High temperature superconductivity in dimer array systems

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Superconductivity in the Hubbard model is studied on a series of lattices in which dimers are coupled in various types of arrays. Using fluctuation exchange method and solving the linearized Eliashberg equation, the transition temperature $T_c$ of these systems is estimated to be much higher than that of the Hubbard model on a simple square lattice, which is a model for the high $T_c$ cuprates. We conclude that these ‘dimer array’ systems can generally exhibit superconductivity with very high $T_c$. Not only $d$-electron systems, but also $p$-electron systems may provide various stages for realizing the present mechanism.

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Search for high temperature superconductivity is one of the most challenging problems in solid state physics. Since one of the bottleneck for high $T_c$ is the generally low energy scale of the phonons, purely electronic pairing mechanism have attracted much attention from the early days. The discovery of high $T_c$ superconductivity in the cuprates\textsuperscript{4} has certainly boosted interest along this line. In particular, the possibility of superconductivity in the Hubbard model on a square lattice, a simplest purely electronic model for the cuprates, has been intensively studied, where spin fluctuation theories using fluctuation exchange (FLEX) method have estimated $T_c$ of the $d_{x^2−y^2}$-wave superconductivity to be $O(0.01t)$ ($t$ is the nearest neighbor hopping integral)\textsuperscript{5}. Since $t \sim 0.4\text{eV}$ for the cuprates, this estimation is consistent with the experimentally observed $T_c$ of up to 150K, but at the same time one should note that it is two orders of magnitude lower than the kinetic energy scale $t$.

In our view, one reason for this reduction of $T_c$ is that the $d_{x^2−y^2}$ gap function changes sign, having nodal lines that intersect the Fermi surface. Such a sign change in the gap function is a ‘necessary evil’ for spin fluctuation pairing in that the pair scattering processes $[k \uparrow, −k \downarrow] \rightarrow [k + Q \uparrow, −k − Q \downarrow]$, mediated by the dominant spin fluctuations with wave vector $Q$, have to accompany a sign change in the gap function $\phi$, i.e., $\phi(k)\phi(k + Q) < 0$. In the case of the square lattice, this requirement leads to the $d_{x^2−y^2}$ pairing, where the gap function has nodes that intersect the Fermi surface, thereby resulting in a reduction of $T_c$.

From this viewpoint, two of the present authors have recently proposed that superconductivity with much higher $T_c$ can be achieved in systems having two pocket-like nested Fermi surfaces, where the dominant pair scattering processes take place between the two Fermi surfaces, so that the sign change in the gap function takes place across, not on, the Fermi surfaces\textsuperscript{6}. Along this line, Hubbard models on a two band lattice (Fig. 1) and a four band one\textsuperscript{7} have been studied using FLEX method, where high $T_c$ has been obtained solving the linearized Eliashberg equation.

If we focus on the two band model shown in Fig. 1, the obtained gap function indeed changes sign across the two bands but stays nearly constant within each band\textsuperscript{8}. Such a form of the gap function can be interpreted in terms of a real space picture by looking at the system as dimers coupled in an array. Namely, it is natural to consider that the singlet pairs are mainly formed between electrons residing on different sites within a dimer due to the antiferromagnetic interaction $\propto t^2_d/U$ between the two sites. Then, the gap function has $s$ wave symmetry within each band because the pairing occurs within a unit cell, while it changes sign across the two bands because the pairs are formed between different sites\textsuperscript{9}.

This intuitive picture has led us to consider here the Hubbard model on a series of lattices in which dimers are coupled in various types of arrays. We conclude that these ‘dimer array’ systems can generally exhibit superconductivity with very high $T_c$.

Let us now start with a dimer array Hubbard system

$$H = −t_d \sum_{i,\sigma} (c_{i\sigma}^\dagger d_{i\sigma} + d_{i\sigma}^\dagger c_{i\sigma}) − t’ \sum_{(i,j),\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + d_{i\sigma}^\dagger d_{j\sigma} + \text{H.c}) + U \sum_{i} (n_{i\uparrow} n_{i\downarrow} + n_{i\uparrow}^d n_{i\downarrow}^d)$$

FIG. 1. The two band lattice studied in ref. The thickness of the lines represent the magnitude of hopping integrals.
the overlap of the two bands, and thus the size of the Fermi surfaces, should not be too large for high $T_c$ superconductivity to occur. This is because when the Fermi surfaces are small compared to the spread $\Delta Q$ of the peak in the spin susceptibility, inter-Fermi-surface pair scatterings $\forall \{k \uparrow, -k \downarrow\} \in A \rightarrow \forall \{k + q \uparrow, -k - q \downarrow\} \in B$ all have large contribution, while when the Fermi surfaces are large compared to $\Delta Q$, the pair scattering processes having large contribution will be restricted to a certain combination of initial states $k \in A$ and final states $k + q \in B$.

In order to verify the above expectation, we use the multiband version of FLEX, which is kind of a self-consistent random phase approximation, to obtain the renormalized Green’s function of the Hubbard model. Then, $T_c$ is determined as the temperature at which the eigenvalue $\lambda$ of the Eliashberg equation,

$$\lambda \phi_{lm}(k) = -\frac{T}{N} \sum_{k'} \sum_{l',m'} V_{lm}(k - k') G_{l'l'}^{(\uparrow)}(k') G_{mm'}^{(\downarrow)}(-k') \phi_{m'}(k'),$$

reaches unity. Here, $G$ is the renormalized Green’s function matrix (with $l, m, \text{etc}...$ labeling sites in a unit cell) obtained by FLEX. $V$ is the spin singlet pairing interaction matrix given by $V(q) = \frac{1}{2} V_{sp}(q) - \frac{1}{4} V_{ch}(q)$, where the pairing interaction due to spin fluctuations (sp) and that due to charge fluctuations (ch) are given as $V_{sp(ch)} = U^2 \chi_{sp(ch)}$ using the spin and charge susceptibilities $\chi_{sp(ch)}(q) = \chi_{irr}(q) [1 - (+) U \chi_{irr}(q)]^{-1}$, where $\chi_{irr}(q)$ is the irreducible susceptibility matrix $\chi_{irr}(q) = \frac{1}{N} \sum_k G(k + q) G(k)$ ($N$ is the number of $k$-point meshes). In the present paper, we take up to $64 \times 64 k$-point meshes and up to 4096 Matsubara frequencies.

As mentioned above, the FLEX-Eliashberg equation approach is known to give reasonable $T_c$ of order 0.01$t$ for the single band Hubbard model, which is a model for the high $T_c$ cuprates. The occurrence of superconductivity in the Hubbard model contradicts with some of the numerical studies, but we believe this to be due to finite size effects in the numerical calculations. In fact, a quantum Monte Carlo calculation that pays special attention to the discreteness of the level spacing in finite size systems has detected large enhancement of the pairing correlation function, which is at least qualitatively consistent with the FLEX results.

We have performed FLEX calculation for $n = 0.95$ and $n = 0.9$ with $U = 8$, varying $(t', t_d)$ in a certain range. The gap function obtained by solving the linearized Eliashberg equation (Fig.6) does not change sign in each band, while it changes sign across the two bands, as expected. As a consequence, $T_c$, shown in Fig.6, reaches $\sim 0.13$ for $n = 0.95$, which is 4 ~ 5 times higher than the typical $T_c$ of the Hubbard model, estimated by the same way, on a simple square lattice.
As $t'/t_d$ increases, the Fermi surfaces become large, resulting in a reduction of $\lambda$ due to the reason mentioned above. At the same time, the antiferromagnetic spin fluctuations increase rapidly because the nesting between the two Fermi surfaces becomes better for large Fermi surfaces. Thus, the tendency towards magnetic ordering dominates over superconductivity. On the other hand, when $t'/t_d$ is small, only one band intersects the Fermi level, so that the Fermi surface nesting is degraded and $T_c$ becomes low. Consequently, high $T_c$ is obtained in a certain optimized regime of $(t', t_d)$ as seen in Fig.6. At $n = 0.9$, $T_c$ becomes slightly lower, but still reaches 0.1.

We now show that high $T_c$ superconductivity in dimer array systems is quite general by looking into triangular and honeycomb lattices shown in Fig.6(a) and (b), respectively. $T_c$ for $n = 0.95$ and $U = 8$ on these lattices are shown in Fig.7 as functions of $(t', t_d)$, which again exceed or come close to 0.1. These results suggest that dimer array systems can generally exhibit high $T_c$ superconductivity on various types of lattices.
unhatched orbitals is higher by \( \varepsilon \) than that of the hatched ones. (b) The effective lattice of (a).

**FIG. 8.** (a) Dimer array system (consisting of \( p_x \) orbitals here) on a honeycomb lattice in which the site energy of the unhatched orbitals is higher by \( \varepsilon \) than that of the hatched ones. (b) The effective lattice of (a).

![Diagram](image)

**FIG. 9.** \( T_c \) of the system shown in Fig. 8(a) as a function of \( \varepsilon \) with \( U/t' = 2, t' = 1, t_d = 0.5 \) and \( n = 0.5 \).

So far we have focused on parameter regimes with large \( U/t' \) and \( U/t_d \), where we have \( d \)-electron systems in mind. Namely, if \( t' \) and \( t_d \) are few hundred meV, which is typical for \( d \)-electron systems, \( T_c \sim 0.1t' \) corresponds to a very high temperature of few hundred K. Then our next question is: can we obtain similarly high \( T_c \) in systems with smaller \( U/t' \), as in \( p \)-electron systems? In 2\( p \)-electron systems such as B, C, and/or N compounds, the on-site Coulomb repulsion and the hopping integrals are both typically few eV, so that \( U/t \sim O(1) \).

In such a case, we have found that \( T_c \) estimated by FLEX+Eliashberg equation is very low (or does not exist) not only on conventional lattices, but also on the lattices considered above as well. Nevertheless, we now show that high \( T_c \) can be achieved even for systems with small \( U/t' \) by introducing a level offset between neighboring sites, thus reducing the effective band width. As an example, let us consider a dimer array system on a honeycomb lattice where the site energy differs by \( \varepsilon \) between neighboring sites (Fig. 8(a)). At quarter filling (\( n = 0.5 \)) and in the limit of large \( \varepsilon \), the system becomes equivalent to a half-filled dimer array system on a triangular lattice with an effective hopping \( t_{\text{eff}} = t'^2/\varepsilon \) between the dimers (Fig. 8(b)). Consequently, we can expect high \( T_c \) when the value of \( \varepsilon \) is tuned so that \( U/t_{\text{eff}} \) is optimized. In Fig. 9, we show \( T_c \) for \( U = 2, t' = 1, t_d = 0.5 \) and \( n = 0.5 \) as a function of \( \varepsilon \). \( T_c \) is found to exceed 0.02, which again corresponds to few hundred K if \( t' = 1 \) corresponds to few eV as in \( 2p \) systems.

To summarize, we have shown that 'dimer array' Hubbard systems can generally exhibit superconductivity with very high \( T_c \). Not only \( d \)-electron systems, but also \( p \)-electron systems may provide various stages for realizing the present mechanism.

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The creation operators of bonding (A) and antibonding (B) orbitals can be given as \( c_{A,B}^\dagger \propto c_{\uparrow,\downarrow}^\dagger \) in terms of the creation operators on sites 1 and 2 within a dimer. If the pairing occurs only between sites 1 and 2 (i.e., \( \langle c_1^\dagger c_2^\dagger \rangle = \langle c_2^\dagger c_1^\dagger \rangle = 0 \)), then \( \langle c_A^\dagger c_B^\dagger \rangle = -\langle c_B^\dagger c_A^\dagger \rangle \) holds.

Although this model seems similar to the \( t-J \) model on a coupled plane studied by E. Dagotto et al. in Phys. Rev. B 45, 5744 (1992), an essential difference is that there, the interplane spin-spin coupling is taken to be stronger than the intraplane one, while the interplane hopping \( (t_d \text{ in our model}) \) is considered to be small.

Throughout the paper, the band filling is defined as \( n = \text{[number of electrons]} / \text{[number of sites]} \).

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12. The \( d_{3z^2-r^2} \) orbital may be suitable for our purpose since we need large hopping in the out-of-plane direction.
13. Such an alternation of the \( 2p \) orbital energy in a honeycomb plane is realized, for example, in BN graphite.
14. In taking \( t_d/t' = 0.5 \), we have referred to the ratio between inter- and intraplane hoppings of \( 2p_x \) orbitals in MgB\(_2\).