Annalen der Physik. 7. Folge, Band 47, Heft 2/3, 1990, S. 150—156 J. A. Barth, Leipzig

Derivation of Attractive Electron-Electron Interactions for Superconductivity via Canonical Transformations

By E. KOLLEY and W. KOLLEY

Sektion Physik, Karl-Marx-Universität Leipzig, DDR

Dedicated to Professor Dr. A. Uhlmann on the Occasion of his 60th Birthday

Abstract. Two canonical transformations related to the theory of conventional and high-temperature superconductivity are performed in detail. The BCS Hamiltonian is deduced from the Fröhlich Hamiltonian, and the $t - J$ model with attraction from the Hubbard model in the limit of large on-site Coulomb repulsion. The underlying approximations are pointed out.

Herleitung anziehender Elektron-Elektron-Wechselwirkungen für Supraleitung mittels kanonischer Transformationen

Inhaltsübersicht. Zwei kanonische Transformationen, die mit der Theorie der konventionellen und der Hochtemperatur-Supraleitung in Zusammenhang stehen, werden ausgeführt. Der BCS-Hamilton-Operator wird aus dem Fröhlich-Operator hergeleitet und das $t - J$ -Modell mit Anziehung aus dem Hubbard-Modell im Limes großer Coulomb-Abstoßung am Gitterplatz. Die zugrunde liegenden Näherungen werden aufgezeigt.

1. Introduction

The canonical transformation (CT) [1—6] from an original to an approximate effective Hamiltonian permits to isolate those interactions which dominate the dynamics of the system. In the theory of the conventional superconductivity [7] such a CT can be used [4] to eliminate the electron-phonon interaction at the cost of an attractive electron-electron interaction, giving rise to Cooper pairing. Recently, the CT [5, 6] plays a key role to explain high-T_c superconductivity (see, e.g., [8, 9]) in going over from a large on-site electron-electron repulsion to an effective attraction (kinetic exchange). Such a non-phonon mechanism has been already suggested in connection with heavy-fermion superconductivity [10].

In this paper we perform, within a unified framework, the CT's along both lines mentioned above: from the Fröhlich to the BCS Hamiltonian (Section 3) as well as from the Hubbard model in the large-U limit to the t-J model (Section 4). The purpose is to make transparent in detail the assumptions and approximations used to derive the effective attractive interactions.

2. Concept of the Canonical Transformation

Let us start from a Hamiltonian

$$H = H_0 + H_1 \tag{1}$$

decomposed into the unperturbed part H_0 and the perturbation H_1. The CT is defined by (cf. analogous forms in [1—6])

$$H' = e^{-S} H e^{S} \tag{2}$$

with the anti-Hermitean operator $S^+ = -S$. The transformed Hamiltonian H' can be expanded as

$$\begin{aligned} H' &= \left(1 - S + \frac{1}{2!} S^2 - \ldots\right) H \left(1 + S + \frac{1}{2!} S^2 + \ldots\right) \\ &= H + [H, S] + \frac{1}{2} [[H, S], S] + \ldots \\ &= H_0 + (H_1 + [H_0, S]) + \frac{1}{2} [(H_1 + [H_0, S]), S] + \frac{1}{2} [H_1, S] + \ldots \end{aligned} \tag{3}$$

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

$$H_1 + [H_0, S] = 0. \tag{4}$$

Then, in the lowest order, H' is well approximated by

$$\tilde{H}' = H_0 + \frac{1}{2} [H_1, S]. \tag{5}$$

The last step consists in replacing $\tilde{H}'$ by a suitable effective Hamiltonian H_{eff} describing a new physical situation. Two realizations of the chain $H \to H' \to \tilde{H}' \to H_{\text{eff}}$ are given in the following.

3. Transformation of the Fröhlich- to the BCS-Hamiltonian

Consider an electron-phonon system. According to (1) we decompose $H = H_e + H_{\text{ph}} + H_{e\text{ph}}$ into

$$H_0 = H_e + H_{\text{ph}}, \quad H_1 = H_{e\text{ph}}. \tag{6}$$

More explicitly, in the sense of the Fröhlich model, one has

$$H_e = \sum_{k\sigma} \varepsilon_k c^+_{k\sigma} c_{k\sigma}, \tag{7}$$

$$H_{\text{ph}} = \sum_q \hbar\omega_q \left(b^+_q b_q + \frac{1}{2}\right), \tag{8}$$

$$H_{e\text{ph}} = \sum_{kq\sigma} \tilde{W}_{kq} c^+_{k\sigma} c_{k-q\sigma} (b_q + b^+_{-q}), \tag{9}$$

where $c^+_{k\sigma}(c_{k\sigma})$ are creation (annihilation) operators for electrons in Bloch states with the wave vector k and spin σ; b^+_q, b_q denote the phonon operators at momentum q, ε_k is the one-electron energy and ω_q the phonon frequency. For simplicity, only longitudinal acoustical phonons are taken into account. The matrix element of the electron-phonon interaction reads

$$\tilde{W}_{kq} = -\left(\frac{\hbar N}{2M\omega_q}\right)^{1/2} e_q \cdot \langle k | \nabla_r W(r) | k - q \rangle \tag{10a}$$

$$= -\left(\frac{\hbar}{2MN\omega_q}\right)^{1/2} i q \cdot e_q W_{kq} \tag{10b}$$

with the total number N of atoms (of lattice sites), the ionic mass M, the polarization unit vector $\boldsymbol{e}_{\boldsymbol{q}}$ ($= \boldsymbol{e}_{-\boldsymbol{q}}$), and the electron-ion interaction potential W. There holds $\tilde{W}_{\boldsymbol{kq}} = \tilde{W}^*_{\boldsymbol{k}-\boldsymbol{q},-\boldsymbol{q}}$.

On the other hand, $W_{\boldsymbol{kq}}$ in (10b) is connected with the double Fourier transform of the three-centre integral

$$\langle i \,|\, W(\boldsymbol{r} - \boldsymbol{R}_m^{(0)}) \,|\, j\rangle = \frac{1}{N^2} \sum_{\boldsymbol{k}_1 \boldsymbol{k}_2} W_{\boldsymbol{k}_1 \boldsymbol{k}_2} \, e^{i\boldsymbol{k}_1 (\boldsymbol{R}_i^{(0)} - \boldsymbol{R}_j^{(0)}) + i\boldsymbol{k}_2 (\boldsymbol{R}_j^{(0)} - \boldsymbol{R}_m^{(0)})}, \tag{11}$$

where $\boldsymbol{R}_i^{(0)}$ denotes the equilibrium position of the i-th ion. The matrix element (11) enters the electron-phonon interaction

$$H_{\mathrm{eph}} = -\sum_{ijm\sigma} \langle i \,|\, \nabla_{\boldsymbol{r}} W(\boldsymbol{r} - \boldsymbol{R}_m^{(0)}) \,|\, j\rangle \cdot \boldsymbol{u}_m c_{i\sigma}^{+} c_{j\sigma} \tag{12}$$

written down in Wannier representation instead of (9). The vector

$$\boldsymbol{u}_m = \sum_{\boldsymbol{q}} \left(\frac{\hbar}{2MN\omega_{\boldsymbol{q}}} \right)^{1/2} \boldsymbol{e}_{\boldsymbol{q}} e^{i\boldsymbol{q}\boldsymbol{R}_m^{(0)}} (b_{\boldsymbol{q}} + b_{-\boldsymbol{q}}^{+}) \tag{13}$$

represents a small displacement of the m-th ion from its equilibrium position.

Adopting now the procedure outlined in Section 2, we make in view of (9) the ansatz [4]

$$S = \sum_{\boldsymbol{kq}\sigma} \tilde{W}_{\boldsymbol{kq}} c_{\boldsymbol{k}0}^{+} c_{\boldsymbol{k}-\boldsymbol{q}\sigma} (\alpha b_{\boldsymbol{q}} + \beta b_{-\boldsymbol{q}}^{+}). \tag{14}$$

The coefficients α and β must be determined by (4) on the basis of (6) to (9). By employing the fermionic anticommutator $\{c_{\boldsymbol{k}\sigma}, c_{\boldsymbol{k}'\sigma'}^{+}\} = \delta_{\boldsymbol{kk}'} \delta_{\sigma\sigma'}$ and the bosonic commutator $[b_{\boldsymbol{q}}, b_{\boldsymbol{q}'}^{+}] = \delta_{\boldsymbol{qq}'}$ relations, from (4) one finds

$$\begin{aligned} &\sum_{\boldsymbol{kq}\sigma} \tilde{W}_{\boldsymbol{kq}} c_{\boldsymbol{k}\sigma}^{+} c_{\boldsymbol{k}-\boldsymbol{q}\sigma} \{ b_{\boldsymbol{q}} + b_{-\boldsymbol{q}}^{+} + (\varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}-\boldsymbol{q}}) (\alpha b_{\boldsymbol{q}} + \beta b_{-\boldsymbol{q}}^{+}) \\ &- \hbar\omega_{\boldsymbol{q}} \alpha b_{\boldsymbol{q}} + \hbar\omega_{-\boldsymbol{q}} \beta b_{-\boldsymbol{q}}^{+} \} = 0. \end{aligned} \tag{15}$$

This yields

$$\begin{aligned} \alpha &= -(\varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}-\boldsymbol{q}} - \hbar\omega_{\boldsymbol{q}})^{-1}, \\ \beta &= -(\varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}-\boldsymbol{q}} + \hbar\omega_{\boldsymbol{q}})^{-1}, \end{aligned} \tag{16}$$

provided that $\omega_{\boldsymbol{q}} = \omega_{-\boldsymbol{q}}$.

Next the commutator $\frac{1}{2}[H_{\mathrm{eph}}, S]$ is needed. From (9), (14), and (16) one obtains

$$\begin{aligned} [H_{\mathrm{eph}}, S] = \sum_{\substack{\boldsymbol{kq}\sigma \\ \boldsymbol{k}'\boldsymbol{q}'\sigma'}} &\tilde{W}_{\boldsymbol{kq}} \tilde{W}_{\boldsymbol{k}'\boldsymbol{q}'} \{ c_{\boldsymbol{k}\sigma}^{+} c_{\boldsymbol{k}-\boldsymbol{q}\sigma} c_{\boldsymbol{k}'\sigma'}^{+} c_{\boldsymbol{k}'-\boldsymbol{q}'\sigma'} (b_{\boldsymbol{q}} + b_{-\boldsymbol{q}}^{+}) (\alpha' b_{\boldsymbol{q}'} + \beta' b_{-\boldsymbol{q}'}^{+}) \\ &- c_{\boldsymbol{k}'\sigma'}^{+} c_{\boldsymbol{k}'-\boldsymbol{q}'\sigma'} c_{\boldsymbol{k}\sigma}^{+} c_{\boldsymbol{k}-\boldsymbol{q}\sigma} (\alpha' b_{\boldsymbol{q}'} + \beta' b_{-\boldsymbol{q}'}^{+}) (b_{\boldsymbol{q}} + b_{-\boldsymbol{q}}^{+}) \}, \end{aligned} \tag{17}$$

where $\alpha' \equiv \alpha_{\boldsymbol{k}',\boldsymbol{q}'}$ and $\beta' \equiv \beta_{\boldsymbol{k}',\boldsymbol{q}'}$. In the following we retain only terms with $\boldsymbol{q}' = -\boldsymbol{q}$, i.e. two electrons are scattered from states with $\boldsymbol{k} - \boldsymbol{q}$ and $\boldsymbol{k}' + \boldsymbol{q}$ into such with $\boldsymbol{k}$ and $\boldsymbol{k}'$, implying momentum conservation. Thus (17) can be reduced to

$$\begin{aligned} [H_{\mathrm{eph}}, S] = &\sum_{\substack{\boldsymbol{kk}'\boldsymbol{q} \\ \sigma\sigma'}} \tilde{W}_{\boldsymbol{kq}} \tilde{W}_{\boldsymbol{k}',-\boldsymbol{q}} (\beta' - \alpha')|_{\boldsymbol{q}'=-\boldsymbol{q}} \, c_{\boldsymbol{k}\sigma}^{+} c_{\boldsymbol{k}-\boldsymbol{q}\sigma} c_{\boldsymbol{k}'\sigma'}^{+} c_{\boldsymbol{k}'+\boldsymbol{q}\sigma'} \\ &+ \sum_{\boldsymbol{kq}\sigma} \tilde{W}_{\boldsymbol{kq}} \tilde{W}_{\boldsymbol{k}-\boldsymbol{q},-\boldsymbol{q}} (n_{\boldsymbol{k}\sigma} - n_{\boldsymbol{k}-\boldsymbol{q}\sigma}) (\alpha_{\boldsymbol{k}-\boldsymbol{q},-\boldsymbol{q}} b_{-\boldsymbol{q}} + \beta_{\boldsymbol{k}-\boldsymbol{q},-\boldsymbol{q}} b_{\boldsymbol{q}}^{+}) (b_{\boldsymbol{q}} + b_{-\boldsymbol{q}}^{+}), \end{aligned} \tag{18}$$

where $n_{\boldsymbol{k}\sigma} = c_{\boldsymbol{k}\sigma}^{+} c_{\boldsymbol{k}\sigma}$. Thus we arrive at $\tilde{H}' = H_e + H_{\mathrm{ph}} + \frac{1}{2}[H_{\mathrm{eph}}, S]$.

Because we are interested in terms which describe the electron subsystem with effective interaction induced by phonons, we neglect in $\tilde{H}'$ the free phonon part H_{ph} as well

as the second term in (18). This results in

$$H_{\text{eff}} = \sum_{k\sigma} \tilde{\varepsilon}_k c^+_{k\sigma} c_{k\sigma} + \sum_{\substack{kk'q \\ \sigma\sigma'}} \langle k, k' \,|\, U \,|\, k - q, k' + q \rangle \, c^+_{k\sigma} c^+_{k'\sigma'} c_{k'+q\sigma'} c_{k-q\sigma}, \tag{19}$$

where

$$\tilde{\varepsilon}_k = \varepsilon_k + \sum_{kq\sigma} \tilde{W}_{kq} \tilde{W}_{k-q,-q} \frac{\hbar\omega_q}{(\varepsilon_{k-q} - \varepsilon_k)^2 - (\hbar\omega_q)^2}, \tag{20}$$

$$\langle k, k' \,|\, U \,|\, k - q, k' + q \rangle = \frac{\tilde{W}_{kq} \tilde{W}_{k',-q} \hbar\omega_q}{(\varepsilon_{k'} - \varepsilon_{k'+q})^2 - (\hbar\omega_q)^2}. \tag{21}$$

By additional assumptions H_{eff} can be reduced to the BCS Hamiltonian [7]. Restricting ourselves in (19) to terms with $k' = -k$ only (aimed at Cooper pairing), we get

$$H_{\text{eff}} = \sum_{k\sigma} \tilde{\varepsilon}_k c^+_{k\sigma} c_{k\sigma} + \sum_{\substack{kk' \\ \sigma\sigma'}} U_{kk'} c^+_{k\sigma} c^+_{-k\sigma'} c_{-k'\sigma'} c_{k'\sigma}, \tag{22}$$

where

$$U_{kk'} \equiv \langle k, -k \,|\, U \,|\, k', -k' \rangle = \frac{|\tilde{W}_{kk-k'}|^2 \hbar\omega_{k-k'}}{(\varepsilon_k - \varepsilon_{k'})^2 - (\hbar\omega_{k-k'})^2}. \tag{23}$$

This involves effective attraction between electrons since $U_{kk'} < 0$ if $|\varepsilon_k - \varepsilon_{k'}| < \hbar\omega_{k-k'}$. Hence, H_{eff} given in (22) makes contact to the well-known BCS model

$$H_{BCS} = \sum_{k\sigma} \varepsilon_k c^+_{k\sigma} c_{k\sigma} + \sum_{kk'} U_{kk'} c^+_{k\uparrow} c^+_{-k\downarrow} c_{k'\downarrow} c_{k'\uparrow}, \tag{24}$$

where ε_k is simplified to the Bloch energy and $U_{kk'}$ is parametrized by

$$U_{kk'} = \begin{cases} -U & (U > 0), \quad \text{if } \varepsilon_F - \hbar\omega_D \leq \varepsilon_k, \varepsilon_{k'} \leq \varepsilon_F + \hbar\omega_D \\ 0 & \text{otherwise}. \end{cases} \tag{25}$$

Here a narrow shell of the width $2\hbar\omega_D$ (i.e., $\omega_{k-k'}$ is characterized by the Debye frequency ω_D) around the Fermi energy ε_F contributes to the attractive electron-electron interaction which is responsible for weak-coupling superconductivity [7].

4. From the Hubbard- to the t—J-Model

The Hubbard model Hamiltonian

$$H = -t \sum_{\langle i,j \rangle \sigma} c^+_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_t + H_U \tag{26}$$

describes the motion of tightly bound electrons on a lattice as an interplay between the hopping term H_t and the electron-electron interaction H_U. 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 (n. n.) sites; t is the n. n. hopping integral. U denotes the strength of the on-site Coulomb repulsion between electrons with opposite spins.

From the very beginning we suppose the following situation: the strong correlation limit $U/t \gg 1$ and the nearly-half-filled band case $(1 - n) \ll 1$ with the mean value $n = \langle n_{i\uparrow} \rangle + \langle n_{i\downarrow} \rangle$ (number of electrons per site). As a consequence the band splits into two Hubbard subbands. Correspondingly, one can rewrite identically the hopping part by $H_t = H_{t,h} + H_{t,d} + H_{t,mix}$, where [5]

$$H_{t,h} = -t \sum_{\langle i,j \rangle \sigma} (1 - n_{i,-\sigma}) \, c^+_{i\sigma} c_{j\sigma} (1 - n_{j,-\sigma}), \tag{27}$$

$$H_{t,d} = -t \sum_{\langle i,j \rangle \sigma} n_{i,-\sigma} c^+_{i\sigma} c_{j\sigma} n_{j,-\sigma}, \tag{28}$$

$$H_{t,mix} = -t \sum_{\langle i,j \rangle \sigma} \{ n_{i,-\sigma} c^+_{i\sigma} c_{j\sigma} (1 - n_{j,-\sigma}) + (1 - n_{i,-\sigma}) \, c^+_{i\sigma} c_{j\sigma} n_{j,-\sigma} \}. \tag{29}$$

$H_{t,h}$ ($H_{t,d}$) is ascribed to the transport of holes (double occupied sites), and $H_{t,\mathrm{mix}}$ is the mixing term. In other words, $H_{t,h}$ ($H_{t,d}$) belongs to the lower (upper) subband, whereas $H_{t,\mathrm{mix}}$ mixes the different Hubbard bands.

In the large-U limit real doubly occupied sites are energetically unfavourable [6]. Virtual doubly occupied sites can be handled by a CT. The aim is to eliminate high-energy hopping processes which change the total number of doubly occupied sites. Therefore, we choose for (26) to (29) the decomposition

$$H_0 = H_{t,h} + H_{t,d} + H_U, \qquad H_1 = H_{t,\mathrm{mix}} \tag{30}$$

according to (1). Thus, H_0 includes the low-energy hopping processes which do not change the number of doubly occupied sites.

Applying the CT scheme from Section 2 we make in view of (29) the ansatz

$$S = -t \sum_{\langle i,j\rangle\sigma} \{\alpha n_{i,-\sigma} c_{i\sigma}^{+} c_{j\sigma}(1 - n_{j,-\sigma}) + \beta(1 - n_{i,-\sigma})\, c_{i\sigma}^{+} c_{j\sigma} n_{j,-\sigma}\}. \tag{31}$$

In fulfilling (4) the coefficients α and β must be chosen so that $H_{t,\mathrm{mix}} + [(H_{t,h} + H_{t,d} + H_U), S] = 0$. This leads to

$$\begin{aligned} &-t \sum_{\langle i,j\rangle\sigma} \{(1 + \alpha U)\, n_{i,-\sigma} c_{i\sigma}^{+} c_{j\sigma}(1 - n_{j,-\sigma}) + (1 - \beta U)\,(1 - n_{i,-\sigma})\, c_{i\sigma}^{+} c_{j\sigma} n_{j,-\sigma}\} \\ &+ \text{terms } O(\alpha t^2, \beta t^2) = 0 \end{aligned} \tag{32}$$

having used the anticommutator relations $\{c_{i\sigma}, c_{j\sigma'}^{+}\} = \delta_{ij}\,\delta_{\sigma\sigma'}$ and $\{c_{i\sigma}, c_{j\sigma'}\} = \{c_{i\sigma}^{+}, c_{j\sigma'}^{+}\} = 0$. In (32) the terms of order αt^2 and βt^2 are originated from $[(H_{t,h} + H_{t,d}), S]$, the terms proportional to U stem from $[H_U, S]$, and the remainder comes from $H_{t,\mathrm{mix}}$. With respect to the large-U limit we drop in (32) the terms $O(\alpha t^2, \beta t^2)$ which involve also three-site contributions. Then one obtains $\alpha = -\beta = -1/U$ and (31) becomes (cf. [5])

$$S = \frac{t}{U} \sum_{\langle i,j\rangle\sigma} \{n_{i,-\sigma} c_{i\sigma}^{+} c_{j\sigma}(1 - n_{j,-\sigma}) - (1 - n_{i,-\sigma})\, c_{i\sigma}^{+} c_{j\sigma} n_{j,-\sigma}\}. \tag{33}$$

To construct H_{eff} one has to evaluate the commutator

$$\begin{aligned} \frac{1}{2}[H_{t,\mathrm{mix}}, S] = -\frac{t^2}{2U} \sum_{\langle i,j\rangle\sigma} \sum_{\langle m,n\rangle\sigma'} [\{&n_{m,-\sigma'} c_{m\sigma'}^{+} c_{n\sigma'}(1 - n_{n,-\sigma'}) \\ &+ (1 - n_{m,-\sigma'})\, c_{m\sigma'}^{+} c_{n\sigma'} n_{n,-\sigma'}\}, \\ \{n_{i,-\sigma} c_{i\sigma}^{+} c_{j\sigma}(1 - n_{j,-\sigma}) - (1 - n_{i,-\sigma})\, c_{i\sigma}^{+} c_{j\sigma} n_{j,-\sigma}\}]. \end{aligned} \tag{34}$$

As an intermediate step of the calculation we quote the expression

$$\begin{aligned} \frac{1}{2}[H_{t,\mathrm{mix}}, S] = -\frac{t^2}{2U} \sum_{\langle i,j\rangle\sigma} \sum_{\langle m,n\rangle\sigma'} &\{(1 - 2n_{m,-\sigma'})\,[(c_{m\sigma}^{+} c_{j\sigma}\,\delta_{in} - c_{i\sigma}^{+} c_{n\sigma}\delta_{jm}) \\ &\times n_{n,-\sigma'} n_{i,-\sigma}\,\delta_{\sigma\sigma'} + c_{m\sigma'}^{+} c_{n\sigma'} c_{i\sigma}^{+} c_{j\sigma} n_{i,-\sigma}(\delta_{in} - \delta_{jn})\,\delta_{\sigma,-\sigma'} \\ &+ c_{i\sigma}^{+} c_{j\sigma} c_{m\sigma'}^{+} c_{n\sigma'} n_{n,-\sigma'}(\delta_{in} - \delta_{im})\,\delta_{\sigma,-\sigma'}] - 2c_{i\sigma}^{+} c_{j\sigma} n_{i,-\sigma} c_{m\sigma'}^{+} c_{n\sigma'} n_{n,-\sigma'} \\ &\times (\delta_{im} - \delta_{jm})\,\delta_{\sigma,-\sigma'} - (1 - 2n_{n,-\sigma'})\,[(c_{m\sigma}^{+} c_{j\sigma}\,\delta_{in} - c_{i\sigma}^{+} c_{n\sigma}\,\delta_{jm})\, n_{m,-\sigma'} n_{j,-\sigma}\,\delta_{\sigma\sigma'} \\ &+ c_{m\sigma'}^{+} c_{n\sigma'} c_{i\sigma}^{+} c_{j\sigma} n_{j,-\sigma}(\delta_{im} - \delta_{jm})\,\delta_{\sigma,-\sigma'} + c_{i\sigma}^{+} c_{j\sigma} c_{m\sigma'}^{+} c_{n\sigma'} n_{m,-\sigma'}(\delta_{jn} - \delta_{jm})\,\delta_{\sigma,-\sigma'}] \\ &+ 2c_{i\sigma}^{+} c_{j\sigma} n_{j,-\sigma} c_{m\sigma'}^{+} c_{n\sigma'} n_{m,-\sigma'}(\delta_{in} - \delta_{jn})\,\delta_{\sigma,-\sigma'}\}. \end{aligned} \tag{35}$$

Neglecting the three-centre contributions (such terms are retained in [2, 6]), (35) can be cast in the form

$$\begin{aligned}\frac{1}{2}[H_{t,\mathrm{mix}}, S] = \frac{t^2}{2U}\sum_{\langle i,j\rangle\sigma}\{&n_{i\sigma}n_{i,-\sigma} + n_{j\sigma}n_{j,-\sigma} - n_{i\sigma}n_{j,-\sigma} - n_{j\sigma}n_{i,-\sigma}\\ &+ (1-2n_{j\sigma})\,(c_{i\sigma}^{+}c_{i,-\sigma})\,(c_{j,-\sigma}^{+}c_{j\sigma})\,n_{i,-\sigma} + (1-2n_{i\sigma})\,(c_{i\sigma}^{+}c_{i,-\sigma}^{+})\,(c_{j,-\sigma}c_{j\sigma})\,n_{i,-\sigma}\\ &+ (1-2n_{j\sigma})\,(c_{i\sigma}^{+}c_{i,-\sigma})\,(c_{j,-\sigma}^{+}c_{j\sigma})\,n_{i\sigma} + (1-2n_{i\sigma})\,(c_{i\sigma}^{+}c_{i,-\sigma}^{+})\,(c_{j,-\sigma}c_{j\sigma})\,n_{j\sigma}\\ &+ 2n_{i,-\sigma}\,(c_{i\sigma}^{+}c_{i,-\sigma})\,(c_{j,-\sigma}^{+}c_{j\sigma})\,n_{i\sigma} + 2n_{i,-\sigma}\,(c_{i\sigma}^{+}c_{i,-\sigma}^{+})\,(c_{j,-\sigma}c_{j\sigma})\,n_{j\sigma}\\ &+ (1-2n_{i\sigma})\,(c_{i\sigma}^{+}c_{i,-\sigma})\,(c_{j,-\sigma}^{+}c_{j\sigma})\,n_{j,-\sigma} + (1-2n_{j\sigma})\,(c_{i\sigma}^{+}c_{i,-\sigma}^{+})\,(c_{j,-\sigma}c_{j\sigma})\,n_{j,-\sigma}\\ &+ (1-2n_{i\sigma})\,(c_{i\sigma}^{+}c_{i,-\sigma})\,(c_{j,-\sigma}^{+}c_{j\sigma})\,n_{j\sigma} + (1-2n_{j\sigma})\,(c_{i\sigma}^{+}c_{i,-\sigma}^{+})\,(c_{j,-\sigma}c_{j\sigma})\,n_{i\sigma}\\ &+ 2n_{j,-\sigma}\,(c_{i\sigma}^{+}c_{i,-\sigma})\,(c_{j,-\sigma}^{+}c_{j\sigma})\,n_{j\sigma} + 2n_{j,-\sigma}\,(c_{i\sigma}^{+}c_{i,-\sigma}^{+})\,(c_{j,-\sigma}c_{j\sigma})\,n_{i\sigma}\}.\end{aligned} \tag{36}$$

The contributions on the r.h.s. of (36) can be classified as follows. The first and the second terms, namely

$$H'_H = \frac{t^2}{2U}\sum_{\langle i,j\rangle\sigma}(n_{i\sigma}n_{i,-\sigma} + n_{j\sigma}n_{j,-\sigma}), \tag{37}$$

reflect a repulsive Hubbard-type interaction. The third and fourth terms,

$$H'_{s,l} = -\frac{t^2}{2U}\sum_{\langle i,j\rangle\sigma}(n_{i\sigma}n_{i,-\sigma} + n_{j\sigma}n_{i,-\sigma}) = \frac{4t^2}{U}\sum_{\langle ij\rangle}\left(S_{iz}S_{jz} - \frac{1}{4}n_in_j\right), \tag{38}$$

describe a nonlocal (n. n.) attractive Hubbard-type interaction which can be interpreted as longitudinal spin-spin coupling. The symbol $\langle ij\rangle$ refers to pairs of n. n. sites (links). The six spin-flip terms, which can be summarized as

$$H'_{s,tr} = \frac{t^2}{U}\sum_{\langle i,j\rangle\sigma}(c_{i\sigma}^{+}c_{i,-\sigma})\,(c_{j,-\sigma}^{+}c_{j\sigma}) = \frac{4t^2}{U}\sum_{\langle ij\rangle}(S_{ix}S_{jx} + S_{iy}S_{jy}), \tag{39}$$

produce a transverse spin-spin coupling [3]. The last six terms, which can be reduced to

$$H'_{\mathrm{pair}} = \frac{2t^2}{U}\sum_{\langle i,j\rangle} c_{i\uparrow}^{+}c_{i\downarrow}^{+}c_{j\downarrow}c_{j\uparrow}, \tag{40}$$

represent, in agreement with [3], the hopping of pairs of electrons.

Altogether, the result of the CT becomes $H' = \tilde{H}' + O(t^3/U^2) + \ldots$ with

$$\tilde{H}' = H_{t,h} + H_{t,d} + H_U + H'_H + H'_{s,l} + H'_{s,tr} + H'_{\mathrm{pair}} \tag{41}$$

corresponding to (5). For large U and $(1-n) \ll 1$, one can exclude the doubly occupied states in (41). Then, we are left with the effective Hamiltonian

$$H_{\mathrm{eff}} = H_{t,h} + H'_{s,l} + H'_{s,tr} \tag{42}$$

acting only on the states with no doubly occupied sites. More explicitly, on the basis of (27), (38), and (39) one obtains

$$H_{\mathrm{eff}} = -t\sum_{\langle i,j\rangle\sigma}(1-n_{i,-\sigma})\,c_{i\sigma}^{+}c_{j\sigma}(1-n_{j,-\sigma}) + J\sum_{\langle ij\rangle}(\boldsymbol{S}_i\boldsymbol{S}_j - \frac{1}{4}n_in_j) = H_{t\text{-}J} \tag{43}$$

with the exchange parameter $J = 4t^2/U$; the itinerant spin vector operator $\boldsymbol{S}_i = (S_{ix}, S_{iy}, S_{iz})$ expressed via $S_i^{+} = c_{i\uparrow}^{+}c_{i\downarrow}$, $S_i^{-} = c_{i\downarrow}^{+}c_{i\uparrow}$ by $S_{ix} = \frac{1}{2}(S_i^{+} + S_i^{-})$, $S_{iy} = \frac{1}{2i}(S_i^{+} - S_i^{-})$, and $S_{iz} = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$; and $n_i = n_{i\uparrow} + n_{i\downarrow} = \sum_{\sigma} c_{i\sigma}^{+}c_{i\sigma}$. To sum completely over links $\langle ij\rangle$ instead partially over $\langle i, j\rangle$, the first summand in (43) must be augmented

by its Hermitean conjugate. The final form (43) represents the so-called t-J model being valid in the non-doubly occupied subspace, i.e. in the lower Hubbard band. Especially, (43) involves an antiferromagnetic exchange interaction ($J > 0$) of the Heisenberg-type arising from virtual transitions into states with doubly occupied sites [10]. H_{t-J} can serve as a starting point [8, 9] to study high-T_c superconductivity, in particular by means of the resonating valence bond (RVB) concept [8].

5. Conclusion

The method of the CT was used to establish within a unified framework two different Hamiltonians with effective attraction of electrons on the basis of electron-phonon or purely repulsive electron-electron interactions, respectively. The underlying approximations were pointed out. The resulting H_{BCS} and H_{t-J} are significant models within the theories for conventional and high-T_c superconductivity, respectively. Let us summarize the analogy of the two CT schemes (BCS/$t - J$, respectively) by means of the

(i) formulation: $\boldsymbol{k}$-space/real space (lattice);
(ii) original model: Fröhlich/Hubbard ($U/t \gg 1$);
(iii) elimination: electron-phonon interaction H_{eph}/cross-subband hopping $H_{t,\mathrm{mix}}$;
(iv) subsystem neglected (due to decoupling): phonon/upper Hubbard band;
(v) final model: BCS/$t - J$;
(vi) result of the attraction: Cooper pair/n. n. singlet pair.

Note that the two-body term of H_{BCS} in (24) takes the form $-U \sum_{\boldsymbol{k}\boldsymbol{k}'} b_{\boldsymbol{k}}^{+} b_{\boldsymbol{k}'}$ with $b_{\boldsymbol{k}}^{+} = c_{\boldsymbol{k}\uparrow}^{+} c_{-\boldsymbol{k}\downarrow}^{+}$ creating a Cooper pair; while the J-term of H_{t-J} in (43) can be written as [8] $-J \sum_{\langle ij \rangle} b_{ij}^{+} b_{ij}$, where $b_{ij}^{+} = \frac{1}{\sqrt{2}} (c_{i\uparrow}^{+} c_{j\downarrow}^{+} - c_{i\downarrow}^{+} c_{j\uparrow}^{+})$ creates a singlet spin pair on the n. n. "valence" bond $\langle ij \rangle$.

The BCS model applies mainly to superconductivity in simple metals, whereas the CuO_2 planes in high-T_c superconductors can be treated by the $t - J$ model with states centred on Cu sites.

References

[1] Schrieffer, J. R.; Wolff, P. A.: Phys. Rev. **149** (1966) 491.
[2] Harris, A. B.; Lange, R. V.: Phys. Rev. **157** (1967) 295.
[3] Chao, K. A.; Spałek, J.; Olés, A. M.: J. Phys. C **10** (1977) L271.
[4] Valenta, L.; Jäger, E.: Vorlesungen über Festkörpertheorie, Bd. II. Berlin: VEB Deutscher Verlag der Wissenschaften 1981.
[5] Gros, C.; Joynt, R.; Rice, T. M.: Phys. Rev. B **36** (1987) 381.
[6] Gros, C.: Ann. Phys. (N.Y.) **189** (1989) 53.
[7] Bardeen, J.; Cooper, L. N.; Schrieffer, J. R.: Phys. Rev. **108** (1957) 1175.
[8] Baskaran, G.; Zou, Z.; Anderson, P. W.: Solid State Commun. **63** (1987) 973.
[9] Suzumura, Y.; Hasegawa, Y.; Fukuyama, H.: J. Phys. Soc. Jap. **57** (1988) 401.
[10] Hirsch, J. E.: Phys. Rev. Lett. **54** (1985) 1317.

Bei der Redaktion eingegangen am 16. Juni 1989.

Anschr. d. Verf.: Prof. Dr. E. Kolley
Doz. Dr. W. Kolley
Sektion Physik
Karl-Marx-Universität Leipzig
Linnéstr. 5
Leipzig, DDR-7010