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APPLICATION TO HIGH TEMPERATURE BIPOLARONIC SUPERCONDUCTIVITY

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ABSTRACT

It is desirable to have a better knowledge of direct paths to phonon-mediated high-transition-temperature (Tc) superconductivity since electron-lattice interactions play a significant role in quantum materials. However, it has long been understood that although poor electron-phonon coupling results in low Tc, high electron-phonon coupling causes bipolarons to develop or lattice instability, both of which are thought to be bad for superconductivity. As a result, it has previously seemed that the only way to create high-Tc materials via phonon-mediated processes is to increase the phonon frequency, as in hydrogen sulfides. Here, we provide a straightforward theory for superfluid light bipolaron-based phonon-mediated high-Tc superconductivity. We look at the case where lattice distortions control electron hopping, as opposed to the extensively researched Holstein model where they modify the electron's potential energy. We examine these tiny, light bipolarons using a quantum Monte Carlo method that is accurate sign-problem free, illuminating a novel path to phonon-mediated high-Tc superconductivity. We find that Tc in our model considerably and often surpasses upper constraints derived from the superfluidity of Holstein bipolarons or the Migdal-Eliashberg hypothesis. The combination of the light mass and tiny size of the bipolarons is the essential component in the bipolaronic process that generates high Tc. Through functional material engineering, our study sets guidelines for the design of high-Tc superconductors.

Keywords: *Critical Temperature, Energy Storage System, Superconductivity*

INTRODUCTION

It is desirable to have a better knowledge of direct paths to phonon-mediated high-transition-temperature (Tc) superconductivity since electron-lattice interactions play a significant role in quantum materials. However, it has long been understood that although poor electron-phonon coupling results in low Tc, high electron-phonon coupling causes bipolarons to develop or lattice instability, both of which are thought to be bad for superconductivity. As a result, it has previously seemed that the only way to create high-Tc materials via phonon-mediated processes is to increase the phonon frequency, as in hydrogen sulfides. Here, we provide a straightforward theory for superfluid light bipolaron-based phonon-mediated high-Tc superconductivity. We look at the case where lattice distortions control electron hopping, as opposed to the extensively researched Holstein model where they modify the electron's potential energy. We examine these tiny, light bipolarons using a quantum Monte Carlo method that is accurate sign-problem free, illuminating a novel path to phonon-mediated high-Tc superconductivity. We find that Tc in our model considerably and often surpasses upper constraints derived from the superfluidity of Holstein bipolarons or the Migdal-Eliashberg hypothesis. The combination of the light mass and tiny size of the bipolarons is the essential component in the bipolaronic

process that generates high Tc. Our research sets guidelines for the functional material engineering design of high-Tc superconductors.

Here, we provide a specific, experimentally applicable model for phonon-mediated bipolaronic high-Tc superconductivity with a Tc that can be significantly higher than previously established upper bounds, challenging the widely held belief that bipolaron formation is not favorable for high-transition-temperature superconductivity; see Our research is predicated on the finding that bipolarons behave like interacting bosons in the dilute limit, with a transition temperature that relies on both mass and density. At fixed mass, the transition temperature rises as the density rises, but the theory breaks down and, we believe, the superconducting transition temperature saturates when either the transition temperature reaches the order of the bipolaron binding energy or the density is high enough for the bipolarons to significantly overlap. As a result, the binding strength, inverse mass, and inverse size together determine the maximum transition temperature, with small-size, light-mass, firmly bound bipolarons maximizing the maximum transition temperature. The size saturates to a value on the order of the lattice constant in the extreme strong-coupling domain, although it seems that in all models, the polaronic mass enhancement increases exponentially in. The details and, thus, the maximum value of Tc will rely on the particulars of the underlying microscopic model being researched, despite the fact that these qualitative aspects are general.

Studies of the Holstein model, in which lattice distortions relate to the electron density (potential energy), have provided a general knowledge of this physics. The emphasis has been on the bipolaron mass, with the size getting less attention. As is raised in these models, the mass rises dramatically. Light masses have been discovered in conditions involving the interaction of conflicting forces, but recent studies suggest that this light mass occurs in such a constrained region of parameter space that its relevance to realistic systems is unclear. The Fröhlich or extended-Holstein models, in which the coupling to the electron density is longer ranged, have also been studied. Alternative types of electron-phonon interaction, however, are equally significant. Any substance containing a unit cell made up of many atoms will, in particular, undergo atomic bond distortions that locally modify.

OBJEACTIVES

1. The study phonon-mediated high-transition-temperature (Tc) superconductivity desirable.
2. The study design of high-Tc superconductors via functional material engineering.

RESEARCH METHODOLOGY

It is possible for us to investigate pairing and singlet bipolaron generation in the two-electron sector of the model by using a QMC technique that is based on a path-integral formulation of the electronic sector. This formulation is paired with either a real-space diagrammatic or a Fock-space path-integral representation of the phononic sector. Due to the lack of a sign issue, which is unique to this particular microscopic formulation and sector of the model, it is possible to get numerically correct findings with tiny statistical errors on large lattices even in the problematic regime of all the way to the heavy-mass limit; for more information, please refer to Appendix B. In spite of the fact that the coupling of electronic hopping to phonons may manifest itself in a number of distinct ways, the method that we have taken here enables us to reach generalizations about

high-Tc bipolaronic superconductivity as a result of the modulation of electronic hopping by lattice distortions over the whole parameter space.

Superfluidity Of Bipolarons

At a temperature that is dictated by the bipolaron density and effective mass and that only double-logarithmically weakly relies on the effective bipolaron-bipolaron interactions, bipolarons go through a transition into a superfluid state when considered in two dimensions (2D). If there is no other competing instability, phase separation, or Wigner crystallization, then we are free to disregard bipolaron-bipolaron interactions without fear of consequence. Our previous research leads us to believe that the instabilities in question are unlikely to occur. These considerations bring our issue down to that of the superfluidity of a gas of hard-core bipolarons, where BP denotes the density of bipolarons and mBP denotes the effective mass of bipolarons. As long as there is no overlap between bipolarons, this formula for Tc will continue to hold true throughout a wide density range. Because of this, the highest Tc that can be generated by this process occurs for a BP that corresponds to a liquid composed of bosons and has an interparticle separation that is on the order of the radial dimension of the bipolaron. We establish an estimate for the maximum Tc of the Berezinskii-Kosterlitz model by using RBP, which, after lattice regularization, has to be at least this.-Thouless transition of the bipolaronic liquid, which is determined only by the characteristics of the bipolarons provided by (we will refer to the optimized Tc simply as Tc in what follows and in the pictures)

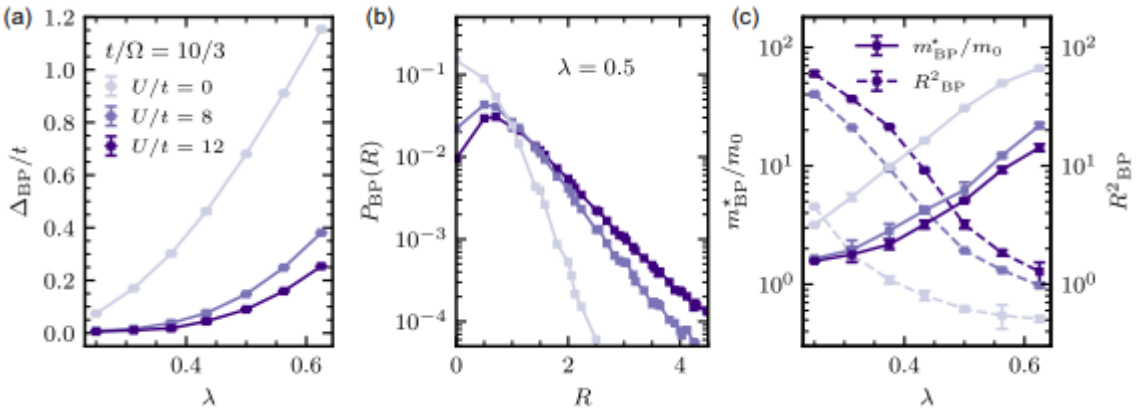

FIG. 1. Bipolaron properties in the bond-Peierls model. Bipolaron properties computed from QMC calculations performed (a) Bipolaron binding energy ΔBP in units of the electron hopping t. (b) Bipolaron radial size probability density distribution (absolute value squared of the bipolaron wave function) pbpðrþ for λ ¼ 0.5. (c) Bipolaron effective mass m⋆ BP in units of the mass of two free electrons.

qualitatively endure and acquire a frequency dependency (retardation), along with a predisposition for the bipolaron mass to rise as the number of phonons in the bipolaronic cloud develops. This is in addition to the fact that bipolarons have a frequency dependence (retardation). The features of bipolaronic superconductivity are determined by a conflict between phonon-mediated kinetic-energy-enhancing electron pair-hopping interactions and a propensity to increase mass. This competition takes place in bipolaronic superconductors. The results of our calculations show that there is a physically significant but parametrically huge zone in which the augmentation of the bipolaron mass is modest to moderate, but the bipolarons still have a relatively

small radial dimension R2 BP and a considerable binding energy. This characteristic is absolutely missing in the traditional Holstein model, which predicts that bipolarons would quickly become heavy in a way that is exponentially dependent on the strength of the electron-phonon interaction. The behavior that is typical of our model, which we believe to be true in a more general sense for Peierls-coupled systems, explains the rise in with up to an ideal beyond which bipolarons enter a domain of exponential mass enhancement that becomes prominent for Despite this, we find that, for a large portion of the parameter space, the simulated results much exceed any and all expectations that were previously held.

DATA ANALYSIS

This appendix provides a summary of the findings achieved by the ME approximation for the H and BP models that were taken into consideration in the main article. Although the approximation and calculations are conventional, the ramifications of the momentum dependent electron-phonon coupling in the BP model have not been examined before. This is because the consequences of this coupling have not been previously discussed. The comparison of the transition temperature Tc calculated within ME theory is presented in the main text of the appendix. The objective of the appendix is to make the comparison as exact as possible by describing the details of the calculations. It cannot be stressed enough that in the research that has been done on the limits of Tc in actual compounds, the physics of those limitations have been described.

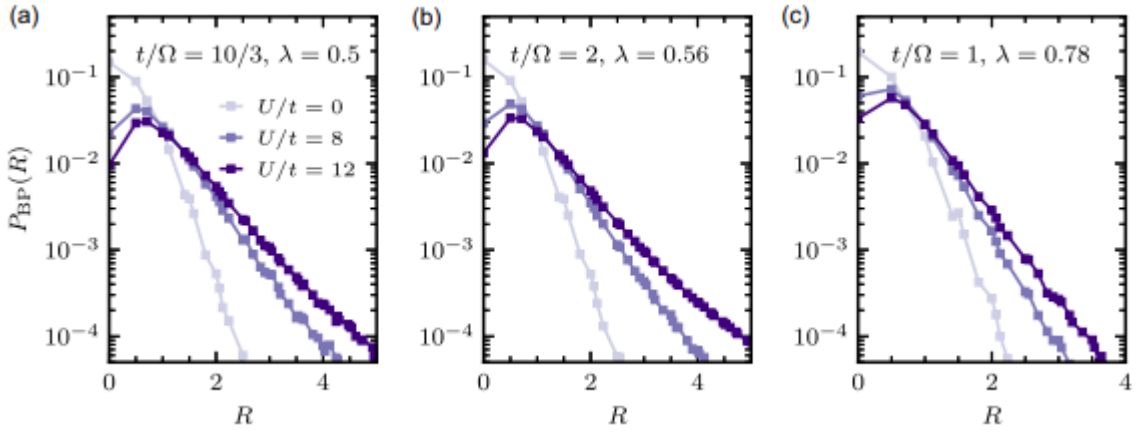

FIG. 2. Bipolaron radial size probability density distribution pbpðrþ in the bond-Peierls model. Pbpðrþ computed from QMC calculations performed on Eq. (1) at various values of the adiabaticity parameter t=Ω for the value of λ ¼ α2=ð2ωtþ which maximizes Tc at on-site Hubbard repulsion U=t ¼ 0; 8; 12; see Fig. 1. Error bars in pbpðrþ correspond to statistical errors smaller than the symbol size and therefore are not shown.

Tc is essentially based on considerations of the highest physically possible electron-phonon coupling strength in realistic models. These models are based on a theory of electrons and ions linked by the physical Coulomb interactions. The electron-phonon interaction is estimated from microscopics in this theory. In this section, we will be concentrating on the characteristics of the model systems that were covered in the primary book, but we will be setting the Hubbard U to zero. The findings for the H model that are reported here are in line with recent research carried out by Esterlis.

$$\hat{V}_H = \tilde{\alpha}_H \sum_{k,q,\sigma} (\hat{c}^\dagger_{k-\frac{q}{2},\sigma} \hat{c}_{k+\frac{q}{2},\sigma}) \hat{X}_q,$$

$$\hat{V}_{\mathrm{BP}} = \tilde{\alpha}_{\mathrm{BP}} \sum_{a=\pm} \sum_{k,q,\sigma} (\hat{c}^\dagger_{k-\frac{q}{2},\sigma} \hat{c}_{k+\frac{q}{2},\sigma}) \Lambda_a(k_x, k_y) \hat{X}_{q,a}.$$

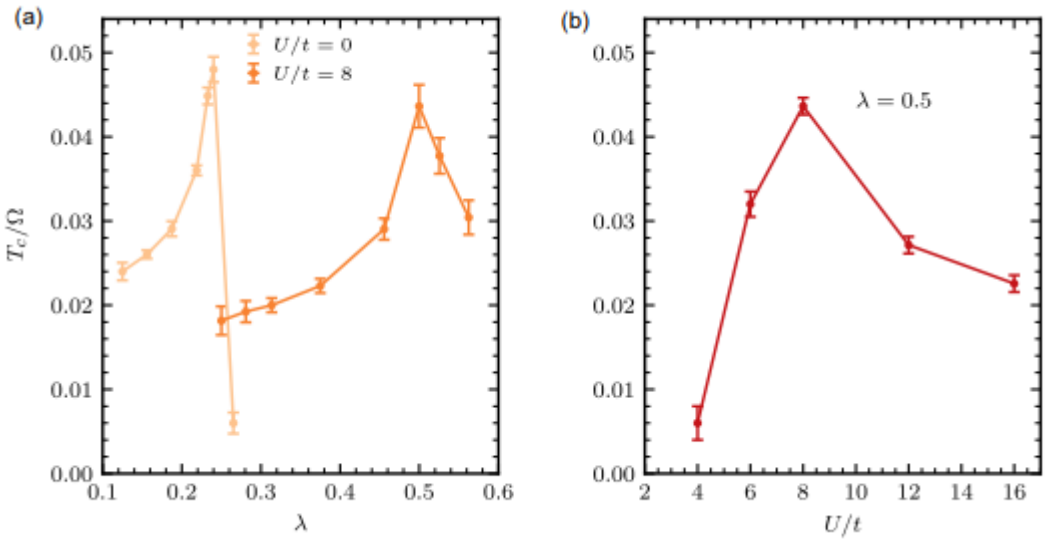

FIG. 3. Bipolaronic superconductivity in the Holstein model. Tc=Ω at adiabaticity parameter t=Ω ¼ 2 as a function of λ ¼ α2=ð8ωtþ for an on-site Hubbard U=t ¼ 0 and 8 (a) and as a function of U=t for λ ¼ 0.5 (b). Error bars represent statistical errors in QMC simulations corresponding to 1 standard deviation.

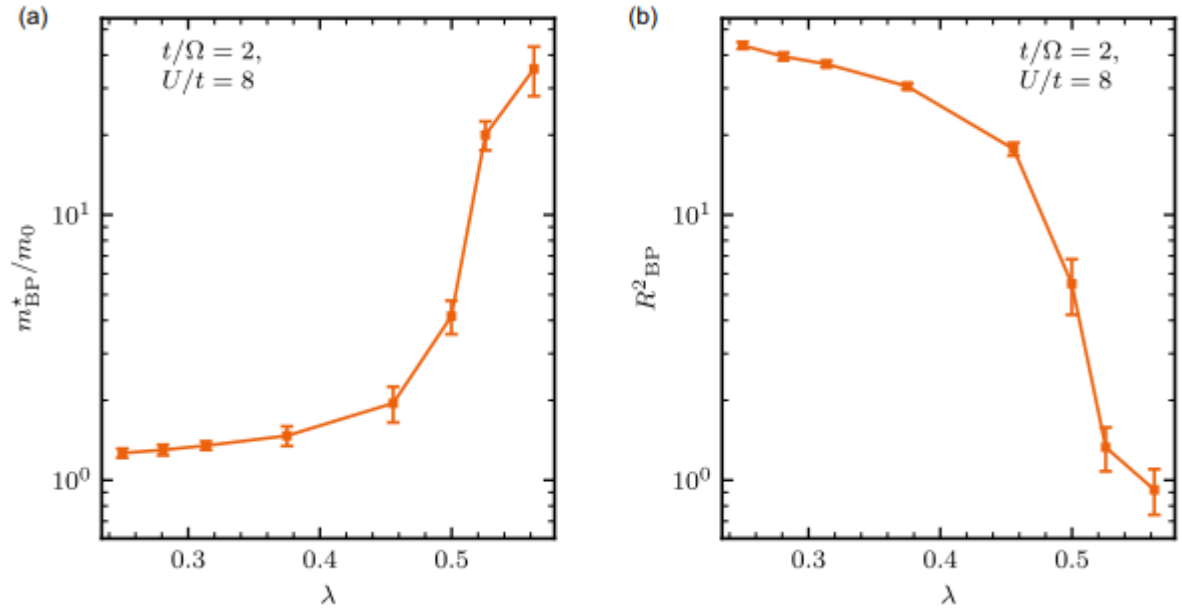

FIG. 4. Bipolaron properties in the Holstein model. Bipolaron properties computed from QMC calculations performed on Eq. (A2) at adiabaticity parameter t=Ω ¼ 2 as a function of the electron-phonon coupling λ ¼ α2=ð8ωtþ for an on-site Hubbard U=t ¼ 8. (a) Bipolaron effective mass m⋆ BP

in units of the mass of two free electrons m0 ¼ 2me ¼ 1=t. (b) Bipolaron mean-squared radius R2 BP. Error bars represent statistical errors in QMC simulations corresponding to 1 standard deviation.

McMillan's Phenomenological Approach To Phonon-Mediated Strong-Coupling Superconductivity

Within the context of Migdal-Eliashberg theory, the method that McMillan developed for studying strong-coupling superconductivity is predicated on a phenomenological analysis of experimental data on ordinary superconducting materials. This treatment is carried out. This method makes use of a coupling constant that is directly estimated from experimental data by taking into account an electron-phonon interaction that is averaged over the Fermi surface. Additionally, this treatment is supplemented by empirical parameters that are used to mimic the effect of the Coulomb interaction in order to better fit the experimental data. The Migdal-Eliashberg theory is sound in its own right inside the adiabatic limit and for moderate values. This is due to the fact that, aside from structural instability, the Fermi liquid transforms into a metastable state that is higher in energy than a state made by bipolarons when it reaches the adiabatic limit. Within the scope of its application, McMillan's formula discovers that a strong electron-phonon coupling may cause a Fermi liquid to exhibit properties of a superconducting instability.

The bond-Peierls electron-phonon coupling is a phenomenon that occurs always in systems in which the orbitals of out-of-plane atoms mingle with the bonding orbitals of in-plane atoms. In this case, transverse variations in the displacement of the out-of-plane atoms are what give rise to modification of the barrier for electron tunneling across bonds. This is exactly how the model described in is implemented. It is interesting to demonstrate that same physics is at work in the iron pnictides, in which case the height of the pnictogen may be modulated in a manner that dramatically affects certain hopping paths. indicates the occurrence of this event. In this particular example, there is one atom of pnictogen located at the apex of an octahedron, and there are four atoms of iron located in the centre of the octahedron. The electronic barrier for tunneling between iron atoms inside the pnictogen crystal is subject to variations as a result of the transverse motion of the pnictogen atom out of plane in the z direction. Overlaps between lobe orbitals with opposite signs on nearby iron atoms in the material that result in a negative hopping are a primary mechanism for direct electronic hopping between iron atoms in this class of materials. This kind of hopping is known as a negative hopping.

The overlap of the px orbital of the apex atom with each lobe of the two dxy orbitals, which results in a net positive hopping potential, is an example of an indirect electronic route that may be attributed to a second-order, super-exchangelike event. Because the magnitudes of t and t 0 are almost similar in FeSe, these two paths almost cancel each other out. On the other hand, the ratio of t to t 0 varies in different pnictide materials, which results in an overall drop in the amplitude of the net electronic hopping between the iron atoms. Because of this interference effect as well as the large modulation of the tunneling barrier caused by the displacement of the pnictogen atom along this particular hopping pathway, the value of the dimensionless electron-bond-phonon coupling strength relevant to this mode in this family of materials can be quite high; for instance, in one member of this family of materials; however, additional research is required to accurately determine the strength of electron-phonon coupling in specific compounds. The transverse phonon frequency is calculated to be in FeSe, and about suggesting a ratio of the relevant phonon frequency to the magnitude of the relevant (net) electron hopping that is approximately in these materials. The ratio of the relevant phonon frequency to the magnitude of the relevant (net) electron hopping is approximately. An "extended s-wave" state that has

some parallels to our bond bipolaron state is a leading contender, as we have already noted, despite the fact that the pairing symmetry in these materials has not yet been completely defined in its entirety.

Based on the findings of this investigation, it seems that the bond-Peierls coupling may be at work in the pnictides. On the other hand, it's possible that these materials include extra electronphonon interaction terms. For example, since a bond between two iron atoms connects two octahedra, the motion of a single pnictogen atom out of plane within one octahedron is correlated with that of another pnictogen atom in the neighboring octahedron, and this correlated pnictogen-pnictogen motion can simultaneously modulate the hopping across two iron-iron bonds, giving rise to yet another electron-phonon coupling term in these materials. To understand the interplay between the electron-phonon interaction terms and other features such as those presented by the multiple electronic bands, Hund's coupling, and the form and range of the effective electron-electron interactions near the Fermi surface, more research is required. This is because the true extent to which the bond-Peierls coupling is important in determining the behavior of these materials requires more work than is currently available.

CONCLUSION

To this point, it has seemed that the only way to get high-Tc materials via phonon-mediated processes was to increase the phonon frequency, as in the hydrogen sulfides. A straightforward model for phonon-mediated high-Tc superconductivity is presented here, and it is predicated on the superfluidity of light bipolarons. In contrast to the commonly researched Holstein model, in which lattice distortions modify the electron's potential energy, the case in which lattice distortions influence the electron's hopping is one that we explore. This physics gives birth to bipolarons that are tiny in size while yet being relatively light. We explore these bipolarons using an exact sign-problem-free quantum Monte Carlo technique, which demonstrates a novel way to phononmediated high-Tc superconductivity. We find that the critical temperature, Tc, in our model surpasses the traditional upper constraints based on the Migdal-Eliashberg theory or the superfluidity of Holstein bipolarons in a large and general way. The combination of light mass and tiny size of bipolarons is the essential component of this bipolaronic process that gives birth to high Tc. This mechanism gives rise to high Tc. Through functional material engineering, the concepts for the design of high-Tc superconductors established.

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