Reformulation of Periodic $s$-$d$ Model

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The periodic $s$-$d$ model is reformulated with four Fermion operators. Localized spins are described by "d" electrons. An unitary transformation transforms the system into a system constructed of new Fermions. Infinite repulsions are introduced to eliminate the extra states. We also show the validity of the treatment by Kato and Tsuneto.

The so-called heavy Fermion systems are investigated both experimentally and theoretically. Recently Kato and Tsuneto have proposed a theory for the periodic $s$-$d$ model which is valid in the strong $s$-$d$ coupling limit. For each lattice site, they introduce four Fermion operators, and describe the singlet state as a vacuum and two doublet states as one "particle" states, where the ket $|n_1,n_2\uparrow(\downarrow)\rangle$ represents the state with $n_1$ spin-up, $n_2$ spin-down conduction electrons and up (down) localized spin. Their reformulation is performed as follows. At first the Hilbert space is truncated to that composed of the singlet and the two doublet states, and then four Fermions are introduced intuitively by observing the matrix elements of the electron transfer term of the hamiltonian.

Finally the infinite repulsion among new Fermions is introduced to guarantee "the exclusion of states". However their method is incomplete because of the following reasons:

1) The correspondence of the new Fermion operators with the original operators is ambiguous.

2) Since four Fermion system needs the wider Hilbert space than that for electron-spin system, the truncation of the Hilbert space must be performed after introducing new Fermions.

3) The relation between the infinite repulsion and the truncation of the Hilbert space is also ambiguous.

In this communication, we will consistently reformulate the periodic $s$-$d$ model with four Fermions by virtue of a unitary transformation. The resultant model is applicable to any range of $W/J$ (where $W$ is the strength of electron transfer and $J$ the $s$-$d$ coupling constant) in principle. The validity of the description by Kato and Tsuneto will also be shown in the last part.

The system under consideration is a cubic lattice. There is a localized spin on each site of the lattice. Conduction electrons are hopping site to site by nearest neighbor transfer interaction, and interact with the localized spins by the $s$-$d$ coupling. The hamiltonian for this system is

$$H = \sum_i h_i + W \sum_{i\neq j} \left( C_i^+ C_j + C_j^+ C_i + (c, c) \right)$$

with $h_i = J \vec{\sigma} \cdot \vec{S}_i$, the site hamiltonian, where $\sigma_i$ and $S_i$ are the spin operators at site $i$ of the conduction electron and the localized spin respectively. $C_i$ is an annihilation operator of a conduction electron at site $i$ with up- (down-) spin. The second term is a sum of all the nearest neighbor pair contributions.

If there is no transfer interaction, the system is composed of independent electron-spin pairs. For each pair, the ground state is a singlet pair with energy $-3J/4$, and there are four states with energy 0 and three triplet states with energy $J/4$. From here to Eq. (5), we restrict our discussion to the one site problem and thus omit the site subscripts. We now describe the localized spin by the virtual $d$-electron in the standard manner. Then the dimension of the Hilbert space becomes 16. We prepare another 16-dimensional Hilbert space constructed from four Fermion operators $\phi_1, \phi_2$ and define a unitary transformation $U$ by the following equations:

$$U \frac{\sqrt{2}}{2} (C_i^+ d_i - C_i d_i^+) |0\rangle = |0\rangle,$$

$$U d_i^+ |0\rangle = \phi_i |0\rangle,$$

$$U C_i^+ C_i d_i^+ |0\rangle = - \phi_i^+ |0\rangle,$$
\[ UC_t^+ C_t^+ d_t^+ |\overline{0}\rangle = - \phi_t^* |0\rangle, \quad Ud_t^+ |\overline{0}\rangle = \phi_t^* |0\rangle, \]
\[ UC_t^+ d_t^+ |\overline{0}\rangle = - \phi_t^* \phi_t^+ |0\rangle, \quad UC_t^+ c_t^+ |\overline{0}\rangle = - \phi_t^* \phi_t^+ |0\rangle, \]
\[ U^{1/2} (C_t^+ d_t^+ + C_t^+ c_t^+ |\overline{0}\rangle) = \sqrt{2} (\phi_t^* \phi_t^* + \phi_t^* \phi_t^+) |0\rangle, \]
\[ UC_t^+ C_t^+ d_t^+ |\overline{0}\rangle = \phi_t^* \phi_t^+ |0\rangle, \quad UC_t^+ d_t^+ |\overline{0}\rangle = \phi_t^* \phi_t^+ |0\rangle, \]
\[ UC_t^+ c_t^+ |\overline{0}\rangle = \phi_t^* \phi_t^+ \phi_t^+ |0\rangle, \quad UC_t^+ |\overline{0}\rangle = \phi_t^* \phi_t^+ \phi_t^+ |0\rangle, \]
\[ Ud_t^+ d_t^+ |\overline{0}\rangle = \sqrt{2} (\phi_t^* \phi_t^* \phi_t^+ + \sqrt{2}/2 (\phi_t^* \phi_t^* - \phi_t^* \phi_t^+)) |0\rangle, \]
\[ UC_t^+ C_t^+ |\overline{0}\rangle = \sqrt{2} (\phi_t^* \phi_t^* - \phi_t^* \phi_t^+) |0\rangle, \quad (2) \]

where \(|\overline{0}\rangle\) is \(C,d\)-vacuum and \(|0\rangle\), \(\phi, \phi\)-vacuum. Because \(U\) transforms a complete orthonormal basis into another one, the unitarity of \(U\) is evident. The transformed states are determined so that,

1) the number of new Fermions in a transformed state increases, as the energy of the original state increases,
2) the transformation conserves the total spin,

\[ \begin{align*}
\hbar &= -\frac{3F}{4} + \frac{3F}{4} (n_t + n_t + \bar{n}_t + \bar{n}_t) - \frac{1}{2} (n_t \bar{n}_t + n_t \bar{n}_t + \phi_t^* \phi_t^* \phi_t^* + \phi_t^* \phi_t^+ \phi_t^+) \\
&= -\frac{3F}{4} (n_t \bar{n}_t + n_t + 1/2 \{ n_t \bar{n}_t + n_t \bar{n}_t - \phi_t^* \phi_t^* \phi_t^* - \phi_t^* \phi_t^+ \phi_t^+ \}) \\
&+ \frac{3F}{8} (\bar{n}_t \bar{n}_t \bar{n}_t + n_t \bar{n}_t + n_t \bar{n}_t + n_t \bar{n}_t + n_t n_t),
\end{align*} \]

\[ (3) \]

3) \(C_t^{(1)}\) can be expressed by new Fermion operators in the simple and symmetric manner.

Among 16 states listed in Eq (2), the former octet is physical but the latter is not. We extend the original operators such that they operate on the unphysical state vectors as null operators. Then the transformed site hamiltonian and \(C\)-operators are

\[ \begin{align*}
C_t &= \frac{\sqrt{2}}{2} (\phi_t^* + \phi_t^*) + \left( \frac{1 - \sqrt{2}}{2} \right) n_t + \frac{1}{2} (\sqrt{2}/2 \bar{n}_t + (\sqrt{2}/2 - 1) n_t \bar{n}_t + (\sqrt{2}/2 n_t \bar{n}_t) \right) \phi_t^* \\
&+ \left( \frac{1 - \sqrt{2}}{2} \right) \bar{n}_t + \frac{1}{2} \left( \frac{\sqrt{2}}{2} - 1 \right) \bar{n}_t + \frac{1}{2} \left( \frac{\sqrt{2}}{2} \bar{n}_t \right) \phi_t^* \\
&+ \frac{1}{2} (1 - n_t) \phi_t^* \phi_t^* \phi_t^* + \frac{1}{2} (1 - \bar{n}_t) \phi_t^* \phi_t^* \phi_t^* + \left( \frac{\sqrt{3}}{2} - \frac{\sqrt{3}}{2} \right) (n_t n_t (1 - \bar{n}_t) \phi_t^* + \bar{n}_t \bar{n}_t (1 - n_t) \phi_t^*),
\end{align*} \]

\[ (4) \]

\[ \begin{align*}
C_t &= \frac{\sqrt{2}}{2} (\phi_t^* - \phi_t^*) + \left( \frac{1 - \sqrt{2}}{2} \right) n_t + \frac{1}{2} (\sqrt{2}/2 \bar{n}_t + (\sqrt{2}/2 - 1) n_t \bar{n}_t + (\sqrt{2}/2 n_t \bar{n}_t) \right) \phi_t^* \\
&+ \frac{1}{2} (1 - n_t) \phi_t^* \phi_t^* \phi_t^* + \frac{1}{2} (1 - \bar{n}_t) \phi_t^* \phi_t^* \phi_t^* + \left( \frac{\sqrt{3}}{2} - \frac{\sqrt{3}}{2} \right) (n_t n_t (1 - \bar{n}_t) \phi_t^* - \bar{n}_t \bar{n}_t (1 - n_t) \phi_t^*),
\end{align*} \]

\[ (5) \]

where \(n_t^{(1)}\) and \(\bar{n}_t^{(1)}\) are the number operators of \(\phi_t^{(1)}\) and \(\phi_t^{(1)}\).

Next we eliminate the unphysical states from the energy eigenvalue problem by introducing an extra term to the site hamiltonian. The result is

\[ \hbar_t = -\frac{3F}{4} + \frac{3F}{4} (n_t + n_t + \bar{n}_t + \bar{n}_t) \]
where \( V \) must go to infinity before the thermodynamic limit is taken. With this Hamiltonian, all the unphysical states have the energy of order \( V \). Thus in the infinite \( V \) limit, they do not appear in the energy eigenstates. Now we simplify the \( C \)-operators in the Hamiltonian as

\[
C_{ti} = \sqrt{2/3} (\phi_{ti} + \phi_{ti}^\dagger) + \left( 1 - \sqrt{2/3} \right) ((\bar{n}_{ti} + \bar{n}_{ti}) \phi_{ti} + (n_{ti} + n_{ti}) \phi_{ti}^\dagger), \\
C_{i} = \sqrt{2/3} (\phi_{i} - \phi_{i}^\dagger) + \left( 1 - \sqrt{2/3} \right) ((\bar{n}_{i} + \bar{n}_{i}) \phi_{i} - (n_{i} + n_{i}) \phi_{i}^\dagger).
\]

Any matrix element of the simplified \( C \)-operators between two physical states is the same as that of the original \( C \)-operators. Although the original \( C \)-operators have no matrix element between a physical state and an unphysical state, the simplified \( C \)-operators do have. The effects of these undesirable matrix elements on energy eigenstates and energy eigenvalues are at most of order \( \max(J,W)/V \) and disappear in the infinite \( V \) limit. Thus the use of simplified \( C \)-operators in the Hamiltonian is valid in the infinite \( V \) limit. Note that the simplification is not allowed in other operators such as a charge density operator.

In conclusion, the model described by the Hamiltonian (Eq. (1)) with \( C_{ti} \), \( C_{i} \), and \( h_{i} \) replaced by the right-hand sides of Eqs. (7), (8) and (6) respectively is equivalent to the periodic \( s-d \) model in the infinite \( V \) limit.

The merit of the present formalism is that it avoids the singular behavior due to the formation of a singlet bound state. This is also the case in the Kato-Tsuneto theory. But the present formalism, in which the triplet states are included, is advantageous to that of Kato and Tsuneto, because the state in which the triplet states play an important role, such as a magnetically ordered state, can also be described.

In the remaining of this communication we show the validity of the treatment by Kato and Tsuneto in case that the triplet states are neglected. To neglect the triplet states, we introduce another repulsion term

\[
h_{s_{i}} = V' \left\{ n_{i} \bar{n}_{i} + n_{i} \bar{n}_{i} + \frac{1}{2} (n_{i} \bar{n}_{i} + n_{i} \bar{n}_{i}) + \phi_{i}^\dagger \phi_{i} - \phi_{i}^\dagger \phi_{i} + \phi_{i}^\dagger \phi_{i} - \phi_{i}^\dagger \phi_{i} \right\}
\]

This is the starting point of the theory of Kato and Tsuneto, and thus their treatment is valid. Incidentally the correspondence between their operators and ours is

\[
\phi_{ti} \leftrightarrow a_{i}, \phi_{i} \leftrightarrow a_{i}, \phi_{i} \leftrightarrow a_{i}, \phi_{i} \leftrightarrow a_{i}.
\]

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1) For example, see G. R. Stewart, Rev. Mod. Phys. 56 (1984), 755 and references therein.