t−J Model Then and Now: a Personal Perspective from the Pioneering Times

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In this overview we sketch briefly the path to the so-called t−J model derived for the first time 30 years ago and provide its original meaning within the theory of strongly correlated magnetic metals with a non-Fermi (non-Landau) liquid ground state. An emergence of the concept of real space pairing is discussed in a historical prospective. A generalization of this model to the many-orbital situation is briefly discussed. The emphasis is put on didactical exposition of ideas, as they were transformed into mathematical language. The concept of hybrid pairing is introduced in the same context at the end.

PACS numbers: 71.27.+a, 74.72.–h, 71.10.Fd

1. Introduction

Before presenting the details, let us first summarize the principal features of the so-called t−J model. This model represents a very nontrivial model of strongly correlated fermions because of the following principal reasons:

1. It represents a system of strongly inter-correlated itinerant fermions which transform into an antiferromagnetic state of localized particles (the Mott–Hubbard insulator); the classic situation takes place at the concentration of one fermion per single-band state (at the half filling, \( n = 1 \)). The half-filled state is an antiferromagnetic insulator modeled by the Anderson kinetic exchange.

2. The itinerant state is represented by particles called the correlated holes or simply the holes in the Mott–Hubbard insulator, which do not have the ordinary fermion properties (their creation and annihilation operators do not obey the fermionic anticommutation rules). In other words, they cannot be represented by the Landau quasiparticles in an exact manner, since they do not represent almost-filled band states.

3. Magnetic interaction between the correlated itinerant particles, again the kinetic exchange, is regarded also as the source of real-space pairing as it is represented as taking place between the nearest neighbors. Hence, antiferromagnetism and this new type of paired state must be regarded on equal footing with the paired state (resonance-valence bond state or superconducting state). This is particularly relevant in the context of high-temperature superconductivity near the band filling, i.e. close to the Mott transition.
4. Because of the nontrivial character of the kinetic- (or residual-band-) energy (the projected hopping part), it can become comparable or even smaller than the kinetic-exchange-energy part. In effect, magnetic polaron or phase-separated states or new type of spin-paired states can be formed, concomitantly with the transition to a localized state for small carrier concentration of holes. Thus the transition in real systems such as La_{2-x}Sr_xCuO_4, YBa_2Cu_3O_{6+x}, La_{1-x}Sr_xTiO_3, takes place even for a non-half-filled band configuration. Although, here the role of atomic disorder is probably also very important, if not crucial.

The four mentioned above features originate from the circumstance that the kinetic (band) energy of the fermionic particles in the correlated systems is relatively small and easily comparable (if not smaller) to the Coulomb interaction energy. Furthermore, both energies are then effectively counted on the Kelvin, rather than on the electronvolt scale and represent competing compensating each other, dynamical contributions to the electron states. Hence, the system is very susceptible to the perturbations such as thermal or atomic disorder, or the electron–lattice coupling. This sensitivity of the strongly correlated metallic (or magnetic-insulating) state leads to an instability with respect to the perturbations on the thermal scale and complicates enormously a reliable solution of the model, in addition to the specific situation that, unlike in the standard quantum mechanics, there is no small parameter in the model, since the potential (interaction) energy is at least comparable to the single-particle (band) energy.

The structure of the paper is as follows. In Sect. 2 we define the limit of strong correlation. In Sect. 3 we discuss the original derivation and the meaning of the \( t-J \) model. In Sect. 4 we rewrite the exchange part in terms of pairing operators and discuss this new aspect briefly, whereas in Sect. 5 we introduce hybrid pairing.

2. The Hubbard model

The Hubbard model (1963) [1] was devised first to describe the single-band magnetism, particularly to understand the so-called itinerant (Stoner–Wolfarth) ferromagnetism and criterion of its appearance in a microscopic manner. It is represented by the Hamiltonian, which in the second-quantization representation has the form

\[
H = \sum_{ij\sigma} t_{ij} \hat{a}_{i\sigma}^{\dagger} \hat{a}_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow},
\]

where the primed summation means that we take only \( i \neq j \) terms in the hopping part. The ingenuity of this expression derives from the fact that we start from the atomic (Wannier) representation rather than from the popular then electron-gas (band) representation of the many-electron state in solid. This representation (and actually, the Hamiltonian) has been invented earlier [2], although the meaning of the model was in the latter case quite different namely, to derive the antiferromagnetic superexchange interaction as an effective \( d-d \) exchange in the Mott insulators (such as NiO, MnO, or CoO), without involving, explicitly the filled \( p \) shells of oxygen \( O^{2-} \) or other chalcogenide ions.
Obviously, one should think that the Bloch \( \{ \Phi_k(r) \} \) and the Wannier \( \{ W_i(r) \} \) single-particle bases are physically equivalent, as they are related by (unitary) Fourier transform on the lattice

\[
\Phi_k(r) = \frac{1}{\sqrt{N}} \sum_i W_i(r) e^{ik \cdot R_i}, \quad W_i(r) = \frac{1}{\sqrt{N}} \sum_k \Phi_k(r) e^{-ik \cdot R_i}.
\] (2)

Likewise, the same unitary equivalence holds between the annihilation operators in the Bloch \( \{ a_k \sigma \} \) and the Wannier \( \{ a_i \sigma \} \) representations, namely

\[
a_k \sigma = \frac{1}{\sqrt{N}} \sum_i a_i \sigma e^{i r \cdot R_i}, \quad a_i \sigma = \frac{1}{\sqrt{N}} \sum_k a_k \sigma e^{-i k \cdot R_i}.
\] (3)

The main (and fundamental) aspect of this problem is that, depending on the value of \( U \), the equivalence between the two representations can be broken and, as \( U \) increases, the atomic representation of electronic states becomes more appropriate than the Bloch one. This fact expresses the so-called Mott–Hubbard or metal–insulator transition, which in this case is associated with the breakdown of the global \( U(1) \) symmetry, as in the Mott–Hubbard insulating phase linear momenta is in an obvious manner not a proper quantum number. Parenthetically, one should say that the Hubbard (1964) method of defining the localization [3] is similar to that of Mott. In essence, the Hubbard approach takes into account both the existence of crystal lattice, as well as the narrow-band structure of the correlated electrons. Explicitly, taking expectation values of the two terms in (1) one sees that in the Hartree–Fock approximation and for one electron per atom we have the ground state energy per site in the form

\[
E_G \simeq -\frac{1}{2} \sum_{i,j} t_{ij} \sum_{\sigma} n_\sigma (1 - n_\sigma) + U n_\sigma n_{\bar{\sigma}} = -\frac{W}{4} + U \frac{4}{4},
\] (4)

where \( W \) is the band width and \( z \) — number of nearest neighbors \( (W = 2z|t|) \). In the paramagnetic state \( (n_\sigma = n_{\bar{\sigma}} = 1/2) \) therefore, the two energies compensate each other when \( U = W \), i.e. when band and the Coulomb energy are comparable. The true value \( U = U_C \) of critical interaction depends on the method selected and the density of states for given system, but it is in the regime \( W \lesssim U_C \lesssim 2W \) [4].

In the limit \( U \ll W \) we have the so-called metallic limit. The question interesting us here is the limit of strong correlations \( U \gg W \). In the case of \( n = 1 \) this limit corresponds to the Mott insulating limit [2, 4, 5]. The question which was posed by us, we believe for the first time [6, 7], was what happens when \( U \gg W \) and \( n \neq 1 \).

The situation for \( n \neq 1 \) (it is sufficient to consider the case \( n < 1 \) only, as that with \( n > 1 \) is related to the former by switching to the hole language). Namely, the Hartree–Fock approximation for \( U \simeq 2W \) we have from (4)

\[
E_G \simeq -\frac{1}{2} W n_\sigma (1 - n_\sigma) + U n_\sigma^2 = -\frac{W}{4} + \frac{U}{4},
\] (5)

Taking \( n = 1 - \delta \), with \( \delta \ll 1 \), we have that \( E_G \sim W \delta / 4 \), i.e. the energy is positive and thus the metallic state is unstable. We show below that this is indeed
the case for \( \delta < \delta_C \sim 0.1 \), but that situation requires a refined analysis. In any case, if we take Eq. (5) literally, then for every \( n \) we can define \( U_C \) at which the two energies cancel out each other, i.e. \( U_C/W = (2 - n)/n \) (\( U_C \) increases as \( n \) decreases). This trivial reasoning teaches us one important thing: the creation of holes in the Mott insulator makes particles effectively less correlated for fixed value of \( U \). In other words the condition \( U \gg W \) valid for a half-filled band system gets softened when we change (diminish) the number of electrons in the same band. In our derivation of the \( t-J \) model [6, 7] and in subsequent papers it is assumed that the particles are strongly correlated in the whole filling range considered. Let us note however that if we take \( n = 0.7 \) then \( U_C/W = 1.86 \), i.e. the critical value is almost doubled, so if we had band states with the value of \( U \) such that \( U/U_C = 1 \) for \( n = 1 \), for \( n = 0.7 \) the particles behave as if they experienced only half of the critical value (are substantially less correlated). This must be remembered particularly in the context of high-temperature superconductors described via a single-band model since then for \( n = 1 \) we have \( U/W \sim 2 \div 3 \) [8].

We provide next our original version of the derivation of \( t-J \) model [6, 7] and dwell on the details, which seemed to us not obvious whatsoever and are usually overlooked in the textbooks or review articles.

3. \( t-J \) model as it was derived then

I became interested in the Hubbard model around 1974 and particularly, in the problem of deriving its ferromagnetic state in the limit \( U \gg W \). This was because, on the one hand, we have a definite result of Anderson from 1959 [2] that the Mott insulators are antiferromagnetic and from the other that of Nagaoka [9] that the ground state of the Mott insulator in the limit \( U = \infty \) is for certain lattices (e.g. fcc) ferromagnetic. The obvious thing was to combine the two. In that manner, the question how to generalize the Anderson kinetic-exchange Hamiltonian to the metallic regime has arisen naturally, but the question was how to do it in detail. As the kinetic exchange is \( \sim t^2/U \), one should get it from the second-order virtual hopping processes, with the doubly occupied site configurations in the intermediate state. For that purpose, one can rewrite the dynamical processes contained in the hopping term as follows:

\[
a_{i\sigma}^\dagger n_{j\sigma} \equiv a_{i\sigma}^\dagger (1 - n_{i\sigma} + n_{j\sigma}) a_{j\sigma} (1 - n_{j\sigma} + n_{j\sigma}) = a_{i\sigma}^\dagger (1 - n_{i\sigma}) a_{j\sigma} (1 - n_{j\sigma}) + a_{i\sigma}^\dagger (1 - n_{i\sigma}) a_{j\sigma} n_{j\sigma} + a_{i\sigma} n_{i\sigma} a_{j\sigma} (1 - n_{j\sigma}) + a_{i\sigma} n_{i\sigma} a_{j\sigma} n_{j\sigma}. \tag{6}
\]

The consecutive terms represent the four restricted types of hopping processes: the first hopping from singly occupied site onto an empty one, the second hopping from singly occupied site and formation of a doubly occupied one, etc. In such manner, the full hopping term looks like

\[
\sum_{ij\sigma}^l t_{ij} a_{i\sigma}^\dagger (1 - n_{i\sigma}) a_{j\sigma} + \sum_{ij\sigma}^l t_{ij} a_{i\sigma}^\dagger (1 - n_{i\sigma}) a_{j\sigma} n_{j\sigma} + \sum_{ij\sigma}^l t_{ij} a_{i\sigma} n_{i\sigma} a_{j\sigma} (1 - n_{j\sigma}) + \sum_{ij\sigma}^l t_{ij} a_{i\sigma} n_{i\sigma} a_{j\sigma} n_{j\sigma}. \tag{7}
\]
But then, there is a problem: all the processes have the same coupling constants (are coming from the same term in the Hamiltonian), so singling out only the second and the third term as perturbation does not sound right. After a few-month deliberation we will not dwell upon, we have realized that the canonical perturbation in the version by Bogolyubov is the right method to follow. This is because of the three following features of the method:

1. You can perform a perturbation in an invariant (operator) form (not only on matrix elements),
2. If $H = H_0 + H_1$ and $H_1$ is a perturbation part, then in order to do the calculations $H_0$ does not have to be diagonal, and you can select the perturbation term according to your wishes,
3. It bears a strong resemblance to the quantum mechanical perturbation approach when Hamiltonian splits into (large) diagonal blocks and (small) off-diagonal blocks, as we learnt earlier from the Stevens lectures [10].

Formally, one can write the full Hamiltonian as operating in four subspaces

$$H_0 = \sum_{ij\sigma} t_{ij} a_i^{\dagger} a_j^\sigma = P_0 H P_0 + P_N H P_N + P_0 H P_N + P_N H P_0,$$  

(8) assuming (intuitively at this point) that $P_0 + P_N = 1$, and that

$$P_0 H P_0 = \sum_{ij\sigma} t_{ij} a_i^{\dagger}(1 - n_i^\sigma a_j^\sigma(1 - n_j^\sigma),$$  

(9)

$$P_N H P_N = \sum_{ij\sigma} t_{ij} a_i^{\dagger} n_i^\sigma a_j^\sigma n_j^\sigma + U n_i^\uparrow n_i^\downarrow,$$  

(10)

$$P_0 H P_N = \sum_{ij\sigma} t_{ij} a_i^{\dagger}(1 - n_i^\sigma) a_j^\sigma n_j^\sigma,$$  

(11)

$$P_N H P_0 = \sum_{ij\sigma} t_{ij} a_i^{\dagger} n_i^\sigma a_j^\sigma(1 - n_j^\sigma) = (P_0 H P_N)^\dagger.$$  

(12)

The explicit form of these projection operators were not specified then and they need not to be. Understanding that took us some time. Since every term contains process $\sim t_{ij}$, it is convenient to define the operator

$$H_\epsilon = H_0 + \epsilon H_1.$$  

(13)

Obviously, $H \equiv H_{\epsilon=1}$ and

$$H_0 = P_0 H P_0 + P_N H P_N, \quad H_1 = P_0 H P_N + P_N H P_0.$$  

(14, 15)

By introducing $\epsilon$ we will collect the terms of the same order in $\epsilon$. In this manner, we will assume that $P_0 H P_0 \sim t$ and $P_N H P_N \sim U$ represent two different energy manifolds (the Hubbard subbands) distant roughly by $U$, whereas $P_0 H P_N$ represents rare hopping process of creating a doubly occupied site from two neighboring singly occupied sites $(i,j)$. Therefore, even though all the hopping terms contain the same hopping matrix element $t_{ij}$, $P_0 H P_0$ will provide contribution $\sim t_{ij}$ while $P_0 H P_N$ will provide the contribution of $\sim t_{ij}/U$ in the first nontrivial order.
The last nontrivial feature is to select the unitary transformation matrix, with the help of which we remove part of the hopping processes in the first order and replace them by virtual processes exemplifying physical processes in higher order. For that purpose, we have also proposed the following canonical transformation of the form

$$\tilde{H}_\epsilon = e^{-i\epsilon S} H e^{i\epsilon S} \approx H_0 + \epsilon (H_1 + i[H_0, S]) - \frac{1}{2} \epsilon^2 (2i[H_1, S] - [H_0, S], S)$$  \hspace{1cm} (16)

with $S = S^\dagger$.

The linear term $\sim \epsilon$ is absent when 

$$H_1 + i[H_0, S] = 0$$  \hspace{1cm} (17)

Under this condition

$$\tilde{H}_\epsilon = H_0 + \frac{1}{2} \epsilon^2 [H_1, S].$$  \hspace{1cm} (18)

Equation (17) has to be solved for $S$. The main problem is that $H_0$ is not diagonal. Therefore, it is more difficult to solve it the way it was treated originally by Bogolyubov (cf. also the treatment of electron–phonon case by Kittel). Thus, in order to proceed one tries to solve (17) projected onto the subspaces. Explicitly, we can write

$$P_0 H_1 P_N + iP_0 [H_0, S] P_N = 0,$$  \hspace{1cm} (19)

$$P_0 (H_0 S - SH_0) P_0 = P_N (H_0 S - SH_0) P_N = 0.$$  \hspace{1cm} (20)

From the first equation we see that while $S$ must have nontrivial form as it contains $H_1$, the next two equations are of trivial character. This is because one can rewrite them in the form

$$\left( P_0 H_0 P_0 \right) (P_0 SP_0) - (P_0 SP_0)(P_0 H_0 P_0) = 0,$$  \hspace{1cm} (21)

$$\left( P_N H_0 P_N \right) (P_N SP_N) - (P_N SP_N)(P_N H_0 P_N) = 0.$$  \hspace{1cm} (22)

In the original version we have taken a particular solution $P_{0,N} SP_{0,N} = \gamma_{0,N} P_{0,N}$. Equally good would be to replace right hand side (r.h.s.) with an arbitrary function $f(P_{0,N})$ which has a Taylor expansion as $f(P_{0,N}) = \alpha_{0,N} 1 + \gamma_{0,N} P_{0,N}$ because of the property $P_{0,N}^2 = P_{0,N}$.

In effect, we are left with Eq. (17), which projected takes one of the two possible forms

$$P_0 SP_N = [-iP_0 H_1 P_N + (P_0 HP_0)(P_0 SP_N)](P_N HP_N)^{-1}.$$  \hspace{1cm} (23)

Obviously this relation is well defined if the operator $(P_N HP_N)^{-1}$ exists, but we leave such problems to mathematical physicists. What is important for us instead is that since the transformation matrix appears on both left hand side (l.h.s.) and r.h.s. of (23), we can try to solve it by iterating the solution. In the zeroth order we assumed that on r.h.s. of (23) $(P_0 S^{(0)} P_N) = 0$ and then

$$P_0 S^{(1)} P_N = -iP_0 H_1 P_N / P_N HP_N.$$  \hspace{1cm} (24)

The solution up to infinite order takes the form

$$P_0 SP_N = -iP_0 H_1 P_N (P_N HP_N - P_0 HP_0)^{-1}.$$  \hspace{1cm} (25)

The simplest approximation of the denominator is to replace it by an average
the Anderson (antiferromagnetic) kinetic exchange Hamiltonian to each site Hubbard insulator when the number of particles is conserved and equal to unity respectively, in the middle (31).

The third term denotes hopping between three sites without and with spin flip, in terms of fermionic operators:

\[
\langle n \rangle = \frac{1}{2} \sum_{ijkl} t_{ij} \tilde{a}_{i\sigma} \tilde{a}_{j\sigma} (1 - n_{i\sigma}) (1 - n_{j\sigma}) + \sum_{ij} \frac{(2\tilde{t}^2/U)}{U} [a_{i\sigma} (1 - n_{i\sigma})]
\]

The first part of (27) describes the dynamics of electrons in the lower Hubbard subband for \( n \neq 1 \), whereas (28) will represent the same for \( 1 < n \neq 2 \). In the following discussion we limit ourselves to the situation with \( n \neq 1 \).

3.1. Meaning of the \( t-J \) model

Substituting (11) and (12) to (27) and (28), respectively, we obtain explicitly [11]

\[
P_0 \tilde{H} P_0 = \sum_{ij} t_{ij} \tilde{a}_{i\sigma} \tilde{b}_{j\sigma} (1 - n_{i\sigma}) (1 - n_{j\sigma}) + \sum_{ij} \frac{(2\tilde{t}^2/U)}{U} [a_{i\sigma} (1 - n_{i\sigma})]
\]

The first term in (29) represents electron hopping from single-occupied site onto an empty site \( i \), the second term represents full kinetic-exchange part in which, in general, the spin operators \( \{ S_i \} \) representing itinerant electrons are expressed in terms of fermionic operators: \( S_i \equiv (S_i^+, S_i^-) = (a_{i\uparrow}^\dagger a_{i\downarrow}, (n_{i\uparrow} - n_{i\downarrow})/2) \). The third term denotes hopping between three sites without and with spin flip, respectively, in the middle (\( j \) site). One can easily see that in the limit of Mott–Hubbard insulator when the number of particles is conserved and equal to unity \( \text{at each site} \) (i.e. \( n_{i\uparrow} + n_{i\downarrow} = 1 \); not only \( \langle n_{i\uparrow} + n_{i\downarrow} \rangle = 1 \)), then (29) reduces properly to the Anderson (antiferromagnetic) kinetic exchange Hamiltonian

\[
P_0 \tilde{H} P_0 = \sum_{ij} \frac{(2\tilde{t}^2/U)}{U} (S_i \cdot S_j - \frac{1}{4}).
\]

In our original work [7, 6] we have already noticed that the dynamics requires introduction of projected fermionic creation, annihilation, and particle-number operators

\[
b_{i\sigma}^\dagger \equiv a_{i\sigma}^\dagger (1 - n_{i\sigma}), \quad b_{i\sigma} \equiv a_{i\sigma} (1 - n_{i\sigma}),
\]

\[
u_{i\sigma} \equiv b_{i\sigma}^\dagger b_{i\sigma} = n_{i\sigma} (1 - n_{i\sigma}),
\]

(32, 33, 34)
which have nonfermionic anticommutation relations
\[
\{ b_{i\sigma}, b^\dagger_{j\sigma'} \} = \left[ (1 - n_{i\sigma}) \delta_{\sigma\sigma'} - S^{-\sigma}_{i} (1 - \delta_{\sigma\sigma'}) \right] \delta_{ij}, \tag{35}
\]
\[
\{ b_{i\sigma}, b_{j\sigma'} \} = \{ b^\dagger_{i\sigma}, b^\dagger_{j\sigma'} \} = 0. \tag{36}
\]

The property (35) poses a problem as there is no reference occupation-number representation. Additionally, the hopping and the exchange parts do not commute with each other, so the motion of single electrons and the spin interactions (e.g. spin flip processes) are entangled with each other and result in a strongly correlated (non-Fermi liquid) metallic state. What is equally important, the kinetic energy (∼t_{ij}) and the exchange (t_{ij}^2/U) can become comparable for a filling close to the half-filling and we can have a transition to the localized state induced by the exchange interaction (see next Section) or to the phase separation into antiferromagnetic insulating islands “floating” in the ferromagnetic sea of (1 − n) holes [9]. This second state is rather unstable as the Coulomb repulsion introduced by the holes i.e. by the positively charged ions of the background (usually neglected in the calculations!) will destabilize the phase-separated configuration.

Few comments are relevant at this point. First, the operators (32)–(34) were introduced by Hubbard [12] under the name of atomic representation. The original Hubbard notation is useful for multi-orbital models [13]. Nonetheless, it is used sometimes also for the present model though, in our view, represents an unnecessary formality. Second, it is sometimes important to include the intersite Coulomb interaction, i.e. the term
\[
\frac{1}{2} \sum_{ij} K_{ij} n_{i} n_{j}. \tag{37}
\]

In that situation [9], the kinetic-exchange integral takes the form J_{ij} = 2t_{ij}^2/(U − K_{ij}) and an additional term (1/2)\sum_{ij} K_{ij} \nu_{i} \nu_{j} appears in (29). Finally, essentially the same formalism has been repeated later by other authors [14]. It is unfortunate for us, those references are often quoted as those, from which the t−J model (i.e. (29), without 3-site terms present) originated. We also comment on the effective t−J model later on when we introduce the two-orbital model.

### 3.2. Localization of holes in doped Mott insulator

Intimately connected with the t−J model is the problem of magnetic polarons [15] and the hole localization induced by the kinetic exchange for the small number of correlated holes, δ = 1 − n ≪ 1. One can address the hole localization by starting from the metallic side. The ground state energy of (29) can be estimated as follows:
\[
E_G = \langle H \rangle = t \sum_{\langle ij \rangle \sigma} \left\langle a^\dagger_{i\sigma} (1 - n_{i\sigma}) a_{j\sigma} (1 - n_{j\sigma}) \right\rangle + J \sum_{\langle ij \rangle} \langle S_i \cdot S_j - \frac{1}{4} \nu_i \nu_j \rangle, \tag{38}
\]
where we have included the terms involving only z nearest neighbors \( \langle i, j \rangle \). In the spirit of the Gutzwiller approach, we can renormalize the hopping term by the band narrowing factor \( \Phi(\lambda) \), with \( \lambda \equiv \langle \nu_i \nu_j / 4 - S_i \cdot S_j \rangle / n^2 \) and thus have
\[
\frac{E_G}{N} = zt \Phi(\lambda) \sum_{j(i)\sigma} \langle a_i^{\dagger} a_j \sigma \rangle_0 - Jz n^2 \lambda, \tag{39}
\]

where \( \langle \ldots \rangle_0 \) denotes the average for an uncorrelated state. Next, let us expand \( \Phi(\lambda) = g_0 + g_1 \lambda + g_2 \lambda^2 \), while \( \langle a_i^{\dagger} a_j \sigma \rangle_0 = n \sigma (1 - n) \) expresses the hopping probability in the reference state without antiferromagnetic correlations (\( \lambda = 1/4 \)). For that value of \( \lambda \) we have \( g_0 + g_1/4 + g_2/16 = 1 \). In the opposite limit (\( \lambda = 1 \)), we have a complete frozen antiferromagnetic (Néel) state, without any hopping, i.e. \( g_0 + g_1 + g_2 = 1 \). Furthermore, writing the energy in the form
\[
\frac{E_G}{zN} = -|t|n(1 - n)(g_0 + g_1 \lambda + g_2 \lambda^2) - Jn^2 \lambda, \tag{40}
\]
and minimizing it with respect to \( \lambda \), we obtain the expression
\[
4g_2 \lambda = -\frac{Jn}{|t|(1 - n)} + g_1. \tag{41}
\]

This equation must also be fulfilled for \( J = 0 \), when there are no antiferromagnetic correlations (i.e. when \( \lambda = 1/4 \)). This means that from the above three conditions we can determine explicitly the coefficients of the expansion of \( \Phi(\lambda) \), which have the values: \( g_0 = -1/9 \), \( g_1 = 8/9 \), and \( g_2 = 16/9 \). Hence, the optimal value of the variational parameter \( \lambda \) is
\[
\lambda = \frac{1 + 9J}{32 |t|(1 - n)}. \tag{42}
\]
This means that the full antiferromagnetic insulating state (\( \lambda = 1 \)) is achieved for
\[
\delta = \delta_C = \left(1 + \frac{8|t|}{3J}\right)^{-1}, \tag{43}
\]
and is of the order \( \delta_C \approx 0.1 \) for \( |t|/J = 3 \), a reasonable value for La_{2−x}Sr_{x}CuO_{4} system. The ground state energy is then
\[
\frac{E_G}{zN} = -|t|n(1 - n) - \frac{1}{4} Jn^2 - \frac{9}{64} |t|(1 - n) \frac{J^2 n^3}{|t|(1 - n)}. \tag{44}
\]
This reasoning represents essentially the simplest mean-field-like description of the transition from the strongly correlated paramagnetic metal to an antiferromagnetic insulator with frozen holes at \( \delta = \delta_C \).

4. \textit{t−J model renewal: kinetic exchange as the source of real space pairing}

Until 1987, the \textit{t−J} model was regarded as a generic model for explaining the antiferromagnetism of the Mott insulators such as the oxides NiO or CoO, and relatively rarely considered for \( n \neq 1 \). Obviously, the real oxides have both 3d and 2p orbital states as the valence-band states, but it was argued strongly (and still is) [2, 15, 16] that the \( p−d \) hybridization can be incorporated into an effective d-band Hubbard model, although there were some exceptions to that idea [17]. The essential new idea, about which we have learnt from the preprint of Ruckenstein et al. [18] was to associate the kinetic exchange part with \textit{real space pairing}, but there were quite few papers appearing at about the same time [19]. Soon, the
slave-boson and slave-fermion mean-field theories have been formulated followed by a flood of papers, also about the stability of d-wave superconducting solution. This is a fascinating story for itself, but we shall leave this to a separate occasion.

4.1. t–J Hamiltonian as pairing Hamiltonian

We would like to raise only one aspect of this story namely, the proper formal expression of the pairing part [11]. As we have seen, we have to express the whole Hamiltonian (29) in terms of projected fermion operators \( b_{i\sigma} \) and \( b_{i\sigma}^\dagger \). First, one notices that the spin operator has the same form in both fermion \( \{a_{i\sigma}, a_{i\sigma}^\dagger\} \) and in the projected \( \{b_{i\sigma}, b_{i\sigma}^\dagger\} \) representations. Explicitly,

\[
S_i = \left( a_{i\uparrow}^\dagger a_{i\downarrow}, a_{i\downarrow}^\dagger a_{i\uparrow}, (n_{i\uparrow} - n_{i\downarrow})/2 \right) \equiv \left( b_{i\uparrow}^\dagger b_{i\downarrow}, b_{i\downarrow}^\dagger b_{i\uparrow}, (n_{i\uparrow} - n_{i\downarrow})/2 \right).
\]

(45)

Therefore, the spin-singlet real-space pairing operators should be selected in the form \( (i \neq j) \):

\[
B_{i j}^{\uparrow \downarrow} \equiv \frac{1}{2} \left( b_{i\uparrow}^\dagger b_{j\downarrow}^\dagger - b_{i\downarrow}^\dagger b_{j\uparrow}^\dagger \right),
\]

\[
B_{i j}^{\uparrow \downarrow} \equiv \frac{1}{2} \left( b_{i\uparrow} b_{j\downarrow} - b_{i\downarrow} b_{j\uparrow} \right) = \frac{1}{\sqrt{2}} \left( a_{i\uparrow} a_{j\downarrow} - a_{i\downarrow} a_{j\uparrow} \right) (1 - n_{i\uparrow})(1 - n_{j\uparrow}).
\]

(46)

(47)

In this representation, we have the following identity:

\[
B_{i j}^{\uparrow \downarrow} B_{i j}^{\uparrow \downarrow} = - \left( S_i \cdot S_j - \frac{1}{4} \sum_{\sigma \sigma'} \nu_{i\sigma} \nu_{j\sigma'} \right).
\]

(48)

One should note at this point that the representation of (48) through the operators \( B_{i j}^{\uparrow \downarrow} \) and \( B_{i j}^{\downarrow \uparrow} \) is completely equivalent to that through the spins and projected particle-number operators. In other words, the spin ordering and the nearest-neighbor pairing should be treated on the same footing.

Substituting (48) to \( P_0 H P_0 \) we obtain the effective t–J Hamiltonian in the following closed form when the 3-site terms are also included [11]:

\[
\tilde{H} \equiv P_0 \tilde{H} P_0 = \sum_{i j \sigma} t_{i j} b_{i \sigma}^\dagger b_{j \sigma} - \sum_{i j k} (2t_{i j} t_{j k} / U) B_{i j} B_{j k}. \]

(49)

Obviously, it is assumed that \( t_{i j} \neq 0 \) only for \( i \neq j \). Furthermore, the pairing part vanishes by itself if \( i = j \) as \( B_{i i}^{\uparrow \downarrow} = 0 \). This means that the pairing order parameter will have a nontrivial dependence in both real and reciprocal \( (k) \) spaces.

Transforming the Hamiltonian (49) to \( k \) space, we obtain pairing Hamiltonian, which takes the following form when there are phase differences between the neighbors from the left and the right sides:

\[
P_0 \tilde{H} P_0 = \sum_{k \sigma} \epsilon_k b_{k \sigma}^\dagger b_{k \sigma} - \frac{2t^2}{U} \sum_{k k'} \gamma_{k k'} B_{k - k'}^{\uparrow \downarrow} B_{-k' k},
\]

(50)

where

\[
B_{k' - k}^{\uparrow \downarrow} \equiv \frac{1}{\sqrt{2}} \left( b_{k\uparrow}^\dagger b_{-k\downarrow} - b_{k\downarrow}^\dagger b_{-k\uparrow} \right)
\]

and

\[
b_{k \sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_{R_i} e^{-i k R_i} a_{i \sigma}^\dagger (1 - n_{i \sigma}).
\]

(51)

(52)
From the form (52) we see that also the operators \( b_{k\sigma}^\dagger \) (and \( b_{k\sigma} \)) have a nontrivial many-particle character. The only simple property here is the separability of the pairing potential, i.e. \( V_{kk'} = -(2t^2/U)\gamma_k\gamma_{k'} \equiv V_kV_{k'} \), where \( \gamma_k \) depends on the solution symmetry (for example, for an extended s-wave solution for the square lattice \( \gamma_k = \epsilon_k/t \); see also below).

The solution of the \( t-J \) model in the forms (49) or (50) is the subject of an intense discussion, but this absolutely fundamental aspect of the model will not be touched upon here. We hope to return to this aspect of the exchange mediated superconductivity elsewhere.

4.2. Three remarks on the pairing Hamiltonian with 3-site terms

First remark concerns the formal form of \( \gamma_k \). Namely, when taking the Fourier transform of the part \( \sim t_{ij}t_{jk} \) in (49) and assuming that for given neighbor (e.g. in the square lattice) the operator \( B_{ij} \) for \( j \) to the right from \( i \) acquires the phase \( \varphi_x \) with respect to that to the left. In effect, the part \( \gamma_k \) of the pairing potential can be expressed as

\[
\gamma_k = e^{i k_x a + \varphi_x} + e^{-i k_x a} + e^{i k_y a + \varphi_y} + e^{-i k_y a},
\]

or equivalently

\[
\gamma_k = 2\cos\left(\frac{k_x}{2}\right)\cos\left(\frac{\varphi_x}{2}\right) + 2i\sin\left(\frac{k_x}{2}\right)\sin\left(\frac{\varphi_x}{2}\right) + 2\cos\left(\frac{k_y}{2}\right)\cos\left(\frac{\varphi_y}{2}\right) + 2i\sin\left(\frac{k_y}{2}\right)\sin\left(\frac{\varphi_y}{2}\right).
\]

This form represents the most general \( k \) dependence of the pairing when the 3-site terms are included.

Second remark concerns the equivalence (48) of spin degrees of freedom and the real-space pairing operators (let us note however, that r.h.s. is nonzero for \( i = j \)). Therefore, when decoupling r.h.s. of (49) we should take into account a possibility of have nonzero both averages. In the Hartree–Fock-like approximation this decoupling for \( k = i \) should take the form

\[
B_{ij}^\dagger B_{ij} = \langle B_{ij}^\dagger B_{ij} \rangle - \langle B_{ij}^\dagger \rangle\langle B_{ij} \rangle - \left[ \langle S_i^z \rangle \langle S_j^z \rangle + \langle S_i^+ \rangle\langle S_j^- \rangle - \langle S_i^\dagger \rangle\langle S_j^\dagger \rangle \right] + \ldots
\]

Therefore, in general, the coexistence of antiferromagnetism (or spin density wave) and the paired state is possible and should be studied carefully.

The last remark concerns mapping of the projected Hamiltonian onto an effective fermionic Hamiltonian, as proposed [11, 20] on early stage of the theory development. Namely, introducing the concept of band narrowing \( \Phi = \Phi(\lambda) \) one can have that

\[
\hat{H} = \Phi \sum_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} - (1 - \Phi) \sum_{ij} (2t_{ij}^2/U) B_{ij}^\dagger B_{ij} - \Phi(1 - \Phi) \sum_{ijk} (2t_{ijk}/U) B_{ij}^\dagger B_{kj},
\]

where \( 0 \leq \Phi \leq 1 \) is the band narrowing factor. Macroscopically \( \Phi \) can be regarded
as a degree of itineracy of electrons. Likewise, \((1 - \Phi)\) is the “fraction” of localized electrons. In (56) the two-site and three-site terms have different renormalization factors. Hence, it is tempting to take, as earlier, \(\langle B_{ij}^\dagger B_{ij}\rangle\) as the variational parameter \(\lambda\). Then, as before \(\Phi = \Phi(\lambda)\). It is also tempting then to associate the pairing only with the 3-site part, but as we are aware of, this possibility has not been studied explicitly as yet. In such model the limit of the antiferromagnetic insulator is reached naturally for \(\delta \to 0\) and the pseudogap appearance is associated with short-range antiferromagnetic correlations.

5. Kondo interaction and real-space hybrid pairing as an extension of the \(t-J\) model concepts

5.1. Deep and shallow impurity cases

Shortly after deriving the effective Hamiltonian (49) and determining the principal features of antiferromagnetic phase we have turned our attention to the Wolff model of magnetic impurity [21] and the corresponding generalization of the canonical transformation [7, 6], as it has been proposed and discussed by us earlier [22]. The Wolff model differs from the original Anderson-impurity model [23] only slightly, as it treats both the impurity electron state and the band states of a metal, the impurity is immersed in, in the tight binding approximation. Explicitly, the Hamiltonian of the system is proposed in the form

\[
H = \sum_{i,j} t_{ij}^\sigma a_i^\dagger \sigma a_j^\sigma + \epsilon_d (n_{0\uparrow} + n_{0\downarrow}) + Un_{0\uparrow}n_{0\downarrow} + (1 + \gamma) \sum_{j^\sigma} t_{0j}^\sigma \left( a_{0\sigma}^\dagger a_{j^\sigma} + a_{j^\sigma}^\dagger a_{0\sigma}^\dagger \right).
\]  

(57)

Here we assume that the impurity is at the 0th site, with \(\epsilon_d\) as the energy for the one-electron impurity state. The intraatomic Coulomb energy for the two-electron impurity state is \(U\) (and zero for the metallic host sites \(j \neq 0\)). The hopping strength between the impurity and the host is specified by \(\gamma\). The double primed summation in (57) excludes the terms with either \(i = 0\) or \(j = 0\); \(\epsilon_d\) is the impurity energy-level position with respect to that for band states, which is taken as \(\epsilon_{jj} = 0\).

We were interested in the strong correlation limit when \(|(1 + \gamma)t_{0j}|\) is much smaller than \(U\). What was (and still is) new in our original approach is that we have considered separately the shallow- and deep-impurity limits. This turned out to have a direct relation respectively to the Kondo and to the mixed-valence (or heavy-fermion) limits of correlated electrons. Also, it has relevance to the concept of \(p-d\) pairing in the high-temperature-superconductivity era [24]. As these reminiscences are probably too long-winded already, we provide only the essence of the argument leading to the pairing. But first, let us summarize the results for the impurity situation.

In the interesting us case of a shallow impurity we have the impurity (correlated) state immersed in the Fermi sea of the metal. In that situation singly occupied impurity state is relatively close to the metal Fermi energy \(\epsilon_F\) but its
doubly occupied state is high in energy and therefore, can be realized via virtual excitations (hence, transformed out again). In effect, the effective Hamiltonian in the second order takes rather complicated form

\[ \hat{H} \equiv P_0 \hat{H} P_0 = \sum_{i,j,\sigma} t_{ij} a^\dagger_{i\sigma} a_{j\sigma} + (1 + \gamma) \sum_{j,\sigma} t_{0j}(1 - n_{0\sigma}) \left(a^\dagger_{0\sigma} a_{j\sigma} + a^\dagger_{j\sigma} a_{0\sigma}\right) \\
+ \epsilon_d(n_{0\uparrow} + n_{0\downarrow}) + \frac{2(1 + \gamma)^2}{U + \epsilon_d} \sum_j t^2_{0j} \left(S^\dagger_0 \cdot S_j - \frac{1}{2} \sum_{\sigma'} n_{0\sigma} n_{j\sigma}\right). \tag{58} \]

This effective interaction contains both the antiferromagnetic impurity–host kinetic exchange interaction (the last term, which can be called the non-local Kondo interaction) and the residual hopping between the impurity and the metallic host. This form, at first look, seems to be of limited use, as there is still part of the hopping left between the host and the impurity. As we show in the following, this type of situation is specific for the heavy fermions and high-\(T_C\) systems, since the valence \((p)\) states play an active role in the electric conductivity.

For the sake of completeness, we provide also the effective Hamiltonian in the deep-impurity case, i.e. when the \(\epsilon_d\) level is deep below the Fermi level. It is

\[ \tilde{H} = \sum_{i,j,\sigma} t_{ij} a^\dagger_{i\sigma} a_{j\sigma} + \epsilon_d(\nu_{0\uparrow} + \nu_{0\downarrow}) - \frac{(1 + \gamma)^2}{\epsilon_d} \sum_j t^2_{0j} n_{j\sigma} - \frac{2(1 + \gamma)^2U}{\epsilon_d(U + \epsilon_d)} \]
\[ \times \left[ t^2_{0j} \left(S^\dagger_0 \cdot S_j - \frac{1}{2} \sum_{\sigma'} n_{j\sigma}\right) + \frac{1}{2} \sum_j t_{0j}^2 S^\dagger_0 \gamma_{j\sigma} a^\dagger_{0\sigma} a_{j\sigma}\right]. \tag{59} \]

This Hamiltonian has a direct correspondence to that derived by Schrieffer and Wolff [25] for the Anderson-impurity model. The last term represents the Kondo interaction, with three-site spin-flip term included (here we explicitly assumed that in the present limit \(n_{0\uparrow} + n_{0\downarrow} = 1\), i.e. we have localized moment at the impurity (0th site).

### 5.2. Hybrid pairing in two-orbital system

After the \(t-J\) model had been interpreted in the categories of electron pairing, a natural question arose if one can do the same for the hybridized (two-orbital) system such as the Anderson-lattice model. This idea has been put into writing subsequently [24] by starting from the Hamiltonian

\[ H = \sum_{m,n} t_{mn} c^\dagger_{m\sigma} c_{n\sigma} + \epsilon_f \sum_{i,\sigma} N_{i\sigma} + U \sum_i N_{i\uparrow} N_{i\downarrow} \]
\[ + \sum_{im} V_{im} \left(a^\dagger_{i\sigma} c_{m\sigma} + c^\dagger_{m\sigma} a_{i\sigma}\right), \tag{60} \]

where the \((i, j)\) label correlated atomic \((a = d \text{ or } f)\) states, \((m, n)\) label delocalized \(c\) states, and \(N_{i\sigma} = a^\dagger_{i\sigma} a_{i\sigma}\). \(V_{im}\) represents hybridization integral. As in the case of shallow impurity, we assume that \(|V_{im}| \ll U\), but \(|\epsilon_f| \sim |V_{im}|\), so not the whole hybridization term can be transformed out. Now, decompose the hybridization term as before, i.e.

\[ a^\dagger_{i\sigma} c_{m\sigma} + c^\dagger_{m\sigma} a_{i\sigma} = (1 - N_{i\sigma}) (a^\dagger_{i\sigma} c_{m\sigma} + c^\dagger_{m\sigma} a_{i\sigma}) + N_{i\sigma} (a^\dagger_{i\sigma} c_{m\sigma} + c^\dagger_{m\sigma} a_{i\sigma}). \tag{61} \]
The first term on r.h.s. represents the interstate \((a-c)\) hopping processes which do not involve \(U\) (double occupancies of atomic states), while the second does involve \(U\) and hence leads to higher-order mixing processes. The basic idea introduced at this point [11] is to canonically transform out the second term only and to replace it by an effective interaction incorporating higher-order virtual processes. Leaving the details [24], the effective Hamiltonian with real-space pairing has the form

\[
\tilde{H} = \sum_{mn\sigma} t_{mn} c_{m\sigma}^\dagger c_{n\sigma} + \epsilon_f \sum_{i\sigma} N_{i\sigma} (1 - N_{i\bar{\sigma}}) + \sum_{i\sigma} V_{im} (1 - N_{i\sigma})
\]

\[
\times (a_{i\sigma}^\dagger c_{m\sigma} + c_{m\sigma}^\dagger a_{i\sigma}) - \sum_{imn} \frac{2V_{im}V_{in}}{U + \epsilon_f} B_{im}^\dagger B_{in},
\]

(62)

where the hybrid-pairing operators are defined as

\[
B_{im}^\dagger = \frac{1}{\sqrt{2}} \left( a_{i\uparrow}^\dagger c_{m\downarrow}^\dagger - a_{i\downarrow}^\dagger c_{m\uparrow}^\dagger \right) (1 - N_{i\bar{\sigma}}).
\]

(63)

This model can be transformed again to the effective Fermi-liquid form and the proper form is

\[
\tilde{H} = \sum_{k\sigma} \epsilon_k n_{k\sigma} + \epsilon_f \sum_{i\sigma} N_{i\sigma} + \sum_{k\sigma} \hat{V}_k \left( a_{k\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger a_{k\sigma} \right)
\]

\[- \frac{2}{U + \epsilon_f} \sum_{kq} V_k V_q B_{k,-k}^\dagger B_{q,-q},
\]

(64)

where the tilted quantities are renormalized by correlation, e.g.

\[
\hat{V}_k \equiv q_\sigma V_k = q_\sigma \sum_{j(m)} e^{ik \cdot R_j} V_{jm},
\]

(65)

and \(q_\sigma = (1 - n_f)/(1 - n_{f\sigma})\), with \(n_{f\sigma} = \langle a_{i\sigma}^\dagger a_{i\sigma} \rangle\). Also, the factor \((1 - N_{i\bar{\sigma}})\) is absent in \(B_{im}^\dagger\) (cf. Eq. (63)). This Hamiltonian can be solved in BCS approximation, but the results will not be reproduced here. Likewise, we will omit here the application of (62) to the description of high-\(T_C\) superconductivity with hybrid \(p-d\) pairing, as it would most probably require the inclusion of the 4th order \((d-d\) or \(f-f\)) interactions.

### 5.3. Kinetic exchange in orbitally degenerate systems and possibility of spin–triplet pairing

This topic grew into an independent discipline of its own after publication of the papers by Kugel and Khomskii [26], Cryot and Lyon-Caen [27], and Inagaki [28]. Some aspects of the topic are reviewed in this issue by Oleš [29]. We have also derived the kinetic-exchange Hamiltonian for a partial filling of the band [30], as well as have applied it to explain ferromagnetism of \(\text{CoS}_2\) [31]. In general, inclusion of the orbital degeneracy allows for a natural explanation of the appearance of ferromagnetic Mott–Hubbard insulators in conjunction with the orbital ordering of antiferromagnetic type in systems such as \(\text{K}_2\text{CuF}_4\).

In connection with this, a question has arisen, whether the ferromagnetic kinetic exchange can produce spin–triplet pairing. This question is particularly important because it has been shown earlier that the Hund rule coupling can lead
not only to ferromagnetism, but also to the superconducting pairing [32]. Such an effective model has been proposed and analyzed in detail in the strong-correlation limit very recently [33]. These last results will be submitted for a publication shortly.

6. Concluding remarks

In this overview we have concentrated on the idea of kinetic exchange as it was derived 30 years ago and its subsequent application to the systems with real space pairing mediated by this exchange interaction. By no means it is a complete survey. For example, we have ignored all the subsequent formal development of the model (see e.g. [34]). Also, we have disregarded the effect of electron–lattice coupling on the effective $t−J$ model with pairing [35]. Nonetheless, what we hope we have sketched here is the analytical structure of the $t−J$ model in various strongly correlated systems, in which magnetism and superconductivity seem to have a common origin, although it has not as yet been proved conclusively that the kinetic exchange is the origin of both of them. Future will show.

Acknowledgments

In addition to my colleagues and students mentioned in the Foreword to this volume, I would like to thank Dr. Robert Podsiadly for his technical help. This work was supported by Foundation of Polish Science (FNP) and the grant No. 1 P03B 001 29 from Ministry of Science and Higher Education. Part of the work mentioned is elaborated under the auspices of COST P-16 Network of European Science Foundation.

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