# Route to phonon-mediated high-temperature unconventional superconductivity

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We investigate the appearance of superconductivity in a model with Peierls electron-phonon coupling for very low carrier concentrations. Superconductivity with very high critical temperatures is found to occur at all carrier concentrations if the electron-phonon coupling is not too weak, with a gap of $s + s^*$ symmetry that closes on the Fermi surface for appropriate parameters. The possibility of finding the elusive $p$-type superconductivity is also revealed, although this turns out not to be stable within the approximations we use.

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## I. INTRODUCTION

Over a century after its discovery [1], superconductivity (SC) remains a central theme in condensed matter and materials research. The main reason for this sustained interest is the challenge of finding whether room-temperature SC at ambient pressure is possible, and if yes, the mechanism(s) that enable it and the materials that exhibit it. A positive resolution to this challenge would result in revolutionary changes in most technology-driven aspects of our lives.

To date, the only universally accepted mechanism for SC is the Bardeen, Cooper, and Schrieffer (BCS) theory [2], according to which the conventional, $s$-wave, low-$T_C$ SC found in most elemental metals and simple alloys is due to weak electron-phonon coupling that overscreens the electron-electron repulsion, turning it into an effective attraction at low energies. In the presence of a large Fermi sea, this weak attraction suffices to bind electrons into Cooper pairs below a low $T_C$, opening a small uniform gap in the density of states at the Fermi energy $E_F$. Given the large density of Cooper pairs and their low mass, they are phase-coherent for all $T < T_C$, and hence they superconduct. An upper limit $T_C \sim 30$ K was proposed for BCS SC [3], although this upper limit keeps being revised because of possible loopholes in various arguments [4].

Ever since the BCS theory was published, theorists have considered ways to boost $T_C$, e.g., by using excitons as the glue [5,6] or by including dynamical effects [7,8]. This field exploded after the experimental discovery of high-$T_C$ superconductivity in the cuprate family [9] and then in the iron-based families [10], which are classified as unconventional (non-BCS, not $s$-wave) superconductors. These are joined by other potentially unconventional (not yet fully understood) superconductors such as $Sr_2RuO_4$ [11] and other heavy-fermion materials [12], $K_xBa_{1-x}BiO_3$ [13], and weakly doped $SrTiO_3$ [14]. Several of these are believed to have a nonphononic glue, although this issue is still under vigorous debate [15].

These findings suggest that nonphononic mechanisms leading to higher-$T_C$ superconductivity at ambient pressure may well exist [16], but they certainly need to be deciphered first before we can attempt to figure out whether they allow for room-temperature $T_C$.

Instead of speculating about new glues, in this article we revisit the old question of whether a phonon glue can mediate high-$T_C$ SC. As mentioned, a lot of work was already dedicated to this issue, however virtually always using a so-called $g(\boldsymbol{q})$ type of electron-phonon coupling, like in the Holstein and Fröhlich models [17,18]. For the strong couplings needed to mediate the strong effective attractions that would increase the temperature below which pairs are stable, these models predict very heavy polarons. This substantial increase in the carriers' effective mass lowers the phase-coherence temperature of the condensate, and thus limits its $T_C$ to low values [19].

A possible way to circumvent this phenomenology was suggested by recent studies of so-called $g(\boldsymbol{k}, \boldsymbol{q})$ electron-phonon couplings like the Peierls model [also known as the BLF-SSH (Barisic-Labbe-Friedel–Su-Schrieffer-Heeger) coupling] [20–23]. These showed that such couplings may promote very light single polarons [28] and bipolarons [29] even at very strong electron-phonon couplings. The reason for this qualitative difference is easily uncovered: $g(\boldsymbol{q})$ couplings are due to the modulation of the potential energy of the carrier by the lattice distortion in its vicinity. A larger distortion (at stronger coupling) results in a deeper potential well for the carrier, which makes it harder for it to tunnel to another site, hence the increased effective mass. By contrast, $g(\boldsymbol{k}, \boldsymbol{q})$ electron-phonon couplings arise from the modulation of the hopping integrals because of lattice vibrations. As a result, the lattice distortion associated with the polaron cloud may actually increase the hopping and thus the polaron's mobility (more discussion is presented below).

In this work, we investigate the possibility of superconductivity in the presence of Peierls electron-phonon coupling.

 

We provide proof-of-principle arguments that this type of coupling mediates unconventional, very high-$T_C$ superconductivity when the effective electron-phonon coupling is not too weak, $\lambda \gtrsim 0.5$, even for extremely small carrier concentrations. For technical reasons detailed below, here we investigate only the antiadiabatic limit $\Omega \gg E_F$, where $\Omega$ is the characteristic phonon frequency (however, we expect similar physics to be found for lower values of $\Omega$ as well, for reasons discussed below). Thus, our work paves the way for investigation of couplings and regimes that were not studied in previous work [24–27] on bipolaronic mechanisms of SC, which were focused entirely on the simpler, $g(\boldsymbol{q})$ couplings, and primarily in the Migdal-Eliashberg limit: $E_F \gg \Omega$ and $\lambda \ll 1$. In particular, the $g(\boldsymbol{k}, \boldsymbol{q})$ coupling is the key ingredient driving the unusual SC phenomenology uncovered below.

The paper is organized as follows: Section II describes the model we use, and Sec. III briefly reviews the BCS approximation when applied to our model. Section IV presents our key results. Section V contains a summary and a discussion of our work.

## II. MODEL

We study a simple-cubic lattice with Peierls-type electron phonon coupling arising from the modulation of the hopping integral between neighbor sites as the distance between them varies. Our starting point is a three-dimensional (3D) generalization of the 1D Su-Schrieffer-Heeger (SSH) model, but with optical phonons:

$$\hat{H} = \hat{H}_{\text{el}} + \hat{H}_{\text{ph}} + \hat{V}_{\text{el-ph}},$$

where

$$\hat{H}_{\text{el}} = -t \sum_{\langle i,j\rangle,\sigma} (c^{\dagger}_{i,\sigma} c_{j,\sigma} + \text{H.c.}) - \mu \sum_i \hat{n}_i$$

describes nearest-neighbor (nn) hopping, $\mu$ is the chemical potential, and $\hat{n}_i = \sum_\sigma c^{\dagger}_{i,\sigma} c_{i,\sigma}$. Here, $c^{\dagger}_{i,\sigma}$ creates an electron with spin $\sigma$ at lattice site $i$.

The second term describes three independent Einstein modes for oscillations of the lattice sites along $\gamma = x, y, z$ axes:

$$\hat{H}_{\text{ph}} = \Omega \sum_{i,\gamma} b^{\dagger}_{i,\gamma} b_{i,\gamma},$$

where $b^{\dagger}_{i,\gamma}$ creates a $\gamma$-mode phonon at site $i$ ($\hbar = 1$).

Finally, the Peierls electron-phonon coupling is

$$\hat{V}_{\text{el-ph}} = g \sum_{i,\sigma,\gamma} (c^{\dagger}_{i,\sigma} c_{i+\gamma,\sigma} + \text{H.c.})(b^{\dagger}_{i+\gamma,\gamma} + b_{i+\gamma,\gamma} - b^{\dagger}_{i,\gamma} - b_{i,\gamma}).$$

Here and in the rest of the paper, we use the short-hand notation $i \pm x$ for the site located at $\boldsymbol{R}_i \pm \boldsymbol{x}$, etc., with the lattice constant set to $a = 1$.

We define the dimensionless parameter $\lambda = 2g^2/(\Omega t)$ to characterize the strength of the electron-phonon coupling. This is identical to the 1D definition [28] because the tripling of the free-electron bandwidth in three dimensions is compensated for by the existence of three phonon modes, which triple the polaron energy. However, we emphasize that within the approximations used below, a carrier only couples to one phonon mode at a time, so $\lambda/3$ might be a more appropriate measure of the actual electron-phonon coupling strength.

In the antiadiabatic limit $\Omega \gg t, g$, we can derive the analytical form of the effective polaron Hamiltonian by integrating out high-energy manifolds with one or more phonons. For a system with just two electrons of opposite spin, this leads to an effective low-energy Hamiltonian that is a direct generalization of that obtained in one dimension [29]:

$$\hat{H} \to \hat{\mathcal{H}} = \hat{T}_{\text{eff}} + \hat{U}_{\text{eff}} + O\left(\frac{1}{\Omega^2}\right). \tag{1}$$

Here, the effective polaron dispersion

$$\hat{T}_{\text{eff}} = \hat{H}_{\text{el}} + t_3 \sum_{i,\gamma,\sigma} (c^{\dagger}_{i,\sigma} c_{i+2\boldsymbol{\gamma},\sigma} + \text{H.c.}) + \epsilon_0 \sum_i \hat{n}_i$$

now includes the polaron formation energy $\epsilon_0 = -12g^2/\Omega$, and the bare nn hopping is supplemented by the phonon-mediated, third-nn hopping with $t_3 = g^2/\Omega$, giving rise to an unusual polaron dispersion at stronger couplings, as discussed further below [28]. Note that in three dimensions, next-nearest-neighbor (nnn) hopping cannot arise from emission and absorption of one phonon, because hopping along different axes is modulated by different phonons; such processes can arise only at higher orders.

The effective, phonon-mediated interaction between polarons is given by $\hat{U}_{\text{eff}} = \hat{U}_{0,2} + \hat{U}_1$ [29], where

$$\begin{aligned}\hat{U}_{0,2} = &- T_0 \sum_{i,\gamma} [c^{\dagger}_{i-\boldsymbol{\gamma},\uparrow} c^{\dagger}_{i-\boldsymbol{\gamma},\downarrow} c_{i,\downarrow} c_{i,\uparrow} + \text{H.c.}] \\ &+ T_2 \sum_{i,\gamma} [(c^{\dagger}_{i+\boldsymbol{\gamma},\uparrow} c^{\dagger}_{i-\boldsymbol{\gamma},\downarrow} - c^{\dagger}_{i+\boldsymbol{\gamma},\downarrow} c^{\dagger}_{i-\boldsymbol{\gamma},\uparrow}) c_{i,\downarrow} c_{i,\uparrow} + \text{H.c.}]\end{aligned}$$

describes nn pair hopping of an on-site pair, with $T_0 = 4g^2/\Omega$, and hybridization between an on-site and a third-nn singlet pair, with $T_2 = 2g^2/\Omega$, respectively, while

$$\begin{aligned}\hat{U}_1 = &T_1 \sum_{i,\gamma,\sigma} [c^{\dagger}_{i+\boldsymbol{\gamma},\sigma} c^{\dagger}_{i+2\boldsymbol{\gamma},-\sigma} c_{i+\boldsymbol{\gamma},-\sigma} c_{i,\sigma} + \text{H.c.}] \\ &- J \sum_{i,\gamma,\sigma} c^{\dagger}_{i+\boldsymbol{\gamma},\sigma} c^{\dagger}_{i,-\sigma} c_{i+\boldsymbol{\gamma},-\sigma} c_{i,\sigma}\end{aligned}$$

describes directional (parallel to its backbone) pair hopping of a nn singlet pair, with $T_1 = 2g^2/\Omega$, and a nn antiferromagnetic exchange with $J = 4g^2/\Omega$, respectively.

The unusual form of this effective interaction is a direct consequence of the $g(\boldsymbol{k}, \boldsymbol{q})$ Peierls coupling. $\hat{U}_{\text{eff}}$ is attractive because polarons can lower their kinetic energy if they are bound into singlet bipolarons that move together, hence remaining light; more discussion of this phenomenology can be found in Ref. [29].

Hereafter, this two-polaron effective Hamiltonian $\hat{\mathcal{H}}$ of Eq. (1), corresponding to zero density for an infinite lattice, is assumed to be a good model for systems with low but finite carrier concentrations. This is because even though the phonon-induced renormalizations of the quasiparticle dispersion and of their effective interactions also depend on the carrier concentration, in the limit of very low concentrations their values must be close to those obtained in the zero-concentration limit. Furthermore, as we show below, small

quantitative changes in the values of these effective parameters will not change our conclusions.

## III. METHODS

The effect of this unusual $\hat{U}_{\rm eff}$ pair-hopping effective attraction on SC was not analyzed before, to the best of our knowledge. We do this in the most straightforward way: we switch to momentum space and keep in the interaction only terms scattering pairs of polarons between $(\boldsymbol{k}\uparrow, -\boldsymbol{k}\downarrow)$ states, as is done in the standard BCS approach [2]. This reduces the Hamiltonian of Eq. (1) to

$$\mathcal{H}_{\rm SC} = \sum_{\boldsymbol{k},\sigma} \xi_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} + \sum_{k,k'} \frac{U_{\rm eff}(\boldsymbol{k},\boldsymbol{k'})}{N^3} c^{\dagger}_{\boldsymbol{k}\uparrow} c^{\dagger}_{-\boldsymbol{k}\downarrow} c_{-\boldsymbol{k'}\downarrow} c_{\boldsymbol{k'}\uparrow},$$

where $N^3 \to \infty$ is the number of lattice sites, $\xi_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} - \mu$ is the single polaron dispersion $\epsilon_{\boldsymbol{k}} = \epsilon_0 - 2t\sum_\gamma \cos(k_\gamma) + 2t_3 \sum_\gamma \cos(2k_\gamma)$ measured from the Fermi energy, and the scattering vertex for pairs with $\boldsymbol{k}_{\rm tot} = 0$ is

$$U_{\rm eff}(\boldsymbol{k},\boldsymbol{k'}) = -6T_0 + 2T_2 \sum_\gamma [\cos(2k_\gamma) + \cos(2k'_\gamma)] + 4T_1 \sum_\gamma \cos(k_\gamma - k'_\gamma) - 2J \sum_\gamma \cos(k_\gamma + k'_\gamma).$$

Note that this vertex depends not just on $\boldsymbol{k} - \boldsymbol{k'}$, as for regular, density-density interactions, but also on $\boldsymbol{k} + \boldsymbol{k'}$. This is a direct consequence of the pair-hopping terms.

We use the Bogoliubov-Valatin transformation

$$\gamma_{\boldsymbol{k}\uparrow} = u_{\boldsymbol{k}} c_{\boldsymbol{k}\uparrow} - v_{\boldsymbol{k}} c^{\dagger}_{-\boldsymbol{k}\downarrow}, \tag{2}$$

$$\gamma_{-\boldsymbol{k}\downarrow} = u_{\boldsymbol{k}} c_{-\boldsymbol{k}\downarrow} + v_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\uparrow} \tag{3}$$

to find the usual mean-field approximation:

$$\mathcal{H}_{\rm SC} \approx E_{\rm GS} + \sum_{\boldsymbol{k}\sigma} E_{\boldsymbol{k}} \gamma^{\dagger}_{\boldsymbol{k}\sigma} \gamma_{\boldsymbol{k}\sigma},$$

where the quasiparticle energies are

$$E_{\boldsymbol{k}} = \sqrt{\xi^2_{\boldsymbol{k}} + \Delta^2_{\boldsymbol{k}}}$$

and the SC gap is given by the standard gap equation:

$$\Delta_{\boldsymbol{k}} = -\frac{1}{2N^3} \sum_{\boldsymbol{k'}} \frac{U_{\rm eff}(\boldsymbol{k},\boldsymbol{k'})\Delta_{\boldsymbol{k'}}}{E_{\boldsymbol{k'}}} \tanh \frac{E_{\boldsymbol{k'}}}{2kT}. \tag{4}$$

The chemical potential determines the $T = 0$ carrier concentration: $n = \frac{2}{N^3}\sum_{\boldsymbol{k}} |v_{\boldsymbol{k}}|^2 = \frac{1}{N^3}\sum_{\boldsymbol{k}} [1 - \frac{\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}]$.

For our $U_{\rm eff}(\boldsymbol{k},\boldsymbol{k'})$, the SC gap has the general form

$$\Delta_{\boldsymbol{k}} = \Delta_s + \Delta_{s^*} \sum_\gamma \cos(2k_\gamma) + \Delta_p \sum_\gamma \sin(k_\gamma), \tag{5}$$

where

$$\Delta_s = \frac{1}{N^3} \sum_{\boldsymbol{k'},\gamma} [T_0 - T_2 \cos(2k'_\gamma)] \frac{\Delta_{\boldsymbol{k'}}}{E_{\boldsymbol{k'}}} \tanh \frac{E_{\boldsymbol{k'}}}{2kT},$$

$$\Delta_{s^*} = -\frac{T_2}{N^3} \sum_{\boldsymbol{k'}} \frac{\Delta_{\boldsymbol{k'}}}{E_{\boldsymbol{k'}}} \tanh \frac{E_{\boldsymbol{k'}}}{2kT},$$

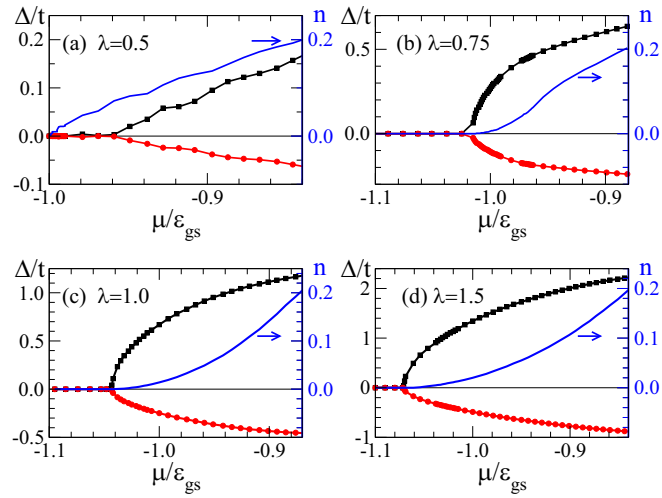


FIG. 1. Magnitudes of the superconducting gaps $\Delta_s/t$ (black squares) and $\Delta_{s^*}/t$ (red circles) vs $\mu/\epsilon_{\rm GS}$, where $\epsilon_{\rm GS}$ is the corresponding polaron GS energy. The blue full line shows the average carrier concentration $n$ (right-side scale). Panels correspond to effective couplings $\lambda = 0.5$, 0.75, 1.0, and 1.5, respectively.

$$\Delta_p = -\frac{2T_1 + J}{N^3} \sum_{\boldsymbol{k'},\gamma} \sin k'_\gamma \frac{\Delta_{\boldsymbol{k'}}}{E_{\boldsymbol{k'}}} \tanh \frac{E_{\boldsymbol{k'}}}{2kT}. \tag{6}$$

We note that another term with extended $s^*$ symmetry, $\propto \sum_\gamma \cos k_\gamma$, vanishes because its prefactor $2T_1 - J = 0$ in this asymptotic antiadiabatic limit, however it could contribute to $\Delta_{\boldsymbol{k}}$ if higher-order terms further renormalize the values of $T_1$ and $J$ in the limit of lower $\Omega$.

We solved these equations iteratively on a lattice with $N^3 = 30^3$ sites, with an accuracy below $10^{-6}t$, for values of $\mu$ near the bottom of the polaron band so that the average carrier concentration $n < 0.20$ is small.

As expected, we find that $s$ and $p$ symmetries do not coexist, and moreover, $\Delta_p = 0$ because of the overall minus sign in its gap equation (6) (we comment more on this below). As a result, we find that within these approximations, the SC gap has $s + s^*$ contributions.

## IV. RESULTS

We begin at $T = 0$. For small $\lambda$ we find no SC for small carrier concentrations $n \to 0$: both $\Delta_s$ and $\Delta_{s^*}$ vanish. This does not contradict the BCS theory, which is valid in the limit $E_F \gg \Omega$, $\lambda \ll 1$. In that case, the phonon-mediated scattering—within an energy shell of width $\Omega$ from the Fermi surface—is effectively a 2D problem, and bound solutions (Cooper pairs) form for arbitrarily weak attractive interactions. Our calculation, however, is in the opposite limit $\Omega \gg E_F$ where the scattering is 3D and a bound solution is expected only if the attractive potential is strong enough.

As we increase $\lambda$, we find finite $\Delta_s$, $\Delta_{s^*}$ if the carrier concentration goes above a threshold value $n \geqslant n_c$. This is shown in Fig. 1(a), where for $\lambda = 0.5$ we plot the evolution of $\Delta_s$ and $\Delta_{s^*}$ (left-hand vertical axis) with $\mu$; superimposed is the evolution of $n$ (right-hand vertical axis) with $\mu$. When

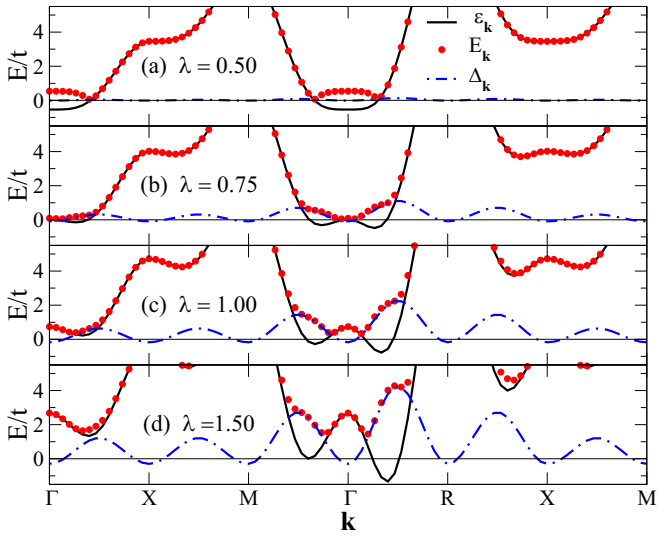


FIG. 2. Polaron energy $\epsilon_{\boldsymbol{k}}$ (solid black line), quasiparticle energy $E_{\boldsymbol{k}}$ (red circles), and SC gap $\Delta_{\boldsymbol{k}}$ (dot-dashed blue line) along high-symmetry lines in the Brillouin zone. All energies are in units of $t$, and $\mu$ is chosen such that $n = 0.1$ for the values $\lambda = 0.5$, 0.75, 1.0, and 1.5 shown.

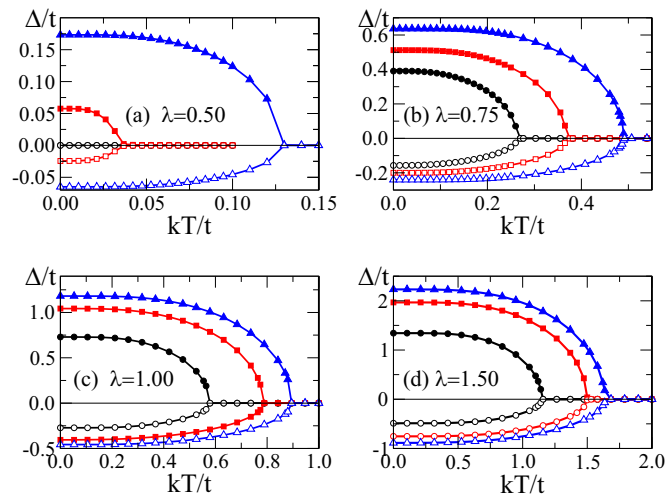


FIG. 3. Superconducting gaps $\Delta_s/t$ (full symbols) and $\Delta_{s^*}/t$ (empty symbols) vs $kT/t$. The three sets of lines correspond to $n = 0.05$ (black circles), 0.10 (red squares), and 0.20 (blue triangles), respectively.

$\mu$ is at the bottom of the polaron band so that $n \to 0$, the gaps vanish. However, for $n > n_c \approx 0.07$, SC appears and the magnitudes of $\Delta_s$ and $\Delta_{s^*}$ increase fast with $n$. The value of $n_c$ decreases with increasing $\lambda$. We do not try to pinpoint it here because even for $\lambda = 0.5$ there are still finite $N$ size effects (small oscillations) in the results, and these become worse as $\lambda$ decreases. Moreover, our focus here is on larger $\lambda$, where $n_c \to 0$, as we show next. For reference, we mention that for $\lambda = 0.25$, we find $n_c \sim 0.2$, which is probably above the low carrier concentrations for which our model is quantitatively accurate.

Figures 1(b)–1(d) show results for $\lambda = 0.75$, 1.0, and 1.5, respectively. We now find robust values for $\Delta_s$ and $\Delta_{s^*}$ at all $n \geqslant 0$. For a fixed $\lambda$, the magnitudes of the gaps increase monotonically with $n$. At a fixed $n$, they increase fast with $\lambda$ so that for $\lambda \sim 1$, both $\Delta_s$ and $\Delta_{s^*}$ are of order $t$, which is an *extremely large* energy scale for SC.

To clarify the origin of this unusual behavior, in Fig. 2 we plot together the polaron dispersion $\epsilon_{\boldsymbol{k}} = \xi_{\boldsymbol{k}} + \mu$ (solid black line), the quasiparticle energy $E_{\boldsymbol{k}}$ (red circles), and the gap $\Delta_{\boldsymbol{k}}$ (dot-dashed blue line) along various lines in the Brillouin zone. The chemical potential is chosen so that $n = 0.1$. Consider first the evolution of $\epsilon_{\boldsymbol{k}}$ with $\lambda$: for $\lambda < 0.5$, the polaron ground state is at the $\Gamma$ point, however for $\lambda > 0.5$ there are eight degenerate ground states at finite momentum $\pm\boldsymbol{k}_{\rm GS}$ lying along the $\Gamma$-$R$ line and its symmetric counterparts. This is because at small $\lambda$ the polaron dispersion is dominated by the nn hopping $t$ term that favors a GS at the $\Gamma$ point, while for $\lambda \geqslant 0.5$ the polaron dispersion is dominated by the third-nn hoping term $t_3$, which favors a GS at the $R$ point [28]. As a result, for $\mu$ near the bottom of the band, the system evolves from having a single, quasispherical Fermi sea when $\lambda$ is small, to having eight Fermi pockets when $\lambda$ is larger (these become connected if $\mu$ is further increased).

This significant change in the polaron dispersion results in the very different nature of the SC gap at small $\lambda$ versus large $\lambda$: in panel (a) we see a BCS-like picture, with a tiny and nearly constant gap opening at the Fermi energy. As $\lambda$ increases, so does the gap magnitude. Because of the opposite signs of $\Delta_s$ and $\Delta_{s^*}$, the gap is negative near the $\Gamma$ point but switches sign and becomes positive and is maximum on the "outer" side of the Fermi pockets, on the $\Gamma$-$R$ lines. For $\lambda = 0.75$ and this $\mu$, the smallest gap magnitude is close to the $\Gamma$ point, on the "inner" side of the Fermi pockets, and its sign is negative, whereas the "outer" side has a significant, positive gap. This shows that by adjusting the parameters, one can find an unconventional gap that closes on the Fermi pocket surface.

The more typical behavior, however, is found for larger $\mu$ and/or $\lambda$, with the Fermi pockets significantly gapped, the gap being positive. Interestingly, we see that the gap is considerable also in the regions lying between two Fermi pockets, on the $\Gamma$-$M$ and $\Gamma$-$X$ lines, even when these regions lie well above $\mu$ in the absence of SC.

The results in Fig. 2 suggest that the SC gap is considerable at $T = 0$ if $\lambda > 0.5$. This is confirmed in Fig. 3, where we plot $\Delta_s$ and $\Delta_{s^*}$ versus $T$ for $n = 0.05$, 0.1, and 0.2. For $\lambda = 0.5$ there is no SC if $n = 0.05$, and $T_C$ for larger $n$ appears small (although if $t$ is in the 100 meV range, even these $T_C$ could be at room temperature). For larger $\lambda$ we find a significant $T_C \sim t$ even for $n = 0.05$, suggesting that even narrowband materials with a $t$ of tens of meV would sustain room-temperature SC.

The appearance of these large values of $T_C$, comparable to the bare carrier hopping $t$, are the main result of this work.

## V. SUMMARY AND DISCUSSION

We used the BCS approximation to study the appearance of superconductivity in a model with Peierls electron-phonon coupling, at low carrier concentrations, and we showed that it promotes very high $T_C$ (comparable with the free-carrier

hopping) if the electron-phonon coupling is not too weak. The fact that for larger $\lambda$ we find SC to occur for all carrier concentrations $n$ shows that it must have BEC nature. The key ingredient is the effective attraction $U_{\rm eff}(\boldsymbol{k},\boldsymbol{k}')$ that strongly binds very light bipolarons at all $\lambda$, so that both the pair binding energy and their coherence energy are large. Bipolarons are light because $U_{\rm eff}$ promotes their mobility by acting on pairs of carriers that hop together. This is a direct consequence of the $g(\boldsymbol{k},\boldsymbol{q})$ electron-phonon coupling. In one dimension, stable bipolarons form for any $\lambda$ [29]; in three dimensions, there is a finite threshold for binding, hence different behavior at small versus large $\lambda$.

Regarding our methodology, we emphasize that these results are in the antiadiabatic limit simply because this is where we can obtain the analytical form of the effective polaron Hamiltonian (1), which allows us to carry out the calculations relatively easily. In one dimension, the bipolaron behavior remains qualitatively similar to that found in the antiadiabatic limit, even for much lower phonon frequencies down to $\Omega \sim 0.5t$ [30], and we expect the same to be true in three dimensions (what happens in the adiabatic limit $\Omega/t \to 0$ is not yet clear). This is why we expect robust SC to appear for most phonon frequencies, and not just in the antiadiabatic limit considered here.

Similarly, we used the BCS variational solution because of its simplicity. It may overestimate $T_C$, as is typical for mean-field methods, but the predicted $T_C$ values are so large that we expect significant values to be found by more accurate methods. We hope that this work will provide a strong motivation for the implementation of costly numerical methods to study such models in the whole parameter space, so as to gain an accurate quantitative understanding of the upper limit for their $T_C$.

Beside high-$T_C$ SC, another very exciting result is the possibility of $p$-wave SC. It does not occur within our approximations due to the lack of a $p^*$ term to interplay with the $p$ term of Eq. (6), the way the $s$ and $s^*$ terms do. A $p^*$ term may arise in a more accurate treatment and/or for different $g(\boldsymbol{k},\boldsymbol{q})$ couplings. Studying such possibilities opens another essential area of investigations, given the need for $p$-type SC in the topological context.

The last question is for which materials may this be relevant. We believe that it is premature to attempt to answer this, given that our work is only a proof-of-principle check that exciting SC physics is expected in materials with $g(\boldsymbol{k},\boldsymbol{q})$ couplings. Nevertheless, we note that both doped $SrTiO_3$ and $BaBiO_3$ exhibit "high"-$T_C$ SC (however in relative, not in absolute terms), believed to arise from $g(\boldsymbol{k},\boldsymbol{q})$ electron-phonon couplings [31]. This is pointing roughly in the same direction as our findings, and it further supports our call for accurate studies of such models.

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