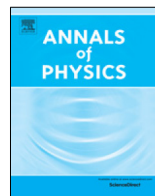




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Phonon-mediated superconductivity in strongly correlated electron systems: A Luttinger–Ward functional approach[☆]

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ARTICLE INFO

Article history:

Received 10 November 2019

Received in revised form 3 February 2020

Accepted 9 February 2020

Available online 15 February 2020

Keywords:

Electron–phonon interaction

Electron–electron interaction

Superconductivity

Eliashberg theory

Strongly correlated electron systems

ABSTRACT

We use a Luttinger–Ward functional approach to study the problem of phonon-mediated superconductivity in electron systems with strong electron–electron interactions (EEl). Our derivation does not rely on an expansion in skeleton diagrams for the EEI and the resulting theory is therefore nonperturbative in the strength of the latter. We show that one of the building blocks of the theory is the irreducible six-leg vertex related to EEIs. Diagrammatically, this implies five contributions (one of the Fock and four of the Hartree type) to the electronic self-energy, which, to the best of our knowledge, have never been discussed in the literature. Our approach is applicable to (and in fact designed to tackle superconductivity in) strongly correlated electron systems described by generic lattice models, as long as the glue for electron pairing is provided by phonons.

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1. Introduction

Our microscopic knowledge of superconductivity relies on the monumental theory laid down between the end of the Fifties and the beginning of the Sixties by Migdal and Eliashberg [1–7], in a

[☆] This article is part of the Special Issue: Eliashberg theory at 60.

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period where significant progress in the theoretical understanding of electron–phonon interactions (EPIs) [8–15] was made.

Interest in the Migdal–Eliashberg theory, which represents one of the first applications of quantum field theory to condensed matter physics, arose out of the need to transcend the Bardeen–Cooper–Schrieffer (BCS) mean-field theory [16]. In brief, BCS theory relies on a quasiparticle reduced Hamiltonian approach, which is inadequate to describe at least three situations [6]: (1) when the quasiparticle damping rate due to EPIs becomes comparable with the excitation energy; (2) when the BCS assumption of an effective two-body instantaneous attractive interaction between quasiparticles does not provide an adequate representation of the retarded nature of electron–phonon interactions; or (3) when normal and pairing correlations must be treated on equal footing.

From the Sixties to the present days, many researchers have invested a truly considerable energy in studying superconductivity in an extremely large number of situations and materials. In what follows we provide a largely incomplete list of past and contemporary research subfields in the realm of superconductivity:

- (i) *Unconventional superconductors*. Huge efforts have been devoted to investigate *unconventional* superconductivity [17–25], i.e. superconductivity unrelated to EPIs but arising from other pairing glues, originating microscopically solely from repulsive electron–electron interactions (EELs). These studies were motivated by the discovery of high-temperature superconductivity in the cuprates [26], which still pose tremendous challenges to theoretical condensed matter physics.
- (ii) *Non-adiabatic effects in the theory of superconductivity*. Since the theory by Eliashberg [2,3] relies on the Migdal theorem [1], many researchers have studied the importance of *non-adiabatic* corrections [27–36], which become important when the Migdal parameter $\hbar\omega_D/E_F$ ceases to be $\ll 1$. Here, ω_D is the Debye frequency and E_F is the Fermi energy.
- (iii) *The Migdal–Eliashberg theory for real materials*. For understanding phonon-mediated superconductivity in real materials, the Eliashberg equations need to be supplemented by first principles calculations of the electronic band structure and EPIs. For a recent review of this vast research field, we invite the reader to consult Ref. [37]. In passing, we note that an *ab initio* theory of phonon-mediated superconductivity (SCDFT)–constructed by generalizing the Hohenberg–Kohn theorem [38] of density functional theory to include the order parameter as an additional “density”–has been recently laid down and applied to a number of materials [39].
- (iv) *High-temperature superconductivity in hydrates*. The discovery of high-temperature superconductivity at high pressures in hydrogen-rich compounds (at 203 K in H_3S [40] and at ~ 250 K in LaH_{10} [41,42]) has re-attracted a great deal of attention to conventional phonon-mediated superconductors. Despite the underlying pairing mechanism in these compounds is conventional, several unconventional processes [43–49] compete in them, such as high phonon frequencies, quantum zero-point motion of H, strong anharmonic effects, and van Hove singularities. In this latter respect, for example, H_3S displays [46–49] a pair of closely spaced van Hove singularities at E_F . As a result, in a significant portion of the Brillouin zone, the quasiparticle velocity vanishes, technically invalidating the applicability of the Migdal theorem – see point (ii) above – and, at the same time, greatly enhancing the role of EELs.
- (v) *Superconductivity in magic-angle twisted bilayer graphene*. The discovery of superconductivity and correlated insulating states in magic-angle twisted bilayer graphene (MATBG) [50,51] has proven this system to be a rich playground for exploring strong correlations [52–58]. While the mechanism of superconductivity is still debated, several theoretical and experimental works point to the importance of electron–phonon interactions [59–63]. On top of this, the electronic structure of MATBG displays nearly flat bands near the charge neutrality point [64–68]. Similarly to the case of the hydrates, these undermine, at least in principle, the applicability of the Migdal–Eliashberg theory and are believed to be responsible for strong EELs.

This work is mainly motivated by the experimental systems mentioned at points (iv) and (v) above. We pose the following simple question: What is the fate of the Migdal–Eliashberg theory in materials where EELs play a dominant role? More precisely: Is it possible to construct a theory

of conventional, phonon-mediated superconductivity in materials where EEs require a nonperturbative treatment? In this work we answer this question affirmatively and present such theory. Our main result is that, in order to produce a consistent theory of EEs to all orders, a building block which has so far been overlooked needs to be taken into account: the irreducible six-leg vertex related to EEs. Under certain approximations discussed below, we derive a set of extended Eliashberg equations.

2. Outline, approximations, and applicability

We here summarize the key features of our theory, which will be detailed in the remainder of this work.

We consider an electron–phonon Hamiltonian (written for an arbitrary set of basis states) where EEs are included in all generality, while EPIs are assumed to be linear in the ion displacements from their equilibrium positions, as in the Fröhlich EPI Hamiltonian (Section 3). By using Matsubara path integrals, in Section 4 we derive the general form of the Luttinger–Ward functional (LWF) [69,70] corresponding to this Hamiltonian, using an exact procedure that is nonperturbative in the EEI. We then make the first approximation, which consists in expanding the LWF in powers of the EPI matrix elements, up to the second order (Section 5). As in any other LWF, the coefficients of such expansion are *fully interacting* many-body quantities, namely Green’s functions (GFs) and interaction vertices. From this approximate LWF, in Section 6 (Section 7) we derive the electronic (phononic) self-energy. In particular, the electronic self-energy consists of the EEI self-energy functional, plus two EPI self-energy functionals (Hartree and Fock contributions). Up to this point, our treatment is very general and can be applied to study the combined effects of EEs and EPIs in any solid-state system. No approximations are made, except for the truncation of the LWF (such a truncation is necessary to develop any practical theory). Our main general results can be found in Eqs. (87)–(89), (92), and (93).

Section 8 is specific to the problem of phonon-mediated superconductivity. Here, we apply the previously developed general formalism to derive a set of *extended Eliashberg equations*. Our aim is to provide a way to compute the anomalous components of the electronic self-energy, accounting as much as possible for the EEI effects derived in Sections 3–6. This task requires some approximations. Most importantly, we need to adopt a tractable, explicit expression for the electronic self-energy functional; this cannot be done exactly, because the functional corresponding to the EEI self-energy is not known analytically (and even if it were, it would be overwhelmingly complicated). In Section 8 we therefore: (1) neglect the EEI vertices appearing in the EPI self-energy functionals and (2) confine ourselves to the regime of temperatures close to the critical temperature, where the expressions can be linearized in the anomalous self-energy. We then assume that the EEI self-energy functional *in the normal state* can be obtained via other theoretical/computational means [71–73], and plugged into the resulting extended Eliashberg Eqs, (135)–(140). These equations include the vertex corrections arising from the EEI self-energy functional, which are not captured by the Tolmachev–Morel–Anderson pseudopotential method [74,75] and the McMillan formula [76].

A brief set of conclusions and future perspectives are reported in Section 9. Numerous technical details are reported in [Appendices A–G](#).

3. Model Hamiltonian

We consider a system of electrons and phonons, in the presence of EEs and EPIs. The Hamiltonian has the following general form

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}(\mathbf{t}, \mathbf{U}, \mathbf{f}, \mathbf{M}) = \hat{\mathcal{H}}_{\text{IE}}(\mathbf{t}) + \hat{\mathcal{H}}_{\text{EEI}}(\mathbf{U}) + \hat{\mathcal{H}}_{\text{IP}}(\mathbf{f}) + \hat{\mathcal{H}}_{\text{EPI}}(\mathbf{M}, \mathbf{f}), \quad (1)$$

where the independent-electron (IE) term is

$$\hat{\mathcal{H}}_{\text{IE}}(\mathbf{t}) = \sum_{\alpha, \beta} t_{\alpha, \beta} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\beta}, \quad (2)$$

the electron–electron interaction (EEI) is

$$\hat{\mathcal{H}}_{\text{EEI}}(\mathbf{U}) = \frac{1}{2} \sum_{\alpha, \beta, \gamma, \delta} U_{\alpha, \beta, \delta, \gamma} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\beta}^{\dagger} \hat{c}_{\gamma} \hat{c}_{\delta}, \quad (3)$$

the independent-phonon (IP) term is

$$\hat{\mathcal{H}}_{\text{IP}}(\mathbf{f}) = \sum_{\kappa, \lambda} f_{\kappa, \lambda} \hat{b}_{\kappa}^{\dagger} \hat{b}_{\lambda}, \quad (4)$$

and the electron–phonon interaction (EPI) is

$$\hat{\mathcal{H}}_{\text{EPI}}(\mathbf{M}, \mathbf{f}) = \sum_{\alpha, \beta, \lambda} M_{\alpha, \beta}^{(\lambda)} \hat{Q}_{\lambda} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\beta}. \quad (5)$$

In the above equations, we have denoted electron and phonon creation operators by $\hat{c}_{\alpha}^{\dagger}$ and $\hat{b}_{\kappa}^{\dagger}$, respectively. Greek indices denote sets of quantum numbers for both electron and phonon single-particle basis functions. For the sake of concreteness, electronic indices are given explicitly by $\alpha = (i_{\alpha}, \sigma_{\alpha})$ in a lattice representation, where i_{α} is the lattice site and σ_{α} is the spin–orbital index. The latter accounts for the component of the spin along a given direction, as well as for an orbital index in the case where two or more orbitals reside on a given lattice site (this also includes the case where the unit cell contains two or more atoms). For phonons, we have $\kappa = (i_{\kappa}, s_{\kappa})$, where i_{κ} is, again, a lattice site, while s_{κ} is a branch index. The full derivation of the EPI Hamiltonian, including the microscopic definition of the coefficients, is given in [Appendix A](#). Without loss of generality, we assume that $M_{\alpha, \beta}^{(\lambda)} = M_{\beta, \alpha}^{(\lambda)}$. This condition, together with $t_{\alpha, \beta} = t_{\beta, \alpha}^*$, $f_{\kappa, \lambda} = f_{\lambda, \kappa}^*$, and $U_{\alpha, \beta, \delta, \gamma} = U_{\delta, \gamma, \alpha, \beta}^*$, guarantees that the Hamiltonian is Hermitian.

Eqs. (1), (2), (3), (4), and (5) explicitly display their dependence on the sets of parameters $\mathbf{t} \equiv \{t_{\alpha, \beta}\}$, $\mathbf{U} \equiv \{U_{\alpha, \beta, \gamma, \delta}\}$, $\mathbf{f} \equiv \{f_{\kappa, \lambda}\}$, and $\mathbf{M} \equiv \{M_{\alpha, \beta}^{(\lambda)}\}$. The phonon displacement operator \hat{Q}_{λ} in (5) is defined as

$$\hat{Q}_{\lambda} = \sum_{\kappa} f_{\lambda, -\kappa}^{-1/2} \frac{1}{\sqrt{2}} (\hat{b}_{\kappa}^{\dagger} + \hat{b}_{\kappa}), \quad (6)$$

where $-\kappa$ is the composite index that results after applying spatial inversion to the position index i_{κ} of the composite index κ (see [Appendix B](#)).

The parameters \mathbf{t} , \mathbf{U} , and \mathbf{f} have dimensions of energy, $[E]$. The field operators \hat{c} and \hat{b} are dimensionless. The operators \hat{Q} have dimensions of $[E^{-1/2}]$, and therefore the \mathbf{M} parameters have dimensions of $[E^{3/2}]$.

Although Eq. (5) makes use of the widely used definition of the \mathbf{M} parameters, for the present derivation of the LWF it is convenient to rewrite it as

$$\hat{\mathcal{H}}_{\text{EPI}}(\mathbf{I}) = \sum_{\alpha, \beta, \kappa} I_{\alpha, \beta}^{(\kappa)} \hat{q}_{\kappa} \hat{c}_{\alpha}^{\dagger} \hat{c}_{\beta}, \quad (7)$$

where we have introduced a dimensionless displacement operator

$$\hat{q}_{\kappa} \equiv \frac{1}{\sqrt{2}} (\hat{b}_{\kappa}^{\dagger} + \hat{b}_{\kappa}), \quad (8)$$

as well as the renormalized EPI parameters $\mathbf{I} \equiv \{I_{\alpha, \beta}^{(\kappa)}\}$ given by

$$I_{\alpha, \beta}^{(\kappa)} \equiv \sum_{\lambda} M_{\alpha, \beta}^{(\lambda)} f_{\lambda, -\kappa}^{-1/2}, \quad (9)$$

with dimensions of energy, $[E]$. In this way, the operators have no hidden dependence on the parameters \mathbf{f} . We will revert to the use of the \mathbf{M} parameters starting from [Section 5.3](#).

We carry out our formal derivations for a general basis of single-particle states. The position (lattice) representation may be particularly useful, e.g., to study the Hubbard model, or any strongly

correlated system. However, in some cases it is useful to switch to the Bloch state representation, which diagonalizes the independent-particle Hamiltonians. We then denote the lattice coordinates by \mathbf{R}_i (while the equilibrium position of a nucleus is, in general, $\mathbf{R}_{i,n} \equiv \mathbf{R}_i + \mathbf{B}_n$, where \mathbf{B}_n is a vector of the unit cell basis), and we introduce the Fourier transform matrix elements,

$$F_{\mathbf{k},i} = \frac{1}{\sqrt{N}} e^{i\mathbf{k}\cdot\mathbf{R}_i}, \quad (10)$$

where N is the number of lattice sites; then

$$\sum_i F_{\mathbf{k},i} F_{\mathbf{k}',i}^* = \delta_{\mathbf{k},\mathbf{k}'}, \quad \sum_{\mathbf{k}} F_{\mathbf{k},i}^* F_{\mathbf{k},j} = \delta_{i,j}. \quad (11)$$

We assume that the matrices \mathbf{t} and \mathbf{f} are diagonal in the spin-orbital or branch indices, respectively:

$$t_{\alpha,\beta} = \delta_{\sigma_\alpha,\sigma_\beta} t_{i_\alpha,i_\beta}(\sigma_\alpha), \quad f_{\kappa,\lambda} = \delta_{s_\kappa,s_\lambda} f_{i_\kappa,i_\lambda}(s_\kappa). \quad (12)$$

They are diagonalized with respect to the lattice index by the Fourier transform matrix,

$$\begin{aligned} \sum_{i,j} F_{\mathbf{k},i}^* t_{i,j}(\sigma) F_{\mathbf{k}',j} &= \delta_{\mathbf{k},\mathbf{k}'} \epsilon_{\mathbf{k},\sigma} \Leftrightarrow t_{i,j}(\sigma) = \sum_{\mathbf{k}} F_{\mathbf{k},i} \epsilon_{\mathbf{k},\sigma} F_{\mathbf{k},j}^*, \\ \sum_{i,j} F_{\mathbf{k},i}^* f_{i,j}(s) F_{\mathbf{k}',j} &= \delta_{\mathbf{k},\mathbf{k}'} \omega_{\mathbf{k},s} \Leftrightarrow f_{i,j}(s) = \sum_{\mathbf{k}} F_{\mathbf{k},i} \omega_{\mathbf{k},s} F_{\mathbf{k},j}^*, \end{aligned} \quad (13)$$

where $\epsilon_{\mathbf{k},\sigma}$ is the electronic spectrum and $\omega_{\mathbf{k},s}$ is the phonon dispersion. The operators are then transformed according to

$$\begin{aligned} \hat{c}_{i,\sigma}^\dagger &= \sum_{\mathbf{k}} F_{\mathbf{k},i}^* \hat{c}_{\mathbf{k},\sigma}^\dagger, \quad \hat{c}_{i,\sigma} = \sum_{\mathbf{k}} F_{\mathbf{k},i} \hat{c}_{\mathbf{k},\sigma}, \\ \hat{b}_{i,s}^\dagger &= \sum_{\mathbf{k}} F_{\mathbf{k},i}^* \hat{b}_{\mathbf{k},s}^\dagger, \quad \hat{b}_{i,s} = \sum_{\mathbf{k}} F_{\mathbf{k},i} \hat{b}_{\mathbf{k},s}. \end{aligned} \quad (14)$$

Because of the complete generality of the notation introduced in Eqs. (1), (2), (3), (4), and (5), the present formalism can be directly applied to both normal and superconducting systems; in the latter case, it is convenient to use the Gor'kov–Nambu representation of the electronic basis set [77], as we will see in Section 8.

4. Derivation of the LWF

The LWF for a purely electronic system was derived in Ref. [78] in a way that is *nonperturbative* in the EEL. Hence, it is suitable for applications to strongly correlated electronic systems, where the skeleton-diagram expansion [69,70], which is typically used in the weakly-interacting regime, may fail to converge. Here, we extend the derivation of Ref. [78] by including the phonon terms $\hat{\mathcal{H}}_{\text{IP}}(\mathbf{f})$ and $\hat{\mathcal{H}}_{\text{EPI}}(\mathbf{I})$ in the Hamiltonian. In our notation, Ref. [78] only treats the electronic subsystem described by $\hat{\mathcal{H}}_{\text{IE}}(\mathbf{t})$ and $\hat{\mathcal{H}}_{\text{EEL}}(\mathbf{U})$.

4.1. Definitions

We start by introducing a number of useful quantities, and the corresponding notations. The grand potential of the system at temperature T is

$$\Omega_{\mathbf{t},\mathbf{U},\mathbf{f},\mathbf{I}} = -T \ln(\mathcal{Z}_{\mathbf{t},\mathbf{U},\mathbf{f},\mathbf{I}}), \quad (15)$$

where the partition function is

$$\mathcal{Z}_{\mathbf{t},\mathbf{U},\mathbf{f},\mathbf{I}} = \text{tr} \exp \left[-\frac{\hat{\mathcal{H}}(\mathbf{t}, \mathbf{U}, \mathbf{f}, \mathbf{I}) - \mu \hat{N}}{T} \right], \quad (16)$$

μ being the electron chemical potential and \hat{N} the total electron number operator; the symbol “tr” denotes the trace over the Fock space associated with the Hamiltonian $\hat{\mathcal{H}}(\mathbf{t}, \mathbf{U}, \mathbf{f}, \mathbf{I})$. In the framework of a path-integral formulation, we introduce the action

$$\begin{aligned}
 A_{\mathbf{t}, \mathbf{U}, \mathbf{f}, \mathbf{I}}^{(c, \bar{c}, b, b^*)} &\equiv \frac{1}{T} \sum_n \sum_{\alpha, \beta} \bar{c}_\alpha(i\omega_n) [(i\omega_n + \mu)\delta_{\alpha, \beta} - t_{\alpha, \beta}] c_\beta(i\omega_n) \\
 &+ \frac{1}{T} \sum_n \sum_{\kappa, \lambda} b_\kappa^*(i\Omega_n) (i\Omega_n \delta_{\kappa, \lambda} - f_{\kappa, \lambda}) b_\lambda(i\Omega_n) \\
 &- \frac{1}{2} \sum_{\alpha, \beta, \gamma, \delta} U_{\alpha, \beta, \delta, \gamma} \int_0^{1/T} d\tau \bar{c}_\alpha(\tau) \bar{c}_\beta(\tau) c_\gamma(\tau) c_\delta(\tau) \\
 &- \sum_{\alpha, \beta, \kappa} l_{\alpha, \beta}^{(\kappa)} \int_0^{1/T} d\tau q_\kappa(\tau) \bar{c}_\alpha(\tau) c_\beta(\tau), \tag{17}
 \end{aligned}$$

where the fermionic and bosonic field operators appearing in the Hamiltonian $\hat{\mathcal{H}}(\mathbf{t}, \mathbf{U}, \mathbf{f}, \mathbf{I})$ have been replaced by the corresponding Grassmann numbers (\bar{c} , c) and complex numbers (b^* , b , q), respectively. Moreover, $\omega_n = (2n + 1)\pi T$ is a fermionic Matsubara frequency, $\Omega_n = 2n\pi T$ is a bosonic Matsubara frequency, and [79]

$$\begin{aligned}
 c_\alpha(i\omega_n) &= T \int_0^{1/T} d\tau e^{i\omega_n \tau} c_\alpha(\tau), & \bar{c}_\alpha(i\omega_n) &= T \int_0^{1/T} d\tau e^{-i\omega_n \tau} \bar{c}_\alpha(\tau), \\
 b_\kappa(i\Omega_n) &= T \int_0^{1/T} d\tau e^{i\Omega_n \tau} b_\kappa(\tau), & b_\kappa^*(i\Omega_n) &= T \int_0^{1/T} d\tau e^{-i\Omega_n \tau} b_\kappa^*(\tau). \tag{18}
 \end{aligned}$$

Finally,

$$q_\kappa(\tau) = \frac{1}{\sqrt{2}} [b_\kappa^*(\tau) + b_\kappa(\tau)] = \sum_{i\Omega_n} \frac{e^{i\Omega_n \tau}}{\sqrt{2}} [b_\kappa^*(i\Omega_n) + b_\kappa(-i\Omega_n)], \tag{19}$$

where we have used Eq. (8).

The partition-function path integral is written as

$$\mathcal{Z}_{\mathbf{t}, \mathbf{U}, \mathbf{f}, \mathbf{I}} \equiv \int D(\bar{c}, c) D(b^*, b) e^{A_{\mathbf{t}, \mathbf{U}, \mathbf{f}, \mathbf{I}}^{(c, \bar{c}, b, b^*)}}. \tag{20}$$

The fully-interacting one-electron and one-phonon Green's functions (GFs) are given, respectively, by

$$G_{\mathbf{t}, \mathbf{U}, \mathbf{f}, \mathbf{I}; \alpha, \beta}(i\omega_n) \equiv \frac{-T^{-1}}{\mathcal{Z}_{\mathbf{t}, \mathbf{U}, \mathbf{f}, \mathbf{I}}} \int D(\bar{c}, c) D(b^*, b) c_\alpha(i\omega_n) \bar{c}_\beta(i\omega_n) e^{A_{\mathbf{t}, \mathbf{U}, \mathbf{f}, \mathbf{I}}^{(c, \bar{c}, b, b^*)}} \tag{21}$$

and

$$P_{\mathbf{t}, \mathbf{U}, \mathbf{f}, \mathbf{I}; \kappa, \lambda}(i\Omega_n) \equiv \frac{-T^{-1}}{\mathcal{Z}_{\mathbf{t}, \mathbf{U}, \mathbf{f}, \mathbf{I}}} \int D(\bar{c}, c) D(b^*, b) b_\kappa(i\Omega_n) b_\lambda^*(i\Omega_n) e^{A_{\mathbf{t}, \mathbf{U}, \mathbf{f}, \mathbf{I}}^{(c, \bar{c}, b, b^*)}}. \tag{22}$$

We also introduce the free one-electron GF,

$$G_{\mathbf{t}, \mathbf{0}, \mathbf{f}, \mathbf{0}; \alpha, \beta}(i\omega_n) = \left(\frac{1}{i\omega_n \mathbb{1} + \boldsymbol{\mu} - \mathbf{t}} \right)_{\alpha, \beta}, \tag{23}$$

and the free one-phonon GF,

$$P_{\mathbf{t}, \mathbf{0}, \mathbf{f}, \mathbf{0}; \kappa, \lambda}(i\Omega_n) = \left(\frac{1}{i\Omega_n \mathbb{1} - \mathbf{f}} \right)_{\kappa, \lambda}, \tag{24}$$

which are obtained from Eqs. (21) and (22), respectively, by setting $\mathbf{U} = \mathbf{0}$ and $\mathbf{I} = \mathbf{0}$. In Eq. (23), we introduced the identity matrix $\mathbb{1}$ and allowed the chemical potential $\boldsymbol{\mu}$ to be a diagonal matrix

in the spin indices. This allows us to describe spin-polarized systems, and/or do calculations in the Nambu-Gor'kov representation.

All GFs are matrices in the particle Greek indices. To denote the full matrices (as opposed to their elements), we use notations such as $\mathbf{G}_{t,u,f,I}(i\omega_n)$ and $\mathbf{P}_{t,u,f,I}(i\Omega_n)$. When the dependence on the frequency is not made explicit, e.g., as in $\mathbf{G}_{t,u,f,I}$ and $\mathbf{P}_{t,u,f,I}$, we mean that the matrix symbols include the dependence on the Matsubara frequencies as well.

The following important identity holds:

$$\Omega_{t,0,f,0} = T \text{Tr} \ln (-T \mathbf{G}_{t,0,f,0}) - T \text{Tr} \ln (-T \mathbf{P}_{t,0,f,0}) , \quad (25)$$

where the notation $\text{Tr} \mathbf{X} \equiv \sum_n \sum_\alpha e^{i\omega_n 0^+} X_{\alpha,\alpha}(i\omega_n)$ was used. The property (25) is proven in Appendix C.

The electronic/phononic self-energy matrices are defined, respectively, as

$$\Sigma_{t,u,f,I}(i\omega_n) \equiv \mathbf{G}_{t,0,f,0}^{-1}(i\omega_n) - \mathbf{G}_{t,u,f,I}^{-1}(i\omega_n) , \quad (26)$$

and

$$\Lambda_{t,u,f,I}(i\Omega_n) \equiv \mathbf{P}_{t,0,f,0}^{-1}(i\Omega_n) - \mathbf{P}_{t,u,f,I}^{-1}(i\Omega_n) . \quad (27)$$

4.2. Auxiliary functionals

We introduce the following functionals:

$$\tilde{\Omega}_{U,I} [\mathbf{G}_0^{-1}; \mathbf{P}_0^{-1}] \equiv -T \ln \tilde{\Xi}_{U,I} [\mathbf{G}_0^{-1}; \mathbf{P}_0^{-1}] , \quad (28)$$

$$\tilde{\Xi}_{U,I} [\mathbf{G}_0^{-1}; \mathbf{P}_0^{-1}] \equiv \int D(\bar{c}, c) D(b^*, b) e^{\tilde{A}_{U,I}^{(c,\bar{c},b,b^*)} [\mathbf{G}_0^{-1}; \mathbf{P}_0^{-1}]} , \quad (29)$$

and

$$\begin{aligned} \tilde{A}_{U,I}^{(c,\bar{c},b,b^*)} [\mathbf{G}_0^{-1}; \mathbf{P}_0^{-1}] &\equiv \frac{1}{T} \sum_n \sum_{\alpha,\beta} \bar{c}_\alpha(i\omega_n) G_{0;\alpha,\beta}^{-1}(i\omega_n) c_\beta(i\omega_n) \\ &+ \frac{1}{T} \sum_n \sum_{\kappa,\lambda} b_\kappa^*(i\Omega_n) P_{0;\kappa,\lambda}^{-1}(i\Omega_n) b_\lambda(i\Omega_n) \\ &- \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} U_{\alpha,\beta,\delta,\gamma} \int_0^{1/T} d\tau \bar{c}_\alpha(\tau) \bar{c}_\beta(\tau) c_\gamma(\tau) c_\delta(\tau) \\ &- \sum_{\alpha,\beta,\lambda} I_{\alpha,\beta}^{(\lambda)} \int_0^{1/T} d\tau q_\lambda(\tau) \bar{c}_\alpha(\tau) c_\beta(\tau) . \end{aligned} \quad (30)$$

The above quantities are functionals of the matrices \mathbf{G}_0^{-1} and \mathbf{P}_0^{-1} , which ought to be considered as *free variables*. They should not be confused with the quantities $\mathbf{G}_{t,0,f,0}^{-1}(i\omega_n)$ and $\mathbf{P}_{t,0,f,0}^{-1}(i\Omega_n)$, which have a precise physical meaning. If the substitution $[\mathbf{G}_0^{-1}; \mathbf{P}_0^{-1}] \rightarrow [\mathbf{G}_{t,0,f,0}^{-1}; \mathbf{P}_{t,0,f,0}^{-1}]$ is made, then

$$\tilde{\Omega}_{U,I} [\mathbf{G}_{t,0,f,0}^{-1}; \mathbf{P}_{t,0,f,0}^{-1}] = \Omega_{t,u,f,I} \quad (31)$$

follows by construction (this explains the adopted notation).

We now define the following functional,

$$\tilde{\mathbf{G}}_{U,I} [\mathbf{G}_0^{-1}; \mathbf{P}_0^{-1}](i\omega_n) \equiv -\frac{1}{T} \frac{\delta \tilde{\Omega}_{U,I} [\mathbf{G}_0^{-1}; \mathbf{P}_0^{-1}]}{\delta \mathbf{G}_0^{-1T}(i\omega_n)} , \quad (32)$$

where \mathbf{G}_0^{-1T} denotes the transpose [80] of the matrix \mathbf{G}_0^{-1} . The functional $\tilde{\mathbf{G}}_{U,I}$ has the following property:

$$\tilde{\mathbf{G}}_{U,I} [\mathbf{G}_{t,0,f,0}^{-1}; \mathbf{P}_{t,0,f,0}^{-1}](i\omega_n) = \mathbf{G}_{t,u,f,I}(i\omega_n) . \quad (33)$$

Analogously, we introduce the functional

$$\tilde{\mathbf{P}}_{U,I} [\mathbf{G}_0^{-1}; \mathbf{P}_0^{-1}] (i\Omega_n) \equiv \frac{1}{T} \frac{\delta \tilde{\Omega}_{U,I} [\mathbf{G}_0^{-1}; \mathbf{P}_0^{-1}]}{\delta \mathbf{P}_0^{-1T} (i\Omega_n)}, \quad (34)$$

with the property

$$\tilde{\mathbf{P}}_{U,I} [\mathbf{G}_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0}}^{-1}; \mathbf{P}_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0}}^{-1}] (i\Omega_n) = \mathbf{P}_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0}} (i\Omega_n). \quad (35)$$

Importantly, the functionals $\tilde{\mathbf{G}}_{U,I}$ and $\tilde{\mathbf{P}}_{U,I}$ do not depend on the parameters \mathbf{t} and \mathbf{f} , characterizing the independent-particle system.

4.3. Variable substitutions

The functionals introduced above depend on the variables $\mathbf{G}_0^{-1}, \mathbf{P}_0^{-1}$. We now make two variable substitutions, choosing $\mathbf{G}, \Sigma, \mathbf{P}$, and Λ in such a way that

$$\tilde{\mathbf{G}}_{U,I} [\mathbf{G}^{-1} + \Sigma; \mathbf{P}^{-1} + \Lambda] (i\omega_n) = \mathbf{G} (i\omega_n) \quad (36)$$

and

$$\tilde{\mathbf{P}}_{U,I} [\mathbf{G}^{-1} + \Sigma; \mathbf{P}^{-1} + \Lambda] (i\Omega_n) = \mathbf{P} (i\Omega_n). \quad (37)$$

These two relations can be used to define the following functionals of the new independent variables Σ and Λ ,

$$\tilde{\mathbf{G}}_{U,I} [\Sigma; \Lambda] (i\omega_n) \equiv \tilde{\mathbf{G}}_{U,I} [\tilde{\mathbf{G}}_{U,I}^{-1} [\Sigma; \Lambda] + \Sigma; \tilde{\mathbf{P}}_{U,I}^{-1} [\Sigma; \Lambda] + \Lambda] (i\omega_n), \quad (38)$$

$$\tilde{\mathbf{P}}_{U,I} [\Sigma; \Lambda] (i\Omega_n) \equiv \tilde{\mathbf{P}}_{U,I} [\tilde{\mathbf{G}}_{U,I}^{-1} [\Sigma; \Lambda] + \Sigma; \tilde{\mathbf{P}}_{U,I}^{-1} [\Sigma; \Lambda] + \Lambda] (i\Omega_n). \quad (39)$$

When the substitution $[\Sigma; \Lambda] \rightarrow [\Sigma_{\mathbf{t},\mathbf{U},\mathbf{f},\mathbf{I}}; \Lambda_{\mathbf{t},\mathbf{U},\mathbf{f},\mathbf{I}}]$ is made, the relations

$$\tilde{\mathbf{G}}_{U,I} [\Sigma_{\mathbf{t},\mathbf{U},\mathbf{f},\mathbf{I}}; \Lambda_{\mathbf{t},\mathbf{U},\mathbf{f},\mathbf{I}}] (i\omega_n) = \mathbf{G}_{\mathbf{t},\mathbf{U},\mathbf{f},\mathbf{I}} (i\omega_n) \quad (40)$$

and

$$\tilde{\mathbf{P}}_{U,I} [\Sigma_{\mathbf{t},\mathbf{U},\mathbf{f},\mathbf{I}}; \Lambda_{\mathbf{t},\mathbf{U},\mathbf{f},\mathbf{I}}] (i\Omega_n) = \mathbf{P}_{\mathbf{t},\mathbf{U},\mathbf{f},\mathbf{I}} (i\Omega_n) \quad (41)$$

follow by construction.

4.4. Functional of the self-energies

We now introduce the functional

$$\begin{aligned} \tilde{F}_{U,I} [\Sigma; \Lambda] &\equiv \tilde{\Omega}_{U,I} [\tilde{\mathbf{G}}_{U,I} [\Sigma; \Lambda]^{-1} + \Sigma; \tilde{\mathbf{P}}_{U,I} [\Sigma; \Lambda]^{-1} + \Lambda] \\ &\quad - T \text{Tr} \ln (-T \tilde{\mathbf{G}}_{U,I} [\Sigma; \Lambda]) + T \text{Tr} \ln (-T \tilde{\mathbf{P}}_{U,I} [\Sigma; \Lambda]), \end{aligned} \quad (42)$$

which is written in terms of the other functionals introduced above.

The following important properties hold:

$$-\frac{1}{T} \frac{\delta \tilde{F}_{U,I} [\Sigma; \Lambda]}{\delta \Sigma^T (i\omega_n)} = \tilde{\mathbf{G}}_{U,I} [\Sigma; \Lambda] (i\omega_n) \quad (43)$$

and

$$\frac{1}{T} \frac{\delta \tilde{F}_{U,I} [\Sigma; \Lambda]}{\delta \Lambda^T (i\Omega_n)} = \tilde{\mathbf{P}}_{U,I} [\Sigma; \Lambda] (i\Omega_n). \quad (44)$$

The proof of Eqs. (43) and (44) is given in [Appendix D](#).

4.5. Generalized LWF

We assume that the pair of functionals $(\tilde{\mathbf{G}}_{U,I}[\Sigma; \Lambda], \tilde{\mathbf{P}}_{U,I}[\Sigma; \Lambda])$ can be inverted, yielding the pair $(\tilde{\Sigma}_{U,I}[\mathbf{G}; \mathbf{P}], \tilde{\Lambda}_{U,I}[\mathbf{G}; \mathbf{P}])$. We then define the generalized LWF as the Legendre transform of \tilde{F} , i.e.

$$\tilde{\Phi}_{U,I}[\mathbf{G}; \mathbf{P}] \equiv \tilde{F}_{U,I}[\tilde{\Sigma}_{U,I}[\mathbf{G}; \mathbf{P}]; \tilde{\Lambda}_{U,I}[\mathbf{G}; \mathbf{P}]] + T\text{Tr}(\tilde{\Sigma}_{U,I}[\mathbf{G}; \mathbf{P}]\mathbf{G}) - T\text{Tr}(\tilde{\Lambda}_{U,I}[\mathbf{G}; \mathbf{P}]\mathbf{P}) . \quad (45)$$

Taking Eq. (42) into account, we write $\tilde{\Phi}_{U,I}[\mathbf{G}; \mathbf{P}]$ as

$$\begin{aligned} \tilde{\Phi}_{U,I}[\mathbf{G}; \mathbf{P}] &= \tilde{\Omega}_{U,I}[\mathbf{G}^{-1} + \tilde{\Sigma}_{U,I}[\mathbf{G}; \mathbf{P}]; \mathbf{P}^{-1} + \tilde{\Lambda}_{U,I}[\mathbf{G}; \mathbf{P}]] - T\text{Tr} \ln(-T\mathbf{G}) \\ &\quad + T\text{Tr}(\tilde{\Sigma}_{U,I}[\mathbf{G}; \mathbf{P}]\mathbf{G}) + T\text{Tr} \ln(-T\mathbf{P}) - T\text{Tr}(\tilde{\Lambda}_{U,I}[\mathbf{G}; \mathbf{P}]\mathbf{P}) . \end{aligned} \quad (46)$$

By construction, $\tilde{\Phi}_{U,I}[\mathbf{G}; \mathbf{P}]$ is independent of \mathbf{t} and \mathbf{f} . It has the following properties:

- (1) When the replacement $[\mathbf{G}; \mathbf{P}] \rightarrow [\mathbf{G}_{\mathbf{t},U,\mathbf{f},I}; \mathbf{P}_{\mathbf{t},U,\mathbf{f},I}]$ is made, the grand potential of the electron-phonon system is obtained as

$$\begin{aligned} \Omega_{\mathbf{t},U,\mathbf{f},I} &= \tilde{\Phi}_{U,I}[\mathbf{G}_{\mathbf{t},U,\mathbf{f},I}; \mathbf{P}_{\mathbf{t},U,\mathbf{f},I}] + T\text{Tr} \ln(-T\mathbf{G}_{\mathbf{t},U,\mathbf{f},I}) - T\text{Tr}(\Sigma_{\mathbf{t},U,\mathbf{f},I} \mathbf{G}_{\mathbf{t},U,\mathbf{f},I}) \\ &\quad - T\text{Tr} \ln(-T\mathbf{P}_{\mathbf{t},U,\mathbf{f},I}) + T\text{Tr}(\Lambda_{\mathbf{t},U,\mathbf{f},I} \mathbf{P}_{\mathbf{t},U,\mathbf{f},I}) . \end{aligned} \quad (47)$$

- (2) The functionals corresponding to the self-energies are obtained from the LWF via functional differentiation, i.e.

$$\frac{1}{T} \frac{\delta \tilde{\Phi}_{U,I}[\mathbf{G}; \mathbf{P}]}{\delta \mathbf{G}^T} = \tilde{\Sigma}_{U,I}[\mathbf{G}; \mathbf{P}] \quad (48)$$

and

$$-\frac{1}{T} \frac{\delta \tilde{\Phi}_{U,I}[\mathbf{G}; \mathbf{P}]}{\delta \mathbf{P}^T} = \tilde{\Lambda}_{U,I}[\mathbf{G}; \mathbf{P}] . \quad (49)$$

The proof of Eqs. (48) and (49) is given in [Appendix E](#). These properties are often referred to as the Φ -derivability of the self-energies. Any approximation on $\tilde{\Phi}_{U,I}[\mathbf{G}; \mathbf{P}]$ that preserves its symmetry properties (such as invariance under gauge transformations and time translations) yields a conserving approximation for the self-energy [70,81,82].

- (3) From the definitions of Σ and Λ , we have $\Sigma_{\mathbf{t},0,\mathbf{f},0} = \mathbf{0}$ and $\Lambda_{\mathbf{t},0,\mathbf{f},0} = \mathbf{0}$. Therefore, in the non-interacting case we have

$$\Omega_{\mathbf{t},0,\mathbf{f},0} = \tilde{\Phi}_{0,0}[\mathbf{G}_{\mathbf{t},0,\mathbf{f},0}; \mathbf{P}_{\mathbf{t},0,\mathbf{f},0}] + T\text{Tr} \ln(-T\mathbf{G}_{\mathbf{t},0,\mathbf{f},0}) - T\text{Tr} \ln(-T\mathbf{P}_{\mathbf{t},0,\mathbf{f},0}) . \quad (50)$$

Substituting Eq. (25) into (50), we find that the LWF vanishes for a non-interacting system:

$$\tilde{\Phi}_{0,0}[\mathbf{G}_{\mathbf{t},0,\mathbf{f},0}; \mathbf{P}_{\mathbf{t},0,\mathbf{f},0}] = 0 . \quad (51)$$

5. Expansion of the LWF

We now study the dependence of the LWF on the parameters \mathbf{I} , by means of a perturbative expansion in the EPI, close to $\mathbf{I} = \mathbf{0}$. We expand the LWF in powers of \mathbf{I} , up to second order:

$$\tilde{\Phi}_{U,I}[\mathbf{G}; \mathbf{P}] \approx \tilde{\Phi}_{U,0}[\mathbf{G}; \mathbf{P}] + \tilde{\Phi}_{U,I}^{(1)}[\mathbf{G}; \mathbf{P}] + \tilde{\Phi}_{U,I}^{(2)}[\mathbf{G}; \mathbf{P}] , \quad (52)$$

where

$$\tilde{\Phi}_{U,I}^{(1)}[\mathbf{G}; \mathbf{P}] = \sum_{\lambda,\alpha,\beta} I_{\alpha,\beta}^{(\lambda)} \left. \frac{\partial \tilde{\Phi}_{U,I}[\mathbf{G}; \mathbf{P}]}{\partial I_{\alpha,\beta}^{(\lambda)}} \right|_{\mathbf{I}=\mathbf{0}} , \quad (53)$$

and

$$\tilde{\Phi}_{U,I}^{(2)}[\mathbf{G}; \mathbf{P}] = \frac{1}{2} \sum_{\lambda,\alpha,\beta} \sum_{\lambda',\alpha',\beta'} I_{\alpha,\beta}^{(\lambda)} I_{\alpha',\beta'}^{(\lambda')} \left. \frac{\partial^2 \tilde{\Phi}_{U,I}[\mathbf{G}; \mathbf{P}]}{\partial I_{\alpha,\beta}^{(\lambda)} \partial I_{\alpha',\beta'}^{(\lambda')}} \right|_{\mathbf{I}=\mathbf{0}} . \quad (54)$$

It should be noted that the LWF depends on \mathbf{I} via the parametric dependences of $\tilde{\Sigma}_{U,\mathbf{I}}$, $\tilde{\Lambda}_{U,\mathbf{I}}$, and $\tilde{\Omega}_{U,\mathbf{I}}$ —see Eq. (46).

In the following, we derive the three terms of Eq. (52). We first note that, in the absence of EPIs (i.e. for $\mathbf{I} = \mathbf{0}$), the electronic system is totally decoupled from the phonons. It follows that

$$\tilde{\Lambda}_{U,\mathbf{0}}[\mathbf{G}; \mathbf{P}] \equiv \mathbf{0}, \quad \tilde{\Sigma}_{U,\mathbf{0}}[\mathbf{G}; \mathbf{P}] \equiv \tilde{\Sigma}_U[\mathbf{G}], \quad (55)$$

where $\tilde{\Sigma}_U[\mathbf{G}]$ is the *universal* self-energy functional for a system of electrons interacting via the Hamiltonian defined in (3).

5.1. Zeroth-order term

The zeroth-order term is

$$\begin{aligned} \tilde{\Phi}_{U,\mathbf{0}}[\mathbf{G}; \mathbf{P}] &= -T \ln \tilde{\mathcal{Z}}_{U,\mathbf{0}}[\mathbf{G}^{-1} + \tilde{\Sigma}_{U,\mathbf{0}}[\mathbf{G}; \mathbf{P}]; \mathbf{P}^{-1} + \tilde{\Lambda}_{U,\mathbf{0}}[\mathbf{G}; \mathbf{P}]] \\ &\quad + T \text{Tr}(\tilde{\Sigma}_{U,\mathbf{0}}[\mathbf{G}; \mathbf{P}]\mathbf{G}) - T \text{Tr} \ln(-T\mathbf{G}) - T \text{Tr}(\tilde{\Lambda}_{U,\mathbf{0}}[\mathbf{G}; \mathbf{P}]\mathbf{P}) + T \text{Tr} \ln(-T\mathbf{P}). \end{aligned} \quad (56)$$

At $\mathbf{I} = \mathbf{0}$, we have

$$\begin{aligned} \tilde{\mathcal{Z}}_{U,\mathbf{0}}[\mathbf{G}_0^{-1}; \mathbf{P}_0^{-1}] &= \int D(\bar{c}, c) D(b^*, b) e^{\tilde{\Lambda}_{U,\mathbf{0}}^{(c,\bar{c},b,b^*)}[\mathbf{G}_0^{-1}; \mathbf{P}_0^{-1}]} \\ &= \frac{1}{\prod_{\Omega_n} \det[-\frac{1}{T}\mathbf{P}_0^{-1}(i\Omega_n)]} \tilde{\mathcal{Z}}_U[\mathbf{G}_0^{-1}], \end{aligned} \quad (57)$$

where

$$\tilde{\mathcal{Z}}_U[\mathbf{G}_0^{-1}] \equiv \int D(\bar{c}, c) e^{\tilde{\Lambda}_{U,\mathbf{0}}^{(c,\bar{c},0,0)}[\mathbf{G}_0^{-1}; \mathbf{0}]} \quad (58)$$

is the partition-function functional for the system of interacting electrons alone. We now apply the identity $\ln \det = \text{tr} \ln$, as well as Eq. (55), and we obtain

$$\begin{aligned} \tilde{\Phi}_{U,\mathbf{0}}[\mathbf{G}; \mathbf{P}] &= -T \ln \tilde{\mathcal{Z}}_U[\mathbf{G}^{-1} + \tilde{\Sigma}_U[\mathbf{G}]] + T \text{Tr}(\tilde{\Sigma}_U[\mathbf{G}]\mathbf{G}) - T \text{Tr} \ln(-T\mathbf{G}) \\ &\equiv \tilde{\Phi}_U^{(\text{E})}[\mathbf{G}], \end{aligned} \quad (59)$$

which is the LWF for the system of interacting electrons, completely decoupled from the phonon system. This is equivalent to the LWF for the electronic system derived in Ref. [78]. In this limit, where the EPI is absent, the properties of the non-interacting phonon system still enter the physical grand potential via the term $-T \text{Tr} \ln(-T\mathbf{P}_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0}})$, as can be seen from Eq. (50).

5.2. First-order term

We observe that

$$\begin{aligned} &\frac{\partial \tilde{\Omega}_{U,\mathbf{I}}[\mathbf{G}^{-1} + \tilde{\Sigma}_{U,\mathbf{I}}[\mathbf{G}; \mathbf{P}]; \mathbf{P}^{-1} + \tilde{\Lambda}_{U,\mathbf{I}}[\mathbf{G}; \mathbf{P}]]}{\partial I_{\alpha,\beta}^{(\lambda)}} \\ &= -T \text{Tr} \left(\mathbf{G} \frac{\partial \tilde{\Sigma}_{U,\mathbf{I}}[\mathbf{G}; \mathbf{P}]}{\partial I_{\alpha,\beta}^{(\lambda)}} - \mathbf{P} \frac{\partial \tilde{\Lambda}_{U,\mathbf{I}}[\mathbf{G}; \mathbf{P}]}{\partial I_{\alpha,\beta}^{(\lambda)}} \right) \\ &\quad + T \frac{1}{\tilde{\mathcal{Z}}_{U,\mathbf{I}}[\mathbf{G}^{-1} + \tilde{\Sigma}_{U,\mathbf{I}}[\mathbf{G}; \mathbf{P}]; \mathbf{P}^{-1} + \tilde{\Lambda}_{U,\mathbf{I}}[\mathbf{G}; \mathbf{P}]]} \\ &\quad \times \int D(\bar{c}, c) D(b^*, b) \int_0^{1/T} d\tau q_\lambda(\tau) \bar{c}_\alpha(\tau) c_\beta(\tau) e^{\tilde{\Lambda}_{U,\mathbf{I}}^{(c,\bar{c},b,b^*)}[\mathbf{G}^{-1} + \tilde{\Sigma}_{U,\mathbf{I}}[\mathbf{G}; \mathbf{P}]; \mathbf{P}^{-1} + \tilde{\Lambda}_{U,\mathbf{I}}[\mathbf{G}; \mathbf{P}]]}. \end{aligned} \quad (60)$$

Therefore, the first derivative of Eq. (46) is

$$\begin{aligned} \frac{\partial \tilde{\Phi}_{U,I}[\mathbf{G}; \mathbf{P}]}{\partial I_{\alpha,\beta}^{(\lambda)}} &= T \frac{1}{\tilde{\mathcal{Z}}_{U,I}[\mathbf{G}^{-1} + \tilde{\Sigma}_{U,I}[\mathbf{G}; \mathbf{P}]; \mathbf{P}^{-1} + \tilde{\Lambda}_{U,I}[\mathbf{G}; \mathbf{P}]} \\ &\times \int D(\bar{c}, c) D(b^*, b) \int_0^{1/T} d\tau q_\lambda(\tau) \bar{c}_\alpha(\tau) c_\beta(\tau) \\ &\times e^{\tilde{\Lambda}_{U,I}^{(c,\bar{c},b,b^*)}[\mathbf{G}^{-1} + \tilde{\Sigma}_{U,I}[\mathbf{G}; \mathbf{P}]; \mathbf{P}^{-1} + \tilde{\Lambda}_{U,I}[\mathbf{G}; \mathbf{P}]} . \end{aligned} \tag{61}$$

At $\mathbf{I} = \mathbf{0}$, this functional vanishes. In fact, it is proportional to the ensemble average of $q_\lambda(\tau)$, which is linear in the bosonic fields [see Eq. (8)], evaluated with an action that is quadratic in the boson fields. Therefore,

$$\tilde{\Phi}_{U,I}^{(1)}[\mathbf{G}; \mathbf{P}] = 0 . \tag{62}$$

5.3. Second-order term

Starting from Eq. (61), we directly evaluate the second derivative of the LWF at $\mathbf{I} = \mathbf{0}$, using the fact that the average of an odd-power combination of bosonic operators vanishes if the bosonic action is quadratic. We obtain

$$\begin{aligned} \left. \frac{\partial^2 \tilde{\Phi}_{U,I}[\mathbf{G}; \mathbf{P}]}{\partial I_{\alpha,\beta}^{(\lambda)} \partial I_{\alpha',\beta'}^{(\lambda')}} \right|_{\mathbf{I}=\mathbf{0}} &= -T \frac{1}{\tilde{\mathcal{Z}}_{U,0}[\mathbf{G}^{-1} + \tilde{\Sigma}_U[\mathbf{G}]; \mathbf{P}^{-1}]} \\ &\times \int D(\bar{c}, c) D(b^*, b) \int_0^{1/T} d\tau q_\lambda(\tau) \bar{c}_\alpha(\tau) c_\beta(\tau) \\ &\times \int_0^{1/T} d\tau' q_{\lambda'}(\tau') \bar{c}_{\alpha'}(\tau') c_{\beta'}(\tau') e^{\tilde{\Lambda}_{U,0}^{(c,\bar{c},b,b^*)}[\mathbf{G}^{-1} + \tilde{\Sigma}_U[\mathbf{G}]; \mathbf{P}^{-1}]} , \end{aligned} \tag{63}$$

where the partition-function functional at $\mathbf{I} = \mathbf{0}$ can be factorized as shown in Eq. (57) as

$$\tilde{\mathcal{Z}}_{U,0}[\mathbf{G}^{-1} + \tilde{\Sigma}_U[\mathbf{G}]; \mathbf{P}^{-1}] = \frac{\tilde{\mathcal{Z}}_U[\mathbf{G}^{-1} + \tilde{\Sigma}_U[\mathbf{G}]]}{\prod_{\Omega_n} \det[-\frac{1}{T} \mathbf{P}^{-1}(i\Omega_n)]} . \tag{64}$$

We now perform the functional integration over the bosonic fields in Eq. (63):

$$\begin{aligned} &\frac{1}{\prod_{\Omega_n} \det[-\frac{1}{T} \mathbf{P}^{-1}(i\Omega_n)]} \int D(b^*, b) q_\lambda(\tau) q_{\lambda'}(\tau') e^{\frac{1}{T} \sum_n \sum_{\kappa,\lambda} b_\kappa^*(i\Omega_n) P_{\kappa,\lambda}^{-1}(i\Omega_n) b_\lambda(i\Omega_n)} \\ &= \frac{1}{\prod_{\Omega_n} \det[-\frac{1}{T} \mathbf{P}^{-1}(i\Omega_n)]} \sum_{i\Omega_n} \frac{e^{i\Omega_n(\tau-\tau')}}{2} \\ &\times \int D(b^*, b) [b_\lambda^*(i\Omega_n) b_{\lambda'}(i\Omega_n) + b_\lambda(-i\Omega_n) b_{\lambda'}^*(-i\Omega_n)] e^{\frac{1}{T} \sum_m \sum_{\kappa'',\lambda''} b_{\kappa''}^*(i\Omega_m) P_{\kappa'',\lambda''}^{-1}(i\Omega_m) b_{\lambda''}(i\Omega_m)} \\ &= -T \sum_{i\Omega_n} e^{i\Omega_n(\tau-\tau')} \frac{1}{2} [P_{\lambda',\lambda}(i\Omega_n) + P_{\lambda,\lambda'}(-i\Omega_n)] . \end{aligned} \tag{65}$$

Replacing this result into Eq. (63), transforming the fermionic fields to the Matsubara frequency representation, and performing the integrals over the time variables τ and τ' , we arrive at the following result:

$$\begin{aligned} \left. \frac{\partial^2 \tilde{\Phi}_{U,I}[\mathbf{G}; \mathbf{P}]}{\partial I_{\alpha,\beta}^{(\lambda)} \partial I_{\alpha',\beta'}^{(\lambda')}} \right|_{\mathbf{I}=\mathbf{0}} &= \frac{1}{\tilde{\mathcal{Z}}_U[\mathbf{G}^{-1} + \tilde{\Sigma}_U[\mathbf{G}]]} \sum_{i\Omega_n} \sum_{n',m} \int D(\bar{c}, c) c_\beta(i\omega_m) c_{\beta'}(i\omega_{n'} - i\Omega_n) \\ &\times \bar{c}_{\alpha'}(i\omega_{n'}) \bar{c}_\alpha(i\omega_m - i\Omega_n) e^{\tilde{\Lambda}_{U,0}^{(c,\bar{c})}[\mathbf{G}^{-1} + \tilde{\Sigma}_U[\mathbf{G}]]} \frac{1}{2} [P_{\lambda',\lambda}(i\Omega_n) + P_{\lambda,\lambda'}(-i\Omega_n)] , \end{aligned} \tag{66}$$

where we have introduced the electronic action functional in the absence of phonons,

$$\begin{aligned} \tilde{A}_{\mathbf{U}}^{(c,\bar{c})} [\mathbf{G}^{-1} + \tilde{\Sigma}_{\mathbf{U}}[\mathbf{G}]] &\equiv \tilde{A}_{\mathbf{U},\mathbf{0}}^{(c,\bar{c},0,0)} [\mathbf{G}^{-1} + \tilde{\Sigma}_{\mathbf{U}}[\mathbf{G}; \mathbf{0}]] \\ &= \frac{1}{T} \sum_n \sum_{\alpha,\beta} \bar{c}_{\alpha}(i\omega_n) \{ G_{\alpha,\beta}^{-1}(i\omega_n) + \tilde{\Sigma}_{\mathbf{U};\alpha,\beta}[\mathbf{G}](i\omega_n) \} c_{\beta}(i\omega_n) \\ &\quad - \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} U_{\alpha,\beta,\delta,\gamma} \int_0^{1/T} d\tau \bar{c}_{\alpha}(\tau) \bar{c}_{\beta}(\tau) c_{\gamma}(\tau) c_{\delta}(\tau). \end{aligned} \quad (67)$$

Eq. (66) requires the evaluation of a two-particle correlator, in the presence of a non-Gaussian weight. Due to the form of the action, this correlator is equivalent to a two-electron GF. More precisely, its functional dependence on \mathbf{G} (here an independent variable of arbitrary value) is the same as the functional dependence of the two-electron GF on the one-electron GF. We can then apply the usual concepts of many-body perturbation theory, provided that the GF is replaced by the independent variable \mathbf{G} . Only at the end of the derivation, \mathbf{G} will be identified with the physical one-electron GF. Using a compact notation, we write

$$\begin{aligned} &T^{-2} \langle c_{\beta}(i\omega_m) c_{\beta'}(i\omega_{n'} - i\Omega_n) \bar{c}_{\alpha'}(i\omega_{n'}) \bar{c}_{\alpha}(i\omega_m - i\Omega_n) \rangle \\ &= \delta_{n,0} G_{\beta,\alpha}(i\omega_m) G_{\beta',\alpha'}(i\omega_{n'}) - \delta_{m,n'} G_{\beta,\alpha}(i\omega_m) G_{\beta',\alpha'}(i\omega_m - i\Omega_n) \\ &\quad + \delta_{n,0} \sum_{v,\mu,v',\mu'} G_{\beta,v}(i\omega_m) G_{\mu',\alpha'}(i\omega_{n'}) G_{\mu,\alpha}(i\omega_m) G_{\beta',v'}(i\omega_{n'}) \tilde{\Gamma}_{\mathbf{U};(v,\mu;v',\mu')}[\mathbf{G}](i\omega_m, i\omega_{n'}) \\ &\quad - \delta_{m,n'} \sum_{v,\mu,v',\mu'} G_{\beta,v}(i\omega_m) G_{\mu,\alpha}(i\omega_m - i\Omega_n) G_{\mu',\alpha'}(i\omega_m) G_{\beta',v'}(i\omega_m - i\Omega_n) \\ &\quad \times \tilde{\Gamma}_{\mathbf{U};(v,\mu';v',\mu)}[\mathbf{G}](i\omega_m, i\omega_m - i\Omega_n), \end{aligned} \quad (68)$$

where $\tilde{\Gamma}_{\mathbf{U};(v,\mu;v',\mu')}[\mathbf{G}](i\omega_m, i\omega_{n'})$ is the *reducible* four-leg vertex, a functional of \mathbf{G} , which depends parametrically on \mathbf{U} . By inserting this expansion into Eq. (66), and inserting the result into Eq. (54), we finally obtain

$$\begin{aligned} \tilde{\Phi}_{\mathbf{U},\mathbf{I}}^{(2)}[\mathbf{G}; \mathbf{P}] &= \frac{T^2}{2} \sum_{\alpha,\beta} \sum_{\alpha',\beta'} \sum_{\kappa,\kappa'} I_{\alpha,\beta}^{(\kappa)} I_{\alpha',\beta'}^{(\kappa')} \frac{1}{2} [P_{\kappa,\kappa'}(i\Omega_n) + P_{\kappa,\kappa'}(-i\Omega_n)] \\ &\quad \times \sum_{i\Omega_n} \sum_{i\omega_{n'}, i\omega_m} \left\{ \delta_{n,0} G_{\beta,\alpha}(i\omega_m) G_{\beta',\alpha'}(i\omega_{n'}) - \delta_{m,n'} G_{\beta,\alpha}(i\omega_m) G_{\beta',\alpha'}(i\omega_m - i\Omega_n) \right. \\ &\quad + \delta_{n,0} \sum_{v,\mu,v',\mu'} G_{\beta,v}(i\omega_m) G_{\mu',\alpha'}(i\omega_{n'}) G_{\mu,\alpha}(i\omega_m) G_{\beta',v'}(i\omega_{n'}) \\ &\quad \times \tilde{\Gamma}_{\mathbf{U};(v,\mu;v',\mu')}[\mathbf{G}](i\omega_m, i\omega_{n'}) \\ &\quad - \delta_{m,n'} \sum_{v,\mu,v',\mu'} G_{\beta,v}(i\omega_m) G_{\mu,\alpha}(i\omega_m - i\Omega_n) G_{\mu',\alpha'}(i\omega_m) G_{\beta',v'}(i\omega_m - i\Omega_n) \\ &\quad \left. \times \tilde{\Gamma}_{\mathbf{U};(v,\mu';v',\mu)}[\mathbf{G}](i\omega_m, i\omega_m - i\Omega_n) \right\}. \end{aligned} \quad (69)$$

It is now convenient to make a change of variables: from now on, instead of (\mathbf{I}, \mathbf{P}) , we will use (\mathbf{M}, \mathbf{D}) , where

$$D_{\lambda,\lambda'}(i\Omega_n) \equiv \sum_{\kappa,\kappa'} f_{\lambda,-\kappa}^{-1/2} f_{\lambda',-\kappa'}^{-1/2} \frac{1}{2} [P_{\kappa,\kappa'}(i\Omega_n) + P_{\kappa,\kappa'}(-i\Omega_n)], \quad (70)$$

and the \mathbf{M} parameters are the EPI parameters introduced in Section 3. The following property holds,

$$D_{\lambda,\lambda'}(i\Omega_n) = D_{\lambda',\lambda}(-i\Omega_n). \quad (71)$$

The quantity in the first line of Eq. (69) transforms as

$$\sum_{\kappa, \kappa'} f_{\alpha, \beta}^{(\kappa)} f_{\alpha', \beta'}^{(\kappa')} \frac{1}{2} [P_{\kappa, \kappa'}(i\Omega_n) + P_{\kappa, \kappa'}(-i\Omega_n)] = \sum_{\lambda, \lambda'} M_{\alpha, \beta}^{(\lambda)} M_{\alpha', \beta'}^{(\lambda')} D_{\lambda, \lambda'}(i\Omega_n). \quad (72)$$

When evaluated at the physical *non-interacting* phonon GF [see Eq. (24)], Eq. (70) yields

$$\begin{aligned} & \sum_{\kappa} f_{\lambda, -\kappa}^{-1/2} \sum_{\kappa'} f_{\lambda', -\kappa'}^{-1/2} \frac{1}{2} [P_{\mathbf{t}, \mathbf{0}, \mathbf{f}, \mathbf{0}; \kappa, \kappa'}(i\Omega_n) + P_{\mathbf{t}, \mathbf{0}, \mathbf{f}, \mathbf{0}; \kappa, \kappa'}(-i\Omega_n)] \\ &= \sum_{\kappa} f_{\lambda, -\kappa}^{-1/2} \sum_{\kappa'} f_{\lambda', -\kappa'}^{-1/2} \frac{1}{2} \left[\left(\frac{1}{i\Omega_n \mathbb{1} - \mathbf{f}} \right)_{\kappa', \kappa} + \left(\frac{1}{-i\Omega_n \mathbb{1} - \mathbf{f}} \right)_{\kappa, \kappa'} \right] \\ &= \delta_{s_\lambda, s_{\lambda'}} \sum_i f_{i\lambda, -i}^{-1/2}(s_\lambda) \sum_j f_{i\lambda', -j}^{-1/2}(s_{\lambda'}) \frac{1}{2} \sum_{\mathbf{q}} \left[F_{\mathbf{q}, j}^* \left(\frac{1}{i\Omega_n - \omega_{\mathbf{q}, s_\lambda}} \right) F_{\mathbf{q}, i} \right. \\ & \quad \left. + F_{\mathbf{q}, i}^* \left(\frac{1}{-i\Omega_n - \omega_{\mathbf{q}, s_{\lambda'}}} \right) F_{\mathbf{q}, j} \right] \\ &= -\delta_{s_\lambda, s_{\lambda'}} \sum_{ij} \sum_{\mathbf{q}, \mathbf{q}', \mathbf{q}''} F_{\mathbf{q}', i\lambda}^* \omega_{\mathbf{q}', s_\lambda}^{-1/2} F_{\mathbf{q}', i}^* F_{\mathbf{q}'', i\lambda'}^* \omega_{\mathbf{q}'', s_{\lambda'}}^{-1/2} F_{\mathbf{q}'', j}^* \frac{\omega_{\mathbf{q}, s_\lambda}}{\Omega_n^2 + \omega_{\mathbf{q}, s_\lambda}^2} F_{\mathbf{q}, i}^* F_{\mathbf{q}, j} \\ &= -\delta_{s_\lambda, s_{\lambda'}} \sum_{\mathbf{q}} F_{\mathbf{q}, i\lambda} F_{\mathbf{q}, i\lambda'}^* \frac{1}{\Omega_n^2 + \omega_{\mathbf{q}, s_\lambda}^2}, \end{aligned} \quad (73)$$

where we have used the Fourier coefficients defined in Eqs. (10), (13), and the property $\omega_{\mathbf{q}, s_\lambda} = \omega_{-\mathbf{q}, s_\lambda}$. In the last line, we recognize the bare phonon GF associated with the displacement operator,

$$D_{\lambda, \lambda'}^{(0)}(i\Omega_n) \equiv -\delta_{s_\lambda, s_{\lambda'}} \frac{1}{N} \sum_{\mathbf{q}} e^{i\mathbf{q}(\mathbf{R}_{i\lambda} - \mathbf{R}_{i\lambda'})} \frac{1}{\Omega_n^2 + \omega_{\mathbf{q}, s_\lambda}^2} \equiv D_{\mathbf{t}, \mathbf{0}, \mathbf{f}, \mathbf{0}; \lambda, \lambda'}(i\Omega_n), \quad (74)$$

which motivates our notation.

The second-order term of the LWF is finally written as

$$\tilde{\Phi}_{\mathbf{U}, \mathbf{M}}^{(2)}[\mathbf{G}; \mathbf{D}] \equiv \tilde{\Phi}_{\mathbf{U}, \mathbf{M}}^{(F)}[\mathbf{G}; \mathbf{D}] + \tilde{\Phi}_{\mathbf{U}, \mathbf{M}}^{(H)}[\mathbf{G}; \mathbf{D}], \quad (75)$$

where we have separated a Fock term,

$$\begin{aligned} \tilde{\Phi}_{\mathbf{U}, \mathbf{M}}^{(F)}[\mathbf{G}; \mathbf{D}] &= -\frac{T^2}{2} \sum_{\lambda, \alpha, \beta} \sum_{\lambda', \alpha', \beta'} M_{\alpha, \beta}^{(\lambda)} M_{\alpha', \beta'}^{(\lambda')} \sum_{i\Omega_n} D_{\lambda, \lambda'}(i\Omega_n) \sum_{i\omega_m} \left\{ G_{\beta, \alpha'}(i\omega_m) G_{\beta', \alpha}(i\omega_m - i\Omega_n) \right. \\ & \quad \left. + \sum_{v, \mu, v', \mu'} G_{\beta, v}(i\omega_m) G_{\mu, \alpha}(i\omega_m - i\Omega_n) G_{\mu', \alpha'}(i\omega_m) G_{\beta', v'}(i\omega_m - i\Omega_n) \right. \\ & \quad \left. \times \tilde{\Gamma}_{\mathbf{U}; (v, \mu'; v', \mu)}[\mathbf{G}](i\omega_m, i\omega_m - i\Omega_n) \right\}, \end{aligned} \quad (76)$$

and a Hartree term,

$$\begin{aligned} \tilde{\Phi}_{\mathbf{U}, \mathbf{M}}^{(H)}[\mathbf{G}; \mathbf{D}] &= \frac{T^2}{2} \sum_{\lambda, \alpha, \beta} \sum_{\lambda', \alpha', \beta'} M_{\alpha, \beta}^{(\lambda)} M_{\alpha', \beta'}^{(\lambda')} D_{\lambda, \lambda'}(0) \sum_{i\omega_m, i\omega_n} \left\{ G_{\beta, \alpha}(i\omega_m) G_{\beta', \alpha'}(i\omega_n) \right. \\ & \quad \left. + \sum_{v, \mu, v', \mu'} G_{\beta, v}(i\omega_m) G_{\mu', \alpha'}(i\omega_n) G_{\mu, \alpha}(i\omega_m) G_{\beta', v'}(i\omega_n) \right. \\ & \quad \left. \times \tilde{\Gamma}_{\mathbf{U}; (v, \mu; v', \mu')}[\mathbf{G}](i\omega_m, i\omega_n) \right\}. \end{aligned} \quad (77)$$

Functionals analogous to (76) and (77) were first derived in Ref. [77] for the problem of phonon-mediated superconductivity in a *non-interacting* but disordered electron system. The most profound difference between our results (76) and (77) and those of Ref. [77] is in the nature of the reducible

four-leg vertex $\tilde{\Gamma}_{\mathbf{U};(v,\mu;v',\mu')}[\mathbf{G}](i\omega_m, i\omega_n)$. In our case, this is the universal reducible four-leg vertex for a system of electrons interacting via the Hamiltonian defined in (3). In the case of Ref. [77], the analogous four-leg vertex refers to a system of *non-interacting* disordered electrons. The four-leg vertex functional introduced in our work is therefore fundamentally different from that introduced in Ref. [77]. Evident implications of this difference will be discussed below when we calculate the electronic self-energies—see below Section 6.1. One minor difference between our formulas and the corresponding ones in Ref. [77] lies in the temperature prefactors in Eqs. (76) and (77), which stem from the use of a different convention. (In this work we have followed the convention of Ref. [78].)

In summary, in this Section we have been able to prove that the LWF for the fully interacting electron–phonon system is given, up to the second order in the EPI matrix elements, by

$$\tilde{\Phi}_{\mathbf{U},M}[\mathbf{G}; \mathbf{D}] \approx \tilde{\Phi}_{\mathbf{U}}^{(E)}[\mathbf{G}] + \tilde{\Phi}_{\mathbf{U},M}^{(F)}[\mathbf{G}; \mathbf{D}] + \tilde{\Phi}_{\mathbf{U},M}^{(H)}[\mathbf{G}; \mathbf{D}]. \quad (78)$$

6. Electronic self-energy from the expansion of the LWF

We now derive the electronic self-energy by applying Eq. (48) to the terms of the LWF listed in Eq. (78). We obtain

$$\tilde{\Sigma}_{\mathbf{U},M;\phi,\theta}[\mathbf{G}; \mathbf{D}](i\omega_n) \approx \tilde{\Sigma}_{\mathbf{U};\phi,\theta}^{(E)}[\mathbf{G}](i\omega_n) + \tilde{\Sigma}_{\mathbf{U},M;\phi,\theta}^{(F)}[\mathbf{G}; \mathbf{D}](i\omega_n) + \tilde{\Sigma}_{\mathbf{U},M;\phi,\theta}^{(H)}[\mathbf{G}; \mathbf{D}](i\omega_n), \quad (79)$$

where

$$\begin{aligned} \tilde{\Sigma}_{\mathbf{U};\phi,\theta}^{(E)}[\mathbf{G}](i\omega_n) &\equiv \frac{1}{T} \frac{\delta \tilde{\Phi}_{\mathbf{U}}^{(E)}[\mathbf{G}]}{\delta G_{\theta,\phi}(i\omega_n)}, \quad (80) \\ \tilde{\Sigma}_{\mathbf{U},M;\phi,\theta}^{(F)}[\mathbf{G}; \mathbf{D}](i\omega_n) &\equiv \frac{1}{T} \frac{\delta \tilde{\Phi}_{\mathbf{U},M}^{(F)}[\mathbf{G}; \mathbf{D}]}{\delta G_{\theta,\phi}(i\omega_n)} \\ &= -T \sum_{\lambda,\lambda'} \sum_{i\Omega} D_{\lambda,\lambda'}(i\Omega) \left\{ \sum_{\alpha,\beta} M_{\phi,\alpha}^{(\lambda)} M_{\beta,\theta}^{(\lambda')} G_{\alpha,\beta}(i\omega_n - i\Omega) \right. \\ &\quad + \sum_{\alpha,\beta,\alpha'} M_{\alpha,\beta}^{(\lambda)} M_{\alpha',\theta}^{(\lambda')} \sum_{\mu,\nu,\mu'} G_{\mu,\alpha}(i\omega_n) G_{\nu,\alpha'}(i\omega_n - i\Omega) G_{\beta,\mu'}(i\omega_n - i\Omega) \\ &\quad \times \tilde{\Gamma}_{\mathbf{U};(\phi,\mu;\mu',\nu)}[\mathbf{G}](i\omega_n, i\omega_n - i\Omega) \\ &\quad + \sum_{\beta,\alpha',\beta'} M_{\phi,\beta}^{(\lambda)} M_{\alpha',\beta'}^{(\lambda')} \sum_{\nu,\nu',\mu'} G_{\beta,\mu'}(i\omega_n - i\Omega) G_{\nu,\alpha'}(i\omega_n - i\Omega) G_{\beta',\nu'}(i\omega_n) \\ &\quad \times \tilde{\Gamma}_{\mathbf{U};(\mu',\nu;\nu',\theta)}[\mathbf{G}](i\omega_n - i\Omega, i\omega_n) \\ &\quad + \frac{1}{2} \sum_{i\omega_m} \sum_{\alpha,\beta} \sum_{\alpha',\beta'} M_{\alpha,\beta}^{(\lambda)} M_{\alpha',\beta'}^{(\lambda')} \sum_{\nu,\mu,\nu',\mu'} G_{\beta,\mu}(i\omega_m) G_{\mu',\alpha}(i\omega_m - i\Omega) G_{\nu,\alpha'}(i\omega_m) G_{\beta',\nu'}(i\omega_m - i\Omega) \\ &\quad \left. \times \frac{\delta \tilde{\Gamma}_{\mathbf{U};(\mu,\nu;\nu',\mu')}[\mathbf{G}](i\omega_m, i\omega_m - i\Omega)}{\delta G_{\theta,\phi}(i\omega_n)} \right\}, \quad (81) \end{aligned}$$

and

$$\begin{aligned} \tilde{\Sigma}_{\mathbf{U},M;\phi,\theta}^{(H)}[\mathbf{G}; \mathbf{D}](i\omega_n) &\equiv \frac{1}{T} \frac{\delta \tilde{\Phi}_{\mathbf{U},M}^{(H)}[\mathbf{G}; \mathbf{D}]}{\delta G_{\theta,\phi}(i\omega_n)} \\ &= T \sum_{\lambda,\lambda'} D_{\lambda,\lambda'}(0) \sum_{i\omega_m} \left\{ \sum_{\alpha,\beta} M_{\phi,\theta}^{(\lambda)} M_{\alpha,\beta}^{(\lambda')} G_{\beta,\alpha}(i\omega_m) \right. \\ &\quad + \sum_{\alpha,\alpha',\beta} M_{\alpha,\beta}^{(\lambda)} M_{\alpha',\theta}^{(\lambda')} \sum_{\mu,\nu,\mu'} G_{\beta,\nu}(i\omega_m) G_{\mu',\alpha'}(i\omega_n) G_{\mu,\alpha}(i\omega_m) \tilde{\Gamma}_{\mathbf{U};(\phi,\mu';\nu,\mu)}[\mathbf{G}](i\omega_n, i\omega_m) \\ &\quad \left. + \sum_{\beta,\alpha',\beta'} M_{\phi,\beta}^{(\lambda)} M_{\alpha',\beta'}^{(\lambda')} \sum_{\nu,\mu,\nu'} G_{\beta',\nu'}(i\omega_m) G_{\mu,\alpha'}(i\omega_m) G_{\beta,\nu}(i\omega_n) \tilde{\Gamma}_{\mathbf{U};(\nu',\mu;\nu,\theta)}[\mathbf{G}](i\omega_m, i\omega_n) \right\} \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{2} \sum_{i\omega_s} \sum_{\alpha, \beta, \alpha', \beta'} M_{\alpha, \beta}^{(\lambda)} M_{\alpha', \beta'}^{(\lambda')} \sum_{v, \mu, v', \mu'} G_{\beta, \mu}(i\omega_m) G_{\mu', \alpha'}(i\omega_s) G_{v, \alpha}(i\omega_m) G_{\beta', v'}(i\omega_s) \\
& \times \left. \frac{\delta \tilde{\Gamma}_{\mathbf{U}; (\mu, v; v', \mu')}[\mathbf{G}](i\omega_m, i\omega_s)}{\delta G_{\theta, \phi}(i\omega_n)} \right\}. \tag{82}
\end{aligned}$$

6.1. Hartree and Fock terms: simplifications

Eqs. (81) and (82) require the evaluation of the functional derivative of the reducible four-leg vertex, i.e.

$$\tilde{\Gamma}_{\mathbf{U}; (\mu, v; \phi, \theta; v', \mu')}^{[6]}[\mathbf{G}](i\omega_m, i\omega_n, i\omega_s) \equiv \frac{\delta \tilde{\Gamma}_{\mathbf{U}; (\mu, v; v', \mu')}[\mathbf{G}](i\omega_m, i\omega_s)}{\delta G_{\theta, \phi}(i\omega_n)}. \tag{83}$$

We hasten to emphasize that the quantity $\tilde{\Gamma}_{\mathbf{U}; (\mu, v; \phi, \theta; v', \mu')}^{[6]}[\mathbf{G}](i\omega_m, i\omega_n, i\omega_s)$ introduced in Eq. (83), which is the *reducible* six-leg vertex, contains three distinct frequency arguments, in contrast to the analogous quantity for a system of *non-interacting* disordered electrons [77]. Its expression can be simplified by means of the Bethe–Salpeter equation, which connects the four-leg reducible (Γ) and four-leg *irreducible* ($U^{[4]}$) kernels of the two-particle GFs [70,83,84]:

$$\begin{aligned}
\tilde{\Gamma}_{\mathbf{U}; (\mu, v; v', \mu')}[\mathbf{G}](i\omega_m, i\omega_s) & = \tilde{U}_{\mathbf{U}; (\mu, v; v', \mu')}^{[4]}[\mathbf{G}](i\omega_m, i\omega_s) \\
& + \sum_{\xi, \xi', \eta, \eta'} \tilde{U}_{\mathbf{U}; (\mu, \xi; \xi', \mu')}^{[4]}[\mathbf{G}](i\omega_m, i\omega_s) G_{\xi, \eta}(i\omega_m) G_{\eta', \xi'}(i\omega_s) \\
& \times \tilde{\Gamma}_{\mathbf{U}; (\eta, v; v', \eta')}[\mathbf{G}](i\omega_m, i\omega_s). \tag{84}
\end{aligned}$$

By applying the functional derivative in Eqs. (83) to (84), and carrying out a few algebraic steps detailed in Appendix F, we can express Eq. (83) in terms of Γ and the irreducible quantities $U^{[4]}$ and $U^{[6]}$ only, where

$$\tilde{U}_{\mathbf{U}; (\mu, v; \phi, \theta; v', \mu')}^{[6]}[\mathbf{G}](i\omega_m, i\omega_n, i\omega_s) \equiv \frac{\delta \tilde{U}_{\mathbf{U}; (\mu, v; v', \mu')}^{[4]}[\mathbf{G}](i\omega_m, i\omega_s)}{\delta G_{\theta, \phi}(i\omega_n)}. \tag{85}$$

The result is given in Appendix F. Applying it to Eq. (81), and using the property

$$\tilde{\Gamma}_{\mathbf{U}; (\mu, v; v', \mu')}[\mathbf{G}](i\omega_m, i\omega_s) = \tilde{\Gamma}_{\mathbf{U}; (v', \mu'; \mu, v)}[\mathbf{G}](i\omega_s, i\omega_m) \tag{86}$$

of the two-particle reducible vertex, we obtain the Fock self-energy

$$\begin{aligned}
& \tilde{\Sigma}_{\mathbf{U}, \mathbf{M}; \phi, \theta}^{(F)}[\mathbf{G}; \mathbf{D}](i\omega_n) \\
& = -T \sum_{\lambda, \lambda'} \sum_{i\Omega} D_{\lambda, \lambda'}(i\Omega) \left\{ \sum_{\alpha, \beta} \tilde{M}_{\mathbf{U}; (\phi, \alpha)}^{(\lambda)}[\mathbf{G}](i\omega_n, i\omega_n - i\Omega) G_{\alpha, \beta}(i\omega_n - i\Omega) \right. \\
& \quad \times \tilde{M}_{\mathbf{U}; (\beta, \theta)}^{(\lambda')}[\mathbf{G}](i\omega_n - i\Omega, i\omega_n) \\
& \quad + \frac{1}{2} \sum_{i\omega_m} \sum_{\alpha, \beta} \sum_{\alpha', \beta'} \tilde{M}_{\mathbf{U}; (\alpha, \beta)}^{(\lambda)}[\mathbf{G}](i\omega_m - i\Omega, i\omega_m) \tilde{M}_{\mathbf{U}; (\alpha', \beta')}^{(\lambda')}[\mathbf{G}](i\omega_m, i\omega_m - i\Omega) \\
& \quad \times \sum_{v, \mu, v', \mu'} G_{\beta, \mu}(i\omega_m) G_{\mu', \alpha}(i\omega_m - i\Omega) G_{v, \alpha'}(i\omega_m) G_{\beta', v'}(i\omega_m - i\Omega) \\
& \quad \left. \times \tilde{U}_{\mathbf{U}; (\mu, v; \phi, \theta; v', \mu')}^{[6]}[\mathbf{G}](i\omega_m, i\omega_n, i\omega_m - i\Omega) \right\}, \tag{87}
\end{aligned}$$

where we have introduced the renormalized EPI vertex,

$$\tilde{M}_{\mathbf{U};(\alpha,\beta)}^{(\lambda)}[\mathbf{G}](i\omega_m, i\omega_s) \equiv M_{\alpha,\beta}^{(\lambda)} + \sum_{v,v',\mu,\mu'} \tilde{\Gamma}_{\mathbf{U};(\alpha,v;v',\beta)}[\mathbf{G}](i\omega_m, i\omega_s) G_{v,\mu}(i\omega_m) G_{\mu',v'}(i\omega_s) M_{\mu,\mu'}^{(\lambda)}. \quad (88)$$

The same treatment, applied to Eq. (82), yields the Hartree self-energy

$$\begin{aligned} & \tilde{\Sigma}_{\mathbf{U},\mathbf{M};\phi,\theta}^{(\text{H})}[\mathbf{G}; \mathbf{D}](i\omega_n) \\ &= T \sum_{\lambda,\lambda'} D_{\lambda,\lambda'}(0) \sum_{i\omega_m} \left\{ \sum_{\alpha,\beta} M_{\phi,\theta}^{(\lambda)} M_{\alpha,\beta}^{(\lambda')} G_{\beta,\alpha}(i\omega_m) \right. \\ &+ \sum_{\alpha,\alpha',\beta} M_{\alpha,\beta}^{(\lambda)} M_{\alpha',\theta}^{(\lambda')} \sum_{\mu,\nu,\mu'} G_{\beta,\mu}(i\omega_m) G_{\mu',\alpha'}(i\omega_n) G_{\nu,\alpha}(i\omega_m) \tilde{\Gamma}_{\mathbf{U};(\phi,\mu';\mu,\nu)}[\mathbf{G}](i\omega_n, i\omega_m) \\ &+ \sum_{\beta,\alpha',\beta'} M_{\phi,\beta}^{(\lambda)} M_{\alpha',\beta'}^{(\lambda')} \sum_{v,\mu,v'} G_{\beta',\mu}(i\omega_m) G_{v',\alpha'}(i\omega_m) G_{\beta,v}(i\omega_n) \tilde{\Gamma}_{\mathbf{U};(v,\theta;\mu,v')}[\mathbf{G}](i\omega_n, i\omega_m) \\ &+ \sum_{\alpha,\beta,\alpha',\beta'} M_{\alpha,\beta}^{(\lambda)} M_{\alpha',\beta'}^{(\lambda')} \sum_{v,\mu,v',\mu'} G_{\beta,\mu}(i\omega_n) G_{\mu',\alpha'}(i\omega_m) G_{v,\alpha}(i\omega_n) G_{\beta',v'}(i\omega_m) \\ &\times \sum_{\xi',\eta'} \tilde{\Gamma}_{\mathbf{U};(\mu,\theta;\xi',\mu')}[\mathbf{G}](i\omega_n, i\omega_m) G_{\eta',\xi'}(i\omega_m) \tilde{\Gamma}_{\mathbf{U};(\phi,v;v',\eta')}[\mathbf{G}](i\omega_n, i\omega_m) \\ &+ \frac{1}{2} \sum_{i\omega_s} \sum_{\alpha,\beta,\alpha',\beta'} M_{\alpha,\beta}^{(\lambda)} M_{\alpha',\beta'}^{(\lambda')} \sum_{v,\mu,v',\mu'} G_{\beta,\mu}(i\omega_m) G_{\mu',\alpha'}(i\omega_s) G_{v,\alpha}(i\omega_m) G_{\beta',v'}(i\omega_s) \\ &\times \sum_{\xi,\xi',\eta,\eta'} \tilde{U}_{\mathbf{U};(\mu,\xi;\phi,\theta;\xi',\mu')}^{[6]}[\mathbf{G}](i\omega_m, i\omega_n, i\omega_s) G_{\xi,\eta}(i\omega_m) G_{\eta',\xi'}(i\omega_s) \tilde{\Gamma}_{\mathbf{U};(\eta,v;v',\eta')}[\mathbf{G}](i\omega_m, i\omega_s) \\ &+ \frac{1}{2} \sum_{i\omega_s} \sum_{\alpha,\beta,\alpha',\beta'} M_{\alpha,\beta}^{(\lambda)} M_{\alpha',\beta'}^{(\lambda')} \sum_{v,\mu,v',\mu'} G_{\beta,\mu}(i\omega_m) G_{\mu',\alpha'}(i\omega_s) G_{v,\alpha}(i\omega_m) G_{\beta',v'}(i\omega_s) \\ &\times \sum_{\xi,\xi',\eta,\eta'} \tilde{\Gamma}_{\mathbf{U};(\mu,\xi;\xi',\mu')}[\mathbf{G}](i\omega_m, i\omega_s) G_{\xi,\eta}(i\omega_m) G_{\eta',\xi'}(i\omega_s) \tilde{U}_{\mathbf{U};(\eta,v;\phi,\theta;v',\eta')}^{[6]}[\mathbf{G}](i\omega_m, i\omega_n, i\omega_s) \\ &+ \frac{1}{2} \sum_{i\omega_s} \sum_{\alpha,\beta,\alpha',\beta'} M_{\alpha,\beta}^{(\lambda)} M_{\alpha',\beta'}^{(\lambda')} \sum_{v,\mu,v',\mu'} G_{\beta,\mu}(i\omega_m) G_{\mu',\alpha'}(i\omega_s) G_{v,\alpha}(i\omega_m) G_{\beta',v'}(i\omega_s) \\ &\times \sum_{\xi,\xi',\eta,\eta',\zeta,\zeta',\chi,\chi'} \tilde{\Gamma}_{\mathbf{U};(\mu,\xi;\xi',\mu')}[\mathbf{G}](i\omega_m, i\omega_s) G_{\xi,\eta}(i\omega_m) G_{\eta',\xi'}(i\omega_s) \\ &\times \tilde{U}_{\mathbf{U};(\eta,\zeta;\phi,\theta;\zeta',\eta')}^{[6]}[\mathbf{G}](i\omega_m, i\omega_n, i\omega_s) G_{\zeta,\chi}(i\omega_m) G_{\chi',\zeta'}(i\omega_s) \tilde{\Gamma}_{\mathbf{U};(\chi,v;v',\chi')}[\mathbf{G}](i\omega_m, i\omega_s) \\ &+ \frac{1}{2} \sum_{i\omega_s} \sum_{\alpha,\beta,\alpha',\beta'} M_{\alpha,\beta}^{(\lambda)} M_{\alpha',\beta'}^{(\lambda')} \sum_{v,\mu,v',\mu'} G_{\beta,\mu}(i\omega_m) G_{\mu',\alpha'}(i\omega_s) G_{v,\alpha}(i\omega_m) G_{\beta',v'}(i\omega_s) \\ &\times \tilde{U}_{\mathbf{U};(\mu,v;\phi,\theta;v',\mu')}^{[6]}[\mathbf{G}](i\omega_m, i\omega_n, i\omega_s) \left. \right\}. \quad (89) \end{aligned}$$

It is useful to look at the diagrammatic representation of the quantities that we have just derived. In Fig. 1, we represent the renormalized EPI vertex as a triangle with two oriented sides (corresponding to two distinct fermionic frequencies), and we give its diagrammatic equation. In Fig. 2, we represent the two terms contributing to the Fock self-energy in Eq. (87). We want to stress the representation of the $U^{[6]}$ term as a hexagon with three oriented sides and *three distinct fermionic frequencies*. This is different from the analogous term derived in Ref. [77] for the case of a disordered electron system in the absence of EEs. In the latter, two sides of the hexagon have the same fermionic frequency [77]. In the case of EEs, which we are treating here, we cannot make such an assumption, and the

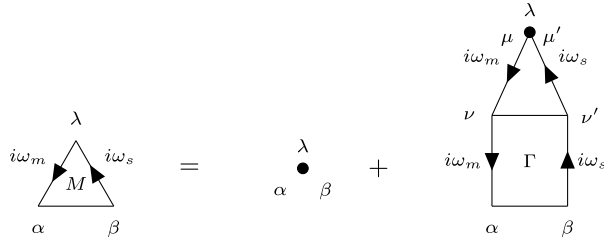


Fig. 1. Diagrammatic representation of the renormalized EPI vertex, Eq. (88). The dot with three Greek indices in the right-hand side represents the bare EPI vertex $M_{\alpha,\beta}^{(\lambda)}$. Oriented lines connecting two Greek indices and carrying a frequency label represent fully-dressed (interacting) fermionic propagators; for example, in the second term on the right-hand side, the line connecting μ to ν with frequency label $i\omega_m$ represents the GF $G_{\nu,\mu}(i\omega_m)$ [compare with Eq. (88)]. These oriented lines are also features of vertex functionals with fermionic character (i.e. that should be connected to fermionic propagators), such as $\tilde{M}_{U;(\alpha,\beta)}^{(\lambda)}[\mathbf{G}](i\omega_m, i\omega_s)$ and $\tilde{\Gamma}_{U;(\alpha,\nu;\nu',\beta)}[\mathbf{G}](i\omega_m, i\omega_s)$. For simplicity, in all diagrams we remove the $\tilde{\cdot}$ symbols over the functionals, so we write, e.g., M for \tilde{M} and Γ for $\tilde{\Gamma}$.

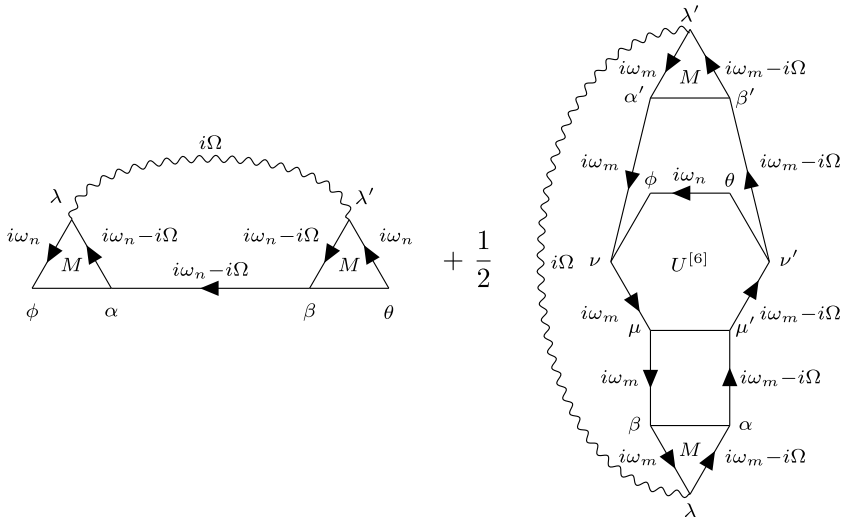


Fig. 2. Diagrammatic representation of the Fock self-energy, $\Sigma_{\phi,\theta}^{(F)}(i\omega_n)$ —see Eq. (87). The wavy line appearing in both diagrams corresponds to a fully-dressed (interacting) phonon propagator, namely, $D_{\lambda,\lambda'}(i\Omega)$ [compare with Eq. (87)]. In order to recover the algebraic expression for the Fock self-energy, Eq. (87), the diagram in this figure must be intended to be multiplied by a factor $-T$.

three frequencies can, in principle, be all different [recall the definition in Eq. (85)]. For this reason, we need a different diagrammatic representation of the six-leg vertex, which produces Feynman diagrams with distinct topological features with respect to those of Ref. [77]. This is evident also in the representation of the Hartree self-energy terms, Figs. 3 and 4. In Fig. 3, we represent the first four terms of Eq. (89): these are topologically equivalent to the analogous ones derived in Ref. [77], since they do not involve $U^{[6]}$. The last four terms of Eq. (89), represented in Fig. 4, are instead topologically different from their counterparts in Ref. [77]. Their structure is a peculiar effect of EEIs.

It should be emphasized that the expansion of the LWF and self-energy functionals up to the second order in the EPI matrix elements effectively produces infinite-order approximations for the

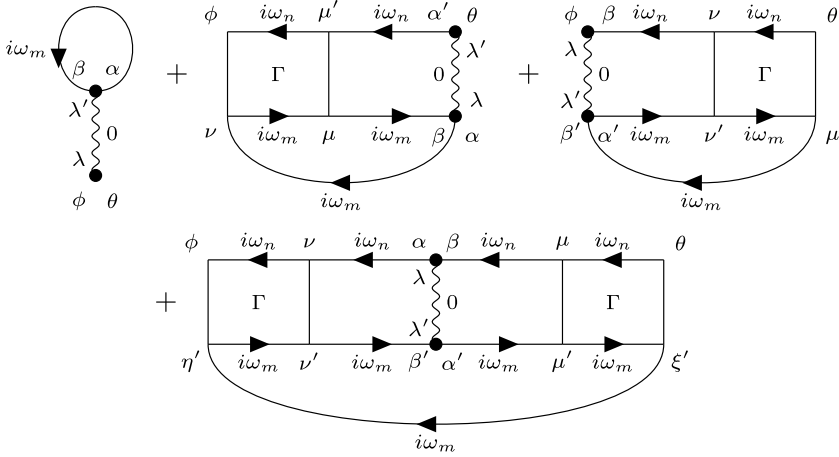


Fig. 3. Diagrammatic representation of the first four terms of the Hartree self-energy, $\Sigma_{\phi,\theta}^{(H)}(i\omega_n)$ —see Eq. (89). In order to recover the algebraic expression for the Hartree self-energy, Eq. (89), the diagram in this figure must be intended to be multiplied by a factor T . The different sign with respect to the Fock case is due to the presence of an additional fermionic loop. This remark applies to the diagrams of Fig. 4 as well.

corresponding *physical quantities*. In fact, the physical self-energy depends on the physical GF, which should be inserted in the place of the independent variable G into Eqs. (80), (87), and (89). As the physical GF depends on the EPI matrix elements up to all orders, so does the physical self-energy. This is a common feature of many-body perturbation theory schemes based on the LWF, which when used with the physical GFs yields self-consistent equations that lead formally to all-order results. An example in the context of electron systems interacting via long-range Coulomb interactions is the so-called GW self-consistent scheme.

Before concluding this Section, we note that our treatment of the electronic self-energy is different from the one presented in Ref. [37]. It is worthwhile to comment on the differences between the two approaches. The author of Ref. [37] introduces the electronic self-energy evaluated at clamped nuclei (Σ^{cn}), which leads to the definition of the electronic GF at clamped nuclei (G^{cn}). The two are connected via the corresponding Dyson equation. These quantities are evaluated within the context of the most general (Hedin–Baym) formalism, by setting to zero all the GFs associated with the phonon displacement D . This procedure corresponds to switching off the EPI completely. As a second step, a higher-level Dyson equation is written for the full problem (in the presence of EPIs), by considering G^{cn} as the “non-interacting” GF, and introducing a self-energy that connects it to the fully interacting GF.

Our approach is different, as we write a single electronic GF (and the corresponding Dyson equation) for the fully interacting problem, and our partition of the self-energy results from an expansion of the LWF in powers of the EPI matrix elements. Therefore, our electronic self-energy term $\Sigma^{(E)}$, given by Eq. (80), does not coincide with the quantity Σ^{cn} introduced in Ref. [37], since the former—as well as the other terms that we have derived, $\Sigma^{(H)}$ and $\Sigma^{(F)}$ —is a functional of the fully interacting GF, while the latter is a functional of G^{cn} . The complicated structure of our Hartree and Fock self-energy terms does not appear in Ref. [37]. It would probably appear in a treatment of the explicit form of the quantity $\Sigma^{(dGW)}$ introduced in Ref. [37] (which is not discussed there). Establishing the exact correspondence between the partition introduced in Ref. [37] and ours is well beyond the scope of this work.

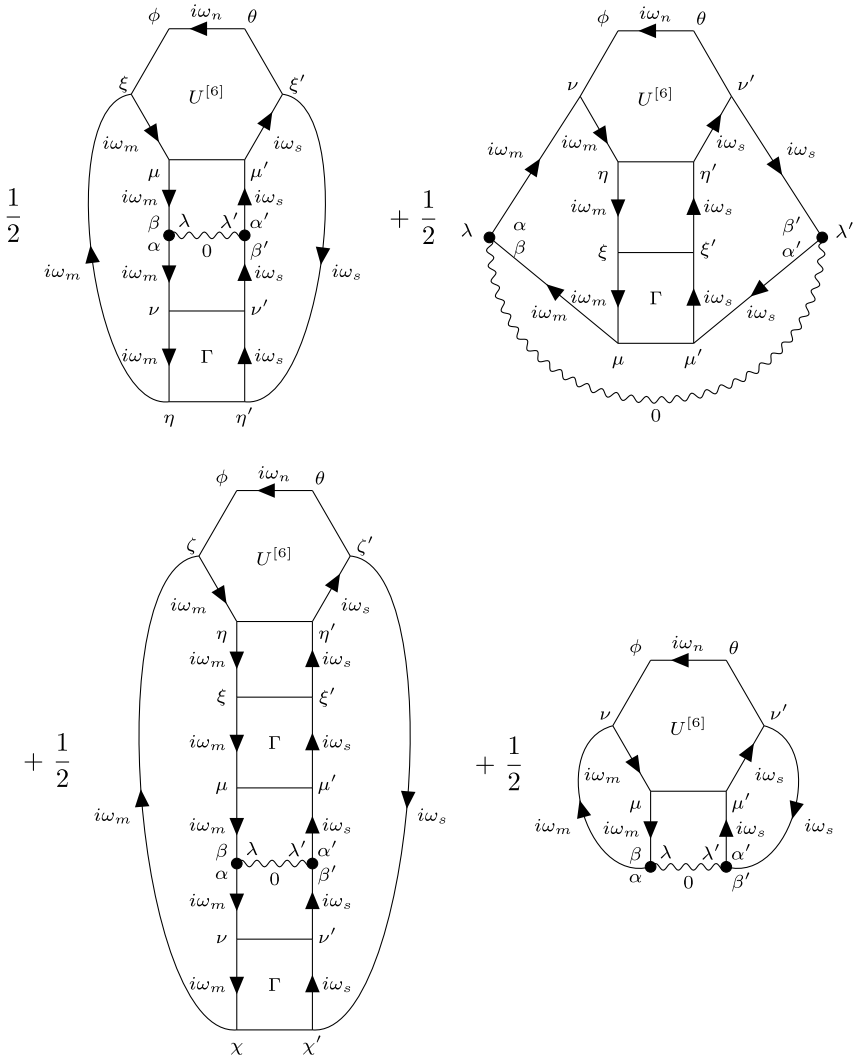


Fig. 4. Diagrammatic representation of the last four terms of the Hartree self-energy, $\Sigma_{\phi,\theta}^{(H)}(i\omega_n)$ —see Eq. (89).

7. Phononic self-energy from the expansion of the LWF

We now derive the phononic self-energy, by applying Eq. (49) to the terms of the LWF listed in Eq. (78). We first restore the (\mathbf{I}, \mathbf{P}) representation, by rewriting Eq. (78) as

$$\tilde{\Phi}_{U,I}[\mathbf{G}; \mathbf{P}] \approx \tilde{\Phi}_U^{(E)}[\mathbf{G}] + \tilde{\Phi}_{U,I}^{(F)}[\mathbf{G}; \mathbf{P}] + \tilde{\Phi}_{U,I}^{(H)}[\mathbf{G}; \mathbf{P}]. \tag{90}$$

The corresponding phononic self-energy functionals are given by

$$\tilde{\Lambda}_{U,I;\phi,\theta}[\mathbf{G}; \mathbf{P}](i\Omega_n) \approx \tilde{\Lambda}_{U,I;\phi,\theta}^{(F)}[\mathbf{G}](i\Omega_n) + \tilde{\Lambda}_{U,I;\phi,\theta}^{(H)}[\mathbf{G}](i\Omega_n), \tag{91}$$

where

$$\begin{aligned}
\tilde{\Lambda}_{\mathbf{U},\mathbf{I};\phi,\theta}^{(\text{F})}[\mathbf{G}](i\Omega_n) &\equiv -\frac{1}{T} \frac{\delta \tilde{\Phi}_{\mathbf{U},\mathbf{I}}^{(\text{F})}[\mathbf{G}; \mathbf{P}]}{\delta P_{\theta,\phi}(i\Omega_n)} \\
&= \frac{T}{2} \sum_{\alpha,\beta} \sum_{\alpha',\beta'} \sum_{i\Omega_{n'}} \frac{1}{2} \left(\delta_{n',n} I_{\alpha,\beta}^{(\phi)} I_{\alpha',\beta'}^{(\theta)} + \delta_{n',-n} I_{\alpha,\beta}^{(\theta)} I_{\alpha',\beta'}^{(\phi)} \right) \sum_{i\omega_m} \left\{ G_{\beta,\alpha'}(i\omega_m) G_{\beta',\alpha}(i\omega_m - i\Omega_{n'}) \right. \\
&\quad + \sum_{v,\mu,v',\mu'} G_{\beta,v}(i\omega_m) G_{\mu,\alpha}(i\omega_m - i\Omega_{n'}) \tilde{\Gamma}_{\mathbf{U};(v,\mu';v',\mu)}[\mathbf{G}](i\omega_m, i\omega_m - i\Omega_{n'}) \\
&\quad \left. \times G_{\mu',\alpha'}(i\omega_m) G_{\beta',v'}(i\omega_m - i\Omega_{n'}) \right\}, \tag{92}
\end{aligned}$$

and

$$\begin{aligned}
\tilde{\Lambda}_{\mathbf{U},\mathbf{I};\phi,\theta}^{(\text{H})}[\mathbf{G}](i\Omega_n) &\equiv -\frac{1}{T} \frac{\delta \tilde{\Phi}_{\mathbf{U},\mathbf{I}}^{(\text{H})}[\mathbf{G}; \mathbf{P}]}{\delta P_{\theta,\phi}(i\Omega_n)} \\
&= -\delta_{n,0} \frac{T}{2} \sum_{\alpha,\beta} \sum_{\alpha',\beta'} \frac{1}{2} \left(I_{\alpha,\beta}^{(\phi)} I_{\alpha',\beta'}^{(\theta)} + I_{\alpha,\beta}^{(\theta)} I_{\alpha',\beta'}^{(\phi)} \right) \sum_{i\omega_n, i\omega_m} \left\{ G_{\beta,\alpha}(i\omega_m) G_{\beta',\alpha'}(i\omega_n) \right. \\
&\quad \left. + \sum_{v,\mu,v',\mu'} G_{\beta,v}(i\omega_m) G_{\mu',\alpha'}(i\omega_n) \tilde{\Gamma}_{\mathbf{U};(v,\mu';v',\mu)}[\mathbf{G}](i\omega_m, i\omega_n) G_{\mu,\alpha}(i\omega_m) G_{\beta',v'}(i\omega_n) \right\}. \tag{93}
\end{aligned}$$

The following properties hold:

$$\tilde{\Lambda}_{\mathbf{U},\mathbf{I};\phi,\theta}^{(\text{F/H})}[\mathbf{G}](i\Omega_n) = \tilde{\Lambda}_{\mathbf{U},\mathbf{I};\theta,\phi}^{(\text{F/H})}[\mathbf{G}](-i\Omega_n). \tag{94}$$

8. Extended Eliashberg equations

We now derive the extended Eliashberg equations for the anomalous components of the electronic GF and self-energy. We consider the particular case of a crystal with a single orbital per unit cell. In this case the spin-orbital index σ introduced for fermions reduces to the spin index, $\sigma = \pm 1$. We neglect magnetic impurities and relativistic effects (such as spin-orbit and magnetic anisotropies). We then choose a basis of real single-electron wave functions for the definition of the Hamiltonian parameters.

For the sake of simplicity, in this Section we drop the functional notation that we have adopted in the previous Sections. It is intended that self-energies and vertex functions are functionals of the GFs.

For the derivation of extended Eliashberg equations, we use the Gor'kov–Nambu (G–N) representation for the fermionic sector of the Hamiltonian. As discussed in detail in [Appendix G](#), the G–N Hamiltonian can be directly obtained from our general formulation provided that the following choices are made:

$$U_{\alpha,\beta,\delta,\gamma} \rightarrow U_{i\alpha,i\beta,i\delta,i\gamma} \delta_{\sigma\alpha,\sigma\delta} \delta_{\sigma\beta,\sigma\gamma} \sigma_\alpha \sigma_\beta, \tag{95}$$

$$M_{\alpha,\beta}^{(\lambda)} \rightarrow M_{i\alpha,i\beta}^{(i\lambda)}(s_\lambda) \delta_{\sigma\alpha,\sigma\beta} \sigma_\alpha, \tag{96}$$

and

$$\begin{aligned}
t_{\alpha,\beta} &\rightarrow \left[t_{i\alpha,i\beta} + \sum_k U_{i\alpha,k,i\beta,k} - \sum_{k,s} I_{i\alpha,i\beta}^{(k)}(s) \sum_m f_{k,m}^{-1}(s) \sum_l I_{l,l}^{(m)}(s) \right] \delta_{\sigma\alpha,\sigma\beta} \sigma_\alpha \\
&\equiv h_{i\alpha,i\beta} \delta_{\sigma\alpha,\sigma\beta} \sigma_\alpha. \tag{97}
\end{aligned}$$

Therefore, our derivation of the LWF and related self-energies holds in the G–N representation as well. GFs and self-energies acquire a 2×2 matrix structure in spin space; the non-zero solutions of the equations for the non-diagonal matrix elements signal the onset of the superconducting phase.

Although we will keep using, for the sake of brevity, the word *electrons* (as well as terms such as EEI and EPI), it should be kept in mind that the fermions appearing in this derivation are actually *Nambu fermions*.

In the G–N formalism, it is natural to introduce a 2×2 matrix representation for the spin sector. We denote such matrices by means of double-underlined symbols, i.e.,

$$\begin{aligned} \underline{\underline{G}}_{i,j}(i\omega_n) &\equiv \begin{pmatrix} G_{(i,\uparrow),(j,\uparrow)}(i\omega_n) & G_{(i,\uparrow),(j,\downarrow)}(i\omega_n) \\ G_{(i,\downarrow),(j,\uparrow)}(i\omega_n) & G_{(i,\downarrow),(j,\downarrow)}(i\omega_n) \end{pmatrix}, \\ \underline{\underline{\Sigma}}_{i,j}(i\omega_n) &\equiv \begin{pmatrix} \Sigma_{(i,\uparrow),(j,\uparrow)}(i\omega_n) & \Sigma_{(i,\uparrow),(j,\downarrow)}(i\omega_n) \\ \Sigma_{(i,\downarrow),(j,\uparrow)}(i\omega_n) & \Sigma_{(i,\downarrow),(j,\downarrow)}(i\omega_n) \end{pmatrix}, \end{aligned} \quad (98)$$

where the matrix elements $G_{(i,\sigma),(j,\sigma')}(i\omega_n)$ and $\Sigma_{(i,\sigma),(j,\sigma')}(i\omega_n)$ are shorthands for the quantities $G_{\mathbf{r},\mathbf{r}',\alpha,\beta}(i\omega_n)$ and $\Sigma_{\mathbf{r},\mathbf{r}',\alpha,\beta}(i\omega_n)$ introduced earlier, respectively, where $\alpha = (i, \sigma)$ and $\beta = (j, \sigma')$.

We switch to the reciprocal lattice representation, by applying various Fourier transforms (see Section 3). Namely, the transformations from direct to reciprocal lattice for the GF and the self-energy read, respectively, as

$$\begin{aligned} \underline{\underline{G}}_{i,j}(i\omega_n) &\equiv \sum_{\mathbf{k}} F_{\mathbf{k},i} F_{\mathbf{k},j}^* \underline{\underline{G}}_{\mathbf{k}}(i\omega_n), \\ \underline{\underline{\Sigma}}_{i,j}(i\omega_n) &\equiv \sum_{\mathbf{k}} F_{\mathbf{k},i} F_{\mathbf{k},j}^* \underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n). \end{aligned} \quad (99)$$

We expand the matrices in Eq. (99) over the set of standard spin-1/2 Pauli matrices:

$$\underline{\underline{\tau}}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \underline{\underline{\tau}}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \underline{\underline{\tau}}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \underline{\underline{\tau}}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (100)$$

The electronic Dyson equation reads as

$$\underline{\underline{G}}_{\mathbf{k}}^{-1}(i\omega_n) = i\omega_n \underline{\underline{\tau}}_0 - \xi_{\mathbf{k}} \underline{\underline{\tau}}_3 - \underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n), \quad (101)$$

where $\xi_{\mathbf{k}} = h_{\mathbf{k}} - \mu$, and $h_{\mathbf{k}}$ is an eigenvalue of the matrix $h_{i,j}$ introduced in Eq. (97). For the electronic self-energy, we take Eq. (79), which we rewrite in the Nambu representation as

$$\underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n) = \underline{\underline{\Sigma}}_{\mathbf{k}}^{(E)}(i\omega_n) + \underline{\underline{\Sigma}}_{\mathbf{k}}^{(H)}(i\omega_n) + \underline{\underline{\Sigma}}_{\mathbf{k}}^{(F)}(i\omega_n) \equiv \underline{\underline{\Sigma}}_{\mathbf{k}}^{(E)}(i\omega_n) + \underline{\underline{\Sigma}}_{\mathbf{k}}^{(EP)}(i\omega_n), \quad (102)$$

where “E” refers to the purely electronic contribution in Eq. (80), while “H” and “F” label the Hartree and Fock terms due to the EPI, respectively. Finally, “EP” labels the total term due to the EPI.

The self-energy terms are decomposed similarly to what is done in Ref. [77], except that we are here considering the case of EEIs rather than disorder. With respect to their derivation, we also include the terms $\propto \underline{\underline{\tau}}_2$. We write

$$\underline{\underline{\Sigma}}_{\mathbf{k}}^{(E)}(i\omega_n) \equiv i\omega_n [1 - \gamma_{\mathbf{k}}(i\omega_n)] \underline{\underline{\tau}}_0 + \phi_{\mathbf{k}}^{(E)}(i\omega_n) \underline{\underline{\tau}}_1 + \overline{\phi}_{\mathbf{k}}^{(E)}(i\omega_n) \underline{\underline{\tau}}_2 + \chi_{\mathbf{k}}^{(E)}(i\omega_n) \underline{\underline{\tau}}_3 \quad (103)$$

and

$$\underline{\underline{\Sigma}}_{\mathbf{k}}^{(EP)}(i\omega_n) \equiv i\omega_n \gamma_{\mathbf{k}}(i\omega_n) [1 - Z_{\mathbf{k}}(i\omega_n)] \underline{\underline{\tau}}_0 + \phi_{\mathbf{k}}^{(EP)}(i\omega_n) \underline{\underline{\tau}}_1 + \overline{\phi}_{\mathbf{k}}^{(EP)}(i\omega_n) \underline{\underline{\tau}}_2 + \chi_{\mathbf{k}}^{(EP)}(i\omega_n) \underline{\underline{\tau}}_3. \quad (104)$$

The total self-energy therefore reads as follows:

$$\underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n) \equiv i\omega_n [1 - \gamma_{\mathbf{k}}(i\omega_n) Z_{\mathbf{k}}(i\omega_n)] \underline{\underline{\tau}}_0 + \phi_{\mathbf{k}}(i\omega_n) \underline{\underline{\tau}}_1 + \overline{\phi}_{\mathbf{k}}(i\omega_n) \underline{\underline{\tau}}_2 + \chi_{\mathbf{k}}(i\omega_n) \underline{\underline{\tau}}_3, \quad (105)$$

where

$$\begin{aligned} \phi_{\mathbf{k}}(i\omega_n) &\equiv \phi_{\mathbf{k}}^{(E)}(i\omega_n) + \phi_{\mathbf{k}}^{(EP)}(i\omega_n), \\ \overline{\phi}_{\mathbf{k}}(i\omega_n) &\equiv \overline{\phi}_{\mathbf{k}}^{(E)}(i\omega_n) + \overline{\phi}_{\mathbf{k}}^{(EP)}(i\omega_n), \\ \chi_{\mathbf{k}}(i\omega_n) &\equiv \chi_{\mathbf{k}}^{(E)}(i\omega_n) + \chi_{\mathbf{k}}^{(EP)}(i\omega_n). \end{aligned} \quad (106)$$

The quantities introduced above can be expressed in terms of the self-energy components as follows:

$$\begin{aligned}
\gamma_{\mathbf{k}}(i\omega_n) &= 1 - \frac{\Sigma_{\mathbf{k};\uparrow,\uparrow}^{(E)}(i\omega_n) + \Sigma_{\mathbf{k};\downarrow,\downarrow}^{(E)}(i\omega_n)}{2i\omega_n}, \\
Z_{\mathbf{k}}(i\omega_n) &= 1 - \frac{\Sigma_{\mathbf{k};\uparrow,\uparrow}^{(EP)}(i\omega_n) + \Sigma_{\mathbf{k};\downarrow,\downarrow}^{(EP)}(i\omega_n)}{2i\omega_n\gamma_{\mathbf{k}}(i\omega_n)}, \\
\chi_{\mathbf{k}}^{(E/EP)}(i\omega_n) &= \frac{\Sigma_{\mathbf{k};\uparrow,\uparrow}^{(E/EP)}(i\omega_n) - \Sigma_{\mathbf{k};\downarrow,\downarrow}^{(E/EP)}(i\omega_n)}{2}, \\
\phi_{\mathbf{k}}^{(E/EP)}(i\omega_n) &= \frac{\Sigma_{\mathbf{k};\uparrow,\downarrow}^{(E/EP)}(i\omega_n) + \Sigma_{\mathbf{k};\downarrow,\uparrow}^{(E/EP)}(i\omega_n)}{2}, \\
\bar{\phi}_{\mathbf{k}}^{(E/EP)}(i\omega_n) &= \frac{\Sigma_{\mathbf{k};\uparrow,\downarrow}^{(E/EP)}(i\omega_n) - \Sigma_{\mathbf{k};\downarrow,\uparrow}^{(E/EP)}(i\omega_n)}{-2i}.
\end{aligned} \tag{107}$$

We now insert Eq. (105) into Eq. (101), and solve for the GF via matrix inversion. This yields the expression for the GF as a function of the self-energy components,

$$\underline{\underline{G}}_{\mathbf{k}}(i\omega_n) = \frac{1}{\Theta_{\mathbf{k}}(i\omega_n)} \left\{ i\omega_n\gamma_{\mathbf{k}}(i\omega_n)Z_{\mathbf{k}}(i\omega_n)\underline{\underline{\tau}}_0 + \phi_{\mathbf{k}}(i\omega_n)\underline{\underline{\tau}}_1 + \bar{\phi}_{\mathbf{k}}(i\omega_n)\underline{\underline{\tau}}_2 + [\xi_{\mathbf{k}} + \chi_{\mathbf{k}}(i\omega_n)]\underline{\underline{\tau}}_3 \right\}, \tag{108}$$

where

$$\Theta_{\mathbf{k}}(i\omega_n) \equiv [i\omega_n\gamma_{\mathbf{k}}(i\omega_n)Z_{\mathbf{k}}(i\omega_n)]^2 - [\xi_{\mathbf{k}} + \chi_{\mathbf{k}}(i\omega_n)]^2 - \phi_{\mathbf{k}}^2(i\omega_n) - \bar{\phi}_{\mathbf{k}}^2(i\omega_n). \tag{109}$$

The quantity in Eq. (105) must be identified with the total electronic self-energy, which we have derived as a functional of the GF, see Eq. (79).

The Eliashberg equations are obtained by inserting the expansion (108) into Eq. (79). In principle, this procedure yields a self-consistent set of eight equations that determine the eight unknown quantities listed in Eq. (107).

8.1. Explicit form of the EPI self-energy functional

To make further progress, we need to adopt an explicit expression for the self-energy $\underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n)$ as a functional of the (fully interacting) electronic GF. Historically, the work of Scalapino, Schrieffer and Wilkins [5] has been a fundamental milestone with respect to the inclusion of EEs in the Eliashberg equations. However, the self-energy that we have derived here from the LWF has a much more complicated form than the simple one that they postulated in their work. As we will see momentarily, this leads to several difficulties in our case. In brief, if the self-energy functional is too complicated, it is impossible to derive a set of self-consistent equations that can be used in practice, unless further approximations are adopted.

We start by separating the self-energy according to Eq. (102). We deal with the EPI self-energy first: in our derivation, this is given by the sum of Fock and Hartree contributions. As we have seen in Section 6.1, our derivation based on the LWF produces (1) a Hartree self-energy that includes various terms depending on the reducible four-leg and irreducible six-leg vertices related to EEs (see Figs. 3 and 4), and (2) a Fock self-energy that contains both EEI-renormalized EPI vertices and a new term that depends on the six-leg irreducible vertex related to EEs (see Fig. 2). We note that the expression that is usually assumed for the EPI self-energy functional [5,6] is of the Fock type but does not include the second term, i.e. the one that depends on the six-leg irreducible vertex. Furthermore, usual theories [5,6] neglect all Hartree-type contributions and rely on a static approximation for the renormalized vertex (analogous to the approximation made on the screened potential) [6], without taking into account explicitly the full functional dependence of the vertex on the electronic GFs. On the other hand, all the new features we have discovered in the electronic self-energy cannot be taken into account in a derivation of extended Eliashberg equations, as there

is no closed-form expression for the four-leg reducible and six-leg irreducible EEI vertices. Further progress could be made, for example, by adopting an explicit expression – based e.g. on Dynamical Mean-Field Theory (DMFT) [71] – for the EEI self-energy functional $\underline{\Sigma}_{\mathbf{k}}^{(E)}(i\omega_n)$ and, consequently, for the EEI vertices. This is well beyond the scope of this work.

In this work, in order to derive Eliashberg-type equations, we make the simplest approximation: we neglect all the EEI vertices terms appearing in the Hartree and Fock self-energy terms. (This is analogous to the approximation made in Ref. [77] for the case of non-interacting electrons in the presence of disorder.) The Hartree and Fock self-energies reduce, respectively, to

$$\begin{aligned} \underline{\Sigma}_{\mathbf{k}}^{(H)}(i\omega_n) &\approx \underline{\tau}_3 T \sum_s M_{\mathbf{k}}^{(0,s)} D_{\mathbf{0},s}(0) \sum_{\mathbf{k}', i\omega_m} M_{\mathbf{k}'}^{(0,s)} \left[G_{\mathbf{k}', \uparrow \uparrow}(i\omega_m) - G_{\mathbf{k}', \downarrow \downarrow}(i\omega_m) \right] \\ &\equiv \underline{\tau}_3 \underline{\Sigma}_{\mathbf{k}}^{(H)} \end{aligned} \quad (110)$$

and

$$\underline{\Sigma}_{\mathbf{k}}^{(F)}(i\omega_n) \approx -T \sum_{i\Omega} \sum_{\mathbf{q}, s} M_{\mathbf{k}}^{(-\mathbf{q}, s)} M_{\mathbf{k}-\mathbf{q}}^{(\mathbf{q}, s)} D_{\mathbf{q}, s}(i\Omega) \underline{\tau}_3 \cdot \underline{G}_{\mathbf{k}-\mathbf{q}}(i\omega_n - i\Omega) \cdot \underline{\tau}_3, \quad (111)$$

where we have used the Fourier representation of the EPI matrix elements, as discussed in detail in [Appendix A](#) [see, in particular, Eq. (A.20)]. In the approximation we made, the Hartree self-energy (110) retains its non-local nature in space, but loses its non-locality in time.

Eqs. (110) and (111) are sufficient to carry out the derivation of *four* out of the eight Eliashberg equations, which connect the unknown quantities listed in Eq. (107). We proceed with this first part of the derivation in Section 8.2, and defer the discussion of the EEI self-energy to the second part of the derivation, reported in Section 8.3.

8.2. Derivation of extended Eliashberg equations: first part

We now substitute Eq. (108) into Eqs. (110) and (111), sum the resulting expressions, and set the result equal to the right-hand side of Eq. (104). This gives a 2×2 matrix equation, equivalent to the following set of four equations:

$$\begin{aligned} i\omega_n \gamma_{\mathbf{k}}(i\omega_n) [1 - Z_{\mathbf{k}}(i\omega_n)] &= -T \sum_{i\omega_m} \sum_{\mathbf{q}, s} M_{\mathbf{k}}^{(\mathbf{q}-\mathbf{k}, s)} M_{\mathbf{q}}^{(\mathbf{k}-\mathbf{q}, s)} D_{\mathbf{k}-\mathbf{q}, s}(i\omega_n - i\omega_m) \\ &\quad \times \frac{i\omega_m \gamma_{\mathbf{q}}(i\omega_m) Z_{\mathbf{q}}(i\omega_m)}{\Theta_{\mathbf{q}}(i\omega_m)}, \end{aligned} \quad (112)$$

$$\chi_{\mathbf{k}}^{(\text{EP})}(i\omega_n) = \Sigma_{\mathbf{k}}^{(H)} - T \sum_{i\omega_m} \sum_{\mathbf{q}, s} M_{\mathbf{k}}^{(\mathbf{q}-\mathbf{k}, s)} M_{\mathbf{q}}^{(\mathbf{k}-\mathbf{q}, s)} D_{\mathbf{k}-\mathbf{q}, s}(i\omega_n - i\omega_m) \frac{\xi_{\mathbf{q}} + \chi_{\mathbf{q}}(i\omega_m)}{\Theta_{\mathbf{q}}(i\omega_m)}, \quad (113)$$

$$\phi_{\mathbf{k}}^{(\text{EP})}(i\omega_n) = T \sum_{i\omega_m} \sum_{\mathbf{q}, s} M_{\mathbf{k}}^{(\mathbf{q}-\mathbf{k}, s)} M_{\mathbf{q}}^{(\mathbf{k}-\mathbf{q}, s)} D_{\mathbf{k}-\mathbf{q}, s}(i\omega_n - i\omega_m) \frac{\phi_{\mathbf{q}}(i\omega_m)}{\Theta_{\mathbf{q}}(i\omega_m)}, \quad (114)$$

and

$$\bar{\phi}_{\mathbf{k}}^{(\text{EP})}(i\omega_n) = T \sum_{i\omega_m} \sum_{\mathbf{q}, s} M_{\mathbf{k}}^{(\mathbf{q}-\mathbf{k}, s)} M_{\mathbf{q}}^{(\mathbf{k}-\mathbf{q}, s)} D_{\mathbf{k}-\mathbf{q}, s}(i\omega_n - i\omega_m) \frac{\bar{\phi}_{\mathbf{q}}(i\omega_m)}{\Theta_{\mathbf{q}}(i\omega_m)}, \quad (115)$$

where the term

$$\Sigma_{\mathbf{k}}^{(H)} \equiv 2T \sum_s M_{\mathbf{k}}^{(0,s)} M_{\mathbf{q}}^{(0,s)} D_{\mathbf{0},s}(0) \sum_{\mathbf{q}, i\omega_m} \frac{\xi_{\mathbf{q}} + \chi_{\mathbf{q}}(i\omega_m)}{\Theta_{\mathbf{q}}(i\omega_m)} \quad (116)$$

appears only in Eq. (113). We note that Eqs. (113), (114) and (115) relate EP self-energy terms (on the left-hand sides) to the respective total self-energy terms (on the right-hand sides). Therefore, these are not yet self-consistent equations. To complete the derivation, we need to take into account the EEI self-energy. This is done in the next Section.

8.3. Derivation of extended Eliashberg equations: second part

For temperatures larger than the critical temperature, $T > T_c$, the anomalous terms of the self-energy and GF vanish. For $T \rightarrow T_c^-$, the anomalous terms are very small, and the Eliashberg equations can be linearized in the quantities $\phi_{\mathbf{k}}(i\omega_n)$ and $\bar{\phi}_{\mathbf{k}}(i\omega_n)$. Namely, we put

$$\underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n) \equiv \underline{\underline{\Sigma}}_{\mathbf{k}}^{(N)}(i\omega_n) + \delta \underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n), \quad (117)$$

where

$$\underline{\underline{\Sigma}}_{\mathbf{k}}^{(N)}(i\omega_n) \equiv i\omega_n \left[1 - \gamma_{\mathbf{k}}^{(N)}(i\omega_n) Z_{\mathbf{k}}^{(N)}(i\omega_n) \right] \underline{\underline{\tau}}_0 + \chi_{\mathbf{k}}^{(N)}(i\omega_n) \underline{\underline{\tau}}_3. \quad (118)$$

The superscript ‘‘N’’ denotes quantities that are evaluated in the normal state. The anomalous correction $\delta \underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n)$ vanishes for $T > T_c$; for $T < T_c$ it includes, in general, both finite off-diagonal and diagonal terms. For $T \rightarrow T_c^-$, the change in the self-energy in going from the superconducting to the normal phase can be approximated as

$$\delta \underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n) \approx \sum_{\mathbf{q}, i\omega_m} \sum_{\sigma, \sigma'} \frac{\delta \underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n)}{\delta G_{\mathbf{q}; \sigma, \sigma'}(i\omega_m)} \Big|_{G=G^{(N)}} \delta G_{\mathbf{q}; \sigma, \sigma'}(i\omega_m), \quad (119)$$

where $\delta G_{\mathbf{q}; \sigma, \sigma'}(i\omega_m)$ denotes the term of the GF which is linear in the anomalous components of the self-energy. We now express this quantity in terms of $\delta \Sigma$, by using the following relations, which are consequences of the Dyson equation:

$$\begin{aligned} G^{-1} &= G_0^{-1} - \Sigma \Rightarrow \delta \Sigma = -\delta G^{-1}, \\ G^{-1} \cdot G &= 1 \Rightarrow \delta G^{-1} \cdot G + G^{-1} \cdot \delta G = 0 \Rightarrow \delta G^{-1} = -G^{-1} \cdot \delta G \cdot G^{-1} \\ &\Rightarrow \delta \Sigma = G^{-1} \cdot \delta G \cdot G^{-1} \Rightarrow \delta G = G \cdot \delta \Sigma \cdot G, \end{aligned} \quad (120)$$

where we have used a compact notation. We obtain

$$\begin{aligned} \delta \underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n) &= \sum_{\mathbf{q}, i\omega_m} \sum_{\sigma, \sigma'} \frac{\delta \underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n)}{\delta G_{\mathbf{q}; \sigma, \sigma'}(i\omega_m)} \Big|_{G=G^{(N)}} \left[\underline{\underline{G}}_{\mathbf{q}}^{(N)}(i\omega_m) \cdot \delta \underline{\underline{\Sigma}}_{\mathbf{q}}(i\omega_m) \cdot \underline{\underline{G}}_{\mathbf{q}}^{(N)}(i\omega_m) \right]_{\sigma, \sigma'} \\ &= \sum_{\mathbf{q}, i\omega_m} G_{\mathbf{q}; \uparrow, \uparrow}^{(N)}(i\omega_m) G_{\mathbf{q}; \downarrow, \downarrow}^{(N)}(i\omega_m) \sum_{\sigma} \frac{\delta \underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n)}{\delta G_{\mathbf{q}; \sigma, -\sigma}(i\omega_m)} \Big|_{G=G^{(N)}} \delta \Sigma_{\mathbf{q}; \sigma, -\sigma}(i\omega_m) \\ &\quad + \sum_{\mathbf{q}, i\omega_m} \sum_{\sigma} \left[G_{\mathbf{q}; \sigma, \sigma}^{(N)}(i\omega_m) \right]^2 \frac{\delta \underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n)}{\delta G_{\mathbf{q}; \sigma, \sigma}(i\omega_m)} \Big|_{G=G^{(N)}} \delta \Sigma_{\mathbf{q}; \sigma, \sigma}(i\omega_m), \end{aligned} \quad (121)$$

where we have used the fact that $\underline{\underline{G}}_{\mathbf{q}}^{(N)}(i\omega_m)$ is diagonal.

We should now derive an expression for $\delta \underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n)/\delta G_{\mathbf{q}; \sigma, \sigma}(i\omega_m)$. Referring to the partition of the self-energy given in Eq. (102), and using the approximations (110) and (111), we obtain

$$\frac{\delta \Sigma_{\mathbf{k}; \mu, \mu'}^{(H)}(i\omega_n)}{\delta G_{\mathbf{q}; \sigma, \sigma'}(i\omega_m)} \Big|_{G=G^{(N)}} \approx \delta_{\mu, \mu'} \mu \delta_{\sigma, \sigma'} \sigma T \sum_s M_{\mathbf{k}}^{(0, s)} M_{\mathbf{q}}^{(0, s)} D_{\mathbf{0}, s}^{(N)}(0) \quad (122)$$

and

$$\frac{\delta \Sigma_{\mathbf{k}; \mu, \mu'}^{(F)}(i\omega_n)}{\delta G_{\mathbf{q}; \sigma, \sigma'}(i\omega_m)} \Big|_{G=G^{(N)}} \approx -\delta_{\sigma, \mu} \delta_{\sigma', \mu'} \sigma \sigma' T \sum_s M_{\mathbf{k}}^{(q-k, s)} M_{\mathbf{q}}^{(k-q, s)} D_{\mathbf{k}-\mathbf{q}, s}^{(N)}(i\omega_n - i\omega_m). \quad (123)$$

Next, we consider the EEI self-energy functional, for which we write the Ward identity

$$\frac{\delta \Sigma_{\mathbf{k}; \mu, \mu'}^{(E)}(i\omega_n)}{\delta G_{\mathbf{q}; \sigma, \sigma'}(i\omega_m)} \Big|_{G=G^{(N)}} \equiv U_{\mathbf{k}, \mathbf{q}; \mu, \sigma; \sigma', \mu'}^{[4](N)}(i\omega_n, i\omega_m), \quad (124)$$

where $U_{\mathbf{k},\mathbf{q};\mu,\sigma;\sigma',\mu'}^{[4](N)}(i\omega_n, i\omega_m)$ is the irreducible four-leg vertex related to EEIs [see Eq. (84)]. In this case, it must be evaluated in the normal state, at $G = G^{(N)}$. By comparison, in Ref. [5] the EEI self-energy was taken in the GW approximation [84], with a statically screened interaction potential. Such potential is itself, in principle, a functional of the electronic GF through the dielectric function; however, in order to obtain tractable equations, in Ref. [5] this dependence is neglected, and the effect of the screened potential is finally embedded in a ‘‘pseudopotential’’ that does not depend on energy and momentum. By contrast, we keep the more general four-leg irreducible vertex in our derivation. Our procedure leads to a tractable system of equations if the EEI self-energy functional (and the related EEI vertices) can be determined *in the normal state* via independent means appropriate e.g. to strongly correlated electron systems, such as DMFT [71].

Substituting all these expressions back into (121), and using the identity

$$G_{\mathbf{q};\uparrow,\uparrow}^{(N)}(i\omega_m) G_{\mathbf{q};\downarrow,\downarrow}^{(N)}(i\omega_m) = 1/\Theta_{\mathbf{q}}^{(N)}(i\omega_m), \quad (125)$$

we obtain

$$\begin{aligned} & \delta \Sigma_{\mathbf{k};\mu,\mu'}(i\omega_n) \\ &= \sum_{\mathbf{q},i\omega_m} \frac{1}{\Theta_{\mathbf{q}}^{(N)}(i\omega_m)} \sum_{\sigma} U_{\mathbf{k},\mathbf{q};\mu,\sigma;-\sigma,\mu'}^{[4]N}(i\omega_n, i\omega_m) \delta \Sigma_{\mathbf{q};\sigma,-\sigma}(i\omega_m) \\ &+ \sum_{\mathbf{q},i\omega_m} \sum_{\sigma} \left[G_{\mathbf{q};\sigma,\sigma}^{(N)}(i\omega_m) \right]^2 U_{\mathbf{k},\mathbf{q};\mu,\sigma;\sigma,\mu'}^{[4]N}(i\omega_n, i\omega_m) \delta \Sigma_{\mathbf{q};\sigma,\sigma}(i\omega_m) \\ &+ \delta_{\mu,\mu'} \mu \sum_{\mathbf{q},i\omega_m} \sum_{\sigma} \left[G_{\mathbf{q};\sigma,\sigma}^{(N)}(i\omega_m) \right]^2 \sigma T \sum_s M_{\mathbf{k}}^{(0,s)} M_{\mathbf{q}}^{(0,s)} D_{0,s}^{(N)}(0) \delta \Sigma_{\mathbf{q};\sigma,\sigma}(i\omega_m) \\ &+ \delta_{\mu,-\mu'} \sum_{\mathbf{q},i\omega_m} \frac{1}{\Theta_{\mathbf{q}}^{(N)}(i\omega_m)} T \sum_s M_{\mathbf{k}}^{(q-k,s)} M_{\mathbf{q}}^{(k-q,s)} D_{\mathbf{k}-\mathbf{q},s}^{(N)}(i\omega_n - i\omega_m) \delta \Sigma_{\mathbf{q};\mu,-\mu}(i\omega_m) \\ &- \delta_{\mu,\mu'} \sum_{\mathbf{q},i\omega_m} \left[G_{\mathbf{q};\mu,\mu}^{(N)}(i\omega_m) \right]^2 T \sum_s M_{\mathbf{k}}^{(q-k,s)} M_{\mathbf{q}}^{(k-q,s)} D_{\mathbf{k}-\mathbf{q},s}^{(N)}(i\omega_n - i\omega_m) \delta \Sigma_{\mathbf{q};\mu,\mu}(i\omega_m). \end{aligned} \quad (126)$$

Regarding the four-leg EEI vertex, it holds that

$$U_{\mathbf{k},\mathbf{q};\mu,\sigma;\sigma',\mu'}^{[4](N)}(i\omega_n, i\omega_m) \equiv \delta_{\sigma,\mu} \delta_{\sigma',\mu'} U_{\mathbf{k},\mathbf{q};\mu,\mu'}^{[4](N)}(i\omega_n, i\omega_m). \quad (127)$$

The previous result stems from the fact that in the normal state all interaction vertices conserve spin and, therefore, the spin indices along the same propagator line must be equal. The self-energy corrections $\delta \Sigma_{\mathbf{q};\mu,\mu}(i\omega_m)$ and $\delta \Sigma_{\mathbf{q};\mu,-\mu}(i\omega_m)$ are then decoupled: the diagonal terms satisfy

$$\begin{aligned} \delta \Sigma_{\mathbf{k};\mu,\mu}(i\omega_n) &= \sum_{\mathbf{q},i\omega_m} \left[G_{\mathbf{q};\mu,\mu}^{(N)}(i\omega_m) \right]^2 \left\{ U_{\mathbf{k},\mathbf{q};\mu,\mu}^{[4](N)}(i\omega_n, i\omega_m) \right. \\ &- T \sum_s M_{\mathbf{k}}^{(q-k,s)} M_{\mathbf{q}}^{(k-q,s)} D_{\mathbf{k}-\mathbf{q},s}^{(N)}(i\omega_n - i\omega_m) \left. \right\} \delta \Sigma_{\mathbf{q};\mu,\mu}(i\omega_m) \\ &+ \mu \sum_{\mathbf{q},i\omega_m} \sum_{\sigma} \left[G_{\mathbf{q};\sigma,\sigma}^{(N)}(i\omega_m) \right]^2 \sigma T \sum_s M_{\mathbf{k}}^{(0,s)} M_{\mathbf{q}}^{(0,s)} D_{0,s}^{(N)}(0) \delta \Sigma_{\mathbf{q};\sigma,\sigma}(i\omega_m), \end{aligned} \quad (128)$$

while the nondiagonal terms satisfy

$$\begin{aligned} \delta \Sigma_{\mathbf{k};\mu,-\mu}(i\omega_n) &= \sum_{\mathbf{q},i\omega_m} \frac{1}{\Theta_{\mathbf{q}}^{(N)}(i\omega_m)} \left\{ U_{\mathbf{k},\mathbf{q};\mu,-\mu}^{[4](N)}(i\omega_n, i\omega_m) \right. \\ &+ T \sum_s M_{\mathbf{k}}^{(q-k,s)} M_{\mathbf{q}}^{(k-q,s)} D_{\mathbf{k}-\mathbf{q},s}^{(N)}(i\omega_n - i\omega_m) \left. \right\} \delta \Sigma_{\mathbf{q};\mu,-\mu}(i\omega_m). \end{aligned} \quad (129)$$

Note that the normal solution, corresponding to $\delta \Sigma_{\mathbf{k};\mu,\mu'}(i\omega_n) = 0$ for every choice of μ, μ' , is always possible. Moreover, we can choose $\delta \Sigma_{\mathbf{k};\mu,\mu}(i\omega_n) = 0$, while the off-diagonal components

must be non-zero. These choices correspond to setting

$$\delta \underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n) \equiv \phi_{\mathbf{k}}(i\omega_n) \underline{\underline{\tau}}_1 + \bar{\phi}_{\mathbf{k}}(i\omega_n) \underline{\underline{\tau}}_2, \quad (130)$$

which conveniently allows to identify the full correction $\delta \underline{\underline{\Sigma}}_{\mathbf{k}}(i\omega_n)$ with the anomalous (off-diagonal) components of the self-energy. We adopt Eq. (130) in the rest of the derivation.

Applying Eqs. (130) to (129), we obtain the following Eliashberg-type equations for the total anomalous components of the self-energy:

$$\begin{aligned} \phi_{\mathbf{k}}(i\omega_n) = & \sum_{\mathbf{q}, i\omega_m} \frac{\phi_{\mathbf{q}}(i\omega_m)}{\Theta_{\mathbf{q}}^{(N)}(i\omega_m)} \left[\frac{1}{2} U_{\mathbf{k}, \mathbf{q}; \uparrow, \downarrow}^{[4](N)}(i\omega_n, i\omega_m) + \frac{1}{2} U_{\mathbf{k}, \mathbf{q}; \downarrow, \uparrow}^{[4](N)}(i\omega_n, i\omega_m) \right. \\ & \left. + T \sum_s M_{\mathbf{k}}^{(\mathbf{q}-\mathbf{k}, s)} M_{\mathbf{q}}^{(\mathbf{k}-\mathbf{q}, s)} D_{\mathbf{k}-\mathbf{q}, s}^{(N)}(i\omega_n - i\omega_m) \right] \\ & - \frac{i}{2} \sum_{\mathbf{q}, i\omega_m} \frac{\bar{\phi}_{\mathbf{q}}(i\omega_m)}{\Theta_{\mathbf{q}}^{(N)}(i\omega_m)} \left[U_{\mathbf{k}, \mathbf{q}; \uparrow, \downarrow}^{[4](N)}(i\omega_n, i\omega_m) - U_{\mathbf{k}, \mathbf{q}; \downarrow, \uparrow}^{[4](N)}(i\omega_n, i\omega_m) \right] \end{aligned} \quad (131)$$

and

$$\begin{aligned} \bar{\phi}_{\mathbf{k}}(i\omega_n) = & \sum_{\mathbf{q}, i\omega_m} \frac{\bar{\phi}_{\mathbf{q}}(i\omega_m)}{\Theta_{\mathbf{q}}^{(N)}(i\omega_m)} \left[\frac{1}{2} U_{\mathbf{k}, \mathbf{q}; \uparrow, \downarrow}^{[4](N)}(i\omega_n, i\omega_m) + \frac{1}{2} U_{\mathbf{k}, \mathbf{q}; \downarrow, \uparrow}^{[4](N)}(i\omega_n, i\omega_m) \right. \\ & \left. + T \sum_s M_{\mathbf{k}}^{(\mathbf{q}-\mathbf{k}, s)} M_{\mathbf{q}}^{(\mathbf{k}-\mathbf{q}, s)} D_{\mathbf{k}-\mathbf{q}, s}^{(N)}(i\omega_n - i\omega_m) \right] \\ & + \frac{i}{2} \sum_{\mathbf{q}, i\omega_m} \frac{\phi_{\mathbf{q}}(i\omega_m)}{\Theta_{\mathbf{q}}^{(N)}(i\omega_m)} \left[U_{\mathbf{k}, \mathbf{q}; \uparrow, \downarrow}^{[4](N)}(i\omega_n, i\omega_m) - U_{\mathbf{k}, \mathbf{q}; \downarrow, \uparrow}^{[4](N)}(i\omega_n, i\omega_m) \right]. \end{aligned} \quad (132)$$

Eqs. (131) and (132), together with (114) and (115), completely determine the anomalous components of the self-energy, for temperatures $T \approx T_c$. If we assume that $U_{\mathbf{k}, \mathbf{q}; \uparrow, \downarrow}^{[4](N)}(i\omega_n, i\omega_m) = U_{\mathbf{k}, \mathbf{q}; \downarrow, \uparrow}^{[4](N)}(i\omega_n, i\omega_m)$, Eqs. (131) and (132) achieve a simplification that effectively decouples the equation for $\phi_{\mathbf{k}}(i\omega_n)$ from that for $\bar{\phi}_{\mathbf{k}}(i\omega_n)$. Combining these simplified equations with (114) and (115) evaluated at $\Theta_{\mathbf{q}}(i\omega_m) \approx \Theta_{\mathbf{q}}^{(N)}(i\omega_m)$ and $D_{\mathbf{k}-\mathbf{q}, s}(i\omega_n - i\omega_m) \approx D_{\mathbf{k}-\mathbf{q}, s}^{(N)}(i\omega_n - i\omega_m)$, we obtain

$$\phi_{\mathbf{k}}^{(E)}(i\omega_n) = \sum_{\mathbf{q}, i\omega_m} U_{\mathbf{k}, \mathbf{q}; \uparrow, \downarrow}^{[4](N)}(i\omega_n, i\omega_m) \frac{\phi_{\mathbf{q}}(i\omega_m)}{\Theta_{\mathbf{q}}^{(N)}(i\omega_m)} \quad (133)$$

and

$$\phi_{\mathbf{k}}^{(EP)}(i\omega_n) = T \sum_{i\omega_m} \sum_{\mathbf{q}, s} M_{\mathbf{k}}^{(\mathbf{q}-\mathbf{k}, s)} M_{\mathbf{q}}^{(\mathbf{k}-\mathbf{q}, s)} D_{\mathbf{k}-\mathbf{q}, s}^{(N)}(i\omega_n - i\omega_m) \frac{\phi_{\mathbf{q}}(i\omega_m)}{\Theta_{\mathbf{q}}^{(N)}(i\omega_m)}, \quad (134)$$

which connect $\phi_{\mathbf{k}}^{(E)}(i\omega_n)$ and $\phi_{\mathbf{k}}^{(EP)}(i\omega_n)$, respectively, to their sum $\phi_{\mathbf{k}}(i\omega_n) = \phi_{\mathbf{k}}^{(E)}(i\omega_n) + \phi_{\mathbf{k}}^{(EP)}(i\omega_n)$, thus forming a system of two coupled matrix equations in two unknown functions. An identical system is obtained for the $\underline{\underline{\tau}}_2$ components of the self-energy, with the replacements $\phi^{(E)} \rightarrow \bar{\phi}^{(E)}$, $\phi^{(EP)} \rightarrow \bar{\phi}^{(EP)}$, and $\phi \rightarrow \bar{\phi}$. Therefore, the $\underline{\underline{\tau}}_1$ components of the self-energy are equal to the $\underline{\underline{\tau}}_2$ components up to a constant, which can also be zero. It is possible to set $\bar{\phi}^{(E)} = \bar{\phi}^{(EP)} = 0 = \bar{\phi}$, while retaining a nonzero solution for ϕ [77].

In the present framework, the remaining ingredients for the total determination of the self-energy are Eqs. (112) and (113) evaluated in the normal state, plus the two equations for $\gamma_{\mathbf{k}}(i\omega_n)$ and $\chi_{\mathbf{k}}^{(E)}(i\omega_n)$ taken from (107), also evaluated in the normal state. In fact, we recall that our working hypothesis is that the EEI self-energy is known in the normal state; therefore, the latter two equations are to be considered as solved.

To summarize, we put together all the above results, and present a set of six equations – not eight, because of the gauge choice $\bar{\phi}^{(E)} = \bar{\phi}^{(EP)} = 0$ – that allow to determine the anomalous corrections to the self-energy in the linearized regime that applies for $T \approx T_c$:

$$\phi_{\mathbf{k}}^{(E)}(i\omega_n) = \sum_{\mathbf{q}, i\omega_m} U_{\mathbf{k}, \mathbf{q}; \uparrow, \downarrow}^{[4](N)}(i\omega_n, i\omega_m) \frac{\phi_{\mathbf{q}}^{(E)}(i\omega_m) + \phi_{\mathbf{q}}^{(EP)}(i\omega_m)}{\Theta_{\mathbf{q}}^{(N)}(i\omega_m)}, \quad (135)$$

$$\phi_{\mathbf{k}}^{(EP)}(i\omega_n) = T \sum_{i\omega_m} \sum_{\mathbf{q}, s} M_{\mathbf{k}}^{(\mathbf{q}-\mathbf{k}, s)} M_{\mathbf{q}}^{(\mathbf{k}-\mathbf{q}, s)} D_{\mathbf{k}-\mathbf{q}, s}^{(N)}(i\omega_n - i\omega_m) \frac{\phi_{\mathbf{q}}^{(E)}(i\omega_m) + \phi_{\mathbf{q}}^{(EP)}(i\omega_m)}{\Theta_{\mathbf{q}}^{(N)}(i\omega_m)}, \quad (136)$$

$$\gamma_{\mathbf{k}}(i\omega_n) = 1 - \frac{\Sigma_{\mathbf{k}; \uparrow, \uparrow}^{(E, N)}(i\omega_n) + \Sigma_{\mathbf{k}; \downarrow, \downarrow}^{(E, N)}(i\omega_n)}{2i\omega_n}, \quad (137)$$

$$\chi_{\mathbf{k}}^{(E)}(i\omega_n) = \frac{\Sigma_{\mathbf{k}; \uparrow, \uparrow}^{(E, N)}(i\omega_n) - \Sigma_{\mathbf{k}; \downarrow, \downarrow}^{(E, N)}(i\omega_n)}{2}, \quad (138)$$

$$i\omega_n \gamma_{\mathbf{k}}(i\omega_n) [1 - Z_{\mathbf{k}}(i\omega_n)] = -T \sum_{i\omega_m} \sum_{\mathbf{q}, s} M_{\mathbf{k}}^{(\mathbf{q}-\mathbf{k}, s)} M_{\mathbf{q}}^{(\mathbf{k}-\mathbf{q}, s)} D_{\mathbf{k}-\mathbf{q}, s}^{(N)}(i\omega_n - i\omega_m) \frac{i\omega_m \gamma_{\mathbf{q}}(i\omega_m) Z_{\mathbf{q}}(i\omega_m)}{\Theta_{\mathbf{q}}^{(N)}(i\omega_m)}, \quad (139)$$

$$\begin{aligned} \chi_{\mathbf{k}}^{(EP)}(i\omega_n) = & -T \sum_{i\omega_m} \sum_{\mathbf{q}, s} \left[M_{\mathbf{k}}^{(\mathbf{q}-\mathbf{k}, s)} M_{\mathbf{q}}^{(\mathbf{k}-\mathbf{q}, s)} D_{\mathbf{k}-\mathbf{q}, s}^{(N)}(i\omega_n - i\omega_m) - 2M_{\mathbf{k}}^{(\mathbf{0}, s)} M_{\mathbf{q}}^{(\mathbf{0}, s)} D_{\mathbf{0}, s}(0) \right] \\ & \times \frac{\xi_{\mathbf{q}} + \chi_{\mathbf{q}}(i\omega_m)}{\Theta_{\mathbf{q}}^{(N)}(i\omega_m)}. \end{aligned} \quad (140)$$

In all of the above,

$$\Theta_{\mathbf{k}}^{(N)}(i\omega_n) \equiv [i\omega_n \gamma_{\mathbf{k}}(i\omega_n) Z_{\mathbf{k}}(i\omega_n)]^2 - [\xi_{\mathbf{k}} + \chi_{\mathbf{k}}(i\omega_n)]^2. \quad (141)$$

The equation for the total anomalous component of the electronic self-energy is obtained by summing Eqs. (135) and (136):

$$\phi_{\mathbf{k}}(i\omega_n) = \sum_{\mathbf{q}, i\omega_m} \left[\sum_s T M_{\mathbf{k}}^{(\mathbf{q}-\mathbf{k}, s)} M_{\mathbf{q}}^{(\mathbf{k}-\mathbf{q}, s)} D_{\mathbf{k}-\mathbf{q}, s}^{(N)}(i\omega_n - i\omega_m) + U_{\mathbf{k}, \mathbf{q}; \uparrow, \downarrow}^{[4](N)}(i\omega_n, i\omega_m) \right] \frac{\phi_{\mathbf{q}}(i\omega_m)}{\Theta_{\mathbf{q}}^{(N)}(i\omega_m)}. \quad (142)$$

The inclusion of the four-leg irreducible vertex $U^{[4]}$ formally allows for a part of the EEI effects that are not captured in widely used approximation schemes, such as the Tolmachev–Morel–Anderson method [74,75], where the Coulomb potential entering the self-energy equations is approximated as a momentum- and frequency-independent pseudopotential. While the Tolmachev–Morel–Anderson method has allowed for great progress in the history of superconductivity (in particular, it laid the foundation for the derivation of the McMillan formula for T_c [76]), it is based on an uncontrolled approximation that neglects Coulomb vertex corrections and the associated retardation effects [85]. Within the stated approximations (i.e. linearization of the self-energy functional for T close to T_c , Eq. (119)), our formulas include the formally exact contributions from the EEI self-energy functional; we remind the reader that the rest of our approximations affects the EPI self-energy functional only, see Eqs. (110) and (111).

9. Summary and conclusions

In summary, in this work we have derived the Luttinger–Ward functional for a system of electrons in the presence of both electron–electron and electron–phonon interactions – see Eqs. (76) – (78). Without relying on a weak-coupling skeleton-diagram expansion, we have demonstrated that this functional generates two types of contributions to the electronic self-energy: (i) a Fock-type contribution, which is reported in Eq. (87) and, diagrammatically, in Fig. 2; and (ii) a Hartree-type contribution, which can be found in Eq. (89) and Figs. 3–4. In both classes of contributions, which are

due to electron–phonon interactions, entirely new terms appear, containing the irreducible six-leg vertex related to electron–electron interactions. To the best of our knowledge, these contributions have never been discussed in the literature on electron–phonon interactions and related phonon-mediated superconductivity. Under certain approximations, we have used these results to derive extended Eliashberg equations—see Eqs. (135)–(140). These include vertex corrections due to electron–electron interactions, which are not accounted for by the Tolmachev–Morel–Anderson pseudopotential [74,75].

As emphasized throughout this work, much more work is needed to shed light on the physical implications of our theory, especially in the realm of phonon-mediated superconductivity in strongly correlated electron systems (SCESs). In this case, approximations such as DMFT [71] and beyond-DMFT approaches [72], such as dual fermion/bosons [73], which have been proven to be very useful in dealing with SCESs, may also be used in this context to examine $U^{[6]}$, as well as the functionals $\Sigma^{(E)}$ and $U^{[4]}$ which are needed as inputs in our extended Eliashberg equations. Another possibility is to rely on a large- N approximation, using $1/N$ as small parameter to select leading diagrams contributing to $U^{[6]}$, $\Sigma^{(E)}$, and $U^{[4]}$, where N is the number of fermion flavors.

We believe that the theory presented in this work could provide tools for the study of EPIs and phonon-mediated superconductivity in materials where the applicability of Migdal theorem is disputed because of features such as, e.g., large phonon frequencies, van Hove singularities, and strong EEs. Relevant modern examples of these materials include hydrates [40–49] and magic-angle twisted bilayer graphene [50–68]. We mention, in passing, that our theory can be generalized to systems of electrons interacting with cavity photons [86], paying particular attention to the \mathbf{A}^2 term and gauge invariance [87].

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Andrea Secchi: Formal analysis, Writing - original draft, Writing - review & editing. **Marco Polini:** Conceptualization, Supervision, Writing - review & editing. **Mikhail I. Katsnelson:** Conceptualization, Supervision, Writing - review & editing.

Acknowledgments

It has been a great pleasure and honor to contribute to the special issue of *Annals of Physics* dedicated to G. M. Eliashberg, one of the founding fathers of the microscopic theory of superconductivity, on the occasion of his ninetieth birthday.

This work was supported by the European Union’s Horizon 2020 research and innovation programme under grant agreement No. 785219 - GrapheneCore2. M. I. K. also acknowledges support from FLAG-ERA JTC2017 Project GRANSPORT.

Appendix A. Derivation of the Hamiltonian

Since the conventions used for the definition of the EPI parameters are not universal in the literature, we present here a full derivation of the electron–phonon Hamiltonian that we have used in this work. This allows to identify the physical definition of the parameters $\{M_{\alpha,\beta}^{(\lambda)}\}$, and to put them in correspondence with the parameters used by other authors.

We use some concepts borrowed from the derivations given in Refs. [33,88,89]. We write the Hamiltonian for a general system of electrons and nuclei in first quantization, in the position

representation, as

$$\begin{aligned}
H &= T_e + V_{ee} + V_{eN} + T_N + V_{NN} \\
&= \sum_{\mathbf{r}} \frac{-\hbar^2 \nabla_{\mathbf{r}}^2}{2m} + \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}' \neq \mathbf{r}} V_{ee}(\mathbf{r} - \mathbf{r}') + \sum_{\mathbf{r}, \mathbf{R}} V_{eN}(\mathbf{r} - \mathbf{R}) + \sum_{\mathbf{R}} \frac{-\hbar^2 \nabla_{\mathbf{R}}^2}{2m_{\mathbf{R}}} \\
&\quad + \frac{1}{2} \sum_{\mathbf{R}, \mathbf{R}' \neq \mathbf{R}} V_{NN}(\mathbf{R} - \mathbf{R}'), \tag{A.1}
\end{aligned}$$

where \mathbf{r} is an electron coordinate, and \mathbf{R} is a nucleus coordinate; m (without subscript) is the electron mass, while $m_{\mathbf{R}}$ is the mass of the nucleus at position \mathbf{R} .

The standard Born–Oppenheimer derivation goes as follows. We introduce the set of nuclear equilibrium position vectors $\mathbf{R}_{i,n} \equiv \mathbf{R}_i + \mathbf{B}_n$, where \mathbf{R}_i is a lattice vector and \mathbf{B}_n is a basis vector that distinguishes the atoms inside a given unit cell. The equilibrium positions satisfy the following set of equations,

$$\sum_{\mathbf{R}' \neq \mathbf{R}} \nabla_{\mathbf{R}} V_{NN}(\mathbf{R} - \mathbf{R}') = \mathbf{0}, \quad \forall \mathbf{R}. \tag{A.2}$$

Displacements of the nuclei with respect to the equilibrium positions are denoted as $\mathbf{Q}_{i,n} \equiv \mathbf{R} - \mathbf{R}_{i,n}$. If they are assumed to be small, then the Hamiltonian can be expanded in powers of $\mathbf{Q}_{i,n}$ up to the second order. Denoting with μ, ν the Cartesian coordinates, we obtain

$$\begin{aligned}
H &\approx \sum_{\mathbf{r}} \frac{-\hbar^2 \nabla_{\mathbf{r}}^2}{2m} + \sum_{\mathbf{r}, (i,n)} V_{eN}(\mathbf{r} - \mathbf{R}_{i,n}) + \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}' \neq \mathbf{r}} V_{ee}(\mathbf{r} - \mathbf{r}') \\
&\quad - \sum_{\mathbf{r}, (i,n)} \sum_{\mu} Q_{(i,n),\mu} \left[\frac{\partial V_{eN}(\mathbf{R})}{\partial R_{\mu}} - \frac{1}{2} \sum_{\nu} Q_{(i,n),\nu} \frac{\partial^2 V_{eN}(\mathbf{R})}{\partial R_{\mu} \partial R_{\nu}} \right] \Bigg|_{\mathbf{R}=\mathbf{r}-\mathbf{R}_{i,n}} \\
&\quad + \sum_{(i,n)} \left[\frac{-\hbar^2 \nabla_{\mathbf{Q}_{i,n}}^2}{2m_n} + \frac{1}{4} \sum_{(i',n') \neq (i,n)} \sum_{\mu,\nu} (Q_{(i,n),\mu} - Q_{(i',n'),\mu}) \right. \\
&\quad \times \left. (Q_{(i,n),\nu} - Q_{(i',n'),\nu}) \frac{\partial^2 V_{NN}(\mathbf{R})}{\partial R_{\mu} \partial R_{\nu}} \Bigg|_{\mathbf{R}=\mathbf{R}_{i,n}-\mathbf{R}_{i',n'}} \right] \\
&\quad + \frac{1}{2} \sum_{(i,n), (i',n') \neq (i,n)} V_{NN}(\mathbf{R}_{i,n} - \mathbf{R}_{i',n'}), \tag{A.3}
\end{aligned}$$

where m_n is the mass of the nucleus at position \mathbf{B}_n within a unit cell (due to the lattice periodicity, it does not depend on the unit cell i). On the right-hand side of Eq. (A.3): (1) the first line is the Hamiltonian for the electronic subsystem alone, including the kinetic energy, a spatially-periodic external potential given by the interaction with the lattice, and the EEI; (2) the second line is the EPI, including a linear and a quadratic term in the nuclear displacements (we neglect the latter, as is usually done); (3) the third and fourth lines constitute the Hamiltonian for the phonon subsystem alone, in the harmonic approximation; (4) the fifth line is a constant with respect to the dynamical coordinates associated with the fixed equilibrium configuration.

The first line can be written in second quantization as the sum of the terms (2) and (3) of the main text, for a general single-electron basis set of wave functions labeled by the index $\alpha = (i_{\alpha}, \sigma_{\alpha})$.

The displacement operators are quantized as [89]

$$\hat{\mathbf{Q}}_{i,n} = i \sum_{\mathbf{q},s} \sqrt{\frac{\hbar}{2N\omega_{\mathbf{q},s}}} \frac{\eta_{\mathbf{q},s,n}}{\sqrt{m_n}} (\hat{b}_{\mathbf{q},s} + \hat{b}_{-\mathbf{q},s}^{\dagger}) e^{i\mathbf{q}\cdot\mathbf{R}_i} = \hat{\mathbf{Q}}_{i,n}^{\dagger}, \tag{A.4}$$

where s is the branch index, and the polarization vectors satisfy $\eta_{\mathbf{q},s,n} = -\eta_{-\mathbf{q},s,n}$. The polarization vectors and the mass, in general, depend on n , as they might be different for different atoms within the same unit cell (so, they depend on the basis vector \mathbf{B}_n , although not on the lattice vector \mathbf{R}_i). The quantity $\omega_{\mathbf{q},s} = \omega_{-\mathbf{q},s}$ is, at this stage, introduced as a mere parameter. When Eq. (A.4) is replaced into Eq. (A.3), the third and fourth lines of the latter are transformed into the second-quantized IP Hamiltonian given in Eq. (4) of the main text, and $\omega_{\mathbf{q},s}$ acquires the meaning of a phonon (vibrational mode) frequency; it is related to the direct-space matrix $f_{i,j}(s)$ via Eqs. (13).

The linear term of the EPI [second line of Eq. (A.3)] becomes:

$$\begin{aligned} & - \sum_{\mathbf{r},(j,n)} \hat{\mathbf{Q}}_{j,n} \cdot \left. \frac{\partial V_{eN}(\mathbf{R})}{\partial \mathbf{R}} \right|_{\mathbf{R}=\mathbf{r}-\mathbf{R}_{j,n}} \\ & = i \sum_{\mathbf{q},s,(j,n)} \sqrt{\frac{\hbar}{2N\omega_{\mathbf{q},s}}} \frac{e^{-i\mathbf{q}\cdot\mathbf{R}_j}}{\sqrt{m_n}} \eta_{\mathbf{q},s,n} \cdot \left[\sum_{\mathbf{r}} \nabla V_{eN}(\mathbf{R})|_{\mathbf{R}=\mathbf{r}-\mathbf{R}_{j,n}} \right] \left(\hat{b}_{-\mathbf{q},s} + \hat{b}_{\mathbf{q},s}^\dagger \right). \end{aligned} \quad (\text{A.5})$$

We now write the EPI Hamiltonian in second quantization. Let $\sigma = (n, \tau)$, where n denotes the orbital within a unit cell, and τ denotes the electron spin. Let $\psi_{i_\alpha, n_\alpha}(\mathbf{r})$ be the spatial part of the single-electron basis wave function corresponding to the composite index α . We introduce the quantity

$$M_{\alpha,\beta}^{(\mathbf{q},s)} \equiv \delta_{\tau_\alpha, \tau_\beta} i \sum_{j,n} F_{\mathbf{q},j}^* \sqrt{\frac{\hbar}{m_n}} \eta_{\mathbf{q},s,n} \cdot \int d\mathbf{r} \psi_{i_\alpha, n_\alpha}^*(\mathbf{r}) \left[\nabla V_{eN}(\mathbf{R})|_{\mathbf{R}=\mathbf{r}-\mathbf{R}_{j,n}} \right] \psi_{i_\beta, n_\beta}(\mathbf{r}), \quad (\text{A.6})$$

and the operator

$$\hat{Q}_{\mathbf{q},s} = \frac{1}{\sqrt{2\omega_{\mathbf{q},s}}} \left(\hat{b}_{\mathbf{q},s}^\dagger + \hat{b}_{-\mathbf{q},s} \right). \quad (\text{A.7})$$

Using these, we turn Eq. (A.5) into its second-quantized expression,

$$\hat{\mathcal{H}}_{\text{EPI}} = \sum_{\mathbf{q},s} \sum_{\alpha,\beta} M_{\alpha,\beta}^{(\mathbf{q},s)} \hat{Q}_{\mathbf{q},s} \hat{c}_\alpha^\dagger \hat{c}_\beta. \quad (\text{A.8})$$

We turn to the position representation by applying the Fourier transformation, with the coefficients defined in Eq. (10), and we obtain

$$\hat{\mathcal{H}}_{\text{EPI}} = \sum_{(j,s)} \sum_{\alpha,\beta} M_{\alpha,\beta}^{(j,s)} \hat{Q}_{j,s} \hat{c}_\alpha^\dagger \hat{c}_\beta, \quad (\text{A.9})$$

where

$$\begin{aligned} M_{\alpha,\beta}^{(j,s)} & \equiv \sum_{\mathbf{q}} F_{\mathbf{q},j} M_{\alpha,\beta}^{(\mathbf{q},s)} = \delta_{\tau_\alpha, \tau_\beta} i \sum_{j',n} \sqrt{\frac{\hbar}{m_n}} \left(\sum_{\mathbf{q}} F_{\mathbf{q},j} F_{\mathbf{q},j'}^* \eta_{\mathbf{q},s,n} \right) \\ & \cdot \int d\mathbf{r} \psi_{i_\alpha, n_\alpha}^*(\mathbf{r}) \left[\nabla_{\mathbf{r}} V_{eN}(\mathbf{r} - \mathbf{R}_{j',n}) \right] \psi_{i_\beta, n_\beta}(\mathbf{r}), \end{aligned} \quad (\text{A.10})$$

and

$$\hat{Q}_{j,s} \equiv \sum_{\mathbf{q}} F_{\mathbf{q},j} \hat{Q}_{\mathbf{q},s} = \sum_{\mathbf{q}} F_{\mathbf{q},j} \frac{1}{\sqrt{2\omega_{\mathbf{q},s}}} \left(\hat{b}_{\mathbf{q},s}^\dagger + \hat{b}_{-\mathbf{q},s} \right). \quad (\text{A.11})$$

Switching to the Greek-indices notation, we immediately turn Eq. (A.9) into Eq. (5) of the main text.

Let us investigate Eq. (A.10) further. We write the Fourier representation of $V_{\text{eN}}(\mathbf{r} - \mathbf{R}_j - \mathbf{B}_n)$ as

$$\begin{aligned} V_{\text{eN}}(\mathbf{r} - \mathbf{R}_j - \mathbf{B}_n) &= \sum_{\mathbf{q}'} \sum_{\mathbf{K}} \frac{e^{-i(\mathbf{q}'+\mathbf{K})\cdot(\mathbf{r}-\mathbf{R}_j-\mathbf{B}_n)}}{N\sqrt{N}} V_{\text{eN}}(\mathbf{q}'+\mathbf{K}) \\ &= \sum_{\mathbf{q}'} \sum_{\mathbf{K}} F_{\mathbf{q}',j} e^{-i(\mathbf{q}'+\mathbf{K})\cdot(\mathbf{r}-\mathbf{B}_n)} \frac{V_{\text{eN}}(\mathbf{q}'+\mathbf{K})}{N}, \end{aligned} \quad (\text{A.12})$$

where \mathbf{q}' belongs to the first Brillouin zone, while \mathbf{K} is a reciprocal lattice vector. Substituting this into Eq. (A.10), we obtain

$$\begin{aligned} M_{\alpha,\beta}^{(j,s)} &= \delta_{\tau_\alpha,\tau_\beta} \sum_{\mathbf{q}} F_{\mathbf{q},j} \sum_n \sqrt{\frac{\hbar}{m_n}} \eta_{\mathbf{q},s,n} \cdot \sum_{\mathbf{K}} (\mathbf{q}+\mathbf{K}) \frac{V_{\text{eN}}(\mathbf{q}+\mathbf{K})}{N} e^{i(\mathbf{q}+\mathbf{K})\cdot\mathbf{B}_n} \\ &\quad \times \int d\mathbf{r} \psi_{i_\alpha,n_\alpha}^*(\mathbf{r}) e^{-i(\mathbf{q}+\mathbf{K})\cdot\mathbf{r}} \psi_{i_\beta,n_\beta}(\mathbf{r}). \end{aligned} \quad (\text{A.13})$$

We now represent the single-electron wave functions as

$$\psi_{i,n}(\mathbf{r}) = \sum_{\mathbf{k}} F_{i,\mathbf{k}}^* \psi_{\mathbf{k},n}(\mathbf{r}) \equiv \sum_{\mathbf{k}} F_{i,\mathbf{k}}^* e^{i\mathbf{k}\cdot\mathbf{r}} \sum_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} \psi_{\mathbf{k},n}(\mathbf{G}), \quad (\text{A.14})$$

where $\psi_{\mathbf{k},n}(\mathbf{r})$ is a Bloch state, whose Fourier decomposition is written explicitly in the last equality (\mathbf{G} is a reciprocal lattice vector). This allows us to perform the integration over \mathbf{r} , which yields a factor

$$\int d\mathbf{r} e^{-i(\mathbf{k}+\mathbf{G}+\mathbf{q}+\mathbf{K}-\mathbf{k}'-\mathbf{G}')\cdot\mathbf{r}} = N \mathcal{V}_{\text{cell}} \delta_{\mathbf{k}+\mathbf{q}-\mathbf{k}',\mathbf{G}'-\mathbf{G}-\mathbf{K}}, \quad (\text{A.15})$$

where $\mathcal{V}_{\text{cell}}$ is the volume of a unit cell. We obtain

$$\begin{aligned} M_{\alpha,\beta}^{(j,s)} &= \delta_{\tau_\alpha,\tau_\beta} \sum_{\mathbf{q}} F_{\mathbf{q},j} \sum_n \sqrt{\frac{\hbar}{m_n}} \eta_{\mathbf{q},s,n} \cdot \sum_{\mathbf{K}} (\mathbf{q}+\mathbf{K}) V_{\text{eN}}(\mathbf{q}+\mathbf{K}) e^{i(\mathbf{q}+\mathbf{K})\cdot\mathbf{B}_n} \\ &\quad \times \sum_{\mathbf{k},\mathbf{k}'} \sum_{\mathbf{G},\mathbf{G}'} F_{i_\alpha,\mathbf{k}} F_{i_\beta,\mathbf{k}'}^* \psi_{\mathbf{k},n_\alpha}^*(\mathbf{G}) \psi_{\mathbf{k}',n_\beta}(\mathbf{G}') \mathcal{V}_{\text{cell}} \delta_{\mathbf{k}+\mathbf{q}-\mathbf{k}',\mathbf{G}'-\mathbf{G}-\mathbf{K}}. \end{aligned} \quad (\text{A.16})$$

The Kronecker delta allows to eliminate \mathbf{k}' as $\mathbf{k}' = \mathbf{k} + \mathbf{q} - \mathbf{G}' + \mathbf{G} + \mathbf{K}$. Since the vector $-\mathbf{G}' + \mathbf{G} + \mathbf{K}$ belongs to the reciprocal lattice, we have $F_{i_\beta,\mathbf{k}+\mathbf{q}-\mathbf{G}'+\mathbf{G}+\mathbf{K}}^* = F_{i_\beta,\mathbf{k}+\mathbf{q}}^*$. We end up with the following (exact) expression:

$$\begin{aligned} M_{\alpha,\beta}^{(j,s)} &= \delta_{\tau_\alpha,\tau_\beta} \mathcal{V}_{\text{cell}} \sum_{\mathbf{q}} F_{\mathbf{q},j} \sum_n \sqrt{\frac{\hbar}{m_n}} \eta_{\mathbf{q},s,n} \cdot \sum_{\mathbf{K}} (\mathbf{q}+\mathbf{K}) V_{\text{eN}}(\mathbf{q}+\mathbf{K}) \\ &\quad \times e^{i(\mathbf{q}+\mathbf{K})\cdot\mathbf{B}_n} \sum_{\mathbf{k}} \sum_{\mathbf{G},\mathbf{G}'} F_{i_\alpha,\mathbf{k}} F_{i_\beta,\mathbf{k}+\mathbf{q}}^* \psi_{\mathbf{k},n_\alpha}^*(\mathbf{G}) \psi_{\mathbf{k}+\mathbf{q}-\mathbf{G}'+\mathbf{G}+\mathbf{K},n_\beta}(\mathbf{G}'). \end{aligned} \quad (\text{A.17})$$

We briefly mention two approximations which are often applied to the expression for the EPI matrix elements. The first possible approximation consists in neglecting the *Umklapp* processes, i.e. in keeping only the term with $\mathbf{K} = \mathbf{0}$ —an approximation which relies on the fact that $V_{\text{eN}}(\mathbf{q}+\mathbf{K})$ decays quickly with increasing $|\mathbf{K}|$. The resulting expression depends on the scalar product $\eta_{\mathbf{q},s,n} \cdot \mathbf{q}$. Therefore, in this approximation, only longitudinal phonon modes couple with the electrons (see also the discussion in Ref. [37]). Another possible approximation, which can be dubbed “*strong*

“tight-binding” assumption, consists in putting

$$\psi_{i\alpha, n\alpha}^*(\mathbf{r}) \psi_{i\beta, n\beta}(\mathbf{r}) \approx \delta_{i\alpha, i\beta} \delta_{n\alpha, n\beta} |\psi_{i\alpha, n\alpha}(\mathbf{r})|^2 \approx \delta_{i\alpha, i\beta} \delta_{n\alpha, n\beta} \delta(\mathbf{r} - \mathbf{R}_{i\alpha} - \mathbf{B}_{n\alpha}) \quad (\text{A.18})$$

in Eq. (A.13). This yields

$$\begin{aligned} M_{\alpha, \beta}^{(j, s)} &\approx \delta_{\alpha, \beta} \sum_{\mathbf{q}} F_{\mathbf{q}, j-i\alpha} \sum_n \sqrt{\frac{\hbar}{m_n}} \eta_{\mathbf{q}, s, n} \cdot \sum_{\mathbf{K}} (\mathbf{q} + \mathbf{K}) \frac{V_{\text{eN}}(\mathbf{q} + \mathbf{K})}{N} e^{i(\mathbf{q} + \mathbf{K}) \cdot (\mathbf{B}_n - \mathbf{B}_{n\alpha})} \\ &\equiv \delta_{\alpha, \beta} M_{(i\alpha, \sigma\alpha)}^{(j, s)}. \end{aligned} \quad (\text{A.19})$$

For the purposes of our derivation, we do not need to apply these approximations, and we can just use Eq. (A.17). We write it as

$$M_{\alpha, \beta}^{(j, s)} \equiv \delta_{\tau\alpha, \tau\beta} \sum_{\mathbf{q}} \sum_{\mathbf{k}} F_{\mathbf{q}, j} F_{i\alpha, \mathbf{k}} F_{i\beta, \mathbf{k} + \mathbf{q}}^* M_{\mathbf{k}; n\alpha, n\beta}^{(\mathbf{q}, s)}, \quad (\text{A.20})$$

emphasizing its Fourier representation. The definition of $M_{\mathbf{k}; n\alpha, n\beta}^{(\mathbf{q}, s)}$ can be determined by comparison with Eq. (A.17); in the case of a single orbital at each lattice site, it bears no dependence on n_α and n_β , and we write it as $M_{\mathbf{k}}^{(\mathbf{q}, s)}$, as we have done in Section 8.

Appendix B. Phonon displacement operator in the position representation

From Eq. (13), it follows that

$$\frac{1}{\sqrt{\omega_{\mathbf{q}, s}}} = \sum_{ij} F_{\mathbf{q}, i}^* [f^{-1/2}(s)]_{ij} F_{\mathbf{q}, j} \equiv \sum_{ij} F_{\mathbf{q}, i}^* f_{ij}^{-1/2}(s) F_{\mathbf{q}, j}. \quad (\text{B.1})$$

Also, using

$$\hat{b}_{\mathbf{q}, s}^\dagger = \sum_{i'} F_{\mathbf{q}, i'} \hat{b}_{i', s}^\dagger, \quad \hat{b}_{-\mathbf{q}, s} = \sum_{i'} F_{\mathbf{q}, i'} \hat{b}_{i', s}, \quad (\text{B.2})$$

we obtain

$$\begin{aligned} \hat{Q}_{\mathbf{q}, s} &= \frac{1}{\sqrt{2}} \sum_{\mathbf{q}} F_{\mathbf{q}, l} \sum_{ij, i'} F_{\mathbf{q}, i}^* f_{ij}^{-1/2}(s) F_{\mathbf{q}, j} F_{\mathbf{q}, i'} (\hat{b}_{i', s}^\dagger + \hat{b}_{i', s}) \\ &= \frac{1}{N} \sum_{ij, i'} f_{ij}^{-1/2}(s) \delta_{\mathbf{R}_i - \mathbf{R}_j, \mathbf{R}_i + \mathbf{R}_{i'}} \frac{1}{\sqrt{2}} (\hat{b}_{i', s}^\dagger + \hat{b}_{i', s}). \end{aligned} \quad (\text{B.3})$$

It is convenient to abbreviate $\mathbf{R}_i - \mathbf{R}_j$ as $i - j$. Since $f_{ij}(s) = f_{i-j}(s)$, we also have $f_{ij}^{-1/2}(s) = f_{i-j}^{-1/2}(s)$, and we obtain:

$$\hat{Q}_{\mathbf{q}, s} = \sum_j f_{i+j}^{-1/2}(s) \frac{1}{\sqrt{2}} (\hat{b}_{j, s}^\dagger + \hat{b}_{j, s}). \quad (\text{B.4})$$

Using Greek indices, this can be rewritten as in Eq. (6), with $f_{\lambda, -\kappa}^{-1/2} \equiv \delta_{s\lambda, s\kappa} f_{i_\lambda + i_\kappa}^{-1/2}$.

Appendix C. Proof - non-interacting grand potential as a function of the non-interacting GFs

In the absence of EEs and EPIs, the action reduces to

$$\begin{aligned} A_{\mathbf{t}, \mathbf{0}, \mathbf{f}, \mathbf{0}}^{(c, \bar{c}, b, b^*)} &= \frac{1}{T} \sum_n \sum_{\alpha, \beta} \bar{c}_\alpha(i\omega_n) G_{\mathbf{t}, \mathbf{0}, \mathbf{f}, \mathbf{0}; \alpha, \beta}^{-1}(i\omega_n) c_\beta(i\omega_n) \\ &\quad + \frac{1}{T} \sum_n \sum_{\kappa, \lambda} b_\kappa^*(i\Omega_n) P_{\mathbf{t}, \mathbf{0}, \mathbf{f}, \mathbf{0}; \kappa, \lambda}^{-1}(i\Omega_n) b_\lambda(i\Omega_n). \end{aligned} \quad (\text{C.1})$$

The partition function can therefore be evaluated analytically:

$$\begin{aligned}
 \mathcal{Z}_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0}} &= \int D(\bar{c}, c) D(b^*, b) e^{A_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0}}^{(c,\bar{c},b,b^*)}} \\
 &= \int D(\bar{c}, c) \exp \left[\frac{1}{T} \sum_n \sum_{\alpha,\beta} \bar{c}_\alpha(i\omega_n) G_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0};\alpha,\beta}^{-1}(i\omega_n) c_\beta(i\omega_n) \right] \\
 &\quad \times \int D(b^*, b) \exp \left[\frac{1}{T} \sum_n \sum_{\kappa,\lambda} b_\kappa^*(i\Omega_n) P_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0};\kappa,\lambda}^{-1}(i\Omega_n) b_\lambda(i\Omega_n) \right] \\
 &= \frac{\prod_{\omega_n} \det \left[-\frac{1}{T} \mathbf{G}_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0}}^{-1}(i\omega_n) \right]}{\prod_{\Omega_n} \det \left[-\frac{1}{T} \mathbf{P}_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0}}^{-1}(i\Omega_n) \right]}.
 \end{aligned} \tag{C.2}$$

From Eq. (C.2), we evaluate the non-interacting grand potential as

$$\begin{aligned}
 \Omega_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0}} &= -T \ln \mathcal{Z}_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0}} \\
 &= -T \sum_n \ln \det \left[-\frac{1}{T} \mathbf{G}_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0}}^{-1}(i\omega_n) \right] + T \sum_n \ln \det \left[-\frac{1}{T} \mathbf{P}_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0}}^{-1}(i\Omega_n) \right] \\
 &= T \sum_n \ln \det \left[-T \mathbf{G}_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0}}(i\omega_n) \right] - T \sum_n \ln \det \left[-T \mathbf{P}_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0}}(i\Omega_n) \right] \\
 &= T \text{Tr} \ln \left(-T \mathbf{G}_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0}} \right) - T \text{Tr} \ln \left(-T \mathbf{P}_{\mathbf{t},\mathbf{0},\mathbf{f},\mathbf{0}} \right),
 \end{aligned} \tag{C.3}$$

which is Eq. (25). This is used in the main text to derive Eq. (51).

Appendix D. Proof - GF functionals as functional derivatives

In this Appendix we prove Eqs. (43) and (44).

Denoting by $\delta F_{\mathbf{U},\mathbf{M}}[\Sigma; \Lambda]$ the variation of the functional $\tilde{F}_{\mathbf{U},\mathbf{M}}[\Sigma; \Lambda]$ with respect to variations of Σ and Λ (while keeping fixed the parameters \mathbf{U} and \mathbf{M}), we have

$$\begin{aligned}
 &-\frac{1}{T} \delta \tilde{F}_{\mathbf{U},\mathbf{M}}[\Sigma; \Lambda] \\
 &= -\frac{1}{T} \delta \tilde{\Omega}_{\mathbf{U},\mathbf{M}} \left[\tilde{\mathbf{G}}_{\mathbf{U},\mathbf{M}}[\Sigma; \Lambda]^{-1} + \Sigma; \tilde{\mathbf{P}}_{\mathbf{U},\mathbf{M}}[\Sigma; \Lambda]^{-1} + \Lambda \right] \\
 &\quad + \delta \sum_n \sum_\alpha e^{i\omega_n 0^+} \left\{ \ln \left(T \tilde{\mathbf{G}}_{\mathbf{U},\mathbf{M}}[\Sigma; \Lambda](i\omega_n) \right) \right\}_{\alpha,\alpha} \\
 &\quad - \delta \sum_n \sum_\alpha e^{i\Omega_n 0^+} \left\{ \ln \left(T \tilde{\mathbf{P}}_{\mathbf{U},\mathbf{M}}[\Sigma; \Lambda](i\Omega_n) \right) \right\}_{\alpha,\alpha} \\
 &= \sum_n \sum_{\alpha,\beta} \tilde{\mathbf{G}}_{\mathbf{U},\mathbf{M};\alpha,\beta}[\Sigma; \Lambda](i\omega_n) \left\{ \delta \tilde{\mathbf{G}}_{\mathbf{U},\mathbf{M};\beta,\alpha}^{-1}[\Sigma; \Lambda](i\omega_n) + \delta \Sigma_{\beta,\alpha}(i\omega_n) \right\} \\
 &\quad - \sum_n \sum_{\alpha,\beta} \tilde{\mathbf{P}}_{\mathbf{U},\mathbf{M};\alpha,\beta}[\Sigma; \Lambda](i\Omega_n) \left\{ \delta \tilde{\mathbf{P}}_{\mathbf{U},\mathbf{M};\beta,\alpha}^{-1}[\Sigma; \Lambda](i\Omega_n) + \delta \Lambda_{\beta,\alpha}(i\Omega_n) \right\} \\
 &\quad + \sum_n \sum_{\alpha,\beta} \tilde{\mathbf{G}}_{\mathbf{U},\mathbf{M};\alpha,\beta}^{-1}[\Sigma; \Lambda](i\omega_n) \left\{ \delta \tilde{\mathbf{G}}_{\mathbf{U},\mathbf{M};\beta,\alpha}[\Sigma; \Lambda](i\omega_n) \right\} \\
 &\quad - \sum_n \sum_{\alpha,\beta} \tilde{\mathbf{P}}_{\mathbf{U},\mathbf{M};\alpha,\beta}^{-1}[\Sigma; \Lambda](i\Omega_n) \left\{ \delta \tilde{\mathbf{P}}_{\mathbf{U},\mathbf{M};\beta,\alpha}[\Sigma; \Lambda](i\Omega_n) \right\}
 \end{aligned}$$

$$= \sum_n \sum_{\alpha, \beta} \left\{ \tilde{\mathcal{C}}_{\mathbf{U}, \mathbf{M}; \alpha, \beta}[\boldsymbol{\Sigma}; \boldsymbol{\Lambda}](i\omega_n) \delta \Sigma_{\beta, \alpha}(i\omega_n) - \tilde{\mathcal{P}}_{\mathbf{U}, \mathbf{M}; \alpha, \beta}[\boldsymbol{\Sigma}; \boldsymbol{\Lambda}](i\Omega_n) \delta \Lambda_{\beta, \alpha}(i\Omega_n) \right\}, \quad (\text{D.1})$$

where we have used that (in condensed notation)

$$\text{Tr} [X^{-1} \cdot (\delta X) + (\delta X^{-1}) \cdot X] = \text{Tr} \delta(X^{-1} \cdot X) = \text{Tr} \delta(1) = 0. \quad (\text{D.2})$$

The result in the last line of (D.1) is equivalent to Eqs. (43)–(44).

Appendix E. Proof - self-energy functionals as functional derivatives

In this Appendix, we prove Eqs. (48) and (49) by using Eq. (45) together with (43) and (44).

Denoting by $\delta \tilde{\Phi}_{\mathbf{U}, \mathbf{I}}[\mathbf{G}; \mathbf{P}]$ the variation of the functional $\tilde{\Phi}_{\mathbf{U}, \mathbf{I}}[\mathbf{G}; \mathbf{P}]$ with respect to variations of \mathbf{G} and \mathbf{P} (while keeping fixed the parameters \mathbf{U} and \mathbf{I}), we have

$$\begin{aligned} \frac{1}{T} \delta \tilde{\Phi}_{\mathbf{U}, \mathbf{I}}[\mathbf{G}; \mathbf{P}] &= \sum_n \sum_{\alpha, \beta} \left\{ -G_{\beta, \alpha}(i\omega_n) \delta \tilde{\Sigma}_{\mathbf{U}, \mathbf{I}; \alpha, \beta}[\mathbf{G}; \mathbf{P}](i\omega_n) + P_{\beta, \alpha}(i\Omega_n) \delta \tilde{\Lambda}_{\mathbf{U}, \mathbf{I}; \alpha, \beta}[\mathbf{G}; \mathbf{P}](i\Omega_n) \right. \\ &\quad \left. + \delta \left[\tilde{\Sigma}_{\mathbf{U}, \mathbf{I}; \alpha, \beta}[\mathbf{G}; \mathbf{P}](i\omega_n) G_{\beta, \alpha}(i\omega_n) \right] - \delta \left[\tilde{\Lambda}_{\mathbf{U}, \mathbf{I}; \alpha, \beta}[\mathbf{G}; \mathbf{P}](i\Omega_n) P_{\beta, \alpha}(i\Omega_n) \right] \right\} \\ &= \sum_n \sum_{\alpha, \beta} \left\{ \tilde{\Sigma}_{\mathbf{U}, \mathbf{I}; \alpha, \beta}[\mathbf{G}; \mathbf{P}](i\omega_n) \delta G_{\beta, \alpha}(i\omega_n) - \tilde{\Lambda}_{\mathbf{U}, \mathbf{I}; \alpha, \beta}[\mathbf{G}; \mathbf{P}](i\Omega_n) \delta P_{\beta, \alpha}(i\Omega_n) \right\}, \end{aligned} \quad (\text{E.1})$$

which leads directly to Eqs. (48) and (49).

Appendix F. Simplification of the functional derivative of the four-leg reducible vertex

By applying the functional derivative to Eq. (84), we obtain

$$\begin{aligned} &\tilde{\Gamma}_{\mathbf{U}; (\mu, \nu; \phi, \theta; \nu', \mu')}^{[6]}[\mathbf{G}](i\omega_m, i\omega_n, i\omega_s) \\ &= \tilde{U}_{\mathbf{U}; (\mu, \nu; \phi, \theta; \nu', \mu')}^{[6]}[\mathbf{G}](i\omega_m, i\omega_n, i\omega_s) \\ &\quad + \delta_{n, m} \sum_{\xi', \eta'} \tilde{U}_{\mathbf{U}; (\mu, \nu; \xi', \mu')}^{[4]}[\mathbf{G}](i\omega_n, i\omega_s) G_{\eta', \xi'}(i\omega_s) \tilde{\Gamma}_{\mathbf{U}; (\phi, \nu; \nu', \eta')}[\mathbf{G}](i\omega_n, i\omega_s) \\ &\quad + \delta_{n, s} \sum_{\xi, \eta} \tilde{U}_{\mathbf{U}; (\mu, \xi; \phi, \mu')}^{[4]}[\mathbf{G}](i\omega_m, i\omega_n) G_{\xi, \eta}(i\omega_m) \tilde{\Gamma}_{\mathbf{U}; (\eta, \nu; \nu', \theta)}[\mathbf{G}](i\omega_m, i\omega_n) \\ &\quad + \sum_{\xi, \xi', \eta, \eta'} \tilde{U}_{\mathbf{U}; (\mu, \xi; \phi, \theta; \xi', \mu')}^{[6]}[\mathbf{G}](i\omega_m, i\omega_n, i\omega_s) G_{\xi, \eta}(i\omega_m) G_{\eta', \xi'}(i\omega_s) \tilde{\Gamma}_{\mathbf{U}; (\eta, \nu; \nu', \eta')}[\mathbf{G}](i\omega_m, i\omega_s) \\ &\quad + \sum_{\xi, \xi', \eta, \eta'} \tilde{U}_{\mathbf{U}; (\mu, \xi; \xi', \mu')}^{[4]}[\mathbf{G}](i\omega_m, i\omega_s) G_{\xi, \eta}(i\omega_m) G_{\eta', \xi'}(i\omega_s) \tilde{\Gamma}_{\mathbf{U}; (\eta, \nu; \phi, \theta; \nu', \eta')}^{[6]}[\mathbf{G}](i\omega_m, i\omega_n, i\omega_s), \end{aligned} \quad (\text{F.1})$$

where we have introduced the functional derivative of the irreducible four-leg vertex as in Eq. (85).

We proceed to simplify Eq. (F.1), with the aim of expressing its right-hand side in terms of the irreducible functionals $U^{[4]}$ and $U^{[6]}$, and the reducible functional Γ , analogously to what was done in Ref. [77] (i.e. we eliminate the reducible six-leg vertex $\Gamma^{[6]}$). It should be noted that Ref. [77] considered quenched disorder, while here we are considering EELs in clean systems as the source of the electronic self-energy in the absence of EPI. Because of this difference, although our final expression is similar to their Eq. (40), some important details are different. Here, in particular, the six-leg vertices depend on three distinct fermionic frequencies, while, in their case, two of the three frequencies coincide, in all vertices. This produces some topologically distinct structures in the final expressions.

We now go through the derivation by employing Feynman diagrams. First, we represent Eq. (F.1) by means of Feynman diagrams, obtaining Fig. F.5, where we explicitly label the internal vertices as

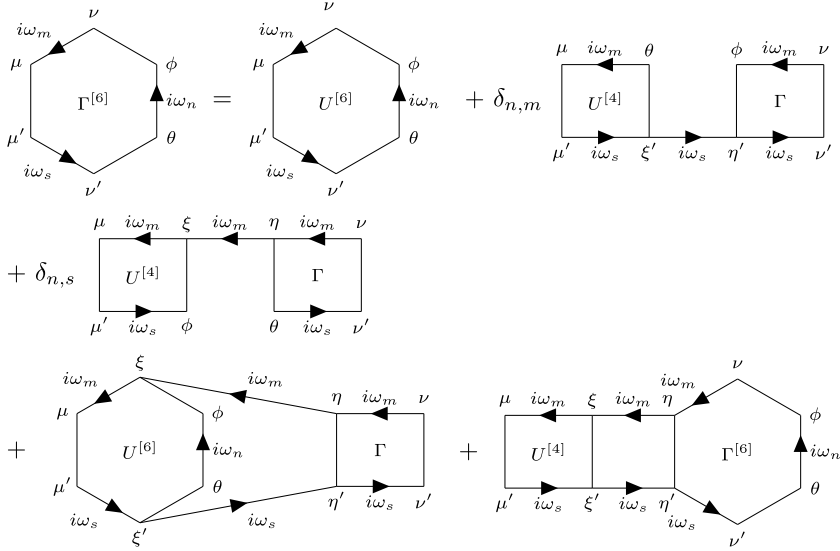


Fig. F.5. Diagrammatic representation of Eq. (F.1).

well as the external vertices (it is intended that internal indices are summed over). In the following steps, we will omit the dummy labels of the internal vertices. Moreover, to avoid cluttering the figures with redundant information, we will indicate only one frequency argument for each fermionic oriented line, with the understanding that it applies to all the connected segments that form that line.

The first step of the derivation consists in applying a Γ diagram from the left, by attaching it (via two GFs) to the μ and μ' vertices in Fig. F.5. After renaming the vertices so that μ and μ' remain the labels of the external vertices on the left of the diagrams, we obtain Fig. F.6.

We then use the Bethe–Salpeter equation, Eq. (84), which relates the reducible four-leg vertex Γ to the irreducible four-leg vertex $U^{[4]}$. In our diagrammatic notation, Eq. (84) is translated into Fig. F.7. By substituting it into Fig. F.6, we obtain Fig. F.8.

We now observe that the last line of Fig. F.8 contains a term which is identical to the quantity on the left-hand side of the same diagrammatic equation (so they cancel out), and another term, which depends on $U^{[4]}$ and $\Gamma^{[6]}$, which appears in the last line of Fig. F.5. We then solve Fig. F.8 for this quantity, substitute into Fig. F.5, and we obtain the result, Fig. F.9.

Finally, we convert the result displayed in Fig. F.9 into the following algebraic expression:

$$\begin{aligned}
 & \tilde{T}_{\mathbf{U};(\mu,\nu;\phi,\theta;\nu',\mu')}^{[6]}[\mathbf{G}](i\omega_m, i\omega_n, i\omega_s) \\
 &= \tilde{U}_{\mathbf{U};(\mu,\nu;\phi,\theta;\nu',\mu')}^{[6]}[\mathbf{G}](i\omega_m, i\omega_n, i\omega_s) \\
 &+ \delta_{n,m} \sum_{\xi',\eta'} \tilde{T}_{\mathbf{U};(\mu,\nu;\xi',\eta';\mu')}[\mathbf{G}](i\omega_m, i\omega_s) G_{\eta',\xi'}(i\omega_s) \tilde{T}_{\mathbf{U};(\phi,\nu;\nu',\eta')}[\mathbf{G}](i\omega_m, i\omega_s) \\
 &+ \delta_{n,s} \sum_{\xi,\eta} \tilde{T}_{\mathbf{U};(\mu,\xi;\phi,\theta;\mu')}[\mathbf{G}](i\omega_m, i\omega_s) G_{\xi,\eta}(i\omega_m) \tilde{T}_{\mathbf{U};(\eta,\nu;\nu',\theta)}[\mathbf{G}](i\omega_m, i\omega_s) \\
 &+ \sum_{\xi,\xi',\eta,\eta'} \tilde{U}_{\mathbf{U};(\mu,\xi;\phi,\theta;\xi',\mu')}^{[6]}[\mathbf{G}](i\omega_m, i\omega_n, i\omega_s) G_{\xi,\eta}(i\omega_m) G_{\eta',\xi'}(i\omega_s) \tilde{T}_{\mathbf{U};(\eta,\nu;\nu',\eta')}[\mathbf{G}](i\omega_m, i\omega_s) \\
 &+ \sum_{\xi,\xi',\eta,\eta'} \tilde{T}_{\mathbf{U};(\mu,\xi;\xi',\mu')}[\mathbf{G}](i\omega_m, i\omega_s) G_{\xi,\eta}(i\omega_m) G_{\eta',\xi'}(i\omega_s) \tilde{U}_{\mathbf{U};(\eta,\nu;\phi,\theta;\nu',\eta')}^{[6]}[\mathbf{G}](i\omega_m, i\omega_n, i\omega_s)
 \end{aligned}$$

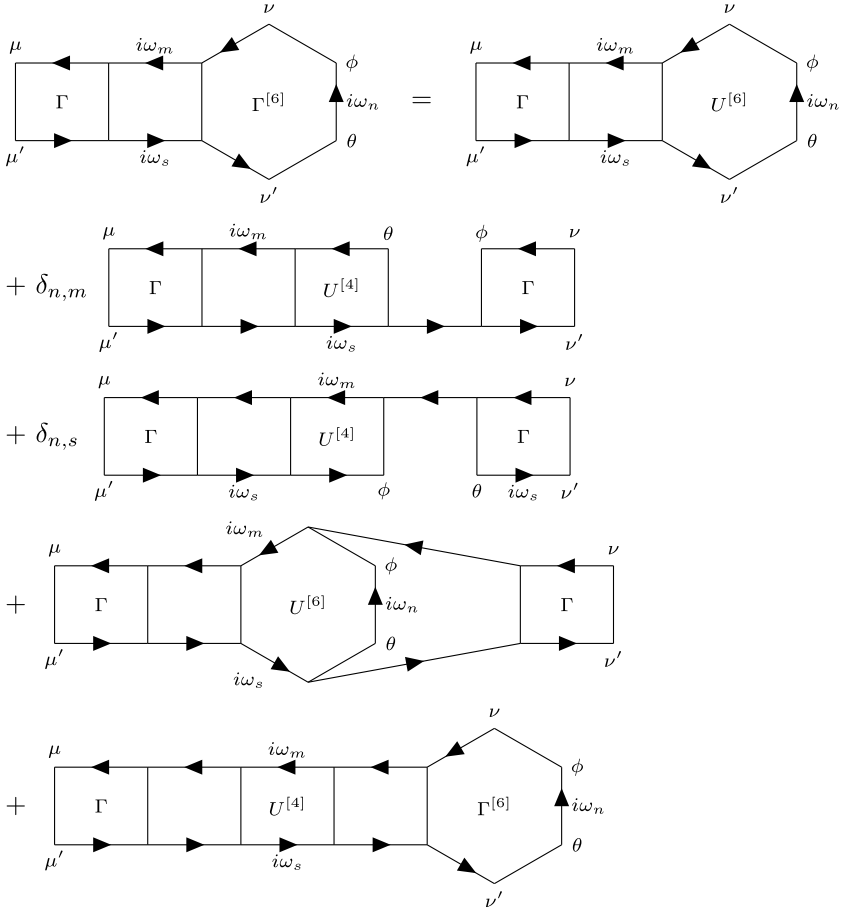


Fig. F.6. First step of the derivation that leads from Eqs. (F.1) to (F.2).

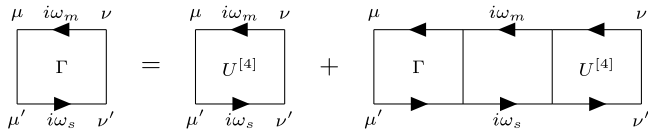


Fig. F.7. Diagrammatic representation of the Bethe-Salpeter equation, Eq. (84). The connected blocks Γ and $U^{[4]}$ on the right-hand side can be interchanged.

$$\begin{aligned}
 &+ \sum_{\xi, \xi', \eta, \eta', \zeta, \zeta', \chi, \chi'} \tilde{\Gamma}_{\mathbf{U}; (\mu, \xi; \xi', \mu')} [\mathbf{G}] (i\omega_m, i\omega_s) G_{\xi, \eta} (i\omega_m) G_{\eta', \xi'} (i\omega_s) \\
 &\times \tilde{U}_{\mathbf{U}; (\eta, \zeta; \phi, \theta; \zeta', \eta')}^{[6]} [\mathbf{G}] (i\omega_m, i\omega_n, i\omega_s) G_{\zeta, \chi} (i\omega_m) G_{\chi', \zeta'} (i\omega_s) \tilde{\Gamma}_{\mathbf{U}; (\chi, \nu; \nu', \chi')} [\mathbf{G}] (i\omega_m, i\omega_s). \quad (\text{F.2})
 \end{aligned}$$

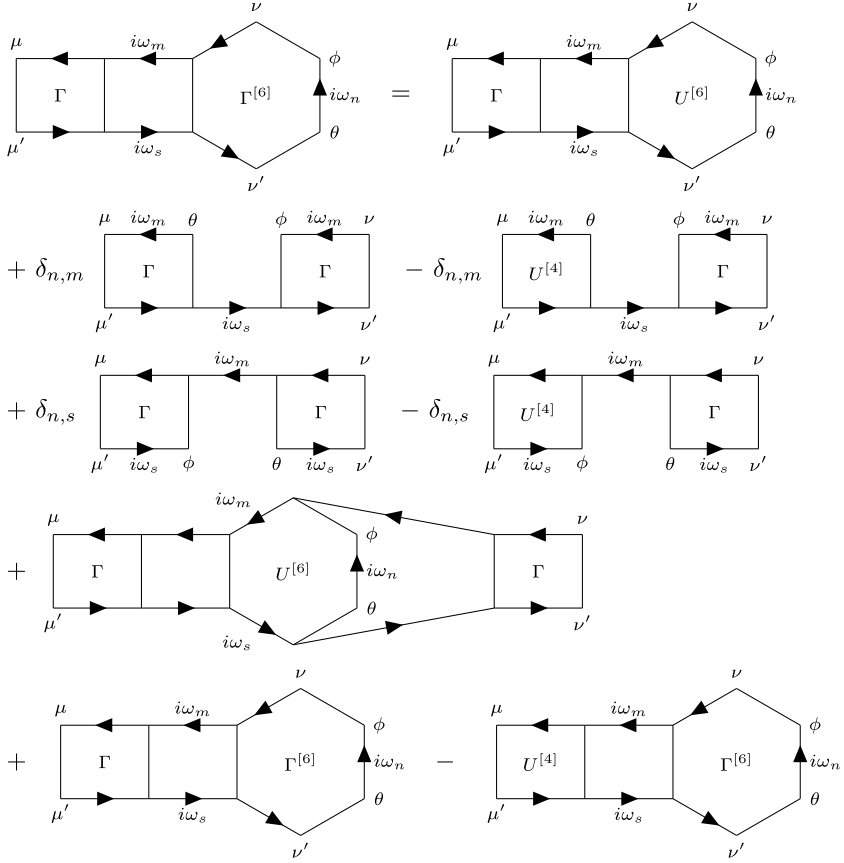


Fig. F.8. Second step of the derivation that leads from Eqs. (F.1) to (F.2).

Appendix G. G-N transformation

Under the assumptions stated at the beginning of Section 8, the total Hamiltonian becomes

$$\begin{aligned}
 \hat{\mathcal{H}} = & \sum_{ij} t_{i,j} \sum_{\sigma} \hat{c}_{i,\sigma}^{\dagger} \hat{c}_{j,\sigma} + \frac{1}{2} \sum_{i,j,k,l} U_{i,j,l,k} \sum_{\sigma,\sigma'} \hat{c}_{i,\sigma}^{\dagger} \hat{c}_{j,\sigma'}^{\dagger} \hat{c}_{k,\sigma'} \hat{c}_{l,\sigma} \\
 & + \sum_{i,j,k} \sum_s I_{ij}^{(k)}(s) \hat{q}_{k,s} \sum_{\sigma} \hat{c}_{i,\sigma}^{\dagger} \hat{c}_{j,\sigma} + \sum_{ij} \sum_s f_{ij}(s) \hat{b}_{i,s}^{\dagger} \hat{b}_{j,s} .
 \end{aligned} \tag{G.1}$$

We perform the G-N transformation on the fermions,

$$\hat{c}_{i,\uparrow} \equiv \hat{d}_{i,\uparrow} , \quad \hat{c}_{i,\downarrow} \equiv \hat{d}_{i,\downarrow}^{\dagger} , \tag{G.2}$$

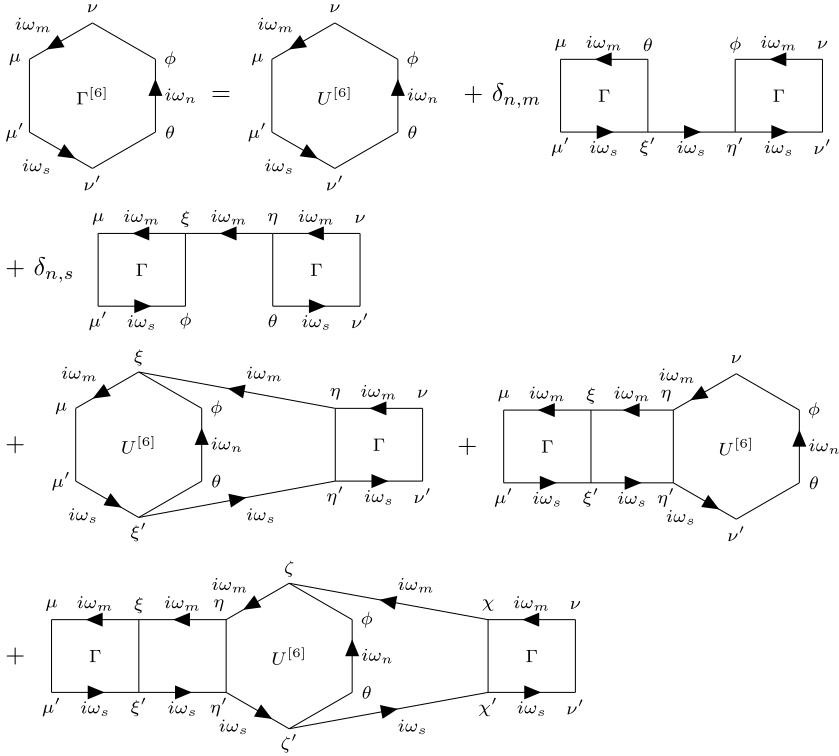


Fig. F.9. Result of the derivation. This is the diagrammatic representation of Eq. (F.2).

and we normal-order the result. Neglecting constant terms, we obtain

$$\begin{aligned}
 \hat{\mathcal{H}} &= \sum_{ij} t_{i,j} \sum_{\sigma} \sigma \hat{a}_{i,\sigma}^{\dagger} \hat{d}_{j,\sigma} + \sum_{ij} \sum_s f_{i,j}(s) \hat{b}_{i,s}^{\dagger} \hat{b}_{j,s} \\
 &+ \frac{1}{2} \sum_{i,j,k,l} U_{i,j,l,k} \sum_{\sigma,\sigma'} \sigma \sigma' \hat{a}_{i,\sigma}^{\dagger} \hat{a}_{j,\sigma'}^{\dagger} \hat{d}_{k,\sigma'} \hat{d}_{l,\sigma} + \sum_{ij} \left(\sum_k U_{i,k,j,k} \right) \sum_{\sigma} \sigma \hat{a}_{i,\sigma}^{\dagger} \hat{d}_{j,\sigma} \\
 &+ \sum_{i,j,k} \sum_s I_{i,j}^{(k)}(s) \hat{q}_{k,s} \sum_{\sigma} \sigma \hat{a}_{i,\sigma}^{\dagger} \hat{d}_{j,\sigma} + \sum_k \sum_s \hat{q}_{k,s} \sum_i I_{i,i}^{(k)}(s). \quad (\text{G.3})
 \end{aligned}$$

Let us examine Eq. (G.3). Notice, in particular, the last term in the second line, which results from the normal-ordering of the transformed EEI Hamiltonian, and the last term in the third line, which results from the normal-ordering of the transformed EPI Hamiltonian. The first of these terms (purely fermionic) can be directly incorporated into a renormalization of the electronic hopping parameters. The second term, instead, which is purely phononic, apparently differs from the other phononic terms. In order to recover the form of the Hamiltonian, we make the bosonic transformation

$$\hat{b}_{i,s} \equiv \hat{a}_{i,s} + K_{i,s}, \quad \hat{b}_{i,s}^{\dagger} \equiv \hat{a}_{i,s}^{\dagger} + K_{i,s}^*, \quad (\text{G.4})$$

where the quantities $K_{i,s}$ are constants that will be determined shortly, and the fields $\hat{a}_{i,s}$ are bosons. When this transformation is done, the first term in the third line of Eq. (G.3) generates an additional purely electronic term, while the second term in the first line generates both quadratic and linear terms in the new bosonic fields. By imposing that the terms which are linear in the bosons (and do

not involve fermionic fields) cancel out, we determine the values of the parameters $K_{i,s}$:

$$K_{i,s} = K_{i,s}^* \equiv -\frac{1}{\sqrt{2}} \sum_j f_{ij}^{-1}(s) \sum_l I_{l,l}^{(j)}(s), \quad (\text{G.5})$$

where we have exploited that $f_{k,i}(s) = f_{i,k}(s)$. Neglecting further constants, the Hamiltonian becomes

$$\begin{aligned} \hat{\mathcal{H}} = & \sum_{ij} \left[t_{i,j} + \sum_k U_{i,k,j,k} - \sum_{k,s} I_{i,j}^{(k)}(s) \sum_m f_{k,m}^{-1}(s) \sum_l I_{l,l}^{(m)}(s) \right] \sum_{\sigma} \sigma \hat{a}_{i,\sigma}^{\dagger} \hat{a}_{j,\sigma} \\ & + \sum_{ij} f_{i,j}(s) \hat{a}_{i,s}^{\dagger} \hat{a}_{j,s} + \sum_{ij} \sum_{k,s} I_{i,j}^{(k)}(s) \frac{1}{\sqrt{2}} \left(\hat{a}_{k,s} + \hat{a}_{k,s}^{\dagger} \right) \sum_{\sigma} \sigma \hat{a}_{i,\sigma}^{\dagger} \hat{a}_{j,\sigma} \\ & + \frac{1}{2} \sum_{ij,k,l} U_{i,j,l,k} \sum_{\sigma,\sigma'} \sigma \sigma' \hat{a}_{i,\sigma}^{\dagger} \hat{a}_{j,\sigma'}^{\dagger} \hat{a}_{k,\sigma'} \hat{a}_{l,\sigma}. \end{aligned} \quad (\text{G.6})$$

This is mathematically equivalent to the initial Hamiltonian (1) of the main text, provided that the fields are renamed and the parameters are specified as in Eqs. (97), (96), and (95).

The transformation (G.4) is equivalent to a fixed displacement of the lattice ions, dependent on the lattice position and on the phonon mode. It can be interpreted as an effect of the interaction between the phonon system and the vacuum of the Nambu fields: when the state of the system contains zero Nambu fermions, the equilibrium positions of the ions are different with respect to those characterizing the state with zero electrons (i.e., the lattice sites). An analogous transformation was discussed in Ref. [90].

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