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LETTER TO THE EDITOR

On a unified canonical transformation of the large-negative-(positive-) U Hubbard model

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Abstract. The Schrieffer–Wolff transformation of the large-negative-U Hubbard model is performed in detail. Similarities to and differences from the canonical transformation of the large-positive-U Hamiltonian into the $t-J$ model are discussed.

Strongly correlated Hubbard models are extensively investigated in view of high-temperature superconductivity. The repulsive case ($U>0$) with its large-positive-U (LPU) limit [1] is discussed in the context of antiferromagnetism and superconductivity.

On the other hand, different versions of attractive ($U<0$) models [2] including the large-negative-U (LNU) limit [3–5] are considered. An effective local attraction of electrons can be caused, e.g. by local phonons, excitons, or acoustic plasmons which overcome the Coulomb repulsion. Earlier work [3, 4] on a semiconductor–superconductor transition within the LNU Hubbard model has been re-analysed and extended [5]. With additional disorder this Hamiltonian was used to study superconducting glasses [3–5].

The method of canonical transformation (CT) of the Schrieffer–Wolff type, which permits us to isolate those interactions dominating the dynamics of the system, has a long history [6–8], but has not, until recently, been under discussion [9–11]. This approach was applied to the single-impurity Anderson Hamiltonian [6] and the LPU Hubbard model [7–11].

The main purpose of this letter is to make transparent the assumptions and approximations used to derive via the CT an effective model from the LNU limit. Additionally, we point out similarities and differences between the CT of the LPU Hubbard model and the $t-J$ model. It is shown that both cases can be treated within a unified scheme.

The simplest Hamiltonian describing negative-U centres is given by

$$H=-t\sum_{\langle i,j\rangle\sigma} c_{i\sigma}^{+}c_{j\sigma}+U\sum_{i} n_{i\uparrow}n_{i\downarrow}=H_t+H_U. \tag{1}$$

Here $c_{i\sigma}^{+}$ ($c_{i\sigma}$) creates (annihilates) an electron in the Wannier state at site i with spin σ; $n_{i\sigma}=c_{i\sigma}^{+}c_{i\sigma}$ is the local particle number operator. The summation $\langle i,j\rangle$ runs over all nearest-neighbour (NN) sites. t is the hopping integral and U denotes the on-site interaction strength between electrons with opposite spins.

First, let us sketch the concept of the CT. The Hamiltonian $H=H_0+H_1$ is decomposed into the unperturbed part H_0 and the perturbation H_1. The CT is defined by

$H' = e^{-S} H\, e^{S}$ (cf analogous forms in [6–10]) with the anti-Hermitian operator $S^+ = -S$. The transformed H' can be expanded as

$$H' = H_0 + (H_1 + [H_0, S]) + \tfrac{1}{2}[(H_1 + [H_0, S]), S] + \tfrac{1}{2}[H_1, S] + \ldots \qquad (2)$$

The aim of the CT is to eliminate H_1 to first order. This can be achieved by choosing the generator S to satisfy the condition $H_1 + [H_0, S] = 0$. Then, in lowest order, H' is well approximated by

$$\tilde{H}' = H_0 + \tfrac{1}{2}[H_1, S]. \qquad (3)$$

The last step consists in replacing $\tilde{H}'$ by a suitable effective Hamiltonian H_{eff} describing a new physical situation.

We suppose the following situation: the LNU limit $|U/t| \gg 1$ with $U < 0$ and an even number of electrons. Then the CT is based on the separation of the hopping part into $H_t = H_{t,\mathrm{h}} + H_{t,\mathrm{d}} + H_{t,\mathrm{mix}}$, where [7, 8]

$$H_{t,\mathrm{h}} = -t \sum_{\langle i,j\rangle\sigma} (1 - n_{i,-\sigma}) c^+_{i\sigma} c_{j\sigma} (1 - n_{j,-\sigma}) \qquad (4a)$$

$$H_{t,\mathrm{d}} = -t \sum_{\langle i,j\rangle\sigma} n_{i,-\sigma} c^+_{i\sigma} c_{j\sigma} n_{j,-\sigma} \qquad (4b)$$

$$H_{t,\mathrm{mix}} = -t \sum_{\langle i,j\rangle\sigma} [n_{i,-\sigma} c^+_{i\sigma} c_{j\sigma} (1 - n_{j,-\sigma}) + (1 - n_{i,-\sigma}) c^+_{i\sigma} c_{j\sigma} n_{j,-\sigma}]. \qquad (4c)$$

$H_{t,\mathrm{h}}$ ($H_{t,\mathrm{d}}$) is ascribed to the transport of holes (doubly occupied sites), whereas $H_{t,\mathrm{mix}}$ describes processes changing the number of doubly occupied or, equivalently, empty sites. In the LNU limit only empty or doubly occupied sites occur. Virtual singly occupied sites can be handled by a CT, which eliminates the high-energy hopping processes in (4*c*). Therefore, we choose for H the decomposition

$$H_0 = H_{t,\mathrm{h}} + H_{t,\mathrm{d}} + H_U \qquad H_1 = H_{t,\mathrm{mix}}. \qquad (5)$$

Applying the CT scheme one obtains

$$S = \frac{t}{U} \sum_{\langle i,j\rangle\sigma} [n_{i,-\sigma} c^+_{i\sigma} c_{j\sigma} (1 - n_{j,-\sigma}) - (1 - n_{i,-\sigma}) c^+_{i\sigma} c_{j\sigma} n_{j,-\sigma}] \qquad (6)$$

having used the anticommutator relations $\{c_{i\sigma}, c_{j\sigma'}\} = \{c^+_{i\sigma}, c^+_{j\sigma'}\} = 0$ and $\{c_{i\sigma}, c^+_{j\sigma'}\} = \delta_{ij}\delta_{\sigma,\sigma'}$. In (6) terms of higher order are neglected which are originated from $[(H_{t,\mathrm{h}} + H_{t,\mathrm{d}}), S]$. As an intermediate step of the calculation we quote explicitly the expression [11]

$$\begin{aligned}
[H_{t,\mathrm{mix}}, S] = -\frac{t^2}{U} \sum_{\substack{\langle i,j\rangle\sigma \\ \langle m,n\rangle\sigma'}} \{ & 2c^+_{i\sigma} c_{j\sigma} n_{j,-\sigma} c^+_{m\sigma'} c_{n\sigma'} n_{m,-\sigma'} (\delta_{in} - \delta_{jn}) \delta_{\sigma,-\sigma'} \\
& -2c^+_{i\sigma} c_{j\sigma} n_{i,-\sigma} c^+_{m\sigma'} c_{n\sigma'} n_{n,-\sigma'} (\delta_{im} - \delta_{jm}) \delta_{\sigma,-\sigma'} \\
& +[(c^+_{m\sigma} c_{j\sigma} \delta_{in} - c^+_{i\sigma} c_{n\sigma} \delta_{jm}) n_{n,-\sigma'} n_{i,-\sigma} \delta_{\sigma\sigma'} \\
& + c^+_{m\sigma'} c_{n\sigma'} c^+_{i\sigma} c_{j\sigma} n_{i,-\sigma} (\delta_{in} - \delta_{jn}) \delta_{\sigma,-\sigma'} \\
& + c^+_{i\sigma} c_{j\sigma} c^+_{m\sigma'} c_{n\sigma'} n_{n,-\sigma'} (\delta_{in} - \delta_{im}) \delta_{\sigma,-\sigma'}](1 - 2n_{m,-\sigma'}) \\
& -[(c^+_{m\sigma} c_{j\sigma} \delta_{in} - c^+_{i\sigma} c_{n\sigma} \delta_{jm}) n_{m,-\sigma'} n_{j,-\sigma} \delta_{\sigma\sigma'} \\
& + c^+_{m\sigma'} c_{n\sigma'} c^+_{i\sigma} c_{j\sigma} n_{j,-\sigma} (\delta_{im} - \delta_{jm}) \delta_{\sigma,-\sigma'} \\
& + c^+_{i\sigma} c_{j\sigma} c^+_{m\sigma'} c_{n\sigma'} n_{m,-\sigma'} (\delta_{jn} - \delta_{jm}) \delta_{\sigma,-\sigma'}](1 - 2n_{n,-\sigma'}) \}.
\end{aligned} \qquad (7)$$

Using (3), $\tilde{H}'$ can be cast into the form

$$\tilde{H}' = H_{t,\mathrm{h}} + H_{t,\mathrm{d}} + H_U + H'_H + H'_{s,\mathrm{l}} + H'_{s,\mathrm{tr}} + H'_{\mathrm{pair}} + H'_3 \tag{8}$$

with

$$H'_H = \frac{t^2}{2U} \sum_{\langle i,j\rangle\sigma} (n_{i\sigma}n_{i,-\sigma} + n_{j\sigma}n_{j,-\sigma}) \tag{9a}$$

$$H'_{s,\mathrm{l}} = -\frac{t^2}{2U} \sum_{\langle i,j\rangle\sigma} (n_{i\sigma}n_{j,-\sigma} + n_{j\sigma}n_{i,-\sigma}) \tag{9b}$$

$$H'_{s,\mathrm{tr}} = \frac{t^2}{U} \sum_{\langle i,j\rangle\sigma} (c^+_{i\sigma}c_{i,-\sigma})(c^+_{j,-\sigma}c_{j\sigma}) \tag{9c}$$

$$H'_{\mathrm{pair}} = \frac{2t^2}{U} \sum_{\langle i,j\rangle} c^+_{i_\uparrow}c^+_{i_\downarrow}c_{j_\downarrow}c_{j_\uparrow}. \tag{9d}$$

The first term (9a) describes as H_U an attractive Hubbard-type interaction, which is neglected in the following because of $|U| \gg t^2/|U|$. The terms $H'_{s,\mathrm{l}}$ and $H'_{s,\mathrm{tr}}$ can be interpreted as a longitudinal and a transversal spin–spin coupling, respectively. The expression in (9d) represents the hopping of pairs of electrons. The term H'_3 in (8) contains three-centre contributions. In the LNU limit one has to exclude singly occupied sites yielding the constraint

$$n_{i_\uparrow} - n_{i_\downarrow} = 0 \tag{10}$$

for each site. Thus we are left with the effective Hamiltonian

$$H_{\mathrm{eff}} = H_U + H'_{s,\mathrm{l}} + H'_{\mathrm{pair}}. \tag{11}$$

Introducing the pair operators $C_i = c_{i_\uparrow}c_{i_\downarrow}$ and $C^+_i = c^+_{i_\downarrow}c^+_{i_\uparrow}$ and the pair number operator $N_i = C^+_iC_i$ one obtains

$$H_{\mathrm{eff}} = U\sum_i N_i - \frac{2t^2}{U}\sum_{\langle i,j\rangle} N_iN_j + \frac{2t^2}{U}\sum_{\langle i,j\rangle} C^+_iC_j \tag{12}$$

in agreement with [3–5]. Here the identities $N_iN_j = n_{i\sigma}n_{j\sigma'}$ and $N_i = n_{i\sigma}$ with arbitrary σ and σ' were employed.

Now we make some remarks on the two performed steps ($H \to \tilde{H}'$ and $\tilde{H}' \to H_{\mathrm{eff}}$) of the CT. Especially, we discuss connections to the CT of the nearly half-filled LPU Hubbard model to the $t-J$ model

$$H_{t-J} = -t\sum_{\langle i,j\rangle\sigma} (1-n_{i,-\sigma})c^+_{i\sigma}c_{j\sigma}(1-n_{j,-\sigma}) - \frac{J}{8}\sum_{\langle i,j\rangle\sigma} (n_{i\sigma}n_{j,-\sigma} + n_{j\sigma}n_{i,-\sigma})$$
$$+\frac{J}{4}\sum_{\langle i,j\rangle\sigma} (c^+_{i\sigma}c_{i,-\sigma})(c^+_{j,-\sigma}c_{j\sigma}) \tag{13}$$

with $J = 4t^2/U$ and written in a form without using the more familiar spin vector operator S_i. The constraint reads now $n_{i_\uparrow} + n_{i_\downarrow} \leq 1$.

Let us summarize our discussion in four points.

(i) In both limits it is not suitable to choose $H_1 = H_t$ as perturbation. Formally, an ansatz for S analogous to that in [11] including all four terms of the decomposed H_t (see (4)) with four free parameters leads to contradictions in solving $H_1 + [H_0, S] = 0$. Only the virtual processes in $H_{t,\mathrm{mix}}$ are the relevant perturbations. Thus the first step of the CT, i.e. $H \to \tilde{H}'$, is identical in both cases.

(ii) Now we point out the main difference between the two limits. Doubly occupied sites are energetically favourable in the LNU but unfavourable in the LPU limit. Thus the second step is quite different. In the LNU (LPU) limit one has to project out all terms containing singly (doubly) occupied sites, namely $H_{t,\mathrm{h}}$, $H_{t,\mathrm{d}}$, H'_H, $H'_{s,\mathrm{tr}}$ and H'_3 ($H_{t,\mathrm{d}}$, H_U, H'_H and H'_{pair}). This leads to different restrictions of the Hilbert space. The following approximations are taken into account. In the LNU limit the term H'_H, which is small compared with H_U, is neglected. Three-centre terms summarized in H'_3 and projected out in the LNU case by the constraint (10), are omitted in the LPU case.

(iii) In deriving the $t-J$ model the large U contribution is transformed into the 'very small' antiferromagnetic exchange interaction ($J>0$) of the Heisenberg type but the small $H_{t,\mathrm{h}}$ term survives. In the LNU case the small hopping contribution goes over to the 'very small' pair hopping and NN interaction terms, whereas the strong on-site attraction is not changed.

(iv) No restrictions on the band filling n are needed to carry out the CT in the LNU limit, whereas the $t-J$ model was derived for $1-n \ll 1$. It is also interesting to note that at half-filling both models can be mapped onto each other. But a hidden local symmetry holding for arbitrary n in the LNU [5] case does not exist for $n \neq 1$ in the LPU limit.

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