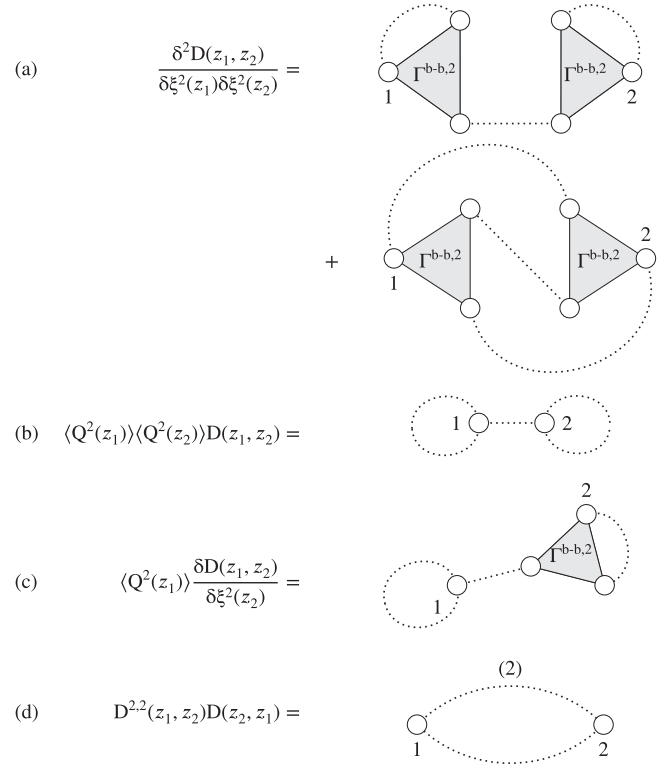

FIG. 14. Diagrammatic representation of the terms in Eq. (89) contributing to $D^{3,3}$.

Equation (86) coincides with the expression that can be derived by using the diagrammatic approach.

3. *The three-bosons case*

In the three-bosons case the calculation of $D^{3,3}$ may appear to be prohibitively complicated. Still, the present scheme allows us, via the functional derivative approach, to derive it in an elegant and compact way. We start by applying Eq. (21) to $D^{3,3}$:

$$D^{3,3}_{\underline{\mu},\underline{\nu}}(z_1,z_2) = \left[i\frac{\delta}{\delta\xi^2_{\underline{\lambda}}(z_1)} + \left\langle \widehat{Q}^2_{\underline{\lambda}}(z_1)\right\rangle \right] D^{1,3}_{t,\underline{\nu}}(z_1,z_2), \quad (87)$$

with $\underline{\mu} \equiv \underline{\lambda} \oplus t$. By using Eq. (21) again we get that

$$\begin{aligned} D^{1,3}_{t,\underline{\nu}}(z_1,z_2) &= D^{3,1}_{\underline{\nu},t}(z_2,z_1) \\ &= \left[i\frac{\delta}{\delta\xi^2_{\underline{\sigma}}(z_2)} + \left\langle \widehat{Q}^2_{\underline{\sigma}}(z_2)\right\rangle \right] D_{s,t}(z_2,z_1), \end{aligned} \quad (88)$$

where $\underline{\nu} \equiv \underline{\sigma} \oplus s$. Equations (87) and (88) show that $D^{3,3}$ is composed of five terms:

$$\begin{aligned} D^{3,3}_{\underline{\mu},\underline{\nu}}(z_1,z_2) = \Bigg[& D^{2,2}_{\underline{\lambda},\underline{\sigma}}(z_1,z_2) - \frac{\delta^2}{\delta\xi^2_{\underline{\lambda}}(z_1)\xi^2_{\underline{\sigma}}(z_2)} \\ & + \left\langle \widehat{Q}^2_{\underline{\lambda}}(z_1)\right\rangle\left\langle \widehat{Q}^2_{\underline{\sigma}}(z_2)\right\rangle + i\left\langle \widehat{Q}^2_{\underline{\sigma}}(z_2)\right\rangle \frac{\delta}{\delta\xi^2_{\underline{\lambda}}(z_1)} \\ & + i\left\langle \widehat{Q}^2_{\underline{\lambda}}(z_1)\right\rangle \frac{\delta}{\delta\xi^2_{\underline{\sigma}}(z_2)} \Bigg] D_{s,t}(z_2,z_1). \end{aligned} \quad (89)$$

The construction of the diagrammatic form of Eq. (89) can be done by using a simple diagrammatic form of Eq. (84), as shown in Fig. 13(a). This shows that any of the functional derivatives appearing in Eq. (89) can be rewritten in terms of a second-order b-b vertex function. In this way it is possible to rewrite $D^{3,3}$ in terms of known quantities, as shown in Fig. 14. All diagrams represented in Fig. 14 reduce when $\Gamma^{\text{b-b},2} \approx \Gamma^{\text{b-b},2}|_0$ to the IBA expression for $D^{3,3}$ which is, indeed, composed of a total of 15 terms.

IX. CONCLUSIONS

In this work we applied Schwinger's variational derivative technique to calculate the coupled electronic and bosonic dynamics induced by an electron-boson Hamiltonian with coupling linearly proportional to the electronic density $\hat{n}(\mathbf{x})$ and to all orders in the bosonic displacement $\widehat{Q}_\nu$.

The complex and coupled electronic and bosonic dynamics is formulated in the form of a system of functional relations between the dressed electronic $G(1,2)$, the *single boson*

$D_{\mu,\nu}(z_1, z_2)$ propagators, and the generalized electronic and bosonic self-energies $\Sigma^{\rm e}(1, 2)$ and $\Sigma^{\rm b}(z_1, z_2)$.

These are expressed as closed functionals of the electron density-density response χ, the multiboson response functions $D^{n,m}$, and four different vertex functions $\Gamma^{\rm e\text{-}e}$, $\Gamma^{\rm b\text{-}e}$, $\Gamma^{\rm e\text{-}b}$, and $\Gamma^{\rm b\text{-}b}$. These vertex functions are shown to have either a mixed electron-boson character ($\Gamma^{\rm b\text{-}e}$ and $\Gamma^{\rm e\text{-}b}$), or a purely electronic ($\Gamma^{\rm e\text{-}e}$) and bosonic ($\Gamma^{\rm b\text{-}b}$) character. The exact equations of motion for all these quantities are formally derived. Sound and controlled approximations are also proposed in order to make the calculations feasible.

The present formulation allows us to tackle the very ambitious problem of deriving using the Schwinger's technique coupled equations of motion for the electronic and bosonic response functions and provide several interesting conclusions and new concepts.

We extend to the nonlinear e-b interaction known concepts like the Debye-Waller potential and the Fan approximation. We further extend the Bethe-Salpeter equation to a 2×2 nonlinear system of integrodifferential equations for the four vertex functions. Thanks to this equation we show that there is no simple way to decouple the electronic and bosonic dynamics. We demonstrate, by using simple diagrammatic examples, that electrons and bosons can equally well mediate the electron-hole and boson-boson interaction. The present scheme, indeed, demonstrates a full and deep symmetry between the electronic and bosonic degrees of freedom.

The final result is an important generalization of the well-known Hedin's equations with a wealth of potential applications in different areas of condensed matter physics, optics, and chemistry.

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APPENDIX A: THE MEAN-FIELD TREATMENT OF THE ELECTRON-ELECTRON INTERACTION

In order to describe how we treat the correlation induced by the electron-electron interaction let us start from the full Hamiltonian in the first quantization and make explicit the distinction between dressed and undressed operators:

$$\widehat{H} = \widehat{H}^0_{\rm e} + \widehat{H}^0_{\rm b} + \widehat{H}^0_{\rm e\text{-}b} + \widehat{H}_{\rm e\text{-}e}, \tag{A1}$$

with the 0 superscript indicating bare operators. Indeed the dressing of the different components of the Hamiltonian (when possible) is a product of the dynamics and cannot be, *a priori*, inserted from the beginning.

In Eq. (A1) we introduced

$$\widehat{H}_{\rm e\text{-}e} = \frac{1}{2}\sum_{i\neq j} v(\mathbf{x}_i - \mathbf{x}_j), \tag{A2}$$

with v the bare Coloumb potential. It is well documented in the literature that one of the effects of $\widehat{H}_{\rm e\text{-}e}$ is to screen itself and all other interactions, including the e-b one. This has been extensively demonstrated, for example, in Ref. [28].

The path we take here is, therefore, to embody $\widehat{H}_{\rm e\text{-}e}$ in a mean-field correction to $\widehat{H}^0_{\rm e}$ and, consequently, dressing of $\widehat{H}^0_{\rm b}$ and $\widehat{H}^0_{\rm e\text{-}b}$:

$$\widehat{H} \Rightarrow \left[\widehat{H}^0_{\rm e} + \widehat{V}_{\rm mf}\right] + \widehat{H}_{\rm b} + \widehat{H}_{\rm e\text{-}b}, \tag{A3}$$

with $\widehat{H}_{\rm e} = \widehat{H}^0_{\rm e} + \widehat{V}_{\rm mf}$. Equation (A3) is the connection with Eq. (1). The specific form of $\widehat{V}_{\rm mf}$ depends on the physical problem. An example is to use DFT, where $\widehat{V}_{\rm mf} = \widehat{V}_{{\rm H}xc}$ is the Hartree plus the Kohn-Sham exchange-correlation potential [61]. In this case also the dressing of $\widehat{H}^0_{\rm e\text{-}b}$ and $\widehat{H}^0_{\rm e\text{-}e}$ is well known and widely documented. In the case of the electron-phonon problem, for example, the self-consistent dressing of the electron-nuclei interaction is described by the density-functional perturbation theory (DFPT) [62,63].

APPENDIX B: CONNECTION WITH THE ELECTRON-PHONON PROBLEM

A specific physical application of the present theoretical scheme is represented by the coupled electron-phonon system. This is a very wide field with a wealth of application in several branches of physics.

The Hamiltonian of the coupled electron-phonon system is obtained by starting from the total Hamiltonian of the system that we divide in its independent bare electronic $\widehat{H}_{\rm e}$, nuclear $\widehat{H}_{\rm n}(\mathbf{R})$, electron-nucleus (e-n) $\widehat{W}_{\rm e\text{-}n}(\mathbf{R})$ parts

$$\widehat{H}(\mathbf{R}) = \widehat{H}_{\rm e} + \widehat{H}_{\rm n}(\mathbf{R}) + \widehat{W}_{\rm e\text{-}n}(\mathbf{R}), \tag{B1}$$

where $\mathbf{R}$ is a generic notation representing positions of the nuclei. The notation used in this paper is the same adopted in Ref. [28].

In introducing Eq. (B1) it is important to stress that $\widehat{H}_{\rm n}(\mathbf{R})$ includes both the kinetic and nuclear-nuclear interaction while $\widehat{W}_{\rm e\text{-}n}(\mathbf{R})$ represents the electron-nuclei interaction, whose expansion in the atomic displacements leads, as well known, to the diagrammatic expansion. Moreover, in the spirit of Appendix A we have assumed, in Eq. (B1), to use DFT to describe the effect of the electron-electron correlation via the well-known exchange-correlation potential.

We split, now, the generic atomic position operator $\widehat{\mathbf{R}}_I$ in its reference plus displacement

$$\widehat{\mathbf{R}}_I \equiv \overline{\mathbf{R}}_I \hat{\mathbf{1}} + \Delta\widehat{\mathbf{R}}_I. \tag{B2}$$

The Cartesian components of $\Delta\widehat{\mathbf{R}}_I$ play the role of the bosonic coordinate operators Q_ν. We can, indeed, write that

$$\Delta\hat{\mathbf{R}}_I = \sum_\nu (N M_I \Omega_\nu)^{-1/2} \boldsymbol{\eta}(\nu|I)\widehat{Q}_\nu, \tag{B3}$$

with N the number of atoms in the system, M_I is the mass of atom I, and $\boldsymbol{\eta}$ is the phonon mode polarization vector. We assume here, for simplicity, a finite system that can be generalized to an periodic solid using periodic boundary conditions.

Our initial system is, therefore, characterized by a set of dressed, electronic, and bosonic single-particle states with energies $\{\mathcal{E}_i\}$ and frequencies $\{\Omega_\nu\}$. We have in total $3N$ bosonic coordinates.

We have now all ingredients to expand the $\widehat{W}_{\text{e-n}}(\mathbf{R})$ in terms of $\hat{\psi}(\mathbf{x})$ and $\widehat{Q}_\nu$. Indeed we can, formally, write that

$$\widehat{W}_{\text{e-n}}(\mathbf{R}) = \sum_n \widehat{W}^{(n)}_{\text{e-n}}(\mathbf{R}) = \sum_n \sum_{\boldsymbol{\nu}} \int d\mathbf{x}\, \hat{\psi}^\dagger(\mathbf{x}) V^{(n)}_{\boldsymbol{\nu}}(\mathbf{x}) \hat{\psi}(\mathbf{x}) \widehat{Q}^n_{\boldsymbol{\nu}}, \tag{B4}$$

with

$$V^{(n)}_{\boldsymbol{\nu}}(\mathbf{x}) = \left(\prod_{i=1}^{n} \partial_{\nu_i} \right)_{\text{eq}} V_{scf}(\mathbf{x} - \mathbf{R}). \tag{B5}$$

In Eq. (B5) V_{scf} is the dressed DFPT electron-nuclei potential and the derivative is taken at the equilibrium position $\mathbf{R} = \overline{\mathbf{R}}$.

APPENDIX C: PROOF OF EQ. (11c)

The equation of motion for $\widehat{P}$ can be derived by using some care. Indeed Eq. (10b) implies that

$$\left[\widehat{P}_\nu(z_1), \widehat{Q}^m_{\underline{\alpha}}(z_1)\right]_- = \left[\widehat{P}_\nu(z_1), \prod_{i=1}^{m} \widehat{Q}_{\alpha_i}(z_1)\right]_- = (-i) \sum_{j=1}^{m} \delta_{\nu,\alpha_j} \prod_{i\neq j, i=1}^{m} \widehat{Q}_{\alpha_i}(z_1). \tag{C1}$$

If we now plug Eq. (C1) into the $[\widehat{P}_\nu(z_1), \widehat{H}(z_1)]_-$ commutator we get

$$(-i)[\widehat{P}_\nu(z_1), \widehat{H}(z_1)]_- = \frac{d}{dz_1} \widehat{P}_\nu(z_1) = -\Omega_\nu \widehat{Q}_\nu(z_1) - \sum_{m,\underline{\alpha}} \sum_{j=1}^{m} \delta_{\nu,\alpha_j} \widehat{\gamma}_{\underline{\alpha}}(z_1) \prod_{i\neq j, i=1}^{m} \widehat{Q}_{\alpha_i}(z_1). \tag{C2}$$

Now we reorder the components of $\underline{\alpha}$ vector (γ is a fully symmetric tensor) so that

$$\delta_{\nu,\alpha_j} \gamma_{\underline{\alpha}}(z_1) = \gamma_{\alpha_1,\ldots,\alpha_{j-1},\nu,\alpha_{j+1},\ldots,\alpha_m}(z_1) = \gamma_{\alpha_1,\ldots,\alpha_{m-1},\nu}(z_1). \tag{C3}$$

We now rename $\underline{\alpha}$ by introducing the $m-1$ dimensional vector $\underline{\mu} \equiv (\alpha_1, \ldots, \alpha_{m-1})$. Thanks to Eq. (C3) we have that

$$\prod_{i\neq j, i=1}^{m} \widehat{Q}_{\alpha_i}(z_1) = \widehat{Q}^{m-1}_{\underline{\mu}}(z_1), \tag{C4}$$

and we finally get

$$\frac{d}{dz_1} \widehat{P}_\nu(z_1) = -\Omega_\nu \widehat{Q}_\nu(z_1) - \sum_{m,\underline{\mu}} m\, \hat{\gamma}^m_{\underline{\mu}\oplus\nu}(z_1) \widehat{Q}^{m-1}_{\underline{\mu}}(z_1). \tag{C5}$$

APPENDIX D: PROOF OF EQ. (21)

We start by observing that

$$\frac{i\delta}{\delta\xi^k_{\underline{\alpha}}(z_1)} D^{m-k,n}_{\underline{\beta},\underline{\nu}}(z_1, z_2) = \frac{\delta}{\delta\xi^k_{\underline{\alpha}}(z_1)} \left[\left\langle \mathcal{T} \widehat{Q}^{m-k}_{\underline{\beta}}(z_1) \widehat{Q}^n_{\underline{\nu}}(z_2) \right\rangle - \left\langle \widehat{Q}^{m-k}_{\underline{\beta}}(z_1) \right\rangle \left\langle \widehat{Q}^n_{\underline{\nu}}(z_2) \right\rangle \right]. \tag{D1}$$

We start by expanding the three terms resulting from the functional derivative of the three components of D:

$$\frac{\delta}{\delta\xi^k_{\underline{\alpha}}(z_1)} \left\langle \mathcal{T} \widehat{Q}^{m-k}_{\underline{\beta}}(z_1) \widehat{Q}^n_{\underline{\nu}}(z_2) \right\rangle = \left\langle \mathcal{T} \widehat{Q}^{m-k}_{\underline{\beta}}(z_1) \widehat{Q}^n_{\underline{\nu}}(z_2) \widehat{Q}^k_{\underline{\alpha}}(z_1) \right\rangle - \left\langle \mathcal{T} \widehat{Q}^{m-k}_{\underline{\beta}}(z_1) \widehat{Q}^n_{\underline{\nu}}(z_2) \right\rangle \left\langle \widehat{Q}^k_{\underline{\alpha}}(z_1) \right\rangle. \tag{D2}$$

The second and third term are due to the derivative of the two single displacement operator averages:

$$\frac{\delta}{\delta\xi^k_{\underline{\alpha}}(z_1)} \left\langle \widehat{Q}^{m-k}_{\underline{\beta}}(z_1) \right\rangle = \left\langle \widehat{Q}^{m-k}_{\underline{\beta}}(z_1) \widehat{Q}^k_{\underline{\alpha}}(z_1) \right\rangle - \left\langle \widehat{Q}^{m-k}_{\underline{\beta}}(z_1) \right\rangle \left\langle \widehat{Q}^k_{\underline{\alpha}}(z_1) \right\rangle \tag{D3}$$

and

$$\frac{\delta}{\delta\xi^k_{\underline{\alpha}}(z_1)} \left\langle \widehat{Q}^n_{\underline{\nu}}(z_2) \right\rangle = \left\langle \mathcal{T} \widehat{Q}^n_{\underline{\nu}}(z_2) \widehat{Q}^k_{\underline{\alpha}}(z_1) \right\rangle - \left\langle \widehat{Q}^n_{\underline{\nu}}(z_2) \right\rangle \left\langle \widehat{Q}^k_{\underline{\alpha}}(z_1) \right\rangle. \tag{D4}$$

If now we put together all components of Eq. (D1) we get

$$\frac{i\delta}{\delta\xi^k_{\underline{\alpha}}(z_1)}D^{m-k,n}_{\underline{\beta},\underline{\nu}}(z_1,z_2)=\langle\mathcal{T}\widehat{Q}^m_{\underline{\beta}\otimes\underline{\alpha}}(z_1)\widehat{Q}^n_{\underline{\nu}}(z_2)\rangle-\langle\widehat{Q}^m_{\underline{\beta}\otimes\underline{\alpha}}(z_1)\rangle\langle\widehat{Q}^n_{\underline{\nu}}(z_2)\rangle-\langle\mathcal{T}\widehat{Q}^{m-k}_{\underline{\beta}}(z_1)\widehat{Q}^n_{\underline{\nu}}(z_2)\rangle\langle\widehat{Q}^k_{\underline{\alpha}}(z_1)\rangle$$
$$+\langle\widehat{Q}^{m-k}_{\underline{\beta}}(z_1)\rangle\langle\widehat{Q}^k_{\underline{\alpha}}(z_1)\rangle\langle\widehat{Q}^n_{\underline{\nu}}(z_2)\rangle-\langle\mathcal{T}\widehat{Q}^n_{\underline{\nu}}(z_2)\widehat{Q}^k_{\underline{\alpha}}(z_1)\rangle\langle\widehat{Q}^{m-k}_{\underline{\beta}}(z_1)\rangle+\langle\widehat{Q}^n_{\underline{\nu}}(z_2)\rangle\langle\widehat{Q}^k_{\underline{\alpha}}(z_1)\rangle\langle\widehat{Q}^{m-k}_{\underline{\beta}}(z_1)\rangle. \quad \text{(D5)}$$

Equation (D5) finally gives

$$\frac{i\delta}{\delta\xi^k_{\underline{\alpha}}(z_1)}D^{m-k,n}_{\underline{\beta},\underline{\nu}}(z_1,z_2)=D^{m,n}_{\underline{\beta}\otimes\underline{\alpha},\underline{\nu}}(z_1,z_2)-\langle\widehat{Q}^k_{\underline{\alpha}}(z_1)\rangle D^{m-k,n}_{\underline{\beta},\underline{\nu}}(z_1,z_2)-\langle\widehat{Q}^{m-k}_{\underline{\beta}}(z_1)\rangle D^{k,n}_{\underline{\alpha},\underline{\nu}}(z_1,z_2). \quad \text{(D6)}$$

In Eq. (D5) we have used the fact that

$$\langle\mathcal{T}\widehat{Q}^{m-k}_{\underline{\beta}}(z_1)\widehat{Q}^n_{\underline{\nu}}(z_2)\widehat{Q}^k_{\underline{\alpha}}(z_1)\rangle=\langle\mathcal{T}\widehat{Q}^m_{\underline{\beta}\otimes\underline{\alpha}}(z_1)\widehat{Q}^n_{\underline{\nu}}(z_2)\rangle. \quad \text{(D7)}$$

Equation (D6) proves Eq. (21).

APPENDIX E: SUMMARY OF DEFINITIONS

a. Bosonic coordinates and the interaction vertex

$$\widehat{Q}^n_{\underline{\nu}}=\prod_{i=1}^n\widehat{Q}_{\nu_i},\quad V^n_{\underline{\nu}}(\mathbf{x})=\frac{1}{n!}\left(\prod_{i=1}^n\partial_{\nu_i}\right)_{\rm eq}V_{\text{e-b}}(\mathbf{x}),\quad \hat{\gamma}^n_{\underline{\nu}}=\int d\mathbf{x}\,\hat{\psi}^\dagger(\mathbf{x})V^n_{\underline{\nu}}(\mathbf{x})\hat{\psi}(\mathbf{x}).$$

b. Auxiliary fields

$$\hat{H}_{\xi,\eta}(z)=\hat{H}+\sum_{n,\,\underline{\nu}}\xi^n_{\underline{\nu}}(z)\widehat{Q}^n_{\underline{\nu}}+\int d\mathbf{x}\,\eta(\mathbf{x},z)\hat{\rho}(\mathbf{x}).$$

c. Correlators and electronic response

$$G(1,2)\equiv-i\langle\mathcal{T}\{\hat{\psi}(1)\hat{\psi}^\dagger(2)\}\rangle,\quad D^{n,m}_{\underline{\mu},\underline{\nu}}(z_1,z_2)\equiv-i\langle\mathcal{T}\{\Delta\widehat{Q}^n_{\underline{\mu}}(z_1)\Delta\widehat{Q}^m_{\underline{\nu}}(z_2)\}\rangle,\quad \chi(1,2)\equiv\frac{\delta\langle\hat{\rho}(1)\rangle}{\delta\eta(2)}.$$

d. Mean-field potentials

$$\Phi(1)=\sum_{m,\,\underline{\mu}}V^m_{\underline{\mu}}(\mathbf{x}_1)\langle\widehat{Q}^m_{\underline{\mu}}(z_1)\rangle,\quad U_{\mu,\nu}(z_1)=\sum_{n,\,\underline{\kappa}}n\,\langle\hat{\gamma}^n_{\mu\oplus\underline{\kappa}\oplus\nu}(z_1)\rangle\langle\widehat{Q}^{n-2}_{\underline{\kappa}}(z_1)\rangle.$$

e. Electronic mass operator

$$M(1,2)=i\sum_{n,\,\underline{\nu}}\sum_{m,\,\underline{\mu}}\int d3\int dz_4\,V^n_{\underline{\nu}}(\mathbf{x}_1)G(1,3)\overline{\Gamma}^{\text{e-b},m}_{\underline{\mu}}(3,2;z_4)D^{m,n}_{\underline{\mu},\underline{\nu}}(z_4,z_1).$$

f. Bosonic mass operator

$$\Pi_{\mu,\nu}(z_1,z_2)=\sum_{I=(1,2a,3,4a,4b,4c,4d)}\Pi^{(I)}_{\mu,\nu}(z_1,z_2)+\Pi^{(2b)}_{\mu,\nu}(z_1)\delta(z_1-z_2).$$

g. Vertex functions

$$\Gamma^{\text{e-e}}(1,2;3)=\frac{\delta G^{-1}(1,2)}{\delta\eta(3)},\quad \Gamma^{\text{e-b},k}_{\underline{\kappa}}(1,2;z_3)=\frac{\delta G^{-1}(1,2)}{\delta\xi^k_{\underline{\kappa}}(3)},\quad \overline{\Gamma}^{\text{e-b},k}_{\underline{\kappa}}(1,2;z_3)=\frac{\delta G^{-1}(1,2)}{\delta\langle Q^m_{\underline{\kappa}}(z_3)\rangle},$$
$$\Gamma^{\text{b-e}}_{\mu,\nu}(z_1,z_2;3)=\frac{\delta D^{-1}_{\mu,\nu}(z_1,z_2)}{\delta\eta(3)},\quad \Gamma^{\text{b-b},k}_{\mu,\nu;\underline{\kappa}}(z_1,z_2;z_3)=\frac{\delta D^{-1}_{\mu,\nu}(z_1,z_2)}{\delta\xi^k_{\underline{\kappa}}(3)}.$$

h. Kernels

$$K^{\text{e-e}}(1,5;2,4)=\frac{\delta\Sigma^e(1,2)}{\delta G(4,5)},\quad K^{\text{e-b}}(1,z_5;z_2,4)=\frac{\delta M(1,2)}{\delta D_{\phi,\psi}(z_4,z_5)},$$
$$K^{\text{b-e}}(z_1,5;2,z_4)=\frac{\delta\Pi_{\mu,\nu}(z_1,z_2)}{\delta G(4,5)},\quad K^{\text{b-b}}(z_1,z_5;z_2,z_4)=\frac{\delta\Sigma^b_{\mu,\nu}(z_1,z_2)}{\delta D_{\phi,\psi}(z_4,z_5)}.$$

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