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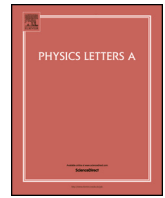
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Letter

Ubiquitous light real-space pairing from long-range hopping and interactions

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ABSTRACT

We systematically examine how long-range hopping and its synergy with extended interactions leads to light bound pairs. Pair properties are determined for a dilute extended Hubbard model with large on-site repulsion (U) and both near- and next-nearest neighbor hopping (t and t') and attraction (V and V'), for cubic and tetragonal lattices. The presence of t' and V' promotes light pairs. For tetragonal lattices, $t' < 0$ pairs can be lighter than non-interacting particles, and d -symmetric pairs form. Close packing transition temperatures, T^* , are estimated for the Bose-Einstein condensation (BEC) of pairs to be $k_B T^* \sim 0.1\bar{t}$, where \bar{t} is the geometric mean of the hoppings on the Cartesian axes. When pairs have d -symmetry, the condensate has d -wave character. Thus, the presence of both t' and V' leads ubiquitously to small strongly bound pairs with an inverse mass that is linear in hopping, which could lead to high temperature BECs.

1. Introduction

The properties of real-space pairs are important in the context of scenarios of superconductivity driven by BEC. Real-space pairs have long been known to adequately describe many aspects of the high- T_c phenomenology [1–5]. Recently, real space pairs were detected in iron-based superconductors [6,7] and in shot noise in copper oxide tunneling junctions [8]. The mass and effective radius of bound pairs define the maximal critical temperature attainable in the system [9–11] making them important quantities to determine. Real-state fermion pairs have also been shown to be stable against further clustering and phase separation [12–18].

In this paper we examine pair properties in dilute extended Hubbard models, concluding that small and light pairs are a ubiquitous consequence of next-nearest neighbor (NNN) interactions and hopping terms in the Hamiltonian, and discuss their contribution to the high transition temperatures in unconventional superconductors. NNN hopping and NNN interaction are often neglected, but longer range effects may be significant for many materials and lattices. Our goal is to examine the relevance of NNN hopping, t' , and interaction, V' , to pairs in a range of lattices.

Both the mass and size of real-space pairs contribute to superconducting transition temperatures in the BEC regime. BEC transition tem-

peratures in the dilute limit (where particles rarely scatter) have the form

$$T_{\text{BEC}} = \frac{3.31\hbar^2 n_b^{2/3}}{k_B \bar{m}^*}. \quad (1)$$

In this equation, the geometric mean of the mass, $\bar{m}^* = (m_{\parallel}^*)^{2/3}(m_{\perp}^*)^{1/3}$ where m_{\parallel}^* is pair mass in the xy plane, m_{\perp}^* is pair mass in the z direction (out of the plane), and n_b is density of pairs. We use subscript \parallel (\perp) to denote properties in the xy - (z -) directions respectively. T_{BEC} increases with n_b until pairs begin to overlap, at which point T_{BEC} first saturates and then starts to decrease. We estimate that T_{BEC} saturates in the vicinity of *close packing*, and define a close packing transition temperature,

$$T^* \sim \frac{3.31\hbar^2}{k_B \bar{m}^* \Omega_p^{2/3}}, \quad (2)$$

where Ω_p is pair volume. Substituting for the bare mass relating to the case of near-neighbor (NN) hopping only ($m_{0,\text{NN}} = \hbar^2/(2ta^2)$ in all cases) this becomes:

$$\frac{k_B T^*}{\bar{t}} \sim \frac{6.62}{\bar{m} \Omega_p^{2/3}}, \quad (3)$$

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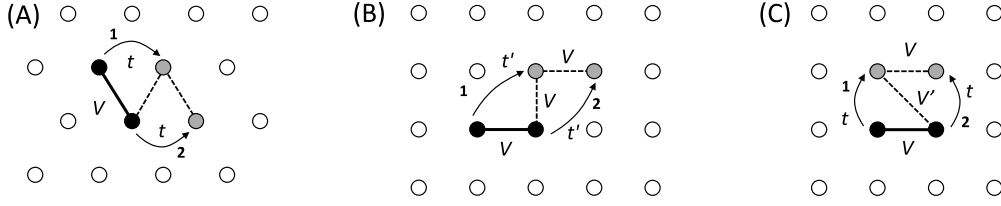


Fig. 1. Schematics of different light pair mechanisms. (A) On the triangular lattice, a pair with NN attraction V moves in the first order of NN hopping t . (B) On the square lattice, a similar pair with NN attraction requires NNN hopping t' to move in the first order. (C) In the resonant case, $V = V'$, the pair can move in the first order of NN hopping t even on the square lattice. Numbers '1' and '2' indicate hopping order.

where $\bar{t} = t_{\parallel}^{2/3} t_{\perp}^{1/3}$, $\bar{m} = m_{\parallel}^{2/3} m_{\perp}^{1/3}$ with dimensionless masses $m_{\parallel} = m_{\parallel}^*/m_{0,\text{NN}}$, $m_{\perp} = m_{\perp}^*/m_{0,\perp}$ and Ω_p' is the pair volume in units of lattice constant a in the xy plane and b in the z direction ($a = b$ for SC and BCC lattices). $m_{0,\perp} = 2b^2t$. For tetragonal cases, t_{\parallel} (t_{\perp}) is hopping parallel (perpendicular) to the xy plane. For isotropic cases (simple and body centered cubic) $t_{\parallel} = t_{\perp} = t$ and $m_{\parallel} = m_{\perp}$. The precise definition of Ω_p' is subtle, as it needs to be sufficiently large that scattering between pairs does not significantly affect Eq. 1. However, some statements can be made: A high T^* requires compact (small Ω_p') and light (small \bar{m}^*) pairs, which in some models leads to a trade off. For example, for large on-site repulsion and NN attraction only, Ω_p decreases with the attractive strength V , but at same time the mass increases as $\bar{m}^* \propto V$ so mass and volume cannot be simultaneously small. It is therefore of interest to examine situations where pair mass and size can be decoupled. In particular, we are interested in systems where the mass remains of the order of bare mass, $\bar{m}^* \sim m_0$, even in the strong coupling regime, $V \rightarrow \infty$ (m_0 is defined for different lattices in Table 1). We shall refer to such real-space pairs as *light*.

There are several physical mechanisms that can lead to light pairs. In some lattices, the pairs remain light for purely geometric reasons. Consider a triangular lattice with a strong NN attraction V , Fig. 1(A). The pair members can hop in turn without ever breaking the attractive bond. The pair mass is limited to $m^* < 6m_0$ even in the $V \rightarrow \infty$ limit [19,20]. Staggered chains [21], staggered square planes [22], and the face-centered-cubic lattice [23] are further examples of this geometric mechanism. In other lattices, the geometric mechanism does not work. For example, on a square lattice with only NN attraction and hopping, the pair can only move via an intermediate, higher-energy state. As a result, the pair mass scales as $m^* \propto m_0^2 V$. The same reasoning applies to simple cubic and body-centered cubic (BCC) lattices with NN V and t , and to the attractive Hubbard model on all lattices.

The situation changes qualitatively with the inclusion of NNN hopping, t' . NNN hopping increases lattice connectivity and the pairs can now move in the *first* order in t' , see Fig. 1(B). Although in general $t' < t$, it is still finite, which means the pair mass no longer scales $\propto V$ but instead saturates at a value defined by t' . One should note that typically NNN hopping is excluded from a model “for simplicity” to make it more tractable. This implicitly assumes that the omission of t' does not change basic physics of the system under study. As we have argued, this is not the case for pair mass. t' is essential for the physics of real-space pairs and for real-space superconductivity in general. The effects of t' are especially prominent in lattices with small NNN-to-NN distance ratios, such as the BCC lattice.

An even more interesting physics emerges if t and t' are of opposite signs. (Typically, $t < 0$ and $t' > 0$.) In this case, destructive interference between NN and NNN hopping can lead to a relatively large *bare* mass m_0 . Pairing disrupts the interference by effectively enhancing t or t' , depending on the details of attraction. With some parameter tuning, one can create a situation where a bound pair is lighter than the bare mass of the constituent particles, $m^* < 2m_0$, and even lighter than one bare mass, $m^* < m_0$. We will refer to such pairs as *superlight*.

Another light pair mechanism (resonant mechanism) is illustrated in Fig. 1(C). In this case, the NNN attraction V' is of the same strength as V . The pair can move with the NN hopping only because now the in-

termediate states have the same energy and the mass remains $m^* \propto m_0$. One might think that this mechanism would be rare since it requires fine tuning of parameters. However, in real systems the inter-particle potential is the combination of a short-range repulsion and a longer-range attraction (mediated by phonons or other mechanisms [24–31]). Such a potential has a shallow minimum that extends over several lattice constants. Thus, the probability of two potential values being close is not small.

The focus of this paper is mechanism (B), i.e., the effects of the NNN hopping t' on the real-space pair mass. The reason is two-fold. First, this mechanism has not been thoroughly discussed in the literature, unlike mechanisms (A) and (C) [19–23,32]. Second, mechanism (B) is *universal*, i.e., it does not require fine tuning. Any system with a nonzero t' will host pairs with $m^* \propto (t')^{-1}$ or lighter. With t' taken into account, the lightness of pairs becomes a common and ubiquitous feature of models with intersite attraction, with important implications for unconventional superconductivity discussed earlier. We also investigate interplay between mechanisms (B) and (C) inspired by the high $k_B T_c / \bar{t}$ ratio in BCC fulleride superconductors where t' and V' are expected to be particularly large.

2. Model and methodology

We examine pairs in the dilute limit of an extended Hubbard model which includes NN and longer-range attractive interactions and hopping, with Hamiltonian,

$$\hat{H} = \sum_{\mathbf{n}, \sigma} t_{\mathbf{b}} c_{\mathbf{n}+\mathbf{b}, \sigma}^{\dagger} c_{\mathbf{n}, \sigma} + U \sum_{\mathbf{n}} \hat{\rho}_{\mathbf{n}\uparrow} \hat{\rho}_{\mathbf{n}\downarrow} + \sum_{\mathbf{n}, \mathbf{b}} \frac{V_{\mathbf{b}}}{2} \hat{\rho}_{\mathbf{n}+\mathbf{b}} \hat{\rho}_{\mathbf{n}}, \quad (4)$$

where the Hubbard repulsion has been separated out from the other interactions. In the above equation, \mathbf{b} are the set of vectors to neighbor sites, $c_{\mathbf{n}\sigma}^{\dagger}$ ($c_{\mathbf{n}\sigma}$) creates (annihilates) an electron of spin σ at site \mathbf{n} , $\hat{\rho}_{\mathbf{n}\sigma} = c_{\mathbf{n}\sigma}^{\dagger} c_{\mathbf{n}\sigma}$, and $\hat{\rho}_{\mathbf{n}} = \hat{\rho}_{\mathbf{n}\uparrow} + \hat{\rho}_{\mathbf{n}\downarrow}$ is the number operator on site \mathbf{n} . One-particle hopping and inter-particle interaction are defined by functions $t_{\mathbf{b}}$ (hopping through a displacement \mathbf{b}) and $V_{\mathbf{b}}$ (interaction at separation \mathbf{b}), respectively. The factor $\frac{1}{2}$ takes account of double counting of the interaction terms. The models described by Eq. (4) are generally known as UV models [22].

A two-particle version of Eq. 4 can be found in two cases. The first case is the dilute limit of the Hamiltonian. Both electron (mostly negative $t_{\mathbf{b}}$) and hole (mostly positive $t_{\mathbf{b}}$) variants have physical meaning. The second, less trivial case occurs close to half filling for the special case $U \gg t_{\mathbf{b}}$. Then two holes interact according to Eq. 4, but with renormalized kinetic energy because movement of holes is restricted by strong correlations [33–35]. As a result, we expect that the bands would be flattened and hopping amplitudes of holes (and thus kinetic energy) would be smaller than the $t_{\mathbf{b}}$ of the original electron Hamiltonian the hole model is derived from. This increases the relative importance of V/t which could be Coulomb or electron-phonon in origin. A NN interaction can originate from a number of sources. Attractive long-range electron-phonon interactions can lead to instantaneous interactions at large phonon frequency, including an intersite V [36] (strong phonon mediated intersite attractions have been measured in 1D cuprates [37,38]). In some materials, attractive V were

predicted from first-principle quantum chemistry calculations [26,27]. Coulomb repulsion can generate a repulsive V . A repulsive Hubbard U can cause an effective intersite Heisenberg interaction J , which while spin dependent could act like V in a dilute system [39]. There are rich phases in extended Hubbard models, including Mott insulators [40], stripe order [41], d -wave superconductivity [36,42], and XY antiferromagnetism [43]. Extended Hubbard models with NN interaction have been applied to superconductors including cuprates [42,44].

We find the exact properties of a pair of spin- $\frac{1}{2}$ fermions in the UV model by solving the following lattice Schrödinger equation:

$$\begin{aligned} & \sum_{\mathbf{b}} t_{\mathbf{b}} \left[\Psi(\mathbf{n}_1 + \mathbf{b}, \mathbf{n}_2) + \Psi(\mathbf{n}_1, \mathbf{n}_2 + \mathbf{b}) \right] \\ & + U \delta_{\mathbf{n}_1, \mathbf{n}_2} \Psi(\mathbf{n}_1, \mathbf{n}_2) + \sum_{\mathbf{b}} V_{\mathbf{b}} \delta_{\mathbf{n}_1 - \mathbf{n}_2, \mathbf{b}} \Psi(\mathbf{n}_1, \mathbf{n}_2) \\ & = E \Psi(\mathbf{n}_1, \mathbf{n}_2), \end{aligned} \quad (5)$$

where E is the total pair energy and δ is the Kronecker delta function. The pair wavefunction is $\Psi(\mathbf{n}_1, \mathbf{n}_2)$. A complete solution methodology can be found in Ref. [22]. Here we outline key steps and features. (i) In momentum space, Eq. (5) becomes an integral equation with a separable kernel. The former is reducible to a system of *linear* equations, thus leading to a mathematically exact solution. The size of the linear system is $(1 + n_{\mathbf{b}})$ where $n_{\mathbf{b}}$ is the number of neighbor vectors with $V_{\mathbf{b}} \neq 0$. The system's matrix elements are two-body lattice Green's functions. The solution's complexity grows sharply with the radius of interaction and lattice dimensionality. (ii) By symmetrizing or antisymmetrizing $\Psi(\mathbf{n}_1, \mathbf{n}_2)$, one can focus the solution either on spin-singlet or spin-triplet pair states. Sizes of the respective systems of linear equations are $(1 + \frac{1}{2}n_{\mathbf{b}})$ and $\frac{1}{2}n_{\mathbf{b}}$. In most cases, this trick significantly reduces the mathematical complexity of the solution. (iii) The linear system includes pair total momentum \mathbf{P} as a parameter. Therefore, the exact solution provides pair dispersion $E(\mathbf{P})$ as well as pair mass m^* defined via a second derivative of $E(\mathbf{P})$. (iv) At the Γ -point of the pair Brillouin zone, $\mathbf{P} = 0$, the full linear system can be further decomposed into blocks corresponding to particular orbital symmetries. Sometimes, the mass can also be obtained from the partial blocks. (v) The eigenvector of the linear system defines the pair wave function $\Psi(\mathbf{n}_1, \mathbf{n}_2)$. From there, the pair effective radius and volume can be computed after proper normalization. The final set of linear equations for specific lattices are given in Supplemental Material.

In addition to the exact solution, we employ an analytical approach to determine pair mass in the strong attraction limit. In this limit, pairs are tightly bound and the basis reduces to a small number of dimer states, which enables a simple derivation of the mass [19,20,22,23,32]. This mass serves as a useful validation check for the all-coupling solution.

3. Qualitative considerations

In this section, we examine the effects of NNN hopping on real-space pairs in a square UV model with NN attraction. The model serves as a good illustration of the physical ideas explored in this paper and is inspired by the unconventional superconductivity in the underdoped cuprates. Two-dimensional copper-oxygen planes host mobile holes at low densities. The multiorbital model describing these can be mapped to a one-orbital model using a variety of reduction schemes [45–48]. Such procedures typically produce long-range hopping, which we wish to study in this work. An attractive V can originate from several physical mechanisms including mediation by phonons [3,31], spin waves [30], and the Jahn-Teller effect [28,29]. An attractive interaction, $V \sim t$ between two holes within a CuO_2 plane was inferred from *ab initio* quantum chemistry calculations [26,27].

The Hamiltonian we wish to study in this section is Eq. 4 with $t_{\mathbf{b}_1} = t$, $t_{\mathbf{b}_2} = t'$, $V_{\mathbf{b}_1} = V$, $V_{\mathbf{b}_2} = V'$, where the four $\mathbf{b}_1 = \{\pm\mathbf{x}; \pm\mathbf{y}\}$ and the four $\mathbf{b}_2 = \{\pm\mathbf{x} \pm \mathbf{y}\}$ are the NN and NNN lattice vectors of the square lattice,

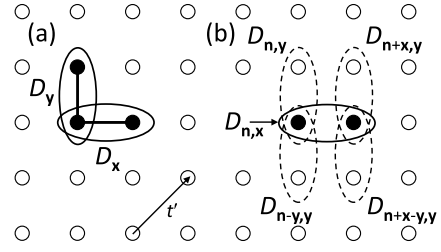


Fig. 2. (a) Two types of spin-singlet dimers in the $|V| \gg t, t'$ limit of Eq. (4). (b) Illustration for the first line in Eq. (9). NNN hopping, t' , connects a starting dimer of type \mathbf{x} with four dimers of type \mathbf{y} . The latter are circled by dashed ovals.

respectively (\mathbf{x} and \mathbf{y} are unit vectors on cartesian axes). Note that we defined hopping amplitudes with negative signs. We are mostly interested in the electron channel, $t, t' > 0$, although we will also consider $t' < 0$ when discussing the superlight effect. The two-particle problem of the square UV model, and of the related $t - J$ model has been considered by several authors [49–53], although the effects of t' have not been fully elaborated yet.

The physical effects discussed below also occur in other lattices with NNN hopping, including the 1D chain and 3D simple cubic lattice. The square UV model serves as a convenient proxy for all hyper-cubic UV models. The non-interacting (one particle) dispersion of Eq. (4) is

$$\epsilon_{\mathbf{k}} = -2t (\cos k_x a + \cos k_y a) - 4t' \cos k_x a \cos k_y a, \quad (6)$$

where a is the lattice constant, k_x and k_y are x and y components of momentum. The bare effective mass for the square lattice is

$$m_0 = \frac{\hbar^2}{2a^2(t + 2t')}. \quad (7)$$

3.1. Strong-coupling limit and light pairs

We first consider the case of *electron*-type NNN hopping with $t' > 0$ (in our sign convention). We begin with considering the strong coupling limit of Eq. (4) with NN attraction only, $V' = 0$, $V < 0$, and $|V| \gg t, t'$. The state basis reduces to tightly bound NN dimers shown in Fig. 2(a). We consider only spin singlets, hence there are only two dimer types

$$D_{\mathbf{n},\mathbf{b}}^s = \frac{1}{\sqrt{2}} (|\uparrow\rangle_{\mathbf{n}} |\downarrow\rangle_{\mathbf{n}+\mathbf{b}} + |\downarrow\rangle_{\mathbf{n}} |\uparrow\rangle_{\mathbf{n}+\mathbf{b}}), \quad (8)$$

where $\mathbf{b} = \mathbf{x}$ or \mathbf{y} and $|\sigma\rangle_{\mathbf{n}} = c_{\mathbf{n}\sigma}^\dagger |0\rangle$ ($\sigma = \uparrow, \downarrow$). The dimer states have energy $-|V|$ and are connected by NNN hopping. Operating by the t' term of \hat{H} (denoted \hat{H}'), one obtains, see Fig. 2(b)

$$\begin{aligned} \hat{H}' D_{\mathbf{n},\mathbf{x}}^s &= -t' \left(D_{\mathbf{n},\mathbf{y}}^s + D_{\mathbf{n}-\mathbf{y},\mathbf{y}}^s + D_{\mathbf{n}+\mathbf{x},\mathbf{y}}^s + D_{\mathbf{n}+\mathbf{x}-\mathbf{y},\mathbf{y}}^s \right) \\ \hat{H}' D_{\mathbf{n},\mathbf{y}}^s &= -t' \left(D_{\mathbf{n},\mathbf{x}}^s + D_{\mathbf{n}+\mathbf{y},\mathbf{x}}^s + D_{\mathbf{n}-\mathbf{x},\mathbf{x}}^s + D_{\mathbf{n}-\mathbf{x}+\mathbf{y},\mathbf{x}}^s \right). \end{aligned} \quad (9)$$

This leads to a Schrödinger equation in momentum space

$$\begin{aligned} & \begin{bmatrix} E(\mathbf{P}) + |V| & t'(1 + e^{iP_x a})(1 + e^{-iP_y a}) \\ t'(1 + e^{-iP_x a})(1 + e^{iP_y a}) & E(\mathbf{P}) + |V| \end{bmatrix} \\ & \times \begin{bmatrix} D_{\mathbf{P},\mathbf{x}}^s \\ D_{\mathbf{P},\mathbf{y}}^s \end{bmatrix} = 0, \end{aligned} \quad (10)$$

where \mathbf{P} is the total pair momentum, with components P_x and P_y . From here, one finds pair dispersion

$$E(\mathbf{P}) = -|V| \pm 4t' \cos \frac{P_x a}{2} \cos \frac{P_y a}{2}, \quad (11)$$

and pair mass

$$m^* = \frac{\hbar^2}{t' a^2}. \quad (12)$$

Table 1

Summary of the properties of a particle in various lattices; the lattice constant is a , z represents the coordination number, and $\eta = d_{\text{NN}}/d_{\text{NNN}}$ the ratio between the NN and NNN distances. For tetragonal case, in-plane m_0 is shown and b is interplane spacing.

Lattice	$\epsilon(\mathbf{k})$	m_0	Distance			z		$E(0) = -W_0 - W'$	
			d_{NN}	d_{NNN}	η	z_{NN}	z_{NNN}	W_0	W'
Square	$-2t(\cos k_x a + \cos k_y a) - 4t' \cos k_x a \cos k_y a$	$\frac{\hbar^2}{2a^2(t+2t')}$	a	$\sqrt{2}a$	$\frac{1}{\sqrt{2}}$	4	4	$8t$	$8t'$
Tetragonal	$-2t(\cos k_x a + \cos k_y a) - 4t' \cos k_x a \cos k_y a - 2t_{\perp} \cos k_z b$	$\frac{\hbar^2}{2a^2(t+2t')}$	a	$\sqrt{2}a$	$\frac{1}{\sqrt{2}}$	4	4	$8t$	$8t' + 4t_{\perp}$
SC	$-2t(\cos k_x a + \cos k_y a + \cos k_z a)$ $-4t'(\cos k_x a \cos k_y a + \cos k_x a \cos k_z a + \cos k_y a \cos k_z a)$	$\frac{\hbar^2}{2a^2(t+4t')}$	a	$\sqrt{2}a$	$\frac{1}{\sqrt{2}}$	6	12	$12t$	$24t'$
BCC	$-8t \cos \frac{k_x a}{2} \cos \frac{k_y a}{2} \cos \frac{k_z a}{2}$ $-2t'(\cos k_x a + \cos k_y a + \cos k_z a)$	$\frac{\hbar^2}{2a^2(t+t')}$	$\frac{\sqrt{3}}{2}a$	a	$\frac{\sqrt{3}}{2}$	8	6	$16t$	$12t'$

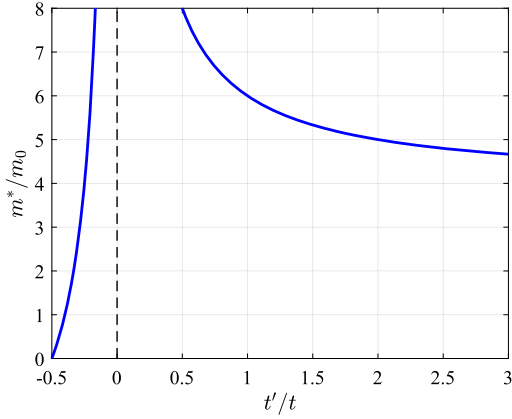


Fig. 3. The mass enhancement function, Eq. (14), in the $V \gg t, t'$ limit. Superlight pairs, $m^* < m_0$, exist near $t'/t = -0.5$. We do not consider the more complex case of $t'/t < -0.5$ where the band minimum is not at $\mathbf{k} = (0, 0)$.

The pair mass only depends on t' and is independent of the binding energy that scales as $|V|$. The pair remains mobile even in the strong coupling limit. This is the *light-pair* effect. On the square lattice, it is entirely due to NNN hopping. We also note that since $t' > 0$, it follows from Eq. (10) near $\mathbf{P} = 0$ that $D_{\mathbf{P},x}^s = D_{\mathbf{P},y}^s$, that is, the pair has s -type orbital symmetry.

When expressed in terms of m_0 , the pair mass becomes

$$\frac{m^*}{m_0} \Big|_{V \rightarrow \infty} = \frac{2(t+2t')}{t'} \quad (13)$$

Although m^* is independent of V , the enhancement relative to m_0 can still be large if $t' \ll t$. The enhancement is small when $t' \gtrsim t$.

3.2. “Superlight” bound pairs

We now consider the case of *hole*-type NNN hopping, i.e., $t' < 0$ with our sign convention. We note that negative t' routinely appears in one-orbital models of CuO_2 planes, that are derived from multi-orbital models [46–48]. Going back to Eq. (9), we now choose the positive sign, which leads to the same ground-state energy $-|V| - 4|t'|$. The pair mass is still given by Eq. (12) but with t' replaced by its absolute value. One important difference concerns the pair symmetry. It follows from Eq. (10) that if $t' < 0$, then $D_{\mathbf{P},x}^s = -D_{\mathbf{P},y}^s$, so the pair has d symmetry.

Another important change occurs in the one-particle dispersion. It can be seen from Eqs. (6) and (7) that if $t > 0$ and $t' < 0$, then destructive interference between NN and NNN hopping flattens the band near $\mathbf{P} = 0$. As a result, m_0 increases and even diverges at $t' \rightarrow -\frac{1}{2}t$. In the following, we do not consider $t' < -\frac{1}{2}t$ because in this parameter region the band bottom shifts from $\mathbf{P} = 0$ to $\mathbf{P} = (\pm\pi, 0)$ and mass near the band bottom is no longer isotropic. Allowing for negative t' , Eq. (13) is generalized as follows

$$\frac{m^*}{m_0} \Big|_{V \rightarrow \infty} = \frac{2(t+2t')}{|t'|}; \quad t' > -\frac{1}{2}t. \quad (14)$$

This mass-enhancement function for $V' = 0$ is plotted in Fig. 3. Remarkably, there is a narrow but finite region, $-\frac{1}{2}t < t' < -\frac{1}{3}t$, where $m^* < 2m_0$, and an even narrower region, $-\frac{1}{2}t < t' < -\frac{2}{5}t$, where $m^* < m_0$, i.e., the tightly bound pair is lighter than one free particle. We call such real-space pairs *superlight*. The physics behind the superlight effect is disruption of the destructive interference by interaction: NN attraction elevates the importance of t' over t . As are result, a bound pair of particles moves more easily than one free particle.

3.3. Interplay with the resonance mechanism

In the preceding sections we showed that a nonzero NNN hopping generally leads to light bound pairs and in some special cases to superlight bound pairs. Additionally, resonance in the attractive potential, illustrated in Fig. 1(c), may also lead to a light mass. In this section we investigate the interplay between the two mechanisms. We consider Eq. (4) with an additional condition, $V' = V$, and take the limit $V, V' \rightarrow -\infty$. In addition to the two dimer states shown in Fig. 2, there will be two more dimer states arranged diagonally. All four dimer types have the same energy and are mixed by t and t' hopping. The dimer Schrödinger equation is an eigenvalue equation derived in the Supplemental Material. On Brillouin zone diagonals, $P_x = \pm P_y \equiv P$, the full dispersion equation factorizes into the following blocks. (i) Dispersionless level, $E = 0$. (ii) $d_{x^2-y^2}$ pair with $E = 2t'(1 + \cos P)$. (iii) $s - d_{xy}$ block with energy defined by

$$E^2 + 2t'(1 + \cos P)E - 8t^2(1 + \cos P) = 0. \quad (15)$$

The s -symmetric ground state is the lowest root of the above equation

$$E_s = -t'(1 + \cos P) - \sqrt{t'^2(1 + \cos P)^2 + 8t^2(1 + \cos P)}. \quad (16)$$

Expanding for small P , the pair effective mass when $V' = V$ is,

$$\frac{m_s^*}{m_0} = \frac{4(t+2t')\sqrt{t'^2+4t^2}}{(t'^2+2t^2)+t'\sqrt{t'^2+4t^2}}, \quad (17)$$

where m_0 is given in Eq. (7). m^*/m_0 varies between 4 and a maximum of ~ 5.2 , depending on t' .

4. Exact pair properties

In this section, we present pair properties obtained from numerical solution of Eq. (4). We study square, quasi-2D tetragonal, 3D simple cubic (SC), and 3D body-centered cubic (BCC) lattices. Study of the tetragonal lattice is inspired by superconductivity in the cuprates while the BCC is inspired by superconductivity in fullerenes [54]. In this section, we limit the parameter space to $|V'| < |V|$ and $t' < t$. The one-particle properties of the model for these systems are summarized in Table 1. For the tetragonal case, we select $t_{\perp} = 0.04$ for hopping between planes.

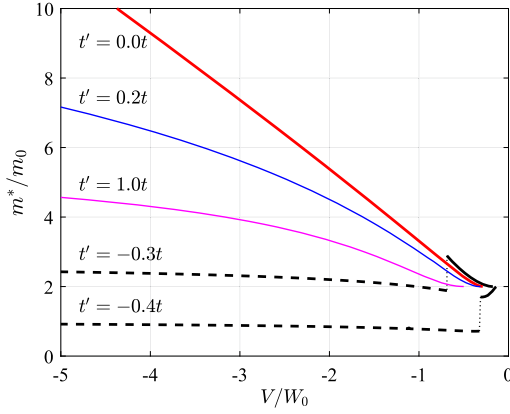


Fig. 4. Mass of the ground state bound state in the square UV model. Note that m_0 is t' -dependent, see Eq. (7). Solid lines correspond to s -symmetric ground states, with thick and thin lines relating to heavy and light states respectively. Dashed lines correspond to d -symmetric superlight states. Notice how the pairs become *superlight*, i.e., lighter than the combined mass of the constituent particles, as $t' \rightarrow -\frac{1}{2}t$.

The specific eigenvalue equations are provided in the Supplemental Material.

Pairs on the square lattice with $V' = 0$ and $t' \neq 0$ may be either heavy (with s symmetry), light (also with s symmetry) or superlight (with d symmetry) depending on the parameters. Fig. 4 shows the spin-singlet ground state for a pair of particles on a square lattice. The parameters for the pairing regimes can be categorized as: (i) NN hopping only, $t' = 0$. In this “heavy pair” regime, the pair only moves in the second order in t , hence the mass grows as $m^* \propto |V|$ as $|V| \rightarrow \infty$. (ii) Nonzero positive (electron-like) t' . The mass starts at $m^* = 2m_0$ at formation. As $|V|$ increases, the mass saturates at a value prescribed by Eq. (13). The pair remains *light* and mobile even in the strong coupling limit, $V \rightarrow -\infty$, as discussed on Sec. 3.1. The ground state has s orbital symmetry in all regimes. (iii) Finally, there is the *superlight* regime, $t' < 0$. In this case, there is level crossing. As $|V|$ increases, s pairs are first to form. The mass either decreases or increases, depending of the value of t' . Upon further increase of V , d pairs form and then become the ground state. This effect has been described by Bak and Micnas [55]. At the crossover, the mass jumps discontinuously. After the crossover, the pairs become superlight (for t' close enough to $-\frac{1}{2}t$), i.e., lighter than two separate free particles. In the $V \rightarrow -\infty$ limit, the mass approaches Eq. (14).

Moving to 3D lattices, the light pair effect can be demonstrated by examining four extremal cases of the parameter space: (i) $V'/V = 0, t'/t = 0$, (ii) $V'/V = 1, t'/t = 0$, (iii) $V'/V = 0, t'/t = 1$, and (iv) $V'/V = 1, t'/t = 1$. The additional cases of (v) $V'/V = 0, t'/t = -0.45$ and (vi) $V'/V = 1, t'/t = -0.45$ are also studied for the tetragonal case. Panels (a)-(c) of Fig. 5 show how the strong-attraction limit is approached for these cases. When $t' = 0$ and $V' = 0$, the “heavy pair” regime is seen with mass increasing proportionally to V . Introduction of t' and V' leads to qualitative changes to the strong coupling mass, which plateaus for strong binding, demonstrating the “light pair” regime. The mass reduces with decreasing V until the pairs unbind. Importantly, pairs related to these light asymptotes at strong coupling also remain light at weak binding. Panel (a) shows how the “superlight” effect, where pairs are *lighter* than the unbound particles is seen for both tetragonal cases with $t'/t = -0.45$. Moreover, in both of those cases, only a small V is required to bind pairs. The d -symmetric pairs found in the square lattice persist in the tetragonal lattice for the case of $V'/V = 0, t'/t = -0.45$, whereas when $V'/V = 1$ pairs have an s -symmetry. Out-of-plane masses are large, for the tetragonal lattice, as shown in the inset of Panel (a). The bare mass m_0 for a particle for each lattice is given in Table 1.

The middle row (panels d-f) of Fig. 5 shows the inverse pair radius, calculated as the inverse root mean square (RMS) pair radius. The radius diverges at small V near the pairing threshold. For the smallest V no pairs are formed. In the strong attraction limit ($V \rightarrow -\infty$) the radius converges to small values of order d_{NN} if only V is present, or between d_{NN} and d_{NNN} if V' is also present. In the tetragonal case, pairs are confined to planes and the out-of-plane radius is small (much less than a lattice spacing), as shown in the inset of Panel (d). We note that similar masses and radii are found for the chain (not shown here).

The close-packing critical temperature $k_B T^*/t$ defined in Eq. 3 is shown in Panels (g)-(i) of Fig. 5, and has a maximum value at small to moderate V depending on lattice and model parameters. We select an estimate of Ω'_p that limits scattering by accounting for the exponentially decaying tails of the pair wavefunction ($\Omega'_p \sim (\alpha R_{\perp}/b + 1)(\alpha R/a + 1)^2$, where R_{\perp} (R_{\parallel}) is the out-of-plane (in-plane) radius. For cubic lattices, $R_{\perp} = R_{\parallel} = R$ and $b = a$). We note that the location of the maximum in T^* is insensitive to the value of α . For the results shown here we selected $\alpha = 5$, to ensure that the exponentially decaying pair tails have very small overlap and scattering is small (essentially eliminating many body effects). A key feature is a maximum in T^* that occurs between $V \sim -0.1W_0$ and $V \sim -3W_0$ and is typically broad. The maximum occurs for the following reason: In the low attraction limit, T^* is dominated by pair radius, with smaller radius leading to higher potential transition temperatures. As attraction increases the pair volume collapses to a minimum before the mass approaches its strong coupling limit, and at this point T^* is maximal. The maximum occurs at small V for tetragonal cases, since the threshold V for binding is small. Depending on whether the strong attraction limit has light pairs, further increase in V either increases the pair mass, which causes a corresponding gradual decrease of T^* , or the pair mass plateaus, in which case T^* also plateaus. For the parameters shown, the overall height of the maximum ranges from $T^* \sim 0.02t$ to $\sim 0.2t$. Large out-of-plane mass in the tetragonal case limits T^* . These calculations illustrate the potential of real-space superconductivity to reach high critical temperatures if scattering between pairs is small.

One must supplement the estimates of the preceding paragraph with a discussion of *phase separation*. Rigorous analysis of pair-pair interaction at the model level [18] indicates that real-space pairs can form clusters when V exceeds the pairing threshold by a few ts , i.e., a fraction of W_0 . This implies that the physical part of Fig. 5 is limited to a narrow interval of V close to the binding threshold. In this interval, pair mass is barely above $2m_0$, but the volume consistently decreases and T^* increases with V as a result. This suggests a route to higher critical temperatures: increase V to make the pairs more compact but without going over the phase separation threshold. The anisotropy in the tetragonal lattice case may be important in this regard, since deep binding occurs for very small V reducing the risk of crossing the phase separation threshold.

The presence of t' and V' lead to reductions in the mass, and there is a range of parameters for which pairs are both small and light with masses of just a few single particle masses and radii of a few lattice spacings. Figs. 6 and 7 supplement the data of Fig. 5 by showing dependence of mass, radius and T^* on V' and t' at a fixed value of $V = -W_0$. Panels (a)-(d) of Fig. 6 show the pair mass and Panels (e)-(h) show the inverse radius. We note a jump around $t' \sim 0.4$ in Panels (a),(d),(e) and (h) where the ground state changes from s to d symmetric character in the tetragonal lattice. Otherwise, the plots show smooth interpolation between the four corner cases, demonstrating a lack of special points in the $t' - V'$ parameter space, and showing that the corner cases are representative of the physical picture above. The inverse radius is typically smallest (radius is largest) for $V' = 0$ and $t'/t = 1$. In the case of the SC lattice (Panel (f)), the zero inverse radius shows that no bound pair is found in that corner of the plot. In the tetragonal case, pairs are bound in-plane, and in the direction perpendicular to the plane, radius is small and the mass is large, because pairs have to break to move be-

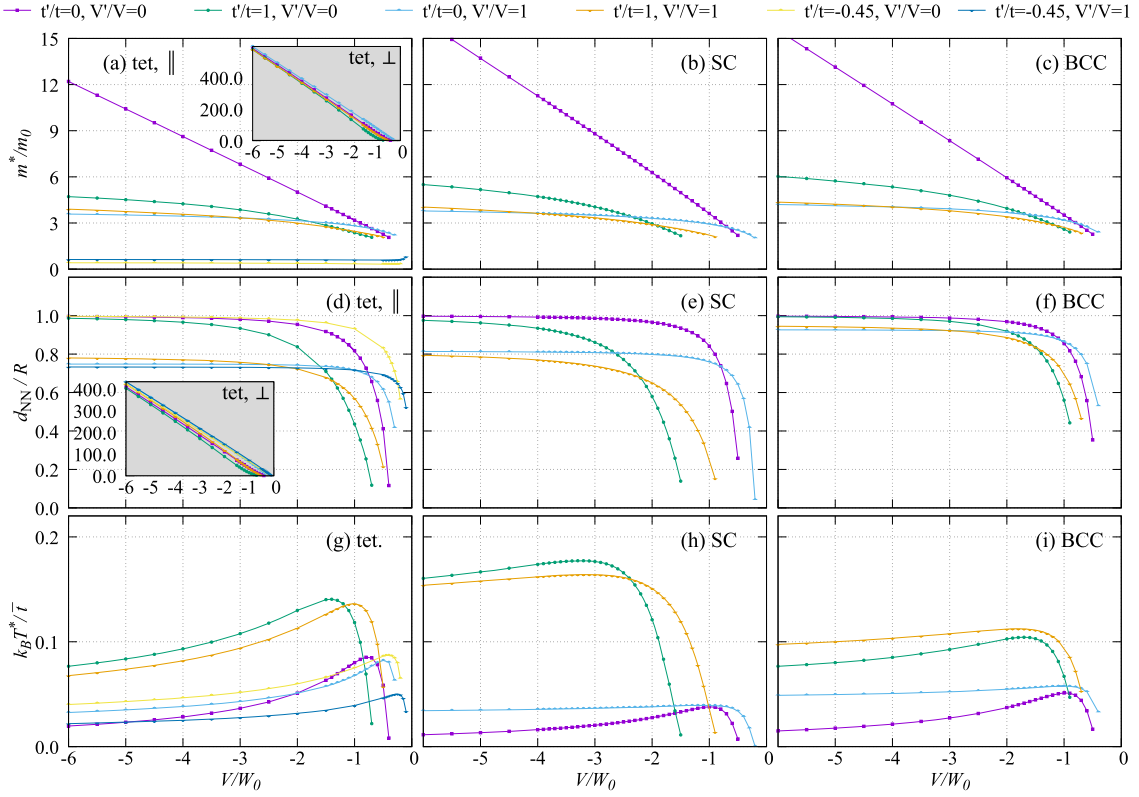


Fig. 5. Scaling of mass, inverse radius, and T^* into the deep potential limit for a subset of the parameter space. The presence of t' or V' leads to light behavior at deep coupling. Such pairs remain lighter in the weak binding limit with small V , and higher predicted transition temperatures also persist to weaker binding. For the tetragonal cases, $t_{\perp}/t = 0.04$. For strong binding, the radius tends to $R \approx a$ and for the tetragonal case, $R_{\perp} \rightarrow 0$ for the parameters shown. Lines are a guide to the eye.

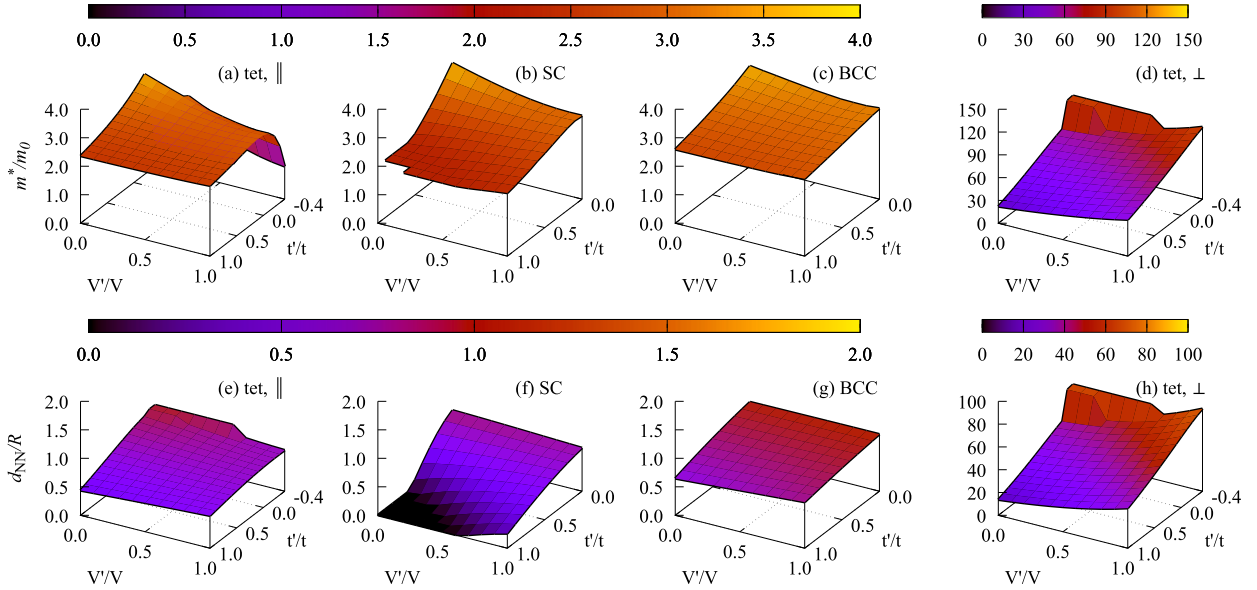


Fig. 6. Mass m^*/m_0 and inverse radius a/R for a range of parameters (V'/V and t'/t) for fixed $U = 2W_0$ with $V = -W_0$. For the tetragonal case, $t_{\perp} = 0.04t$. Panels (a) to (d) show the dependence of the pair mass on V' and t' . Panels (e) to (h) show inverse pair radius. The parameter space is smooth, with the exception of a discontinuity at the boundary between d - and s -pairing.

tween planes. Moreover, Panel (a) shows the superlight regime of $t' < t$, where pairs are lighter than their component particles. Fig. 7 shows that close packing transition temperatures vary smoothly, with the exception of the tetragonal lattice where d -symmetry pairs are associated with a small and discontinuous increase in transition temperature as levels cross.

5. Discussion and conclusions

In this paper we investigated the factors affecting the masses of real-space bound pairs in models with short-range phenomenological attraction V . We showed that inclusion of next-nearest-neighbor (NNN) hopping t' limits m^* to be of the order of bare particle mass m_0 on sev-

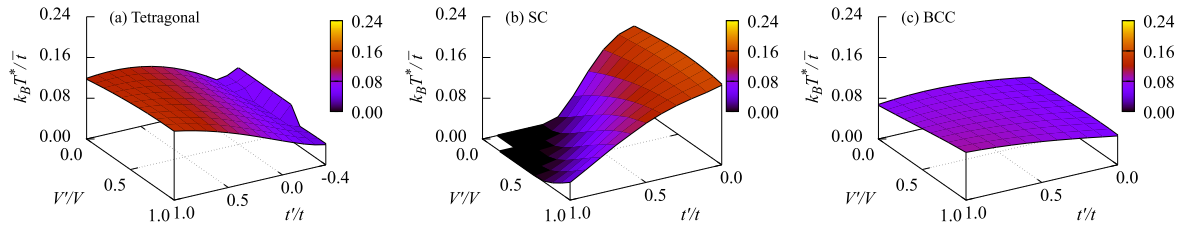


Fig. 7. Plot of close packing (maximum) transition temperature from Eqn (1) as a function of V'/V at varying t' . For the tetragonal case with $t_{\perp} = 0.04$, d -symmetry pairs are associated with a small increase in transition temperature. From left to right: (a) tetragonal lattice, (b) SC lattice, (c) BCC lattice.

eral common lattices. The pairs remain *light* even in the strong-coupling limit because they continue moving via resonant configurations without ever breaking the most attractive bond. In cases of tetragonal lattices where t and t' are of opposite signs, bound pairs can be *superlight*, i.e., lighter than one free particle, $m^* < m_0$. This effect occurs because the negative interference between NN and NNN hopping produces a relatively large m_0 , whereas coupling between particles disrupts the interference and liberates the pair.

Light and superlight pairs are essential for real-space superconductivity because the BEC temperature scales inversely with m^* . The small and V -independent mass offers a recipe for high T_{BEC} : systematically increase V to produce more compact pairs. The latter enable higher packing densities and hence higher T^* s. The model calculations of Section 4 show that the close-packed temperatures can be of the order of tenths of \bar{t} , which in physical units amounts to hundreds of degrees. However, this mechanism is limited by phase separation which occurs at intermediate V . Thus, practically achievable T^* are smaller. Nonetheless, increasing V is a viable route to search for new high-temperature superconductors.

In cuprates, $\bar{t} \sim 0.05$ eV (since $t_{\parallel} \sim 0.1$ eV [56] for holes near half filling and estimating $t_{\perp} \sim 0.04$ eV) so for the cuprates with highest $T_c \sim 133$ K, $k_B T_c / \bar{t} \sim 0.15$. Since the pair size in the cuprates is estimated to be 3-10 unit cells from measurements of the upper critical field [57], the transition temperature is consistent with a close packing picture. Moreover, d -symmetric pairs form condensates with a d -wave character [58]. Phonon mediated momentum space pairing can also lead to d wave superconductivity: d -wave superconducting order parameters can also be found when large U and attractive V with long tails are present [36] and can also be found in dynamical cluster approximation (DCA) studies of the Holstein model of local electron-phonon coupling [59].

We note that the fulleride superconductors are characterized by an unusually high ratio of $k_B T_c / t$. The BCC fulleride Cs_3C_{60} has the record transition temperature $T_c = 38$ K [54]. Models including next-nearest neighbor hopping and interaction may be particularly relevant to BCC lattices, where the ratio of NN to NNN distances is particularly large: $d_{\text{NN}}/d_{\text{NNN}} \sim 0.866$. This ratio is closer to unity in BCC lattices than in any other Bravais lattices. Thus we expect that t'/t and V'/V is larger than in other Bravais lattices. For fullerides, the approximate hopping value ranges from $t \sim 0.02$ eV to 0.04 eV (based on the width of 0.61 eV of the t_{1u} band [60] and using a range of $t \lesssim t'$), so $k_B T_c / t \sim 0.1$ is consistent with the close packing estimates here. We advise that further study of many-body effects (such as phase separation) would be required to obtain values for transition temperatures beyond the close-packing estimates and defer this for future work.

CRedit authorship contribution statement

G.D. Adebajo: Writing – review & editing, Writing – original draft, Methodology, Investigation, Formal analysis, Conceptualization. **J.P. Hague:** Writing – review & editing, Writing – original draft, Supervision, Methodology, Investigation, Formal analysis, Conceptualization. **P.E. Kornilovitch:** Writing – review & editing, Writing – original draft, Supervision, Methodology, Investigation, Formal analysis, Conceptualization.

Declaration of competing interest

The authors declare no competing interests.

Data availability

Data can be found on the ORDO repository. The DOI is: <https://doi.org/10.21954/ou.rd.23653647>.

Appendix A. Supplementary material

Supplementary material related to this article can be found online at <https://doi.org/10.1016/j.physleta.2024.129474>.

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