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Fermion pair formation and condensation in extended Hubbard models in body-centered-cubic optical lattices

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We investigate the formation and condensation of fermion pairs in cold atom quantum simulators for extended Hubbard models (UV models) with body center cubic (BCC) optical lattices, predicting small and light pairs with Bose–Einstein condensation (BEC) temperatures up to the order of 100 nK. Pair mass, radius, and binding conditions are calculated, and then used to compute transition temperatures. We predict that: (a) local pairs can form in BCC optical lattices; (b) for particular cases where the onsite U and intersite V are attractive with similar size, the pairs are both small and light; and (c) that transition temperatures could be as high as 100 nK (50 nK) for 6Li atoms in blue (red) BCC optical lattices. Beyond the application to pairs on BCC optical lattices, we expect our results to be relevant to strong-coupling BCC superconductors.

I. INTRODUCTION

A major success of cold atom quantum simulators formed using optical lattices is the ability to probe models of strong correlation in clean and well-controlled systems. Quantum simulators offer the possibility to implement models of strong correlation, in a way that cannot be achieved in condensed matter. For example single band Hubbard models can be implemented without the complications of interactions between multiple electronic bands. Several milestones have been achieved using cold atoms in optical lattices, including observations of Mott transitions in repulsive Hubbard model. The interactions in cold atom quantum simulators can be tuned such that attractive Hubbard models can be studied, allowing local pairs to be observed. To the best of our knowledge, the low temperature condensation of local fermion pairs has not yet been achieved.

It is the goal of this article to discuss the conditions under which condensation of fermion pairs could occur in cold atom quantum simulators with BCC lattices. In addition to studying the conditions for pairing and condensation in BCC optical lattices, we are also motivated by the observation of superconductivity with high transition temperature (38K) in BCC Au-Cu compound. Optical lattices with BCC structures can be formed using arrays of four laser beams. The aim of this paper is to explore local pairing and condensation originating from strong correlations in BCC optical lattices. The condensation of fermion pairs in cold atom quantum simulators would represent an important step towards understanding of unconventional superconductivity, so finding ways to observe high BEC transition temperatures of fermion pairs in optical lattices is of interest. We therefore wish to investigate whether the high temperature condensates of the BCC superconductors are also found in optical lattices.

A simple extension to the Hubbard model, known as the extended Hubbard model, or (in the low density limit) UV-model includes an onsite Hubbard U and an intersite interaction V. The UV Hamiltonian is defined as:

\[ H = \sum_{\langle n, a \rangle} t_a \hat{c}^\dagger_{n+a, \sigma} \hat{c}_{n,\sigma} + U \sum_n \hat{\rho}_{n\uparrow} \hat{\rho}_{n\downarrow} + \sum_{\langle n, a \rangle} V \hat{\rho}_{n+a} \hat{\rho}_n \]

where \( \hat{c}_{n,\sigma} \) (\( \hat{c}^\dagger_{n,\sigma} \)) creates (annihilates) an atom of spin \( \sigma \) at site \( n \), \( \hat{\rho}_n = \hat{\rho}_{n\uparrow} + \hat{\rho}_{n\downarrow} \), where \( \hat{\rho}_{n\sigma} \) is the number operator for atoms on site \( a \) with spin \( \sigma \), \( V \) the intersite lattice vector, \( t_a \) is the intersite hopping, \( U \) is the onsite interaction and \( \hat{\rho}_n \) is the number of fermions on site \( n \). The site-local Hubbard \( U \) is typically present in any superconductor with low kinetic energy. Since Coulomb repulsion is typically small between sites due to screening (especially in 3D) an effective intersite attraction or repulsion could arise due to phonons, spin fluctuations or other exotic pairing mechanisms.

In optical lattices, very large \( U \) and \( V \) with both attractive and repulsive interactions can be achieved relative to those in condensed matter systems. \( U \) can be changed by orders of magnitude by modifying the magnetic field at the Feshbach resonance. Both polar molecules and Rydberg states are highly polarizable, and therefore can have sizable long range interactions. There are several ways in which \( V \) can be tuned. The simplest is by modifying the principal quantum number of Rydberg states. The dipole-dipole (van der Waals) interaction between Rydberg states increases with the fourth (eleventh) power of the principal quantum number \( n \), leading to a high level of control over the size of long range interaction. By combining Rydberg states with Feshbach resonances, a UV model could be realized on an optical lattice.

In this paper we study the UV model to predict the signatures of local pairing in BCC optical lattices, which to our knowledge have not been studied in this context.
We discuss the properties of local pairs formed in a BCC optical lattice. We calculate the critical pair attraction strength \( U_c \) (\( V_c \)) required for the formation of on-site (intersite) pairs. Pair dispersion, mass and size are determined. We estimate the BEC transition temperature for local fermion pairs. The paper is organized as follows: We describe the methodology used to solve the UV model in the low density limit (Sec. II). In Sec. III we report the properties of local pairs formed in BCC lattices. We conclude this work with discussion in Sec. IV.

II. METHODOLOGY

In this section, we describe the steps required to obtain solutions to the UV model with low particle density. We study the UV model with two spin-\( \frac{1}{2} \) fermions. We solve Hamiltonian \((\vert)\) by constructing a real-space Schrödinger equation. The two-body wave function \( \Psi(n_1, n_2) \) must satisfy the equation:

\[
\sum_a t_a \left[ \Psi(n_1 + a, n_2) + \Psi(n_1, n_2 + a) \right] + \sum_a \hat{V}_a \delta_{n_1 - n_2, a} \Psi(n_1, n_2) = E \Psi(n_1, n_2)
\]

where the interaction terms have been combined into a single function (i.e. \( \hat{V}_{a=0} = U \) and \( \hat{V}_{a \neq 0} = V_a \) as in \((\vert)\)), \( E \) is the total energy of the system.

Equation \((\vert)\) can be solved as follows. We construct the wave function in momentum space using a Fourier transform

\[
\psi_{k_1, k_2} = \frac{1}{N} \sum_{n_1, n_2} \Psi(n_1, n_2) e^{-ik_1 n_1 - i k_2 n_2}
\]

with \( N \) being the total number of lattice points. Then, substituting Equation \((\vert)\) into Equation \((\vert)\), we obtain:

\[
(E - \varepsilon_{k_1} - \varepsilon_{k_2}) \psi_{k_1, k_2} = \frac{1}{N} \sum_{aq} \hat{V}_a e^{iqk_1 a} \psi_{q, k_1 + k_2 - q}
\]

with

\[
\varepsilon_k = \sum_a t_a e^{i k a}
\]

being the one-particle energy dispersion of the model, where \( k \) is the particle’s momentum vector.

We define

\[
\Phi_a(k_1 + k_2) = \Phi_a(P) \equiv \frac{1}{N} \sum_q e^{iqP} \psi_{q, P - q}
\]

where \( P = k_1 + k_2 \) is the total momentum of the particle pair. By using this definition, Equation \((\vert)\) can then be rewritten as

\[
\psi_{k_1, k_2} = \sum_a \hat{V}_a \frac{e^{-ik_1 a}}{E - \varepsilon_{k_1} - \varepsilon_{k_2}} \Phi_a(P)
\]

and finally this expression is substituted into Equation \((\vert)\) which becomes

\[
\Phi_a(P) = - \sum_{a'} \hat{V}_{a'} L_{aa'}(E, P) \Phi_{a'}(P)
\]

where the Green’s function, \( L_{aa'}(E, P) \), is determined from the following sum,

\[
L_{aa'}(E, P) = \frac{1}{N} \sum_q e^{i (a - a') q - \varepsilon_{P - q}}
\]

The set of linear equations \((\vert)\) are solved by

\[
\text{det} \left[ -\hat{V}_{a'} L_{aa'}(E, P) - \delta_{aa'} \right] = 0,
\]

which determines the system energy \( E(P) \) as a function of the total momentum of the pair. Equations \((\vert)\)–\((\vert)\) form the general solution of the two-body problem.

Equation \((\vert)\) generates a \((z + 1)\) square matrix, where \( z \) is the coordination number of the lattice. Hence, we would expect a \((9 \times 9)\) matrix for BCC lattices. It is useful to apply a symmetrized approach which reduces the matrix size as we will demonstrate here. The symmetrization improves numerical stability and speed.

The two-particle wave function has to be symmetric or anti-symmetric under spatial exchange \( \Psi(n_1, n_2) = \pm \Psi(n_2, n_1) \) which translate to singlet (+) and triplet (−) spin states. To express the symmetrized wave functions, we permute \( k_1 \rightarrow k_2 \) in \((\vert)\) and then we add/subtract the resulting equation from the unpermuted version of Equation \((\vert)\). Doing this yields:

\[
(E - \varepsilon_{k_1} - \varepsilon_{k_2}) \psi_{k_1, k_2} \pm \psi_{k_2, k_1} = \frac{1}{N} \sum_{aq} \hat{V}_a \left\{ e^{i (q-k_1) a} \pm e^{i (q-k_2) a} \right\} \psi_{q, k_1 + k_2 - q}
\]

We can rewrite the (anti-)symmetrized pair wave functions on the left-hand-side of Equation \((\vert)\) as

\[
\phi_{k_1, k_2}^+ = \psi_{k_1, k_2} \pm \psi_{k_2, k_1},
\]

where \( \phi_{k_1, k_2}^+ \) and \( \phi_{k_1, k_2}^- \) respectively are the singlet and the triplet wave functions. So, Equation \((\vert)\) becomes

\[
(E - \varepsilon_{k_1} - \varepsilon_{k_2}) \phi_{k_1, k_2}^+ = \frac{1}{N} \sum_{aq} \hat{V}_a \left\{ e^{i (q-k_1) a} \pm e^{i (q-k_2) a} \right\} \psi_{q, k_1 + k_2 - q}
\]

The summation over the lattice vector, \( a \), in Equation \((\vert)\) can be split into two sets \( \{a_+\} \) for singlets, and...
{a_+} for triplets) which thus allows us to write the right-hand side of the equation in terms of \( \phi^\pm \) instead of \( \psi \).

To do this, we define \( \{a_+\} \) and \( \{a_-\} \) to be a set of near-neighbor lattice vectors, and also include the zero vector in the case of singlets:

\[
\{a_+\} = \{(0,0,0), \begin{pmatrix} b \\ b \\ b \end{pmatrix}, \begin{pmatrix} -b \\ b \\ b \end{pmatrix}, \begin{pmatrix} b \\ -b \\ b \end{pmatrix}, \begin{pmatrix} b \\ b \\ -b \end{pmatrix}, \begin{pmatrix} b \\ -b \\ -b \end{pmatrix} \}
\]

\[
\{a_-\} = \{(b \ b \ b), (b \ b \ b), (b \ b \ b), (b \ b \ b), (b \ b \ b), (b \ b \ b) \}
\]

where \( b \) is the lattice constant. It is important that neither set contains pairs of members that are related by inversion, but otherwise there is some freedom in the choice of selecting the new vectors. Then,

\[
(E - \varepsilon_{k_1} - \varepsilon_{k_2}) \phi^{\pm}_{k_1 k_2} = \frac{1}{N} \sum_{q a_z} \hat{V}_{a_z} \left\{ e^{i(q-k_1) a_z \pm} \pm e^{i(q-k_2) a_z} \right\} \phi_{a_z k_1 + k_2 -q}^\pm
\]

Note that the primed summation in Equation (16) above means a factor of \( \frac{1}{2} \) should be included for the case \( a_+ = 0 \). Following similar steps in Equations (6) – (9), we obtain

\[
\Phi_{a_z}^\pm (P) = -\sum_{a_z} \hat{V}_{a_z} L_{a_z a_z}^\pm (E, P) \Phi_{a_z}^\pm (P)
\]

where,

\[
L_{a_z a_z}^\pm (E, P) = \frac{1}{N} \sum_{q} e^{i(qa_z - a_z')} \pm e^{i(qa_z - (P-q)a_z')}
\]

Equations (13) to (18) are used to obtain the (anti)-symmetrized solutions.

III. RESULTS

In this section, we study the properties of pairs in the UV model on the BCC lattice including the total energy, pairing diagram, dispersion, pair mass, radius and finally we estimate the BEC transition temperatures. We focus our attention mainly on the s-states. However, we will briefly discuss other pairing symmetries (p-, d- and f-states).

A. Total Energy

The transition from an unbound (two free particles) to a bound state occurs at a critical value of \( U \) and \( V \) which can be identified using the pair energy. Figure [1] shows plots of the total energy for different pair symmetries. The flat region of the curve corresponds to the total energy of two unbound particles (the threshold energy \( E_{Th} = -2W \), where \( W = 8\varepsilon \) is the half-bandwidth). The energy drops below \(-2W\) as the attraction gets stronger indicating that a bound pair has been formed. Pairs are highly stable (well bound) at large attractive coupling. The p- and d-states are both three-fold degenerate, and s- and f-states have degeneracy 1.

Fig. [1a] and [1b] respectively, show a shift in the critical \( U (V) \) required to form stable s-symmetric pair when modifying the intersite (on-site) repulsion. A stable s-symmetric pair is guaranteed to form if \( U \leq -2W \) or \( V \leq -0.8858W \) (more details in Sec. III B and in the Appendix). For infinite attraction, the particles form deep, localized pairs and the energy of all the pairing symmetries converge, i.e. \( E \to -|V| \) or \( E \to -|U| \), (inset plots in Fig. [1]). For non-s pairing symmetries, the critical interaction is independent of \( U \).

B. Binding Diagram

By identifying the point at which the total energy drops below \(-2W\), the binding diagram at \( P = 0 \) can be constructed (Fig. [2]). A pair of free, unbound particles with zero total momentum has energy \( E = -2W \). So, the threshold energy is \( E_{Th} = -2W \). For any pairing symmetry with a node at the origin, binding is independent of \( U \).

Within the \( U-V \) parameter space, pairing is found at large, attractive \( U/W \) and/or \( V/W \). The kinetic energy of the particles on the BCC optical lattice is large (relative to 1D, 2D and simple cubic lattices) due to the larger coordination number and, as a result, \( U \) or \( V \) must be large and attractive in order to form a bound state. The critical binding values \( U_c \) and \( V_c \) are derived in the Appendix. The critical attraction can be determined via

\[
V_c (U) \leq \frac{UL_0 - 1}{UL_0C - C - 8UL_1^2}
\]

where \( L_0 = -K_0^2/(4\pi^2) \), \( L_1 = L_0 + 1/(16t) \), \( C = 8L_0 + 1/(2t) \) and \( K_0 = K(1/\sqrt{2}) \) is the complete elliptic integral of the first kind. For a negative-\( U \) Hubbard model with no intersite interaction, the critical binding is found to be \( U_c (V=0) \approx -1.4355W \). Similarly, \( V_c (U=0) \approx -0.6358W \) is required to bind particles when the onsite repulsion is absent. As noted in Section IIIA an intersite strength \( V_c (+\infty) \approx -0.8858W \) is sufficient to maintain a bound state even if the Hubbard repulsion is infinite while \( U_c (V \to +\infty) \approx -2W \). Figure [2] also shows the binding thresholds of the p-, d- and f-states respectively occurring at quite large intersite attractions, i.e. \( V_{p} \approx -1.5828W \), \( V_{d} \approx -1.8804W \), \( V_{f} \approx -1.9639W \).
FIG. 1. Ground state energy of pairs. The critical Hubbard attraction for $V = 0$ is $U_{\text{Hub}}(0) = -1.4355W$ and for $U = 0$ $V^c(0) = -0.6358W$. The $p$-, $d$- and $f$- states are independent of $U$ i.e. change in $U$ only affects the total energy of the $s$-state. For large onsite, $|U| \gg |V|$, $t$ (intersite), $|V| \gg |U|$, $t$ attraction, $E \rightarrow -|U|$ ($E \rightarrow -|V|$) for all the states (inset). The corresponding symmetry of each state is also indicated.

C. Dispersion

Estimation of the pair condensation temperature requires the pair effective mass at the $\Gamma$ point, for which it is necessary to calculate the dispersion (pair energy at non-zero momentum). Examples of the dispersion for various $U$ and $V$ are presented in Fig. 3. The dispersion for two free particles is shown for comparison, and lies in the range $-2 \leq E/W \leq 2$. The singlet $s$-symmetric pair has the lowest energy around the Brillouin zone (BZ) center (i.e. $\Gamma$ point) but this is not the case at other high symmetry points. The band structure gets narrower as the intersite attraction, $V$, increases, consistent with an increase in the effective mass. There is a high level of degeneracy on the $\Gamma$-$H$ line. Pairs on the BCC lattice have the following symmetries: $A_1g(s)$, $T_{1u}(p_x, p_y$ and $p_z)$, $T_{2g}(d_{xy}, d_{xz}$ and $d_{yz}$) and $A_{2u}(f)$.

Additionally, the dispersion (Fig. 3) provides further insights into pair stability at different attractive $U$ and $V$ values. Along the $\Gamma$-$H$ line, all states with the same symmetry class are degenerate. The highest excitation occurs at the $H$ point where $P$ is maximum and all states have the same energy. The $s$-state becomes completely independent of the Hubbard $U$ repulsion (Fig. 3) panels (a) and (b)), and as with other pairing symmetries, the total energy of the pair tends to the intersite attraction (i.e. $E = V$). $V$ can be vanishingly small (very weak attraction, $V \rightarrow 0(\sim)$) and still form an $s$ pair (Fig. 3c). In the $H$-$P$ direction, one $d$-state has the highest energy...
FIG. 3. [Color online] Examples of dispersions with increasing intersite attraction and onsite repulsion. The solid line is the $s$-state, the lines with crosses are the $p$-states, the dashed lines are the $d$-states, the line with circles is the $f$-state and the line with triangles represents the energy of two free particles. All the bound states are degenerate at the H point and their energy is equal to $V$. The $s$-state and one of the $p$-states have very close energy along the H-P line. Away from the BZ center, the $s$-state does not necessarily have the lowest energy and the $f$- and $p$-state dispersions cross. and is well-separated from the other two degenerate $d$-states. The $f$-state becomes degenerate with two $p$-states while the $s$-state and the third $p$-state are close in energy.

At point $P$, the three $d$-states are degenerate, with an energy lower than their $\Gamma$ point energy, and all antisymmetric states are degenerate too. $d$-wave pairs are the most stable at points $P$ and $N$. One of the $d$-states reaches a minimum at $N$ and the remaining two $d$-states on the $H$-$P$ line. Along $P$-$N$, two $p$-states are degenerate whereas $f$ and the third $p$ remain degenerate.

FIG. 4. [Color online] Dispersion of $s$-state only. At the symmetry point $H$, the pair (i) shows no effect of repulsive $U$ (ii) can still be formed at very weak attraction [panel (c)] and has an energy $E = V$ even if $U$ is infinite, in contrast to the critical attraction, $V_c$ (refer to Section III B, Fig. 2), required at the $\Gamma$ point.

D. Pair Mass

Pair mass can be calculated from the second derivative of the dispersion within the standard effective mass approximation, as,

$$[m^{*}]^{-1} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial P_i^2}. \quad (20)$$

The resulting effective masses can be seen in Fig. 5.

Weakly bound pairs are light (about $2m_0$ when pair energy approaches the threshold energy $E^{(th)}$) and get heavier as the binding attraction is increased. (Note that $m_0 = \hbar^2/(2b^2t)$ is the bare effective mass of a free particle.)

Pairs with strong intersite attraction are much lighter in comparison to their counterpart pairs with strong onsite attraction (for example, compare the masses at $U = -20W$ in Fig. 5(a) and at $V = -20W$ in Fig. 5(b)). This occurs since large attractive $U$ confines the pair to the same site thereby suppressing the probability of particles hopping to other sites (the suppression is even greater when $V$ is repulsive).

When $U$ and $V$ are both attractive and of similar magnitude, we find superlight pairs (minima in Figs. 5(a) and 5(b)). These correspond to the situation where particles can move without passing through a high energy intermediate state. Figure 5 demonstrates this superlight process on the optical lattice where the pair travels through the lattice in a crawler motion. The process of movement can be summarised in three main steps: (i) the particles interact via attractive $V$; (ii) one particle hops to interact with the other via an attractive $U$; (iii) any of the particles can hop so interaction is intersite again. While it moves around, the pair’s total energy remains unchanged in all the configurations.
FIG. 5. [Color online] The pair mass expressed in unit of a free particle mass. $m_0 = \hbar^2 / (2b^2 t)$ is the bare mass of one free particle on the BCC optical lattice.

E. Pair Radius

The effective radius has been calculated using the relation

$$\langle r^* \rangle = \sqrt{\frac{\sum_n n^2 \Psi^*(n_1, n_2) \Psi(n_1, n_2)}{\sum_n \Psi^*(n_1, n_2) \Psi(n_1, n_2)}}, \tag{21}$$

where $n = n_1 - n_2$ is the spatial separation between the particles and $\Psi(n_1, n_2)$ is the pair wave function.

Figure 6 shows the pair radius. Near the threshold energy ($E \to E^\text{Th}$), the particles form a large pair: a consequence of the delocalization of the pair wave-function. At intermediate $U$ and $V$ (both attractive), the pair’s size is on the order of the near-neighbor distance, $a$ (Fig. 7). In a pairing scenario where $V$ is fixed and $U$ is tuned to be highly attractive, the two bound particles are localized and held on the same site. The pair is also local for large intersite attraction but the size levels off to the nearest neighbor distance at large attractive $V$. By local, we mean bound pairs that are not larger than the lattice constant.

F. Transition Temperature

Bose-Einstein condensation may take place on the optical lattice for well separated, weakly interacting, local pairs at low temperature. The transition temperature can be approximated as:

$$T_{\text{BEC}} = \frac{3.31 \hbar^2}{m^*_p b k_B (n_b \Omega_{\text{site}})^{2/3}}, \tag{22}$$

where $m^*_p$ is the pair mass, $n_b$ is the number of pairs per lattice site, $\Omega_{\text{site}} = b^3 / 2$ is the volume of the Wigner–Seitz cell for a BCC lattice, and $k_B$ is Boltzmann’s constant. Note that $n_b$ is the number of pairs per site and should not be confused with the particle density, which is $n_b / \Omega_{\text{site}} = 2 n_b / b^3$.

Since the pair density is a free parameter, controlled by the experimenter, one could imagine a very high $T_{\text{BEC}}$ could be achieved by increasing the pair density. There are two reasons why this is not possible. Firstly, since we are dealing with pairs of fermions, it is not possible to have $n_b > 1$ since that would require more than two fermions per site which is incompatible with Pauli exclusion. The second is more subtle - if we are to treat pairs of fermions as bosons, their pair wave-functions should not overlap strongly, otherwise corrections would be needed to Equation (22), and this leads to an upper bound on $n_b$. 
FIG. 7. [Color online] Effective radius for various $U$ and $V$.

The thin solid horizontal lines represent the nearest neighbor distance $a = \sqrt{3}b/2$ on a BCC lattice. Note that the radius diverges at low attraction. A shoulder forms in the curves when $U \sim V$.

The upper bound of $n_b$, which we shall denote $n_b^*$, takes into account the pair size via $2n_b^*/b^3 \approx 3/(4R^3)$, where $R' = \alpha r^*$, and $\alpha$ is sufficiently large that the Gaussian tails of the pair wave function are small. Taking into account Pauli exclusion, we estimate the upper bound on $n_b$ to be

$$n_b^* \approx \begin{cases} \frac{3b^3}{2} & \text{when } \frac{3b^3}{2n_b^*} < 1 \\ 1 & \text{otherwise} \end{cases}$$

(23)

We suggest taking $\alpha = 5$ to ensure that the Gaussian tails of the wave functions are small, and thus the overlap between evenly spaced particles is also small. At higher densities we expect that pairs will start to interact and overlap and that would cause the transition temperature to level out and then fall as pairs begin to interact strongly (and potentially clusters form$^{13,15}$).

A four laser scheme can be used to construct a BCC optical lattice (see scheme A from Table 1 of Ref. 7), for which $b/\lambda = \sqrt{3}/2$. Then $\Omega_{\text{site}} = \lambda^3\sqrt{3}/2\hbar$, so we can re-write (22) in terms of the laser beam wavelength $\lambda$, as

$$T_{\text{BEC}}^* = n_b^{*2/3} \frac{701\hbar^2}{m\lambda^6 k_B \lambda^2}. \quad (24)$$

(in our notation, $T_{\text{BEC}}^*$ is calculated at fixed $n_b$, whereas our estimate of the the maximum possible transition temperature, $T_{\text{BEC}}^*$, using the maximum boson occupation $n_b^*$). In the following, we assume either a red laser with wavelength 650 nm or a blue laser with wavelength 450 nm, and fermionic $^6\text{Li}$.

With these considerations, we estimate a maximum $T_{\text{BEC}}^* = 110 \text{ nK}$ (Fig. 8). Figure 8 shows how $T_{\text{BEC}}^*$ varies with $U$ and $V$. In panels $a$ and $b$, $T_{\text{BEC}}^*$ initially rises as attraction increases, before reaching a maximum, after which it declines. At weak coupling, both mass and radius decrease as the superlight regime is approached, leading to an increase in $T_{\text{BEC}}^*$. The mass then reaches a minimum, while the radius continues to decrease, and overall $T_{\text{BEC}}^*$ continues to rise. The peaks occur at $n_b \sim 1$. In the region of greatest attraction, $n_b^* = 1$ and the transition temperature $T_{\text{BEC}}^*$ declines as the mass gets heavier. In panels (c) and (d) the transition temperature quickly rises to a peak on binding, and then decreases on further increase in attraction.

We also explore how transition temperatures vary for fixed $n_b$, showing how there is a peak associated with the superlight behavior (Fig. 9). The colored lines surrounded by the gray-shaded regions indicate cases where the value of $n_b$ is compatible with the conditions on pair overlap. In order to probe the $T_{\text{BEC}}$ of non-overlapping pairs with superlight characteristics in an optical lattice setting, the number of pairs has to be low (say $n_b \sim 0.0015$). In that case, the superlight behavior occurs at roughly 10 nK.

IV. DISCUSSION AND CONCLUSIONS

In this paper, we have investigated the formation and condensation of fermion pairs in cold atom quantum simulators for extended Hubbard models ($UV$ models) with BCC structure, making calculations of BEC transition temperatures and other pair properties, and predicting transition temperatures up to $T_{\text{BEC}}^* \sim 100 \text{ nK}$. This is motivated by: (1) a lack of calculations regarding pairing on BCC optical lattices; (2) BCC superconductors within which fermion pair condensation has been found at high
FIG. 8. [Color online] Plots of the transition temperature taking the pair size $R'$ and the number of boson per site $n_b$ into consideration. Key features in panels (a) and (b) are (i) Solid (purple) curves: $T_{\text{BEC}}^*$ initially increases as pairs bind, which is related to the rapid decrease in pair radius in addition to a rapid decrease in pair mass due to the proximity of the superlight regime. (ii) Once the superlight regime $U = V$ is passed, mass starts to increase, but radius decreases rapidly, leading to an overall increase in transition temperature. (iii) Dotted (green) curves: As pairs become more strongly bound, the pair radius falls below one lattice spacing and bosons act as hard core ($n_b = 1$). Then $T_{\text{BEC}}^*$ decreases since the effective radius cannot decrease, but the mass continues to increase. In panels (c) and (d), the transition temperature quickly rises to a peak on binding, and then decreases on further increase in attraction.

temperatures; and (3) the desire to observe fermion pair condensation in optical lattice systems. We have solved the two particle Schrödinger equation to compute pair mass, radius, transition temperatures and the critical interactions for binding. We predict that local pairs can form in BCC optical lattices with light masses. We have also estimated transition temperatures for Bose-Einstein condensation of pairs for $^6$Li atoms in BCC optical lattice occurring up to approximately 100 nK and 50 nK for blue and red lasers respectively.

A particularly interesting observation is that the pair mass becomes superlight when $U$ and $V$ are of similar magnitude and both attractive. Then pairs can move freely through the optical lattice without the need to access a high energy intermediate state. This low mass state coincides with a change from on-site pairs with very small effective radius to inter-site pairs, and leads to a peak in the transition temperature. Superlight pairs are of particular interest in electron-phonon systems where a retarded self interaction leads to relatively high effective masses even for single particles, and the superlight behavior has been predicted to lead to high superconducting transition temperatures in condensed matter. Thus, the ability to examine superlight behavior in a clean system would be of interest.

We predict that in a cold atom system, a high transition temperature can be achieved for pairs with onsite attraction. Lighter pairs are found at weak pairing and in the superlight regimes, and lead to higher $T_{\text{BEC}}$. We predict that superfluidity could occur around 100 nK and 50 nK for blue and red lasers respectively. Both fermion pairing and BCC optical lattices are still mainly unex-
FIG. 9. [Color online] BEC transition temperatures, $T_{\text{BEC}}$, for $^6\text{Li}$ atoms. Rows are labeled according to the laser color, i.e. either a red or blue beam laser. The number of pairs per site $n_b$ increases from left to right. The horizontal lines in each panel are the corresponding $T_{\text{BEC}}$ value for $m^* = 2m_0$. The colored lines surrounded by the gray-shaded regions indicate situations where the value of $n_b$ is compatible with the conditions on pair overlap. $T_{\text{BEC}}$ peaks when $U = V$ and the pairs are superlight.

explored by the cold atoms community. The high transition temperatures in condensed matter systems raise the question of whether pairing could be observed in BCC optical lattices.

On optical lattices, the sign and magnitude of $U$ can be controlled by the Feshbach resonance, whereas the sign and magnitude of the longer range $V$ can be controlled using (dressed) Rydberg atoms. The technology for using Feshbach resonances to control the Hubbard $U$ is mature. More recently, unprecedented control over inter-site interactions has been demonstrated using Rydberg states. The Rydberg and Feshbach mechanisms are different and thus allow for independent control. Thus the $UV$ model offers a broad general model that could be of interest from a condensed matter perspective and implementable in a clean form by the optical lattices community.
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1. Schrödinger equation

The (anti-)symmetrized Schrödinger equation is given as

\[ (E - \varepsilon_{k_1} - \varepsilon_{k_2}) \phi_{k_1 \bar{k}_2}^\pm = \frac{1}{N} \sum_{qa \bar{q}} \left\{ V_{a \bar{q}} e^{i(q-k_1 \cdot a_\pm) + \varepsilon_{q-k_2}} \right\} \phi_{q, k_1 + k_2 - q}^\pm \]

(A.1)

Appendix: Pair Energy, Dispersion and Binding Conditions

1. Schrödinger equation

The (anti-)symmetrized Schrödinger equation is given as

\[ (E - \varepsilon_{k_1} - \varepsilon_{k_2}) \phi_{k_1 \bar{k}_2}^\pm = \frac{1}{N} \sum_{qa \bar{q}} \left\{ V_{a \bar{q}} e^{i(q-k_1 \cdot a_\pm) + \varepsilon_{q-k_2}} \right\} \phi_{q, k_1 + k_2 - q}^\pm \]

(A.1)
The prime in the sum implies that a factor of $\frac{1}{2}$ is associated with the case $a_+ = 0$. The symmetrized Schrödinger equation corresponds to spin-singlet states and the anti-symmetrized equation to spin-triplets. For the singlets, we define the vectors \( \{ a_+ \} = \{ a_0^+, a_1^+, a_2^+, a_3^+, a_4^+ \} \) \( \{ (0,0,0), \left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right), \left(\frac{1}{2},-\frac{1}{2},\frac{1}{2}\right), \left(\frac{1}{2},\frac{1}{2},-\frac{1}{2}\right), \left(\frac{1}{2},-\frac{1}{2},-\frac{1}{2}\right) \} \) and for triplets, \( \{ a_- \} = \{ a_1^-, a_2^-, a_3^-, a_4^- \} \) \( \{ (1,0,0,0), \left(\frac{1}{2},\frac{1}{2},-\frac{1}{2}\right), \left(\frac{1}{2},-\frac{1}{2},\frac{1}{2}\right), \left(\frac{1}{2},-\frac{1}{2},-\frac{1}{2}\right) \} \). We set $b = 1$ throughout this appendix.

\textit{a. Symmetrized Schrödinger equation}

For the singlets, we use the vectors \( \{ a_+ \} \) in Equation (A.1). Thus we have

\[
(E - \varepsilon_{k_1} - \varepsilon_{k_2})\Phi_{k_1 k_2}^+ = \frac{1}{N} \sum_q \left[ \frac{1}{2} U(e^{i(q-k_1)\alpha_0^+} + e^{i(q-k_2)\alpha_0^+}) + V(e^{i(q-k_1)\alpha_0^+} + e^{i(q-k_2)\alpha_0^+}) \right. \\
+ V(e^{i(q-k_1)\alpha_0^+} + e^{i(q-k_2)\alpha_0^+}) + V(e^{i(q-k_1)\alpha_0^+} + e^{i(q-k_2)\alpha_0^+}) + V(e^{i(q-k_1)\alpha_0^+} + e^{i(q-k_2)\alpha_0^+}) \left. \right] \Phi_{k_1 k_2 - q}^+ (A.2)
\]

We can then represent our basis functions as follows:

\[
\Phi_0^+ (P) = \frac{1}{N} \sum_q \phi_{q-P-q}^+ , \quad \Phi_1^+ (P) = \frac{1}{N} \sum_q e^{i(\frac{\varepsilon_k}{2} + \frac{\varepsilon_p}{2})} \phi_{q-P-q}^+ \\
\Phi_2^+ (P) = \frac{1}{N} \sum_q e^{i(\frac{-\varepsilon_k}{2} + \frac{\varepsilon_p}{2})} \phi_{q-P-q}^+ , \quad \Phi_3^+ (P) = \frac{1}{N} \sum_q e^{i(\frac{-\varepsilon_k}{2} + \frac{-\varepsilon_p}{2})} \phi_{q-P-q}^+ (A.3)
\]

where $P = k_1 + k_2$. Hence, Equation (A.2) can be written in a more generalized form as

\[
\phi_{k_1 k_2}^+ = \frac{1}{(E - \varepsilon_{k_1} - \varepsilon_{k_2})} \left\{ U \Phi_0^+ (P) + V \Phi_1^+ (P)(e^{-ik_1a_0^+} + e^{-ik_2a_0^+}) + V \Phi_2^+ (P)(e^{-ik_1a_0^+} + e^{-ik_2a_0^+}) \right. \\
+ V \Phi_3^+ (P)(e^{-ik_1a_0^+} + e^{-ik_2a_0^+}) \left. + V \Phi_4^+ (P)(e^{-ik_1a_0^+} + e^{-ik_2a_0^+}) \right\} (A.4)
\]

We apply Equation (A.4) to each basis function $\Phi_0^+ (P), \Phi_1^+ (P), \Phi_2^+ (P), \Phi_3^+ (P), \Phi_4^+ (P)$ and transform the variable $q_i$ as: $q_i = q_j + \frac{p_j}{2}$. A simple substitution would yield five equations for $\Phi_i^+ (P): i = 0, 1, 2, 3, 4$ - we give one here as an example.

\[
\Phi_0^+ (P) = \frac{1}{N} \sum_{q'} \frac{1}{E - \varepsilon_{q'} - \varepsilon_{q'}} \left\{ U \Phi_0^+ (P) + V \Phi_1^+ (P) e^{-i\frac{\varepsilon_q}{2} + \frac{\varepsilon_{q'}}{2} + \frac{\varepsilon_{q'}}{2}} \left[e^{i\frac{\varepsilon_q}{2} + \frac{\varepsilon_{q'}}{2} + \frac{\varepsilon_{q'}}{2}} + e^{-i\frac{\varepsilon_q}{2} + \frac{\varepsilon_{q'}}{2} + \frac{\varepsilon_{q'}}{2}} \right] \\
+ V \Phi_2^+ (P) e^{-i\frac{\varepsilon_q}{2} - \varepsilon_{q'}} \left[e^{i\frac{\varepsilon_q}{2} - \varepsilon_{q'}} + e^{-i\frac{\varepsilon_q}{2} - \varepsilon_{q'}} \right] + V \Phi_3^+ (P) e^{-i\frac{\varepsilon_q}{2} - \varepsilon_{q'}} \left[e^{i\frac{\varepsilon_q}{2} - \varepsilon_{q'}} + e^{-i\frac{\varepsilon_q}{2} - \varepsilon_{q'}} \right] \right\} (A.5)
\]

which can be rewritten as

\[
\Phi_0^+ (P) = U L_{(0,0,0)} (P) \Phi_0^+ (P) + V \left[ L_{(x,y,z)} (P) + L_{(-x,y,-z)} (P) \right] \Phi_1^+ (P) + V \left[ L_{(x,-y,-z)} (P) + L_{(-x,y,z)} (P) \right] \Phi_2^+ (P) \\
+ V \left[ L_{(x,y,z)} (P) + L_{(-x,y,-z)} (P) \right] \Phi_3^+ (P) + V \left[ L_{(x,-y,z)} (P) + L_{(-x,y,-z)} (P) \right] \Phi_4^+ (P) (A.6)
\]
Note that the new functions, \( \Phi_i^+ (P) = e^\frac{i}{\hbar} (P q_i^+) \Phi_i^+ \) where \( i = 0, 1, ... 4 \), contain phase factors representing the center-of-mass motion of the pair. In addition, the \( L \) are Green's functions expressed as

\[
L_{lx,my,nz} (P) = \frac{1}{N} \sum_q e^{i (\frac{q}{2} + m \frac{q_y}{2} + n \frac{q_z}{2})} = - \int 2 \pi \int 2 \pi \int 2 \pi dq_x dq_y dq_z \cos(\frac{q_x}{2}) \cos(\frac{q_y}{2}) \cos(\frac{q_z}{2}) (4 \pi)^3 |E| \epsilon + \epsilon q_x + \epsilon q_y + \epsilon q_z (A.7)
\]

where \( l, m \) and \( n \) are integers \( \in [0 \pm 1 \pm 2] \).

For the remaining equations in (A.3), we multiply by \( e^\frac{i}{\hbar} (P q_i^+) \), \( e^\frac{i}{\hbar} (P q_i^+) \), and \( e^\frac{i}{\hbar} (P q_i^+) \) respectively to obtain equations similar to Equation (A.6). Hence, self-consistent equations for all spin-singlets at arbitrary momentum can be written as,

\[
\begin{bmatrix}
UA & V(B_{1} + B_{-1}) & V(C_{1} + C_{-1}) & V(D_{1} + D_{-1}) & V(F_{1} + F_{-1}) \\
UB_{1} & V(A + B_{+1}) & V(G_{1} + I_{+1}) & V(J_{1} + K_{+1}) & V(M_{1} + N_{+1}) \\
UC_1 & V(G_{-1} + L_{+1}) & V(A + C_{-1}) & V(O_{-1} + M_{+1}) & V(Q_{-1} + J_{+1}) \\
UD_{1} & V(J_{-1} + K_{-1}) & V(O_{-1} + M_{+1}) & V(A + D_{+1}) & V(S_{-1} + G_{+1}) \\
UF_{1} & V(M_{-1} + N_{+1}) & V(Q_{+1} + J_{-1}) & V(S_{+1} + G_{+1}) & V(A + F_{+1})
\end{bmatrix}
\begin{bmatrix}
\tilde{\Phi}_0 \\
\tilde{\Phi}_1 \\
\tilde{\Phi}_2 \\
\tilde{\Phi}_3 \\
\tilde{\Phi}_4
\end{bmatrix}
= \begin{bmatrix}
\Phi_0 \\
\Phi_1 \\
\Phi_2 \\
\Phi_3 \\
\Phi_4
\end{bmatrix} (A.8)
\]

where \( A = L_{(0,0,0)}, B_{\pm w} = L_{\pm w(x,y,z)}, C_{\pm w} = L_{\pm w(-x,y,z)}, D_{\pm w} = L_{\pm w(-x,-y,z)}, F_{\pm w} = L_{\pm w(x,y,-z)}, \)

\( G_{\pm w} = L_{\pm w(x,0,0)}, I_{\pm w} = L_{\pm w(y,0,0)}, J_{\pm w} = L_{\pm w(0,y,0)}, K_{\pm w} = L_{\pm w(x,z), M_{\pm w} = L_{\pm w(0,0), N_{\pm w} = L_{\pm w(x,0,0)}} \)

\( O_{\pm w} = L_{\pm w(0,-y)}, Q_{\pm w} = L_{\pm w(0,0,-z)} \) and \( S_{\pm w} = L_{\pm w(0,0,0)} \) are all functions of \( P \).

\( b. \) Anti-symmetrized Schrödinger equation

Using \( \{a\} \) in Equation (A.1), the antisymmetrized equation is

\[
(E - \epsilon_{k_1} - \epsilon_{k_2}) \phi_{k_1k_2}^+ = \frac{1}{N} \sum_q V e^{i(\frac{q}{2} + \frac{q_y}{2} + \frac{q_z}{2})} (e^{-ik_1a_1} - e^{-ik_2a_1})
\]

\[
+ V e^{i(-\frac{q}{2} + \frac{q_y}{2} + \frac{q_z}{2})} (e^{-ik_1a_2} - e^{-ik_2a_2}) + V e^{i(\frac{q}{2} - \frac{q_y}{2} + \frac{q_z}{2})} (e^{-ik_1a_3} - e^{-ik_2a_3})
\]

\[
+ V e^{i(\frac{q}{2} + \frac{q_y}{2} - \frac{q_z}{2})} (e^{-ik_1a_4} - e^{-ik_2a_4}) \phi_{q,k_1+k_2-q}^+ (A.9)
\]

Our spin-triplet basis functions are obtained similar to the singlet case as:

\[
\Phi_1^+ (P) = \frac{1}{N} \sum_q e^{i(\frac{q}{2} + \frac{q_y}{2} + \frac{q_z}{2})} \Phi_{q,P-q}^+, \Phi_2^+ (P) = \frac{1}{N} \sum_q e^{i(-\frac{q}{2} + \frac{q_y}{2} + \frac{q_z}{2})} \Phi_{q,P-q}^-, \Phi_3^+ (P) = \frac{1}{N} \sum_q e^{i(\frac{q}{2} - \frac{q_y}{2} + \frac{q_z}{2})} \Phi_{q,P-q}^-, \Phi_4^+ (P) = \frac{1}{N} \sum_q e^{i(\frac{q}{2} + \frac{q_y}{2} - \frac{q_z}{2})} \Phi_{q,P-q}^-(A.10)
\]

Going through a similar procedure as for the spin-singlets, a set of self-consistent equations for the triplets are obtained. For example,

\[
\Phi_1^+ (P) = \frac{1}{N} \sum_q \frac{1}{E - \epsilon_{q_x} - \epsilon_{q_y} - \epsilon_{q_z}} \left\{ V\Phi_1^+ (P) [1 - e^{2i(\frac{q}{2} + \frac{q_y}{2} + \frac{q_z}{2})}] + V\Phi_2^+ (P) [e^{2i(\frac{q}{2} + \frac{q_y}{2})} - e^{2i(\frac{q}{2} + \frac{q_z}{2})}] e^{2i(\frac{q_z}{2})}
\]

\[
+ V\Phi_3^+ (P) [e^{2i(\frac{q_z}{2})} - e^{2i(\frac{q_y}{2} + \frac{q_z}{2})}] e^{2i(\frac{q_y}{2})} + V\Phi_4^+ (P) [e^{2i(\frac{q_y}{2})} - e^{2i(\frac{q_z}{2} + \frac{q_y}{2})}] e^{2i(\frac{q_z}{2})}
\}
\]

\[
\Phi_1^- (P) = V \left[ L_{(0,0,0)} - L_{2(\pm x,y)} \right] \Phi_1^- + V e^{2i(\frac{q_z}{2})} \left[ L_{2(\pm x,0)} - L_{2(\pm 0,y,z)} \right] \Phi_2^- + V e^{2i(\frac{q_y}{2})} \left[ L_{2(\pm 0,y,0)} - L_{2(\pm x,0,z)} \right] \Phi_3^- + V e^{2i(\frac{q_y}{2})} \left[ L_{2(\pm 0,0,z)} - L_{2(\pm x,y,0)} \right] \Phi_4^- (A.11)
\]

This transforms into

\[
\Phi_1^+ (P) = V \left[ L_{(0,0,0)} (P) - L_{2(x,y,z)} (P) \right] \Phi_1^- (P) + V \left[ L_{2(x,0,0)} (P) - L_{2(0,y,z)} (P) \right] \Phi_2^- (P) + V \left[ L_{2(0,y,0)} (P) - L_{2(x,0,z)} (P) \right] \Phi_3^- (P) + V \left[ L_{2(x,y,0)} (P) - L_{2(0,0,z)} (P) \right] \Phi_4^- (P) (A.12)
\]
The last step is obtained by multiplying through by the phase factor \( e^{\frac{i}{\hbar}(Pa \cdot \tau)} \) such that \( \Phi_1^- (P) = e^{\frac{i}{\hbar}(Pa \cdot \tau)} \Phi_1^- \). Likewise, we multiply Equation (A.10) by \( e^{\frac{i}{\hbar}(Pa \cdot \tau)} \), \( e^{\frac{i}{\hbar}(Pa \cdot \tau)} \) and \( e^{\frac{i}{\hbar}(Pa \cdot \tau)} \) to obtain the respective expressions for \( \Phi_3^- (P) \), \( \Phi_3^- (P) \) and \( \Phi_4^- (P) \) in (A.10). The expression for the Green’s functions, \( L \), is the same as defined in Equation (A.7). Thus, the spin-triplet self-consistent equations at arbitrary momentum can be written as,

\[
\begin{bmatrix}
V(A - B_{+2}) & V(G_{+2} - I_{+2}) & V(J_{+2} - K_{+2}) & V(M_{+2} - N_{+2}) \\
V(G_{-2} - I_{+2}) & V(A - C_{+2}) & V(O_{+2} - M_{+2}) & V(Q_{+2} - J_{+2}) \\
V(J_{+2} - K_{+2}) & V(O_{+2} - M_{+2}) & V(A - D_{+2}) & V(S_{+2} - G_{+2}) \\
V(M_{+2} - N_{+2}) & V(Q_{+2} - J_{+2}) & V(S_{+2} - G_{+2}) & V(A - F_{+2})
\end{bmatrix}
\begin{bmatrix}
\Phi_1^- \\
\Phi_2^- \\
\Phi_3^- \\
\Phi_4^-
\end{bmatrix}
= 
\begin{bmatrix}
\Phi_1^- \\
\Phi_2^- \\
\Phi_3^- \\
\Phi_4^-
\end{bmatrix}
\] (A.13)

and as defined before, \( A = L(0,0,0), B_{\pm w} = L(\pm w(x,y,z), C_{\pm w} = L(\pm w(\mp x,y,z), D_{\pm w} = L(\pm w(x,-y,-z), F_{\pm w} = L(\pm w(\mp x,-y,-z), G_{\pm w} = L(\pm w(x,y,0), I_{\pm w} = L(\pm w(0,y,0), J_{\pm w} = L(\pm w(0,0,z), K_{\pm w} = L(\pm w(0,z,0), M_{\pm w} = L(\pm w(0,0,z), N_{\pm w} = L(\pm w(x,0,0) \), \( O_{\pm w} = L(\pm w(\mp x,0,0), Q_{\pm w} = L(\pm w(x,0,-z) \), \( S_{\pm w} = L(\pm w(\mp x,0,-z) \) and all are functions of \( P \).

Equations (A.8) and (A.13) are both eigenvalue problems that must be solved to obtain pair properties.

2. Pair energy for \( \Gamma \) point

Next, we compute the energies of the singlets and triplets. At the \( \Gamma \) point where \( (P_x = P_y = P_z = 0) \) - there is a further simplification of the Green’s functions (A.7) which can be expressed as an integral,

\[
L_{tx,my,nz}(0) = \frac{1}{N} \sum_{q} \frac{\hbar}{E - \Delta_q} = - \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{\hbar}{4(\pi)^3} \cos(l\frac{\pi}{2}) \cos(m\frac{\pi}{2}) \cos(n\frac{\pi}{2}) |E| - 16t \cos(q_x^0) \cos(q_y^0) \cos(q_z^0)
\]

and the following relations hold

\[
A(0) = L_0 \\
B_{\pm 0} = C_{\pm 0} = D_{\pm 0} = F_{\pm 0} = L_1
\]

Next, we form the matrix equations above can be written in a compact form as

\[
L_{\text{singlet}} \Phi_{\text{singlet}} = \Sigma \Phi_{\text{singlet}}
\]

\[
L_{\text{triplet}} \Phi_{\text{triplet}} = \Sigma \Phi_{\text{triplet}}
\]

thus forming an eigenvalue problem. \( \tilde{L}_s \) and \( \tilde{L}_t \) are the singlet and triplet dispersion matrices, \( \lambda_s \) and \( \lambda_t \) being.

\[
L_{s,t} \Phi_{s,t} = \lambda_{s,t} \Phi_{s,t}
\] (A.18)
the eigenvalues corresponding to singlet $\Phi_s$ and triplet $\Phi_t$ eigenvectors respectively. So, the values of $E$ corresponding to the pair energy are found by searching for eigenvalues of $\lambda_{s,t} = 1$.

3. Further symmetrization at the Brillouin zone center

The system of equations can be significantly simplified at the $\Gamma$ point of the BCC BZ, where the system possesses $O_h$ point symmetry, and this will enable the calculation of binding criteria for pairs at the $\Gamma$ point with $s$, $p$, $d$, and $f$ symmetry. By performing the 48 operations on the system, we determine the linear combinations (excluding the normalization constants) of the eigenvector through the irreducible representations of the $O_h$ group. The eigenfunction $\Phi_{s,t}^{\text{bcc}}$ is located at the center of the BZ and it remains unchanged as all operations are performed (thus forming an s-like molecular orbital).

The sought irreducible representation for both the singlet and triplet states are

$$\Gamma_{\text{singlet}}^{\text{bcc}} = A_{1g} \oplus T_{2g}$$
$$\Gamma_{\text{triplet}}^{\text{bcc}} = T_{1u} \oplus A_{2u}$$

whence $A_{1g}$, $T_{2g}$, $A_{2u}$ and $T_{2u}$ forms the $s$-, $d$-, $p$- and $f$- states respectively. From here, we can find the symmetrized linear combinations for the singlets, $\Gamma_{\text{singlet}}^{\text{bcc}}$, as

$$\chi^{A_{1g}} = \Phi^+_1 + \Phi^+_2 + \Phi^+_3 + \Phi^+_4$$
$$\chi^{T_{2g}} = \Phi^+_1 - \Phi^+_2 - \Phi^+_3 - \Phi^+_4$$

and the triplets, $\Gamma_{\text{triplet}}^{\text{bcc}}$, have the combinations

$$\chi^{T_{1u}} = \Phi^-_1 - \Phi^-_2 + \Phi^-_3 + \Phi^-_4$$
$$\chi^{A_{2u}} = \Phi^-_1 - \Phi^-_2 - \Phi^-_3 - \Phi^-_4$$

If we combine Equation (A.20) with $\Phi_{s,t}^{\text{bcc}}$, we get the transformation to new basis $\hat{\Phi}_{s,t}^{*}$ resulting in $\chi_{s,t} = \hat{\chi}_{s,t}$. Actually, $\hat{\chi}_{i}$ (where $i = s, t$) is derived by performing the symmetry operations and it can help diagonalize the problem further via the equation

$$\hat{L}_{i}^{\text{diag}} = \hat{\chi}_{i} \cdot \hat{L}_{i} \cdot \hat{\chi}_{i}^{-1}$$

By applying the formula above, the new symmetrized bases $\hat{\chi}_{s}$ and $\hat{\chi}_{t}$ respectively block-diagonalizes the dispersion relations $L_s$ and $L_t$ as follows

$$\begin{bmatrix}
UL_{0} & 2VL_{1} & 0 & 0 & 0 & 0 \\
4UL_{1} & K_{s} & 0 & 0 & 0 & 0 \\
0 & 0 & K_{d} & 0 & 0 & 0 \\
0 & 0 & 0 & K_{d} & 0 & 0 \\
0 & 0 & 0 & 0 & K_{f} & 0 \\
0 & 0 & 0 & 0 & 0 & K_{f}
\end{bmatrix}
\begin{bmatrix}
\Phi_{0} \\
\Phi_{s} \\
\Phi_{d1} \\
\Phi_{d2} \\
\Phi_{d3}
\end{bmatrix}
= 
\begin{bmatrix}
\Phi_{0} \\
\Phi_{s} \\
\Phi_{d1} \\
\Phi_{d2} \\
\Phi_{d3}
\end{bmatrix}$$

$$\begin{bmatrix}
K_{p} & 0 & 0 & 0 & 1 \\
0 & K_{p} & 0 & 0 & 0 \\
0 & 0 & K_{p} & 0 & 0 \\
0 & 0 & 0 & K_{f} & 0 \\
0 & 0 & 0 & 0 & K_{f}
\end{bmatrix}
\begin{bmatrix}
\Phi_{p1} \\
\Phi_{p2} \\
\Phi_{p3} \\
\Phi_{f1} \\
\Phi_{f2}
\end{bmatrix}
= 
\begin{bmatrix}
\Phi_{p1} \\
\Phi_{p2} \\
\Phi_{p3} \\
\Phi_{f1} \\
\Phi_{f2}
\end{bmatrix}$$

$K_s = V(L_0 + L_2 + 3L_3 + 3L_4)$, $K_d = V(L_0 + L_2 + L_3 - L_4)$, $K_p = V(L_0 - L_2 + L_3 - L_4)$, $K_f = V(L_0 - L_2 - 3L_3 + 3L_4)$.

In [A.27], the top-left $2 \times 2$ block corresponds to the $s$-symmetrical state while the other three $1 \times 1$ blocks are $d$-symmetrical states which are triply degenerate (when $P = 0$). Similarly in Equation [A.28], the $p$-states are 3-fold degenerate and there is a single $f$-state. We have chosen $t = 1$ for our calculations.

4. Binding criterion at the Brillouin zone center

Once the system of equations has been symmetrized, it is possible to calculate the critical binding threshold by setting $E = -2W = -16t$. For this purpose, it is convenient to re-write the singlet and triplet determinant matrices [A.27] and [A.28], and getting rid of redundant elements

$$s : \begin{bmatrix} 1 - UL_{0} & -2VL_{1} \\
-4UL_{1} & 1 - K_{s}
\end{bmatrix} = 0$$
$$d : \begin{bmatrix} 1 & 0 & 0 \\
-4UL_{1} & 1 & -K_{d}
\end{bmatrix} = 0$$
$$p : \begin{bmatrix} 1 & 0 & 0 \\
-4UL_{1} & 1 & -K_{p}
\end{bmatrix} = 0$$
$$f : \begin{bmatrix} 1 & 0 & 0 \\
-4UL_{1} & 1 & -K_{f}
\end{bmatrix} = 0$$

The Green’s functions [A.15] can be expressed in terms of the elliptic integral of the first kind [B.23] as
\[ L_0 = -\frac{K_0^2}{4\pi^2 t} = -0.087075245605354804 \quad (A.33) \]

\[ L_1 = \frac{1}{16t} - \frac{K_0^2}{4\pi^2 t} = \frac{1}{16t} + L_0 \quad (A.34) \]

\[ L_2 = \frac{1}{2t} - \frac{K_0^2}{\pi^2 t} - \frac{9}{16tK_0^2} = \frac{1}{2t} + 4L_0 + \frac{9}{64\pi^2 t^2 L_0} \quad (A.35) \]

\[ L_3 = -\frac{1}{16tK_0^2} = \frac{1}{64\pi^2 t^2 L_0} \quad (A.36) \]

\[ L_4 = -\frac{K_0^2}{4\pi^2 t} + \frac{1}{4tK_0^2} = L_0 - \frac{1}{16\pi^2 t^2 L_0} = L_0 - 4L_3 \quad (A.37) \]

where \( K_0 = K\left(\frac{1\sqrt{2}}{\sqrt{2}}\right) = 1.85407467\ldots \) is the complete elliptic integral of the first kind.

Expanding the determinant \( (A.29) \) gives the critical binding expression

\[ V^*_c \leq V(U) = \frac{UL_0 - 1}{UL_0C - C - 8UL_1^2} \quad (A.38) \]

where \( C = L_0 + L_2 + 3L_3 + 3L_4 = 8L_0 + \frac{1}{2t} = \frac{-0.19660196484283837}{t} \).

Therefore,

\[ V^*_c (U = 0) = -5.0864191t \quad (A.39) \]

\[ V^*_c (U \rightarrow +\infty) = -7.0864191t \quad (A.40) \]

\[ U_c (V = 0) = -11.4843202t \quad (A.41) \]

\[ U_c (V \rightarrow +\infty) = -16t \quad (A.42) \]

Similarly, \( (A.36) \) - \( (A.32) \) respectively yields

\[ V^d_c = -15.0428185t \quad (A.43) \]

\[ V^p_c = -12.6624416t \quad (A.44) \]

\[ V^f_c = -15.7113739t \quad (A.45) \]