Theoretical study of phonon-mediated superconductivity beyond Migdal-Eliashberg approximation and Coulomb pseudopotential

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In previous theoretical studies of phonon-mediated superconductors, the electron-phonon coupling is treated by solving the Migdal-Eliashberg equations under the bare vertex approximation, whereas the effect of Coulomb repulsion is incorporated by introducing one single pseudopotential parameter. These two approximations become unreliable in low carrier density superconductors in which the vertex corrections are not small and the Coulomb interaction is poorly screened. Here, we go beyond these two approximations and employ the Dyson-Schwinger equation approach to handle the interplay of the electron-phonon interaction and Coulomb interaction in a self-consistent way. We first derive the exact Dyson-Schwinger integral equation of the full electron propagator. Such an equation contains several unknown single-particle propagators and fermion-boson vertex functions, and thus seems to be intractable. To solve this difficulty, we further derive a number of identities satisfied by all the relevant propagators and vertex functions and then use these identities to show that the exact Dyson-Schwinger equation of the electron propagator is actually self-closed. This self-closed equation takes into account not only all the vertex corrections, but also the mutual influence between electron-phonon interaction and Coulomb interaction. Solving it by using proper numerical methods leads to the superconducting temperature T_c and other quantities. As an application of the approach, we compute the T_c of the interfacial superconductivity realized in the one-unit-cell $FeSe/SrTiO_3$ system. We find that T_c can be strongly influenced by the vertex corrections and the competition between phonon-mediated attraction and Coulomb repulsion.

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I. INTRODUCTION

Superconductivity develops in metals as the result of Cooper pairing instability when the attraction between electrons mediated by the exchange of phonons (or other types of bosons) overcomes the static Coulomb repulsion, which is the basic picture of Bardeen-Cooper-Schrieffer (BCS) theory [1]. In principle, the precise values of the pairing gap Δ and the transition temperature T_c should be determined by performing a careful theoretical study of the complicated interplay of electron-phonon interaction (EPI) and Coulomb interaction. This is difficult to achieve. Traditionally, these two interactions are treated by using different methods [1]. The EPI is handled within the Migdal-Eliashberg (ME) theory, and Δ and T_c are computed by solving a set of integral equations satisfied by the electrons' renormalization function and the pairing function. In contrast, the Coulomb interaction is not handled at such a quantitative level: its impact on T_c is approximately measured by one single pseudopotential parameter. Over the last decades, the ME theory and the pseudopotential have been jointly applied [2–5] to evaluate T_c and other quantities in various phonon-mediated superconductors.

That EPI and Coulomb interaction are handled quite differently can be understood by making a field-theoretic analysis. Let us first consider EPI. The EPI describes the mutual influence of the dynamics of electrons and phonons on each other, and hence appears to be very complicated. Within quantum many-body theory [1,2], one needs to compute an infinite number of Feynman diagrams to accurately compute any observable quantity, which is apparently impractical. Fortunately, treatment of EPI can be greatly simplified as the Migdal theorem [6] indicates that the EPI vertex corrections are strongly suppressed by the small factor $\lambda(\omega_D/E_F)$, where λ is a dimensionless coupling parameter, ω_D is the Debye frequency, and E_F is the Fermi energy. For normal metals, $\lambda(\omega_D/E_F) \ll 1$; thus EPI vertex corrections can be safely ignored. Under the bare vertex approximation, Eliashberg [7] derived a set of coupled equations, called ME equations, to study EPI-induced superconducting transition.

We then discuss the influence of Coulomb repulsion. After defining an auxiliary scalar field A to represent the static Coulomb potential, one can map the Coulomb interaction into an equivalent fermion-boson interaction that has a similar field-theoretic structure to EPI. But one cannot naively use the ME theory to handle this fermion-boson interaction since there is no Migdal-like theorem to guarantee the smallness of its vertex corrections. In the absence of a well-controlled method, it seems necessary to make approximations. Tolmachev [8] and Morel and Anderson [9]

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introduced a pseudopotential μ^* to include the impact of Coulomb repulsion. For a three-dimensional metal, the bare Coulomb interaction is described by

$$V_0(\mathbf{q}) = \frac{4\pi e^2}{\mathbf{q}^2}. \tag{1}$$

This bare function is renormalized to become energy-momentum dependent, namely

$$V_R(\omega, \mathbf{q}) = \frac{1}{V_0^{-1}(\mathbf{q}) - \Pi(\omega, \mathbf{q})} = \frac{4\pi e^2}{\mathbf{q}^2 - 4\pi e^2 \Pi(\omega, \mathbf{q})}. \tag{2}$$

The full polarization function $\Pi(\omega, \mathbf{q})$ is hard to compute. A widely used approximation is to calculate $\Pi(\omega, \mathbf{q})$ at the lowest one-loop level, corresponding to the random phase approximation (RPA). The one-loop polarization $\Pi_{1L}(\omega, \mathbf{q})$ is still very complex. Nevertheless, it is easy to reveal that $\Pi_{1L}(\omega, \mathbf{q})$ approaches a constant in the limits of $\omega = 0$ and $\mathbf{q} \to 0$, i.e., $\Pi_{1L}(\omega = 0, \mathbf{q} \to 0) \propto -N_0$, where N_0 is the normal-state density of states (DOS) on Fermi surface. For metals with a large Fermi surface, both E_F and N_0 are fairly large. Thus the Coulomb interaction becomes short ranged and can be roughly described by [9]

$$V_{\text{sim}}(\mathbf{q}) \propto \frac{1}{\mathbf{q}^2 + \kappa_D}, \tag{3}$$

where the static screening factor $\kappa_D \propto 4\pi e^2 N_0$. Morel and Anderson [9] suggested performing an average of $V_{\text{sim}}(\mathbf{q})$ on the Fermi surface, which yields a parameter

$$\mu \propto \langle V_{\text{sim}}(\mathbf{q}) \rangle_{\text{FS}}.$$

The pseudopotential μ^* is related to μ via the relation [9]

$$\mu^* = \frac{\mu}{1 + \mu \ln(E_F/\omega_D)}. \tag{4}$$

Obviously, $\mu^* \ll \mu$ in normal metals where $\omega_D \ll E_F$, rendering the robustness of superconductivity against Coulomb repulsion.

As the above analysis demonstrates, the ME theory of EPI and the Coulomb pseudopotential should be reliable if the condition $\omega_D \ll E_F$ is fulfilled. This condition is violated in phonon-mediated superconductors that have a low carrier density, with dilute $SrTiO_3$ being a famous example [10,11]. In such superconductors, E_F and N_0 are both small. There are no small factors to suppress the EPI vertex corrections, indicating the breakdown of the Migdal theorem. Moreover, the Coulomb interaction is poorly screened due to the smallness of N_0. The time dependence and spatial variation of the Coulomb potential cannot be well described by the oversimplified function $V_{\text{sim}}(\mathbf{q})$ shown in Eq. (3). Accordingly, the pseudopotential defined in Eq. (4) may no longer be valid as it comes directly from Eq. (3). It is more appropriate to adopt an energy-momentum dependent $V_R(\omega, \mathbf{q})$ to replace the static $V_{\text{sim}}(\mathbf{q})$. Another potentially important contribution arises from the mutual influence between EPI and Coulomb interaction. This contribution was ignored in the original work of Morel and Anderson [9] and also in most, if not all, the subsequent studies on the Coulomb repulsion [12–15]. The validity of this approximation is not clear. In principle, we expect that EPI can affect the Coulomb interaction and vice versa, because both EPI and the Coulomb interaction result in a redistribution of all the charges of the system. We should not simply discard their interplay if we cannot prove that such an interplay is negligible. In light of the above analysis, we consider it necessary to establish a more powerful approach to supersede the ME theory of EPI and the pseudopotential treatment of Coulomb repulsion. To achieve this goal, we should take up the challenge of including all the higher-order corrections.

Recently, a nonperturbative Dyson-Schwinger (DS) equation approach [16] was developed to determine the EPI vertex corrections. At the core of this approach is the decoupling of the DS equation of the full electron propagator $G(p)$ from all the rest of the DS equations with the help of several exact identities. It is found [16] that the DS equation of $G(p)$ obtained by using this approach is self-closed and can be solved numerically. This approach was later extended [17] to deal with one single fermion-boson interaction, be it EPI or Coulomb interaction, in the context of Dirac fermion systems. More recently, the approach was further generalized [18] to investigate the coupling of Dirac fermions to two different bosons. According to the results of Refs. [17,18], the DS equation of the full Dirac fermion propagator is self-closed irrespective of whether the fermions are subjected to either EPI or Coulomb interaction, or both.

In this paper, we shall combine the approaches of [16] and [18] to examine how the interplay of EPI and the Coulomb interaction affects the transition temperature T_c of phonon-mediated superconductors. Our analysis will be based on an effective model that describes the couplings of the electron field ψ to a phonon field ϕ and an auxiliary boson A. The EPI is described by the $\psi - \phi$ coupling and the Coulomb interaction is described by the $\psi - A$ coupling. Although there is not any direct coupling between ϕ and A, these two bosons can affect each other since they are both coupled to the same electrons. As a consequence, the DS equation of $G(p)$ becomes formally very complicated. To solve this difficulty, we derive four exact identities after carrying out a series of analytical calculations and then use such identities to show that the exact DS equation of $G(p)$ is still self-closed. The higher-order corrections neglected in the ME theory and the pseudopotential method are properly taken into account in this self-closed DS equation. Solving such an equation leads us to T_c and other quantities.

We shall apply the approach to a concrete example, the interfacial superconductivity of a one-unit-cell (1UC) $FeSe/SrTiO_3$ system. After computing T_c by solving the self-closed DS equation of $G(p)$, we show that the value of T_c depends strongly on the chosen approximations. In particular, T_c obtained under the bare-vertex (ME) approximation is substantially modified when the vertex corrections are included.

The rest of the paper is organized as follows. In Sec. II, we define the effective field theory for phonon-mediated superconductors. In Sec. III, we obtain the DS equation of $G(p)$ and prove its self-closure with the help of four exact identities. In Sec. IV, we present the numerical results of T_c obtained by solving the self-consistent integral equations of two renormalization functions and the pairing function. In

Sec. V, we summarize the results and discuss the limitations of our calculations.

II. MODEL

Our generic method is applicable to systems defined in any spatial dimension. However, for concreteness, we consider a model defined at two spatial dimensions, since later we shall apply the approach to 1UC $FeSe/SrTiO_3$. The interplay of EPI and the Coulomb interaction is described by the following effective Lagrangian density:

$$\mathcal{L} = \mathcal{L}_f + \mathcal{L}_p + \mathcal{L}_A + \mathcal{L}_{fp} + \mathcal{L}_{fA}, \tag{5}$$

$$\mathcal{L}_f = \psi^\dagger(x)\big(i\partial_{x_0}\sigma_0 - \xi_\nabla\sigma_3\big)\psi(x), \tag{6}$$

$$\mathcal{L}_p = \tfrac{1}{2}\phi^\dagger(x)\mathbb{D}(x)\phi(x), \tag{7}$$

$$\mathcal{L}_A = \tfrac{1}{2}A(x)\mathbb{F}(x)A(x), \tag{8}$$

$$\mathcal{L}_{fp} = -g\phi(x)\psi^\dagger(x)\sigma_3\psi(x), \tag{9}$$

$$\mathcal{L}_{fA} = -A(x)\psi^\dagger(x)\sigma_3\psi(x). \tag{10}$$

The electrons are represented by the Nambu spinor [19] $\psi(\mathbf{p}) = (c_{\mathbf{p}\uparrow}, c^\dagger_{-\mathbf{p}\downarrow})^T$ along with four 2×2 matrices, including unit matrix σ_0 and three Pauli matrices $\sigma_{1,2,3}$. Although the system is nonrelativistic, we choose to use a three-dimensional vector $x \equiv (x_0, \mathbf{x}) = (x_0, x_1, x_2)$ for the purpose of simplifying notations. The time x_0 can be either real or imaginary (in Matsubara formalism), and the results hold in both cases. The fermion field $\psi(x)$ is obtained by making the Fourier transformation to $\psi(\mathbf{p})$. For simplicity, here we assume that the kinetic energy operator is $\xi_\nabla = -\frac{1}{2m_e}(\partial^2_{x_1} + \partial^2_{x_2}) - \mu_{\mathrm{F}}$, where m_e is the bare electron mass and μ_{F} is the chemical potential. As demonstrated in Ref. [16], our generic approach remains valid if ξ_∇ takes a different form. Phonons are represented by the scalar field $\phi(x)$, whose equation of free motion is expressed via the operator $\mathbb{D}(x)$ as

$$\mathbb{D}(x)\phi(x) = 0. \tag{11}$$

The EPI strength parameter g appearing in $\mathcal{L}_{fA}$ is not necessarily a constant and could be a function of phonon momentum. $A(x)$ is an auxiliary scalar field. Its equation of free motion is given by

$$\mathbb{F}(x)A(x) = 0. \tag{12}$$

The Coulomb interaction is effectively described by the coupling between $\psi(x)$ and $A(x)$ shown in $\mathcal{L}_{fA}$. Indeed, $\mathcal{L}_A + \mathcal{L}_{fA}$ can be derived by performing a Hubbard-Stratonovich transformation to the following Hamiltonian term for quartic Coulomb interaction:

$$\frac{e^2}{4\pi}\int d^2\mathbf{x}d^2\mathbf{x}'\psi^\dagger(\mathbf{x})\sigma_3\psi_\sigma(\mathbf{x})\frac{1}{|\mathbf{x}-\mathbf{x}'|}\psi^\dagger(\mathbf{x}')\sigma_3\psi(\mathbf{x}'). \tag{13}$$

Notice that the model does not contain self-coupling terms of bosons. The Coulomb interaction originates from the Abelian U(1) gauge principle and the boson field $A(x)$ can be regarded as the time component of the U(1) gauge field (i.e., scalar potential). It is well established that an Abelian gauge boson does not interact with itself. The situation is different for phonons. In principle phonons could interact with themselves. Ignoring the phonon self-couplings is justified only when the lattice vibration is well captured by the harmonic oscillating approximation. When the nonharmonic contributions are not negligible, the self-couplings of phonons need to be explicitly incorporated. Such nonharmonic contributions might lead to a considerable influence on the value of T_c, as shown in a recent work [20]. In this paper, we do not consider the nonharmonic contributions and therefore omit self-coupling terms of ϕ.

Another notable feature of the model is that the two scalar fields $\phi(x)$ and $A(x)$ do not directly interact with each other. Hence there are no such terms as $\phi(x)A(x)$ or $\phi^2(x)A^2(x)$ in the Lagrangian density. However, the mutual influence between $\phi(x)$ and $A(x)$ cannot be simply ignored since both of them are coupled to the same electrons. It will be shown later that the DS equation of the electron propagator has a very complicated form due to the mutual influence between $\phi(x)$ and $A(x)$. Moreover, $\phi(x)$ and $A(x)$ are coupled to the same fermion density operator $\psi^\dagger(x)\sigma_3\psi(x)$. This implies that the vertex function of $\psi - \phi$ coupling has a very similar structure to that of $\psi - A$ coupling. The different behaviors of the ϕ boson and A boson are primarily caused by the difference in the operators $\mathbb{D}(x)$ and $\mathbb{F}(x)$, or equivalently, the difference in the free propagators of the ϕ boson and A boson.

The Lagrangian density $\mathcal{L}$ respects the following two global U(1) symmetries [19]:

$$\psi \to e^{i\chi\sigma_3}\psi, \tag{14}$$

$$\psi \to e^{i\chi\sigma_0}\psi. \tag{15}$$

Here, χ is an infinitesimal constant. The first symmetry leads to charge conservation associated with a conserved current $j^c_\mu(x) \equiv (j^c_t(x), \mathbf{j}^c(x))$, where

$$j^c_t(x) = \psi^\dagger(x)\sigma_3\psi(x), \tag{16}$$

$$\mathbf{j}^c(x) = \frac{1}{2m_e}\{[i\nabla\psi^\dagger(x)]\sigma_0\psi(x) - \psi^\dagger(x)\sigma_0[i\nabla\psi(x)]\}. \tag{17}$$

The second symmetry leads to spin conservation and a conserved current $j^s_\mu(x) \equiv (j^s_t(x), \mathbf{j}^s(x))$, where

$$j^s_t(x) = \psi^\dagger(x)\sigma_0\psi(x), \tag{18}$$

$$\mathbf{j}^s(x) = \frac{1}{2m_e}\{[i\nabla\psi^\dagger(x)]\sigma_3\psi(x) - \psi^\dagger(x)\sigma_3[i\nabla\psi(x)]\}. \tag{19}$$

These two conserved currents obey the identity $i\partial_\mu j^{c,s}_\mu(x) = 0$ in the absence of external sources. As shown in Ref. [35], each conserved current is associated with one Ward-Takahashi identity (WTI).

III. DYSON-SCHWINGER EQUATION OF ELECTRON PROPAGATOR

After defining the effective model, we now are ready to perform a nonperturbative study of the superconducting transition. The following analysis will be largely based on the approaches previously developed in Ref. [16] and Ref. [18]. We will not give all the derivational details and only outline the major steps.

In order to examine the interaction-induced effects, we would like to investigate the properties of various n-point correlation functions. Such correlation functions can be generated from three generating functionals [21,22]. Adding four external sources J, K, η, and $\eta^\dagger$ to the original Lagrangian density leads to

$$\mathcal{L}_T = \mathcal{L} + J\phi + KA + \psi^\dagger\eta + \eta^\dagger\psi. \tag{20}$$

The partition function is defined via $\mathcal{L}_T$ as follows:

$$Z[J, K, \eta, \eta^\dagger] \equiv \int D\phi DAD\psi^\dagger D\psi e^{i\int dx\mathcal{L}_T}. \tag{21}$$

Here, we use notation $\int dx$ to represent $\int d^3x = \int dtd^2\mathbf{x}$. Z is the generating functional for all n-point correlation functions. In this paper, we are mainly interested in connected correlation functions. Connected correlation functions can be generated by the following generating functional:

$$W \equiv W[J, K, \eta, \eta^\dagger] = -i\ln Z[J, K, \eta, \eta^\dagger]. \tag{22}$$

W can be used to generate three two-point correlation functions:

$$G(x-y) = -i\langle\psi(x)\psi^\dagger(y)\rangle = \left.\frac{\delta^2 W}{\delta\eta^\dagger(x)\delta\eta(y)}\right|_{J=0}, \tag{23}$$

$$D(x-y) = -i\langle\phi(x)\phi^\dagger(y)\rangle = -\left.\frac{\delta^2 W}{\delta J(x)\delta J(y)}\right|_{J=0}, \tag{24}$$

$$F(x-y) = -i\langle A(x)A(y)\rangle = -\left.\frac{\delta^2 W}{\delta K(x)\delta K(y)}\right|_{J=0}. \tag{25}$$

Here, $G(x-y)$, $D(x-y)$, and $F(x-y)$ are the full propagators of electron ψ, phonon ϕ, and boson A, respectively. The system is supposed to be homogeneous, so the propagators depend solely on the difference $x-y$. In this paper, we use the abbreviated notation $J=0$ to indicate that all the external sources are removed. All the correlation functions under consideration are defined by the mean value of the time-ordering product of various field operators, but we omit the time-ordering symbols for simplicity. The mutual influence between the properties of two bosons is embodied in two additional two-point correlation functions:

$$D_F(x-y) = -i\langle\phi(x)A(y)\rangle = -\left.\frac{\delta^2 W}{\delta J(x)\delta K(y)}\right|_{J=0}, \tag{26}$$

$$F_D(x-y) = -i\langle A(x)\phi(y)\rangle = -\left.\frac{\delta^2 W}{\delta K(x)\delta J(y)}\right|_{J=0}. \tag{27}$$

As mentioned before, the model does not have such a term as ϕA; thus $D_F = F_D = 0$ at the classic tree level. But the quantum (loop-level) corrections can induce nonzero contributions to D_F and F_D.

The interaction vertex function for a fermion-boson coupling can also be generated from W. In the case of EPI, we consider the following connected three-point correlation function:

$$\begin{aligned}\langle\phi(x)\psi(y)\psi^\dagger(z)\rangle &= \left.\frac{\delta^3 W}{\delta J(x)\delta\eta^\dagger(y)\delta\eta(z)}\right|_{J=0} \\ &= -\int dx'dy'dz'D(x-x')G(y-y') \\ &\quad\times\left.\frac{\delta^3\Xi}{\delta\phi(x')\delta\psi^\dagger(y')\delta\psi(z')}\right|_{J=0} G(z'-z) \\ &\quad-\int dx'dy'dz'D_F(x-x')G(y-y') \\ &\quad\times\left.\frac{\delta^3\Xi}{\delta A(x')\delta\psi^\dagger(y')\delta\psi(z')}\right|_{J=0} G(z'-z),\end{aligned} \tag{28}$$

where the generating functional for proper (irreducible) vertices Ξ is defined via W as

$$\Xi = W - \int dx[J\langle\phi\rangle + K\langle A\rangle + \eta^\dagger\langle\psi\rangle + \langle\psi^\dagger\rangle\eta]. \tag{29}$$

The interaction vertex function for EPI is defined as

$$\Gamma_p(y-x, x-z) = \left.\frac{\delta^3\Xi}{\delta\phi(x)\delta\psi^\dagger(y)\delta\psi(z)}\right|_{J=0}, \tag{30}$$

and that for $\psi - A$ coupling is defined as

$$\Gamma_A(y-x, x-z) = \left.\frac{\delta^3\Xi}{\delta A(x)\delta\psi^\dagger(y)\delta\psi(z)}\right|_{J=0}. \tag{31}$$

It is necessary to emphasize that Γ_p and Γ_A depend on two (not three) free variables, namely $y-x$ and $x-z$. The propagators and interaction vertex functions appearing in Eq. (28) are Fourier transformed as follows:

$$G(p) = \int dxe^{ipx}G(x), \tag{32}$$

$$D(q) = \int dxe^{iqx}D(x), \tag{33}$$

$$D_F(q) = \int dxe^{iqx}D_F(x), \tag{34}$$

$$\begin{aligned}\Gamma_{p,A}(q,p) &= \int dxdye^{i(p+q)(y-x)}e^{ip(x-z)} \\ &\quad\times\Gamma_{p,A}(y-x, x-z).\end{aligned} \tag{35}$$

Here, the electron momentum is $p \equiv (p_0, \mathbf{p}) = (p_0, p_1, p_2)$ and the boson momentum is $q \equiv (q_0, \mathbf{q}) = (q_0, q_1, q_2)$. Performing Fourier transformation to $\langle\phi(x)\psi(y)\psi^\dagger(z)\rangle$, we find

$$\begin{aligned}&\int dxdye^{i(p+q)(y-x)}e^{ip(x-z)}\langle\phi(x)\psi(y)\psi^\dagger(z)\rangle \\ &= -D(q)G(p+q)\Gamma_p(q,p)G(p) \\ &\quad -D_F(q)G(p+q)\Gamma_A(q,p)G(p).\end{aligned} \tag{36}$$

The $\phi - A$ coupling can be investigated using the same procedure. In this case, we need to study another three-point correlation function $\langle A(x)\psi(y)\psi^\dagger(z)\rangle$. Following the calculational steps that lead Eq. (28) to Eq. (36), we obtain

$$\begin{aligned}&\int dxdye^{i(p+q)(y-x)}e^{ip(x-z)}\langle A(x)\psi(y)\psi^\dagger(z)\rangle \\ &= -F(q)G(p+q)\Gamma_A(q,p)G(p) \\ &\quad -F_D(q)G(p+q)\Gamma_p(q,p)G(p),\end{aligned} \tag{37}$$

where $F(q)$ and $F_D(q)$ are transformed from $F(x)$ and $F_D(x)$ respectively as

$$F(q) = \int dxe^{iqx}F(x), \tag{38}$$

$$F_D(q) = \int dx e^{iqx} F_D(x). \tag{39}$$

Making use of derivational procedure presented in Ref. [16] and Ref. [18], we find that the full electron propagator $G(p)$ satisfies the following DS equation:

$$\begin{aligned} G^{-1}(p) = G_0^{-1}(p) &- i\int \frac{d^3q}{(2\pi)^3} g\sigma_3 G(p+q) D(q) \Gamma_p(q,p) \\ &- i\int \frac{d^3q}{(2\pi)^3} \sigma_3 G(p+q) F(q) \Gamma_A(q,p) \\ &- i\int \frac{d^3q}{(2\pi)^3} g\sigma_3 G(p+q) D_F(q) \Gamma_A(q,p) \\ &- i\int \frac{d^3q}{(2\pi)^3} \sigma_3 G(p+q) F_D(q) \Gamma_p(q,p). \end{aligned} \tag{40}$$

The electron self-energy $\Sigma(p) = G^{-1}(p) - G_0^{-1}(p)$ consists of four terms, as shown on the right-hand side of Eq. (40). The first two terms stem from pure EPI and pure Coulomb interaction, respectively. The last two terms arise from the mutual influence between these two interactions. The contributions of such mixing terms to the self-energy were entirely ignored in the original pseudopotential treatment of Morel and Anderson [9]. To the best of our knowledge, such mixing terms have never been seriously incorporated in previous pseudopotential studies [12–15]. While ignoring them might be valid in some normal-metal superconductors, this approximation is not necessarily justified in all cases. It would be better to keep them in calculations.

Unfortunately, retaining all the contributions to the self-energy makes the DS equation of $G(p)$ extremely complex. It appears that Eq. (40) is not even self-closed since $D(q)$, $F(q)$, $D_F(q)$, $F_D(q)$, $\Gamma_p(q,p)$, and $\Gamma_A(q,p)$ are unknown. Technically, one can derive the DS equations fulfilled by these six unknown functions by using the generic rules of quantum field theory [16–18,21,22]. Nevertheless, such equations are coupled to the formally more complicated DS equations of innumerable multipoint correlation functions and hence of little use. Probably, one would have to solve an infinite number of coupled DS equations to completely determine $G(p)$, which is apparently not a feasible scheme.

In order to simplify Eq. (40) and make it tractable, it might be necessary to introduce some approximations by hand. For instance, one could (1) neglect the last two (mixing) terms on the right-hand side; (2) discard all the vertex corrections by assuming that $\Gamma_{p,A}(q,p) \to \sigma_3$; (3) replace the full phonon propagator $D(q)$ with the bare one, i.e., $D(q) \to D_0(q)$; (4) replace the full A-boson propagator $F(q)$ with a substantially simplified expression, such as $F_{\rm sim}(q) = \frac{1}{\mathbf{q}^2+\kappa_{\rm D}}$, or even with one single (pseudopotential) parameter μ^* after carrying out an average on the Fermi surface. Under all of the above approximations, one finds that the original DS equation (40) becomes

$$\begin{aligned} G^{-1}(p) = G_0^{-1}(p) &- i\int \frac{d^3q}{(2\pi)^3} g\sigma_3 G(p+q) D_0(q) \sigma_3 \\ &- i\mu^* \int \frac{d^3q}{(2\pi)^3} \sigma_3 G(p+q) \sigma_3, \end{aligned} \tag{41}$$

which is self-closed and can be solved numerically. The free electron propagator has the form

$$G_0(p) = \frac{1}{i\epsilon_n \sigma_0 - \xi_{\mathbf{p}} \sigma_3}, \tag{42}$$

and the full electron propagator is expanded as

$$G(p) = \frac{1}{A_1(\epsilon_n, \mathbf{p}) i\epsilon_n \sigma_0 - A_2(\epsilon_n, \mathbf{p}) \xi_{\mathbf{p}} \sigma_3 + \Delta(\epsilon_n, \mathbf{p}) \sigma_1}, \tag{43}$$

where $A_1(\epsilon_n, \mathbf{p})$ and $A_2(\epsilon_n, \mathbf{p})$ are two renormalization functions and $\Delta(\epsilon_n, \mathbf{p})$ is a pairing function. Inserting $G(p)$ and $G_0(p)$ into Eq. (41), one would obtain the standard ME equations of $A_1(\epsilon_n, \mathbf{p})$, $A_2(\epsilon_n, \mathbf{p})$, and $\Delta(\epsilon_n, \mathbf{p})$ with the parameter μ^* characterizing the impact of Coulomb repulsion. In the past sixty years, such simplified equations have been extensively applied [1–5] to study a large number of phonon-mediated superconductors. However, the four approximations that lead to Eq. (41) are not always justified. Some, or perhaps all, of them break down in superconductors having a small Fermi energy.

Now we seek to find a more powerful method to deal with the original exact DS equation of $G(p)$ given by Eq. (40) by going beyond the above approximations. We believe that one should not try to determine each of the six functions $D(q)$, $F(q)$, $D_F(q)$, $F_D(q)$, $\Gamma_p(q,p)$, and $\Gamma_A(q,p)$ separately, which can never be achieved. Alternatively, one should make an effort to determine such products as $D(q)\Gamma_p(q,p)$, $F(q)\Gamma_A(q,p)$, $D_F(q)\Gamma_A(q,p)$, and $F_D(q)\Gamma_p(q,p)$. This is the key idea of the approach proposed in Ref. [18], where we have proved the self-closure of the DS equation of the Dirac fermion propagator $G(p)$ in a model describing the coupling of Dirac fermions to two distinct bosons in graphene. Below we show that this same approach can be adopted to prove the self-closure of the DS equation given by Eq. (40). We shall derive two exact identities satisfied by $D(q)$, $F(q)$, $D_F(q)$, $F_D(q)$, $\Gamma_p(q,p)$, and $\Gamma_A(q,p)$.

The derivation of the needed exact identities is based on the invariance of partition function Z under arbitrary infinitesimal changes of ϕ and A. The invariance of Z under an arbitrary infinitesimal change of ϕ gives rise to

$$\langle \mathbb{D}(x)\phi(x) - g\psi^\dagger(x)\sigma_3\psi(x) + J(x)\rangle = 0. \tag{44}$$

Using the relation $\langle\phi(x)\rangle = \delta W/\delta J(x)$, we perform functional derivatives to the above equation with respect to $\eta(z)$ and $\eta^\dagger(y)$ in order and then obtain the following new equation:

$$\mathbb{D}(x)\langle\phi(x)\psi(y)\psi^\dagger(z)\rangle = g\langle\psi^\dagger(x)\sigma_3\psi(x)\psi(y)\psi^\dagger(z)\rangle. \tag{45}$$

Making a Fourier transformation to the left-hand side of Eq. (45) yields

$$\begin{aligned} D_0^{-1}(q)[&-D(q)G(p+q)\Gamma_p(q,p)G(p) \\ &- D_F(q)G(p+q)\Gamma_A(q,p)G(p)], \end{aligned} \tag{46}$$

where the free phonon propagator $D_0(q)$ comes from $\mathbb{D}(x)$. To handle the right-hand side of Eq. (45), we use two bilinear operators $j_t^c(x) = \psi^\dagger(x)\sigma_3\psi(x)$ and $j_t^s(x) = \psi^\dagger(x)\sigma_0\psi(x)$ to define two current vertex functions

$\Gamma_{0,3}(x-z, z-y)$:

$$\langle \psi^\dagger(x)\sigma_{0,3}\psi(x)\psi(y)\psi^\dagger(z)\rangle = -\int d\zeta d\zeta' G(y-\zeta)\Gamma_{0,3}(\zeta - x, x-\zeta')G(\zeta'-z). \tag{47}$$

$\Gamma_{0,3}(x-z, z-y)$ should be Fourier transformed [16,23] as

$$\Gamma_{0,3}(\zeta - x, x-\zeta') = \int dq dp e^{-i(p+q)(\zeta-x)-ip(x-\zeta')}\Gamma_{0,3}(q, p). \tag{48}$$

For more properties of such current vertex functions, see Refs. [16,23]. Then the right-hand side of Eq. (45) is turned into

$$\int dx dy e^{i(p+q)(y-x)}e^{ip(x-z)}g\langle\psi^\dagger(x)\sigma_{0,3}\psi(x)\psi(y)\psi^\dagger(z)\rangle \to -gG(p+q)\Gamma_{0,3}(q, p)G(p). \tag{49}$$

After substituting Eq. (46) and Eq. (49) into Eq. (45), we obtain the following identity:

$$D(q)\Gamma_p(q, p) + D_F(q)\Gamma_A(q, p) = D_0(q)g\Gamma_3(q, p). \tag{50}$$

Similarly, the invariance of Z under an infinitesimal change of A field requires the following equation to hold:

$$\langle \mathbb{F}(x)A(x) - g\psi^\dagger(x)\sigma_3\psi(x) + K(x)\rangle = 0. \tag{51}$$

Carrying out similar analytical calculations generates another identity,

$$F_D(q)\Gamma_p(q, p) + F(q)\Gamma_A(q, p) = F_0(q)\Gamma_3(q, p), \tag{52}$$

where the free propagator of the A boson $F_0(q)$ is computed by performing Fourier transformation to $\mathbb{F}(x)$.

Making use of the two identities given by Eq. (50) and Eq. (52), we rewrite the original DS equation (40) as

$$G^{-1}(p) = G_0^{-1}(p) - i\int \frac{d^3q}{(2\pi)^3}[g^2D_0(q) + F_0(q)]\sigma_3 G(p+q)\Gamma_3(q, p). \tag{53}$$

This equation is still not self-closed if the current vertex function $\Gamma_3(q, p)$ relies on unknown functions other than $G(p)$. As demonstrated in the Supplemental Material [24] (see also Refs. [25–31] therein), the symmetry of Eq. (14) leads to the following WTI:

$$q_0\Gamma_3(q, p) - (\xi_{\mathbf{p}+\mathbf{q}} - \xi_{\mathbf{p}})\Gamma_0(q, p) = G^{-1}(p+q)\sigma_3 - \sigma_3 G^{-1}(p). \tag{54}$$

It is not possible to determine $\Gamma_3(q, p)$ purely based on this single WTI, since $\Gamma_0(q, p)$ is also unknown. Fortunately, from [24] (see also Refs. [25–31] therein) we know that the symmetry of Eq. (15) yields another WTI:

$$q_0\Gamma_0(q, p) - (\xi_{\mathbf{p}+\mathbf{q}} - \xi_{\mathbf{p}})\Gamma_3(q, p) = G^{-1}(p+q)\sigma_0 - \sigma_0 G^{-1}(p). \tag{55}$$

These two WTIs are coupled to each other and can be used to express $\Gamma_3(q, p)$ and $\Gamma_0(q, p)$ purely in terms of $G(p)$. Now $\Gamma_3(q, p)$ can be readily obtained by solving these two WTIs, and its expression is

$$\Gamma_3(q, p) = \frac{q_0[G^{-1}(p+q)\sigma_3 - \sigma_3 G^{-1}(p)] + (\xi_{\mathbf{p}+\mathbf{q}} - \xi_{\mathbf{p}})[G^{-1}(p+q)\sigma_0 - \sigma_0 G^{-1}(p)]}{q_0^2 - (\xi_{\mathbf{p}+\mathbf{q}} - \xi_{\mathbf{p}})^2}. \tag{56}$$

We can see that the DS equation (53) becomes entirely self-closed because it contains merely one unknown function $G(p)$. This equation can be numerically solved to determine $G(p)$, provided that $G_0(p)$, $D_0(q)$, $F_0(q)$, and g are known.

It is useful to make some remarks here:

(1) The two WTIs given by Eq. (54) and Eq. (55) were originally obtained in Ref. [16] based on a pure EPI model. The model considered in this work contains an additional fermion-boson coupling that equivalently represents the Coulomb interaction. We emphasize that such an addition coupling does not alter the WTIs, since the Lagrangian density of pure EPI and the one describing the interplay between EPI and Coulomb interaction preserve the same U(1) symmetries defined by Eq. (14) and Eq. (15).

(2) In many existing publications, it is naively deemed that a symmetry-induced WTI imposes an exact relation between fermion propagator $G(p)$ and interaction vertex function. To understand why this is a misconception, let us take EPI as an example. The EPI vertex function $\Gamma_p(q, p)$ is defined via a three-point correlation function $\langle\phi\psi\psi^\dagger\rangle$, which in itself is not necessarily related to any conserved current. There is no reason to expect $\Gamma_p(q, p)$ to naturally enter into any WTI. To reveal the impact of some symmetry, one should use the symmetry-induced conserved current, say j_μ^c, to define a special correlation function $\langle j_\mu^c\psi\psi^\dagger\rangle$, which, according to Eq. (47) and Eq. (49), is expressed in terms of current vertex functions $\Gamma_0(q, p)$ and $\Gamma_3(q, p)$. After applying the constraint of current conservation $\partial_\mu j_\mu^c = 0$ to $\langle j_\mu^c\psi\psi^\dagger\rangle$, one would obtain a WTI satisfied by $\Gamma_0(q, p)$, $\Gamma_3(q, p)$, and $G(p)$, as shown in Eq. (54).

(3) Our ultimate goal is to determine $G(p)$. Its DS equation (40) contains two interaction vertex functions $\Gamma_p(q, p)$ and $\Gamma_A(q, p)$. On the other hand, it is $\Gamma_0(q, p)$ and $\Gamma_3(q, p)$, rather than $\Gamma_p(q, p)$ and $\Gamma_A(q, p)$, that enter into the WTIs given by

Eq. (54) and Eq. (55). Hence, at least superficially the DS equation of $G(p)$ and the WTIs are not evidently correlated. To find out a natural way to combine the DS equation of $G(p)$ with WTIs, one needs to obtain the relations between interaction vertex functions and current vertex functions. Such relations do exist and are shown in Eq. (50) and Eq. (52).

(4) The appearance of two free boson propagators $D_0(q)$ and $F_0(q)$ in the final DS equation (53) is not an approximation. It should be emphasized that the replacement of the full boson propagators $D(q)$ and $F(q)$ appearing in the original DS equation (40) with their free ones is implemented based on two exact identities given by Eq. (50) and Eq. (52). The interaction-induced effects embodied in such functions as $D(q)$, $F(q)$, $D_F(q)$, $F_D(q)$, $\Gamma_p(q, p)$, and $\Gamma_A(q, p)$ are already incorporated in the current vertex function $\Gamma_3(q, p)$.

Before closing this section, we briefly discuss whether our approach is applicable to four-fermion interactions. The Hubbard model is a typical example of this type. Consider a simple four-fermion coupling term given by

$$U_H \Psi^\dagger \Psi \Psi^\dagger \Psi, \tag{57}$$

where Ψ is a normal (non-Nambu) spinor. Based on this Hubbard model, one can derive DS integral equations and WTIs satisfied by various correlation functions. Actually, it is straightforward to obtain a U(1)-symmetry-induced WTI that connects the fermion propagator $G(p)$ to a current vertex function $\Gamma_H(p, p+q)$ defined through the following correlation function,

$$\langle j_\mu \Psi \Psi^\dagger \rangle \to G(p_1)\Gamma_H(p_1, p_2)G(p_2), \tag{58}$$

where j_μ is a conserved (charge) current operator. The fermion propagator $G(p)$ should be determined by solving its DS integral equation. As demonstrated in Ref. [32], the DS equation of $G(p)$ contains a two-particle kernel function $\Gamma_4(p_1, p_2, p_3, p_4)$, which is defined via a four-point correlation function as follows:

$$\langle \Psi^\dagger \Psi \Psi^\dagger \Psi \rangle \to G(p_1)G(p_2)\Gamma_4(p_1, p_2, p_3, p_4)G(p_3)G(p_4).$$

It is clear that Γ_H is physically distinct from Γ_4. We are not aware of the presence of any simple relation between these two functions. A field-theoretic analysis reveals that the DS integral equation of Γ_4 is strongly coupled to an infinite number of DS integral equations of various n-point correlation functions ($n > 4$). Even though Γ_H can be expressed purely in terms of $G(p)$ after solving a number of WTIs, it cannot be used to simplify the DS equation of $G(p)$ because of our ignorance of the structure of Γ_4. It is therefore unlikely that our approach is directly applicable to Hubbard-type models like Eq. (57).

Alternatively, one could introduce an auxiliary bosonic field φ and then perform a Hubbard-Stratonovich transformation, which turns the original Hubbard model into a Yukawa-type fermion-boson coupling term,

$$\mathcal{L}_Y = -g_Y \varphi \Psi^\dagger \Psi. \tag{59}$$

It seems that this coupling could be treated in the same way as what we have done for the Coulomb interaction. However, we emphasize that this Yukawa coupling alone cannot describe all the physical effects produced by the original Hubbard four-fermion coupling. This is because boson self-interactions cannot be simply neglected. In the case of Coulomb interaction, the Abelian U(1) gauge invariance guarantees the absence of self-interactions of a_0 bosons. In contrast, there is not any physical principle to prevent the auxiliary boson field φ from developing such a self-coupling term:

$$\mathcal{L}_4 = u_4 \varphi^4(x). \tag{60}$$

In quantum field theory, it is well established [22] that the Yukawa interaction cannot be renormalized if the model does not contain an appropriate quartic term. In condensed matter physics, the boson self-interactions have been found [33–36] to play a significant role, especially in the vicinity of a quantum critical point. In fact, even if the Lagrangian originally does not contain any boson self-coupling term, the Yukawa coupling $g_Y \varphi \Psi^\dagger \Psi$ can dynamically generate certain boson self-coupling terms [33,35]. After including the term $\sim\varphi^4$, the invariance of Z under an arbitrary infinitesimal change of φ leads to

$$\langle \mathbb{D}(x)\varphi(x) + 4u_4\varphi^3(x) - g_Y \Psi^\dagger(x)\Psi(x) + J(x)\rangle = 0. \tag{61}$$

Comparing to Eq. (44), there appears an additional term $\sim u_4\varphi^3(x)$ owing to the boson self-interaction. After performing functional derivatives with respect to $\eta(z)$ and $\eta^\dagger(y)$ in order, one obtains

$$\begin{aligned} &\mathbb{D}(x)\langle \varphi(x)\Psi(y)\Psi^\dagger(z)\rangle + 4u_4\langle \varphi^3(x)\Psi(y)\Psi^\dagger(z)\rangle \\ &\quad = g_Y \langle \Psi^\dagger(x)\Psi(x)\Psi(y)\Psi^\dagger(z)\rangle. \end{aligned} \tag{62}$$

Different from Eq. (45), this equation contains an extra correlation function $\langle \varphi^3(x)\Psi(y)\Psi^\dagger(z)\rangle$. This correlation function is formally very complicated and actually makes it impossible to derive a self-closed DS equation of the fermion propagator. Thus, our approach is applicable only when the quartic term $\sim\varphi^4$ can be safely ignored.

IV. NUMERICAL RESULTS OF T_c

In this section, we apply the self-closed DS equation of $G(p)$ given by Eq. (53) along with Eq. (56) to evaluate the pair-breaking temperature T_c of the superconductivity realized in the 1UC FeSe/$SrTiO_3$ system. This material is found [37–39] to possess a surprisingly high T_c. While it is believed by many [38,39] that interfacial optical phonons (IOPs) from the $SrTiO_3$ substrate are responsible for the observed high T_c, other microscopic pairing mechanisms cannot be conclusively excluded. Gor'kov [40] argued that IOPs alone are not capable of causing such a high T_c. If this conclusion (not necessarily the argument itself) is reliable, we would be compelled to invoke at least one additional pairing mechanism, such as magnetic fluctuation or nematic fluctuation, to cooperate with IOPs [39–41]. In recent years, considerable research efforts have been devoted to calculating IOP-induced T_c by using the standard ME theory [42–46] and a slightly corrected version of ME theory [47]. Nevertheless, thus far no consensus has been reached and the accurate value of T_c produced by IOPs alone is still controversial. To get a definite answer, it is important to compute T_c with a sufficiently high precision. This is certainly not an easy task since T_c could be influenced by many factors.

Among all the factors that can potentially affect T_c, the EPI vertex corrections play a major role. Since the ratio ω_D/E_F is at the order of unity, the Migdal theorem becomes invalid. As shown in Ref. [16], including EPI vertex corrections can drastically change the value of T_c obtained under bare vertex approximation. However, the calculations of Ref. [16] were based on two approximations that might lead to inaccuracies and thus still need to be improved. The first approximation is the omission of the influence of Coulomb repulsion [16]. As discussed in Sec. I, the traditional pseudopotential method may not work well in 1UC FeSe/$SrTiO_3$ owing to the smallness of E_F. The impact of the Coulomb interaction on T_c should be examined more carefully. The second approximation is that the electron momentum was supposed [16] to be fixed at the Fermi momentum such that $\xi_{\mathbf{p}} = 0$. Under this second approximation, the DS equation of $G(p)$ has only one integral variable (i.e., frequency). Then the computational time is significantly shortened. For this reason, this kind of approximation has widely been used in the existing calculations of T_c. But the pairing gap Δ and the renormalization factors A_1 and A_2 obtained by solving their single-variable equations depend solely on frequency. The momentum dependence is entirely lost. Since the EPI strength depends strongly on the transferred momentum $\mathbf{q}$, it is important not to neglect the momentum dependence of the DS equation of $G(p)$. We will discard the two approximations adopted in Ref. [16] and directly deal with the self-closed DS equation (53).

We are particularly interested in how T_c is affected by the interplay of EPI and Coulomb repulsion. To avoid the difficulty brought by analytical continuation, we work in the Matsubara formalism and express the electron momentum as $p \equiv (p_0, \mathbf{p}) = (i\epsilon_n, \mathbf{p})$, where $\epsilon_n = (2n+1)\pi T$, and the boson momentum as $q \equiv (q_0, \mathbf{q}) = (i\omega_{n'}, \mathbf{q})$, where $\omega_{n'} = 2n'\pi T$. The free phonon propagator has the form

$$D_0(q) = \frac{2\Omega_{\mathbf{q}}}{(i\omega_{n'})^2 - \Omega_{\mathbf{q}}^2}. \tag{63}$$

The IOPs are found to be almost dispersionless [38,48]; thus $\Omega_{\mathbf{q}}$ can be well approximated by a constant. Here, we choose the value [38,48] $\Omega_{\mathbf{q}} = 81$ meV. The Fermi energy is roughly [39] $E_F = 65$ meV. The EPI strength parameter g is related to phonon momentum $\mathbf{q}$ as [44]

$$g \equiv g(\mathbf{q}) = \sqrt{8\pi\lambda/q_p^2}\,\Omega_{\mathbf{q}} \exp(-|\mathbf{q}|/q_p). \tag{64}$$

The value of λ can be estimated by first-principles calculations [44]. Here we regard λ as a tuning parameter and choose a set of different values in our calculations. The range of EPI is characterized by the parameter q_p [39]. Its precise value relies on the values of other parameters and is hard to determine. For simplicity, we choose to fix its value [44] at $q_p = 0.1p_F$. The free propagator of the A boson is

$$F_0(q) = \frac{2\pi\alpha}{|\mathbf{q}|}, \tag{65}$$

which has the same form as the bare Coulomb interaction function. The fine structure constant is $\alpha = e^2/v_F\varepsilon$. The magnitude of dielectric constant ε depends sensitively on the surroundings (substrate) of the superconducting film. It is not easy to accurately determine ε. To make our analysis more general, we suppose that ε can be freely changed within a certain range.

As the next step, we wish to substitute the free phonon propagator $D_0(q)$ given by Eq. (63), the free A-boson propagator $F_0(q)$ given by Eq. (65), the free electron propagator $G_0(p)$ given by Eq. (42), and the full electron propagator $G(p)$ given by Eq. (43) into the DS equation (53) and also into the function $\Gamma_3(q, p)$ given by Eq. (56). However, we cannot naively do so since here we encounter a fundamental problem. Recall that $\Gamma_3(q, p)$ given by Eq. (56) is derived from two symmetry-induced WTIs. Once the pairing function $\Delta(p)$ develops a finite value, the system enters into superconducting state. The U(1) symmetry of Eq. (15) is preserved in both the normal and superconducting states; thus the WTI of Eq. (55) is not changed. In contrast, the U(1) symmetry of Eq. (14) is spontaneously broken in the superconducting state. If this symmetry breaking does not change the WTI of Eq. (54), one could insert the expression of $G(p)$ given by Eq. (43) into $\Gamma_3(q, p)$. Otherwise, one should explore the modification of the WTI by symmetry breaking. At present, there seems no conclusive answer. Nambu [19] adopted the WTI from charge conservation to prove the gauge invariance of electromagnetic response functions of a superconductor based on a ladder-approximation of the DS equation of vertex function. Following the scheme of Nambu, Schrieffer [1] assumed (without giving a proof) that this WTI is the same in the superconducting and normal phases and used this assumption to show the existence of a gapless Goldstone mode. Nakanishi [49] later demonstrated that, while the WTI for a U(1) gauge field theory has the same form in symmetric and symmetry-broken phases, it might be altered in other field theories. Recently, Yanagisawa [50] revisited this issue and argued that the spontaneous breaking of a continuous symmetry gives rise to an additional term to WTI due to the generation of Goldstone boson(s). However, the expression of such an additional term is unknown. It also remains unclear whether the approach of Ref. [50] still works in superconductors. The superconducting transition is profoundly different from other symmetry-breaking driven transitions. According to the Anderson mechanism [51], the Goldstone boson generated by U(1)-symmetry breaking is eaten by the long-range Coulomb interaction, which lifts the originally gapless mode to a gapped plasmon mode. Thus, the WTI coming from symmetry Eq. (14) is not expected to acquire the additional term derived in Ref. [50] in the superconducting phase. Nevertheless, the absence of the Goldstone boson cannot ensure that the WTI is not changed by the Anderson mechanism.

In order to attain a complete theoretical description of the superconducting transition, one should strive to develop a unified framework to reconcile the nonperturbative DS equation approach with the Anderson mechanism. But such a framework is currently not available. To proceed with our calculations, we have to introduce a suitable approximation. Our purpose is to compute T_c. Near T_c, the pairing function $\Delta(p)$ vanishes and the symmetry Eq. (14) is still preserved. So the WTI of Eq. (54) still holds. Then we substitute the full electron propagator $G(p)$ given by Eq. (43) into Eq. (53) and assume the function $\Gamma_3(q, p)$ to have the following

expression:

$$\Gamma_3(q,p)=\frac{q_0\left[G_s^{-1}(p+q)\sigma_3-\sigma_3G_s^{-1}(p)\right]+(\xi_{\mathbf{p}+\mathbf{q}}-\xi_{\mathbf{p}})\left[G_s^{-1}(p+q)\sigma_0-\sigma_0G_s^{-1}(p)\right]}{q_0^2-(\xi_{\mathbf{p}+\mathbf{q}}-\xi_{\mathbf{p}})^2}, \tag{66}$$

where $G_s(p)$ is a simplified electron propagator of the form

$$G_s(p)=\frac{1}{A_1(p)p_0\sigma_0-A_2(p)\xi_{\mathbf{p}}\sigma_3}. \tag{67}$$

This manipulation leads to three coupled nonlinear integral equations:

$$\begin{aligned}A_1(\epsilon_n,\mathbf{p})=1+\frac{T}{i\epsilon_n}\sum_m\int\frac{d^2\mathbf{q}}{(2\pi)^2}[g^2(\mathbf{q})D_0(\omega_m,\mathbf{q})+F_0(\omega_m,\mathbf{q})]\\ \times\frac{A_1(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})i(\epsilon_n+\omega_m)\Gamma_{33}+A_2(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})\xi_{\mathbf{p}+\mathbf{q}}\Gamma_{30}-\Delta(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})\Gamma_{3d}}{A_1^2(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})(\epsilon_n+\omega_m)^2+A_2^2(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})\xi_{\mathbf{p}+\mathbf{q}}^2+\Delta^2(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})},\end{aligned} \tag{68}$$

$$\begin{aligned}A_2(\epsilon_n,\mathbf{p})=1-\frac{T}{\xi_{\mathbf{p}}}\sum_m\int\frac{d^2\mathbf{q}}{(2\pi)^2}[g^2(\mathbf{q})D_0(\omega_m,\mathbf{q})+F_0(\omega_m,\mathbf{q})]\\ \times\frac{A_1(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})i(\epsilon_n+\omega_m)\Gamma_{30}+A_2(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})\xi_{\mathbf{p}+\mathbf{q}}\Gamma_{33}-\Delta(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})\Gamma_{31}}{A_1^2(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})(\epsilon_n+\omega_m)^2+A_2^2(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})\xi_{\mathbf{p}+\mathbf{q}}^2+\Delta^2(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})},\end{aligned} \tag{69}$$

$$\begin{aligned}\Delta(\epsilon_n,\mathbf{p})=-T\sum_m\int\frac{d^2\mathbf{q}}{(2\pi)^2}[g^2(\mathbf{q})D_0(\omega_m,\mathbf{q})+F_0(\omega_m,\mathbf{q})]\\ \times\frac{A_1(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})i(\epsilon_n+\omega_m)\Gamma_{3d}-A_2(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})\xi_{\mathbf{p}+\mathbf{q}}\Gamma_{31}-\Delta(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})\Gamma_{33}}{A_1^2(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})(\epsilon_n+\omega_m)^2+A_2^2(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})\xi_{\mathbf{p}+\mathbf{q}}^2+\Delta^2(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})}.\end{aligned} \tag{70}$$

Here, we have defined several quantities:

$$\begin{aligned}\Gamma_{30}&=\frac{i\omega_m[A_2(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})\xi_{\mathbf{p}+\mathbf{q}}-A_2(\epsilon_n,\mathbf{p})\xi_{\mathbf{p}}]+(\xi_{\mathbf{p}+\mathbf{q}}-\xi_{\mathbf{p}})[-A_1(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})(i\epsilon_n+i\omega_m)+A_1(\epsilon_n,\mathbf{p})i\epsilon_n]}{\omega_m^2+(\xi_{\mathbf{p}+\mathbf{q}}-\xi_{\mathbf{p}})^2},\\ \Gamma_{33}&=\frac{i\omega_m[-A_1(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})(i\epsilon_n+i\omega_m)+A_1(\epsilon_n,\mathbf{p})i\epsilon_n]+(\xi_{\mathbf{p}+\mathbf{q}}-\xi_{\mathbf{p}})[A_2(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})\xi_{\mathbf{p}+\mathbf{q}}-A_2(\epsilon_n,\mathbf{p})\xi_{\mathbf{p}}]}{\omega_m^2+(\xi_{\mathbf{p}+\mathbf{q}}-\xi_{\mathbf{p}})^2},\\ \Gamma_{31}&=\frac{(\xi_{\mathbf{p}+\mathbf{q}}-\xi_{\mathbf{p}})[-\Delta(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})+\Delta(\epsilon_n,\mathbf{p})]}{\omega_m^2+(\xi_{\mathbf{p}+\mathbf{q}}-\xi_{\mathbf{p}})^2},\\ \Gamma_{3d}&=\frac{i\omega_m[\Delta(\epsilon_n+\omega_m,\mathbf{p}+\mathbf{q})+\Delta(\epsilon_n,\mathbf{p})]}{\omega_m^2+(\xi_{\mathbf{p}+\mathbf{q}}-\xi_{\mathbf{p}})^2}.\end{aligned} \tag{71}$$

It is easy to reproduce the ME equations by replacing the full propagator $G(p)$ appearing in Eq. (56) with the free propagator $G_0(p)$, which is equivalent to the bare vertex approximation $\Gamma_3\to\sigma_3$. Alternatively, one could substitute $A_1=A_2=1$ and $\Delta=0$ into Γ_{30}, Γ_{33}, Γ_{31}, and Γ_{3d}, and then obtain

$$\Gamma_{30}=0,\quad \Gamma_{33}=1,\quad \Gamma_{31}=0,\quad \Gamma_{3d}=0. \tag{72}$$

Such manipulations reduce Eqs. (68)–(70) to the standard ME equations (not shown explicitly).

The self-consistent integral equations of $A_1(\epsilon_n,\mathbf{p})$, $A_2(\epsilon_n,\mathbf{p})$, and $\Delta(\epsilon_n,\mathbf{p})$ can be numerically solved using the iteration method (see Ref. [16] for a detailed illustration of this method). The computational time required to reach convergent results depends crucially on the number of integral variables: adding one variable leads to an exponential increase of the computational time. The coupled equations (68)–(70) have only one variable ϵ_n if all electrons are assumed to reside exactly on the Fermi surface. Such an assumption simplifies the equations and dramatically decreases the computational time, but might not be justified in the present case due to the strong momentum dependence of EPI coupling strength. Therefore, here we consider all the possible values of $\mathbf{p}$ and directly solve Eqs. (68)–(70) without introducing further approximations. But these equations have three integral variables, namely ω_m, q_1, and q_2. Solving them would consume too many computational resources.

The burden of numerical computation can be greatly lightened if the number of integral variables is reduced. We suppose that the system is isotropic and then make an effort to integrate over the angle θ between $\mathbf{p}$ and $\mathbf{q}$ before starting the iterative process. After doing so, only two free variables, namely ω_m and $|\mathbf{q}|$, are involved in the process of performing iterations. The computational time can thus be greatly shortened. Generically, it is not easy to integrate over θ. In our case, however, although the current vertex function $\Gamma_3(q,p)$ is complicated, the free propagators $D_0(q)$ and $F_0(q)$ are simple functions of their variables. The phonon energy $\Omega_{\mathbf{q}}$ is a constant; thus $D_0(q)$ depends solely on the frequency, i.e., $D_0(q)=D_0(\omega_m)$. In comparison, $F_0(\mathbf{q})$ depends solely

on the momentum. To illustrate why θ can be integrated out, it is more convenient to deal with the DS equation shown in Eq. (53) instead of the formally complicated equations (68)–(70). With the redefinitions $\mathbf{p}+\mathbf{q}\to\mathbf{k}$ and $\int d\mathbf{q}\to\int d\mathbf{k}$, we can rewrite Eq. (53) as

$$G^{-1}(\epsilon_n,\mathbf{p}) = G_0^{-1}(\epsilon_n,\mathbf{p}) + T\sum_m \int \frac{kdkd\theta}{(2\pi)}\sigma_3 G(\epsilon_m,\mathbf{k}) \times\left[g^2 D_0(\omega_m) + \frac{e^2}{\varepsilon\sqrt{\mathbf{p}^2+\mathbf{k}^2-2|\mathbf{p}||\mathbf{k}|\cos\theta}}\right] \times\Gamma_3(\epsilon_n,\mathbf{p},\epsilon_n+\omega_m,\mathbf{k}). \quad (73)$$

Both $G_0(\epsilon_n,\mathbf{p})$ and $G(\epsilon_n,\mathbf{p})$ are independent of θ; thus θ is not involved in the iterative process and can be numerically integrated at each step.

$F_0(\mathbf{q})$ is singular at $\mathbf{q}=0$, reflecting the long-range nature of bare Coulomb interaction. If the electrons are treated by the jellium model, the contribution of $\mathbf{q}=0$ must be eliminated since it cancels out the static potential between negative and positive charges. This can be implemented by introducing an infrared cutoff δ. In our calculations, we set $\delta=10^{-6}p_{\rm F}$. We have already confirmed that the final results of T_c are nearly unchanged as δ varies within the range of $[10^{-8}p_{\rm F}, 10^{-3}p_{\rm F}]$. Apart from the infrared cutoff, it is also necessary to introduce an ultraviolet cutoff Λ for the momentum. A natural choice is to set $\Lambda=p_{\rm F}$. Our final results are also insensitive to other choices of Λ, which might be attributed to the dominance of small-$\mathbf{q}$ processes.

To facilitate numerical calculations, it is more convenient to make all the variables become dimensionless. Dimensional parameters can be made dimensionless after performing the following rescaling transformations:

$$\frac{p}{p_{\rm F}}\to p,\quad \frac{k}{p_{\rm F}}\to k,\quad \frac{q}{p_{\rm F}}\to q,\quad \frac{q_{\rm p}}{p_{\rm F}}\to q_{\rm p}, \quad (74)$$

$$\frac{T}{E_{\rm F}}\to T,\quad \frac{\epsilon_n}{E_{\rm F}}\to\epsilon_n,\quad \frac{\omega_m}{E_{\rm F}}\to\omega_m, \quad (75)$$

$$\frac{\Omega_q}{E_{\rm F}}\to\Omega_q,\quad \frac{\xi_p}{E_{\rm F}}\to\xi_p,\quad \frac{g}{E_{\rm F}}\to g. \quad (76)$$

The parameters λ and α are already made dimensionless and thus kept unchanged. The integral interval of the rescaled variable k is $[10^{-6}, 1]$.

After making rescaling transformations, the electron dispersion $\xi_{\mathbf{p}}=\frac{\mathbf{p}^2}{2m_e}-\mu_{\rm F}$ is turned into $\mathbf{p}^2-1$, which is dimensionless. The resulting integral equations of A_1, A_2, and Δ do not explicitly depend on either $p_{\rm F}$ or m_e. Thus, it is not necessary to separately specify the values of $p_{\rm F}$ and m_e, since the final results of the critical temperature only exhibit a dependence on $E_{\rm F}=\frac{p_{\rm F}^2}{2m_e}$. From the numerical solutions of the DS and ME equations, we could obtain an effective dimensionless transition temperature, denoted by T_c', that is equal to $T_c/E_{\rm F}$. The Fermi energy $E_{\rm F}=65$ meV amounts to approximately ∼755 K. Then the actual transition temperature T_c can be readily obtained from T_c' through the relation $T_c\sim T_c'\times(755\ {\rm K})$.

It should be emphasized that the free phonon propagator $D_0(q)$ is used in both the DS-level and ME-level calculations. Thus we are allowed to determine the influence of EPI vertex corrections by comparing the values of T_c obtained under these two approximations. The pairing gap Δ is supposed to have an isotropic s-wave symmetry [44]. To make our analysis more generic, we consider six different values of the strength parameter λ, including $\lambda=0.05$, $\lambda=0.10$, $\lambda=0.15$, $\lambda=0.20$, $\lambda=0.25$, and $\lambda=0.30$. The numerical results of T_c are presented in Fig. 1, where the red and blue curves correspond to the ME and DS results, respectively.

We first consider the simplest case in which the Coulomb interaction is absent. In a previous work [16], it was found that including EPI vertex corrections tends to promote T_c evaluated at the ME level (bare vertex). This conclusion was reached based on the assumption that the electrons always strictly reside on the Fermi surface such that $\xi_{\mathbf{p}}=\xi_{\mathbf{p}_F}=0$ [16]. Here we resolve Eqs. (68)–(70) without making this assumption. From the numerical results presented in Fig. 1, we observe that the impact of EPI vertex corrections on T_c is strongly dependent of the value of EPI strength parameter λ. Specifically, we find that vertex corrections slightly reduce T_c for $\lambda=0.10$, but considerably enhance T_c for $\lambda=0.15$, $\lambda=0.20$, $\lambda=0.25$, and $\lambda=0.30$. The enhancement of T_c due to vertex corrections becomes more significant as λ further increases. The case of $\lambda=0.05$ appears to be peculiar: the vertex corrections play different roles as the effective strength of Coulomb interaction is changed.

The effect of the Coulomb interaction on T_c can be readily investigated by varying the tuning parameter ε. As clearly shown by Fig. 1, T_c drops monotonically as ε decreases. Such a behavior is certainly in accordance with expectation, since the Coulomb repulsion weakens the effective attraction between electrons. In the case of $\lambda=0.05$, T_c is slightly reduced by vertex corrections for weak Coulomb repulsion but is enhanced by vertex corrections when the Coulomb repulsion becomes strong enough. Superconductivity can be completely suppressed, with $T_c\to 0$, once the effective strength of Coulomb repulsion exceeds a certain threshold. For larger values of λ, the Coulomb repulsion has an analogous impact on T_c. However, superconductivity could be entirely suppressed only when the repulsion becomes unrealistically strong.

For any realistic material, ε takes a specific value; so does T_c. T_c is completely determined once all the model parameters are fixed. In a way, our work provides a first-principles study of the superconducting transition, although the role of the Anderson mechanism remains to be ascertained.

V. SUMMARY AND DISCUSSION

In summary, we have performed a nonperturbative study of the interplay of EPI and the Coulomb repulsion by using the DS equation approach. We have shown that the DS equation of the full electron propagator $G(p)$ is self-closed provided that all the higher-order corrections to EPI and the Coulomb interaction are incorporated via a number of exact identities. This self-closed DS equation can be applied to study the superconducting transition beyond the ME approximation of EPI and the pseudopotential approximation of Coulomb repulsion. We have employed this approach to evaluate the pair-breaking temperature T_c for the interfacial superconductivity in the 1UC FeSe/$SrTiO_3$ system and found that the value of T_c could

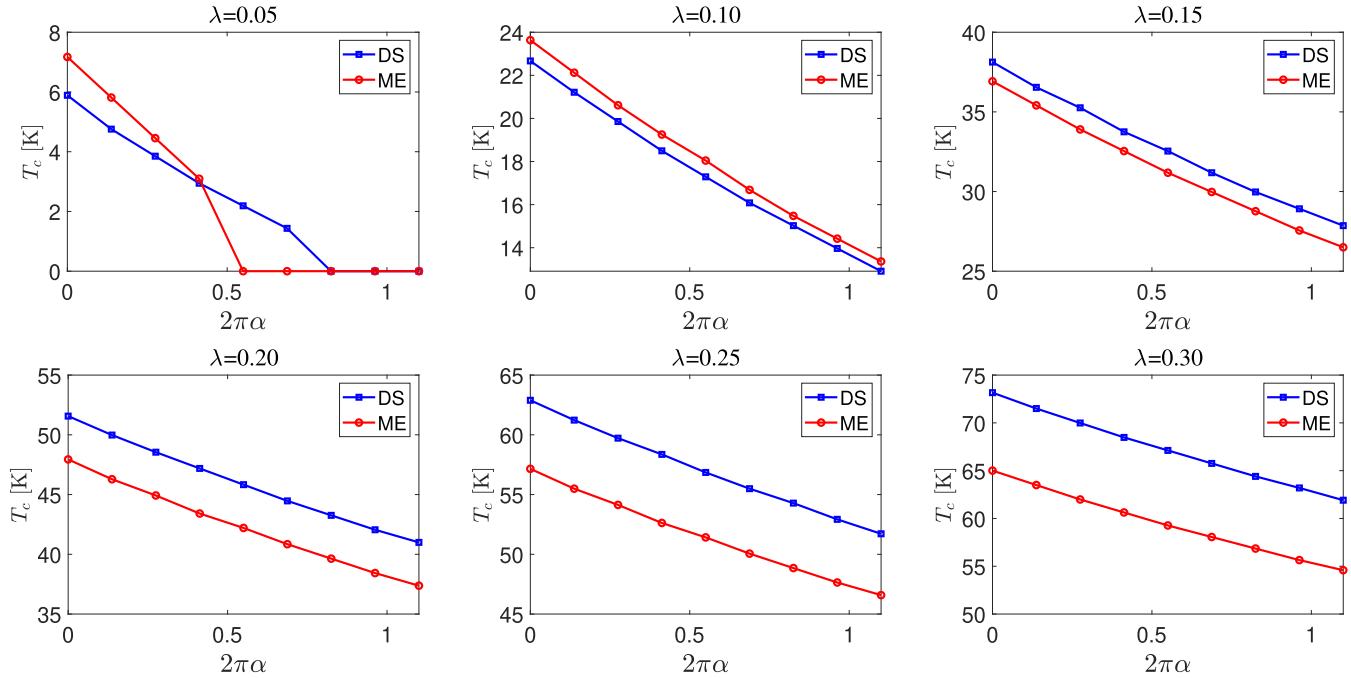

FIG. 1. Comparison between results of T_c obtained by solving ME and DS equations with six different values of λ.

be significantly miscalculated if the vertex corrections and the momentum dependence of relevant quantities are not taken into account in a reliable way.

The calculations of this work ignored several effects that might change the value of T_c and thus need to be improved in the future. First of all, the simple one-band model studied by us should be replaced with a realistic multiband model that embodies the actual electronic structure [46]. The phonon self-coupling terms [20] are entirely neglected in our calculations. Including such self-coupling terms invalidates the two identities given by Eq. (50) and Eq. (52). As a consequence, the DS equation of the electron propagator $G(p)$ can no longer be made self-closed (see Ref. [16] and Ref. [17] for more details). Moreover, we did not consider the quantum geometry effects [52], which could enhance T_c to a certain extent. In this sense, our results of T_c cannot be directly compared to the experimental values. The main achievement of our present work is a methodological advance in the nonperturbative study of the superconducting transition driven by the interplay of EPI and the Coulomb repulsion.

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