Exact ground states of correlated electronic models: heavy-fermion/bilayer systems

1997 J. Phys.: Condens. Matter 9 2471

(http://iopscience.iop.org/0953-8984/9/11/015)

J. Phys.: Condens. Matter **9** (1997) 2471–2483. Printed in the UK PII: S0953-8984(97)73050-9

Exact ground states of correlated electronic models: heavy-fermion/bilayer systems

R Sato†

Department of Physics, Faculty of Science, Osaka University, Toyonaka, Osaka 560, Japan

Received 25 March 1996

Abstract. We construct the exact ground states of a class of models for correlated electronic systems in d dimensions. We introduce generalized models for heavy-fermion systems and those for bilayer systems. By the optimal ground state approach, we show that the models have superconducting ground states via the η-pairing mechanism. We also obtain the criteria for the stability of charge-density-wave states.

1. Introduction

The physics of strongly correlated electronic systems has been a subject of much interest in recent years. Among these systems particular interest is shown in cuprate superconductors and several heavy-fermion systems. One approach to the understanding of the low-temperature physics of these systems is to obtain the exact ground states of the Hamiltonian which describes electronic correlations. In this paper we introduce generalized models for heavy-fermion systems and bilayer systems, the mechanism of whose superconductivity is of current interest. We will then construct the exact ground states of these models. We are mainly interested in superconducting ground states via the so-called η-pairing mechanism [1], which was originally introduced for the construction of the superconducting eigenstates of the Hubbard model. The η-pairing states with momentum P are defined by

$$|\Psi_{\mathrm{P}}^{(\mathrm{N})}\rangle = \left(\eta_P^\dagger\right)^N |0\rangle \qquad \eta_P^\dagger = \sum_{j=1}^{L} \mathrm{e}^{\mathrm{i}Pj} c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger. \tag{1}$$

Here the total number of the conduction electrons is $2N$. These states exhibit off-diagonal long-range order (ODLRO) [2], which implies the Meissner effect and flux quantization [2–4], and are thus superconducting. Electronic models whose ground states are the η-pairing states have recently been intensively studied [5–10].

One simple and effective method for the construction of exact ground states is the optimal ground state (OGS) approach [9]. Suppose a Hamiltonian H is defined by the sum of the local Hamiltonians h_i, $H = \sum_i h_i$. Denote the local ground states of h_i by $|\mathrm{loc}\rangle$. If the lowest eigenvalue of h_i is 0 (by adding a constant term), i.e, $h_i|\mathrm{loc}\rangle = 0$, then a global state $|\Psi\rangle$ constructed from $|\mathrm{loc}\rangle$ states satisfies $H|\Psi\rangle = 0$. Since clearly $\langle\phi|H|\phi\rangle \geqslant 0$ for any eigenstate $|\phi\rangle$ of H, $|\Psi\rangle$ is (at least one of) the (global) ground state(s) and is called an

† Present address: Research Center for Materials Science at Extreme Conditions, Osaka University, 1–3 Machikane, Toyonaka 560, Japan, e-mail address: sato@rcem.osaka-u.ac.jp

0953-8984/97/112471+13$19.50

optimal ground state. In [9] exact ground states of generalized Hubbard models have been obtained by this method.

In section 2, we consider a generalized model for heavy-fermion systems and obtain the exact ground states of it. We will show, in particular, that superconductivity can coexist with various kinds of magnetism (paramagnetic, Néel, and ferromagnetic) via the η-pairing mechanism. We also obtain the criteria for the stability of charge-density-wave (CDW) states with different magnetism. In section 3, we examine the effect of layered structures on the ground states. We introduce the 'multiple' η-pairing states and CDW states for layered systems and obtain the conditions for these states to be optimal ground states. Section 4 is devoted to a summary.

2. A model for heavy-fermion systems

Superconductivity in heavy-fermion systems is of current interest. In Ce- and U-based heavy-fermion materials, superconducting phases are observed at sufficiently low temperatures. For several uranium compounds, the coexistence of superconductivity and antiferromagnetic order is known (for classification of heavy-fermion systems, see [11], for example). Microscopic descriptions of heavy-fermion systems have been made by several lattice models. Though some exact results on the ground states have been found for the Kondo lattice model [12, 13], the periodic Anderson model [14], and the Kondo–Hubbard model [15, 16], no superconducting ground states have been found in these models. In this section we introduce a generalized model for strongly correlated heavy-fermion systems and construct the exact ground states of the model.

We will consider a model which is described by the following Hamiltonian defined on a d-dimensional lattice of L sites ($\langle jl \rangle$ denotes neighbouring sites):

$$H = \sum_{\langle jl \rangle} h_{jl} = \sum_{\langle jl \rangle} (h_{jl}^{(c-c)} + h_{jl}^{(c-l)} + h_{jl}^{(l-l)}) \tag{2}$$

$$h_{jl}^{(c-c)} = \tilde{h}_{jl} + \frac{U}{Z}\left(\left(n_{j\uparrow} - \frac{1}{2}\right)\left(n_{j\downarrow} - \frac{1}{2}\right) + \left(n_{l\uparrow} - \frac{1}{2}\right)\left(n_{l\downarrow} - \frac{1}{2}\right)\right) - \frac{\mu}{Z}(n_j + n_l) \tag{3}$$

$$\begin{aligned}\tilde{h}_{jl} = {} & -t\sum_{\sigma}(c_{j\sigma}^{\dagger}c_{l\sigma} + c_{l\sigma}^{\dagger}c_{j\sigma}) + X\sum_{\sigma}(c_{j\sigma}^{\dagger}c_{l\sigma} + c_{l\sigma}^{\dagger}c_{j\sigma})(n_{j-\sigma} + n_{l-\sigma}) \\ & + V(n_j - 1)(n_l - 1) + Y(c_{j\uparrow}^{\dagger}c_{j\downarrow}^{\dagger}c_{l\downarrow}c_{l\uparrow} + c_{l\uparrow}^{\dagger}c_{l\downarrow}^{\dagger}c_{j\downarrow}c_{j\uparrow}) \\ & + J_{xy}\left(S_j^x S_l^x + S_j^y S_l^y\right) + J_z S_j^z S_l^z\end{aligned} \tag{4}$$

$$\begin{aligned}h_{jl}^{(c-l)} = {} & K_{xy}\left(S_j^x \sigma_j^x + S_j^y \sigma_j^y\right) + K_z S_j^z \sigma_j^z \\ & + K_{xy}\left(S_l^x \sigma_l^x + S_l^y \sigma_l^y\right) + K_z S_l^z \sigma_l^z\end{aligned} \tag{5}$$

$$h_{jl}^{(l-l)} = M_{xy}\left(\sigma_j^x \sigma_l^x + \sigma_j^y \sigma_l^y\right) + M_z \sigma_j^z \sigma_l^z \tag{6}$$

where $c_{j\sigma}^{\dagger}$ ($c_{j\sigma}$) is the creation (annihilation) operator for conduction electrons ($\sigma = \uparrow, \downarrow$), and $\{S^{\alpha}\}$ and $\{\sigma^{\alpha}\}$ ($\alpha = x, y, z$) denote the spin-$\frac{1}{2}$ spin operators for conduction electrons and localized spins, respectively. ($\{\sigma^{\alpha}\}$ are not the Pauli matrices here.) The number operators for conduction electrons are denoted by $n_{j\sigma} = c_{j\sigma}^{\dagger}c_{j\sigma}$ and $n_j = n_{j\uparrow} + n_{j\downarrow}$. μ is the chemical potential and Z is the coordination number of the d-dimensional lattice. The local Hamiltonians $h_{jl}^{(c-c)}$, $h_{jl}^{(c-l)}$, and $h_{jl}^{(l-l)}$ represent the interactions between conduction electrons themselves, between conduction electrons and localized spins, and between localized spins, respectively. $h_{jl}^{(c-c)}$ includes, in addition to the usual Hubbard interaction t and U, correlated hopping term X, nearest-neighbour Coulomb interaction V, pair-hopping term Y, and spin interaction of XXZ type. $h_{jl}^{(c-l)}$ describes the anisotropic Kondo interaction. The effect of $h_{jl}^{(l-l)}$ is usually assumed to be weak, but its contributions are still a matter of interest. If we set $K_{xy} = K_z$ and the other parameters to zero except for t, the model reduces to the usual Kondo lattice model.

Let us apply the OGS method to our Hamiltonian (2). We first determine the region of the interaction parameters where the model exhibits superconductivity via the η-pairing mechanism. First look at the η-pairing states with momentum $P = 0$ and π. The OGS approach reduces the problem of the stability of ground states to the diagonalization of the local Hamiltonian h_{jl} in (2). Write a two-sites state as $|a_\sigma b_\tau\rangle$ where a (b) denotes one of the possible four states at a site for conduction electrons: $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, $|2\rangle = |\uparrow\downarrow\rangle$, and σ (τ) denotes a single-site (spin) state for localized spins. The number of the possible two-site states is then $4^2 \times 2^2 = 64$. One can see that $|\Psi_{\rm P}^{\rm (N)}\rangle$ is constructed from all of (or, some parts of) the following states (among the eigenstates of h_{jl}):

eigenstate	energy		
$\|0_\sigma 0_\sigma\rangle$	$\frac{U}{2Z} + V + \frac{M_z}{4}$		
$\|0_\uparrow 0_\downarrow\rangle \pm \|0_\downarrow 0_\uparrow\rangle$	$\frac{U}{2Z} + V \pm \frac{M_{xy}}{2} - \frac{M_z}{4}$		
$\|2_\sigma 0_\sigma\rangle + \|0_\sigma 2_\sigma\rangle$	$\frac{U}{2Z} - V \pm Y + \frac{M_z}{4} + \frac{2\mu}{Z}$	$(P = 0)$	
$\|2_\sigma 0_\sigma\rangle - \|0_\sigma 2_\sigma\rangle$	$\frac{U}{2Z} - V \pm Y + \frac{M_z}{4} + \frac{2\mu}{Z}$	$(P = \pi)$	(7)
$\|2_\downarrow 0_\uparrow\rangle \pm \|2_\uparrow 0_\downarrow\rangle + \|0_\downarrow 2_\uparrow\rangle \pm \|0_\uparrow 2_\downarrow\rangle$	$\frac{U}{2Z} - V - \frac{M_z}{4} + Y \pm \frac{M_{xy}}{2} + \frac{2\mu}{Z}$	$(P = 0)$	
$\|2_\downarrow 0_\uparrow\rangle \pm \|2_\uparrow 0_\downarrow\rangle - \|0_\downarrow 2_\uparrow\rangle \mp \|0_\uparrow 2_\downarrow\rangle$	$\frac{U}{2Z} - V - \frac{M_z}{4} + Y \pm \frac{M_{xy}}{2} + \frac{2\mu}{Z}$	$(P = \pi)$	
$\|2_\sigma 2_\sigma\rangle$	$\frac{U}{2Z} + V + \frac{M_z}{4} + \frac{4\mu}{Z}$		
$\|2_\uparrow 2_\downarrow\rangle \pm \|2_\downarrow 2_\uparrow\rangle$	$\frac{U}{2Z} + V \pm \frac{M_{xy}}{2} - \frac{M_z}{4} + \frac{4\mu}{Z}$		

where we have imposed the condition $t = X$ upon which all of the states (7) become eigenstates of h_{jl}. (Although this condition is not necessary for η-pairing states with $P = \pi$ to be eigenstates of the Hamiltonian (2), we keep it in mind throughout this section for simplicity.)

Considering the η-pairing states for conduction electrons, we can write the eigenfunctions of the Hamiltonian (2) in the decoupled form of the η-pairing states and various kinds of magnetic (paramagnetic, Néel, and ferromagnetic) state:

$$|\Psi_{\rm P}^{\rm (N)}; \text{para}\rangle = (\eta_P^\dagger)^N \prod_{j\in\mathcal{A}} f_{j\uparrow}^\dagger \prod_{l\in\mathcal{A}'} f_{l\downarrow}^\dagger |0\rangle \tag{8}$$

$$|\Psi_{\rm P}^{\rm (N)}; \text{Néel}\rangle = (\eta_P^\dagger)^N \prod_{j\in\mathcal{B}} f_{j\uparrow}^\dagger \prod_{l\in\mathcal{B}'} f_{l\downarrow}^\dagger |0\rangle \tag{9}$$

$$|\Psi_{\rm P}^{\rm (N)}; \text{ferro}\rangle = \left(\eta_P^\dagger\right)^N \prod_{j} f_{j\uparrow}^\dagger |0\rangle \tag{10}$$

where $\mathcal{A}$ and $\mathcal{A}'$ are an arbitrary disjoint set of lattice sites which together build up the whole lattice, and $\mathcal{B}$ and $\mathcal{B}'$ are even and odd sublattices on a bipartite lattice. The creation and annihilation operators for f-electrons (localized spins) are denoted by $f_{j\sigma}^\dagger$ and $f_{j\sigma}$ ($\sigma =\uparrow, \downarrow$).

The η-pairing states with paramagnetism, $|\Psi_{\rm P}^{\rm (N)}; \text{para}\rangle$, are constructed completely from all of the local eigenstates (7) which have the same eigenvalue $E = U/2Z+V$ for $Y = \pm 2V$ ($+$ for $P = 0$ and $-$ for $P = \pi$), $M_{xy} = M_z = 0$, and $\mu = 0$. Demanding that

$|\Psi_{\rm P}^{(\rm N)}; \text{para}\rangle$ is the optimal ground state, i.e. demanding that all the other eigenvalues of the local Hamiltonian h_{jl} are higher than E leads to the following condition for the interaction parameters:

$$V < 0 \qquad \frac{U}{Z} < \min\left\{ -2|t| - 2V + \frac{K_z}{2}, -V + \frac{J_z}{4} + \frac{K_z}{4}, -V + \frac{J_z}{4} - \frac{K_z}{2}, \right.$$
$$-V - \frac{J_z}{4} - \frac{1}{2}\sqrt{J_{xy}^2 + K_z^2}, -V - \frac{|J_{xy}|}{4} - \frac{1}{4}\sqrt{(J_z + |J_{xy}|)^2 + 4K_{xy}^2},$$
$$\left. \frac{2t}{3} - 2V - \frac{K_z}{6} + 2\xi_1, -\frac{2t}{3} - 2V - \frac{K_z}{6} + 2\xi_2, -V - \frac{J_z}{12} - \frac{K_z}{6} + \xi_3 \right\} \quad (11)$$

where

$$\xi_i = A_i \cos(\theta_i/3) \qquad A_i \cos[(\theta_i + 2\pi)/3] \qquad A_i \cos[(\theta_i + 4\pi)/3] \quad (12)$$

$$A_i = \tfrac{1}{3}\sqrt{p_i} \qquad \cos\theta_i = \tfrac{1}{54} A_i^{-3} q_i \quad (13)$$

with

$$\begin{aligned}
p_1 &= F(t) \equiv 3K_{xy}^2 + (t - K_z)^2 + 15t^2 \\
q_1 &= G(t) \equiv 18K_{xy}^2 K_z - 2K_z^3 - 18K_{xy}^2 t + 6K_z^2 t - 24K_z t^2 + 128t^3 \\
p_2 &= F(-t) \\
q_2 &= G(-t) \\
p_3 &= 12K_{xy}^2 + 3K_z^2 + 3J_{xy}^2 + (J_z - K_z)^2 \\
q_3 &= 2(9J_{xy}^2 J_z - J_z^3 - 18J_z K_{xy}^2 - 9J_{xy}^2 K_z + 3J_z^2 K_z + 72K_{xy}^2 K_z + 6J_z K_z^2 - 8K_z^3).
\end{aligned} \quad (14)$$

For the Néel-ordered η-pairing states $|\Psi_{\rm P}^{(\rm N)}; \text{Néel}\rangle$ we have the restrictions $Y = \pm 2V$ ($+$ for $P = 0$ and $-$ for $P = \pi$), $M_{xy} = 0$, and $\mu = 0$ for which all the constituent local eigenstates have the same energy $U/2Z + V - M_z/4$. The condition for the state $|\Psi_0^{(\rm N)}; \text{Néel}\rangle$ to be the optimal ground state is given by

$$V < 0 \qquad 0 < M_z \qquad \frac{U}{Z} < \min\left\{ -2|t| - 2V + \frac{1}{2}K_z + M_z, \right.$$
$$-V + \frac{J_z}{4} + \frac{K_z}{4} + \frac{M_z}{2}, -V + \frac{J_z}{4} - \frac{K_z}{2} + \frac{M_z}{2},$$
$$-V - \frac{J_z}{4} - \frac{M_z}{2} - \frac{1}{2}\sqrt{J_{xy}^2 + K_z^2}, -V - \frac{|J_{xy}|}{4} - \frac{M_z}{4}$$
$$-\frac{1}{4}\sqrt{(J_z - M_z + |J_{xy}|)^2 + 4K_{xy}^2}, \frac{2t}{3} - 2V - \frac{K_z}{6} + \frac{M_z}{3} + 2\xi_1,$$
$$\left. -\frac{2t}{3} - 2V - \frac{K_z}{6} + \frac{M_z}{3} + 2\xi_2, -V - \frac{J_z}{12} - \frac{K_z}{6} + \frac{M_z}{6} + \xi_3 \right\} \quad (15)$$

where ξ_i is defined in equations (12) and (13) with

$$\begin{aligned}
p_1 &= F(t) \equiv 3K_{xy}^2 + 3K_z^2/4 + 12t^2 + (2t + M_z - K_z/2)^2 \\
q_1 &= G(t) \equiv 18K_{xy}^2 K_z - 2K_z^3 - 9K_{xy}^2 M_z + 3K_z^2 M_z + 3K_z M_z^2 - 2M_z^3 - 18K_{xy}^2 t \\
&\qquad + 6K_z^2 t + 12K_z M_z t - 12M_z^2 t - 24K_z t^2 + 48M_z t^2 + 128t^3 \\
p_2 &= F(-t) \\
q_2 &= G(-t) \\
p_3 &= 12K_{xy}^2 + 3K_z^2 + 3J_{xy}^2 + (J_z + M_z - K_z)^2
\end{aligned} \quad (16)$$

$$q_3 = 2(9J_{xy}^2 J_z - J_z^3 - 18J_z K_{xy}^2 - 9J_{xy}^2 K_z + 3J_z^2 K_z + 72K_{xy}^2 K_z + 6J_z K_z^2 - 8K_z^3 + 9J_{xy}^2 M_z - 3J_z^2 M_z - 18K_{xy}^2 M_z + 6J_z K_z M_z + 6K_z^2 M_z - 3J_z M_z^2 + 3K_z M_z^2 - M_z^3).$$

The η-pairing states with the fully polarized ferromagnetism, $|\Psi_{\mathrm{P}}^{(\mathrm{N})}; \mathrm{ferro}\rangle$, are built from $|0_\sigma 0_\sigma\rangle$, $|2_\sigma 0_\sigma\rangle \pm |0_\sigma 2_\sigma\rangle$ ($+$ for $P = 0$ and $-$ for $P = \pi$), and $|2_\sigma 2_\sigma\rangle$. These local states have the same energy $U/2Z + V + M_z/4$ for $Y = \pm 2V$ ($+$ for $P = 0$ and $-$ for $P = \pi$) and $\mu = 0$. The state $|\Psi_{\mathrm{P}}^{(\mathrm{N})}; \mathrm{ferro}\rangle$ becomes the optimal ground state when the following inequalities are satisfied:

$$V < 0 \qquad M_z < -|M_{xy}| \qquad \frac{U}{Z} < \min\left\{ -2|t| - 2V + \frac{K_z}{2}, -V + \frac{J_z}{4} + \frac{K_z}{4}, -V + \frac{J_z}{4} - \frac{K_z}{2} - V - \frac{J_z}{4} - \frac{M_z}{2} - \frac{1}{2}\sqrt{(J_{xy} - M_{xy})^2 + K_z^2}, -V \pm \frac{1}{4}(J_{xy} + M_{xy}) - \frac{M_z}{4} - \frac{1}{4}\sqrt{[(J_z - M_z) \mp (J_{xy} - M_{xy})]^2 + 4K_{xy}^2}, \frac{2t}{3} - 2V - \frac{K_z}{6} - \frac{2M_z}{3} + 2\xi_1, -\frac{2t}{3} - 2V - \frac{K_z}{6} - \frac{2M_z}{3} + 2\xi_2, -V - \frac{J_z}{12} - \frac{K_z}{6} - \frac{M_z}{3} + \xi_3 \right\} \tag{17}$$

where ξ_i is defined in (12) and (13) with

$$\begin{aligned}
p_1 &= F(t) \equiv 3K_{xy}^2 + 3K_z^2/4 + 3(2t + M_{xy})^2 + (2t + M_z - K_z/2)^2 \\
q_1 &= G(t) \equiv 18K_{xy}^2 K_z - 2K_z^3 - 9K_z M_{xy}^2 - 9K_{xy}^2 M_z + 3K_z^2 M_z + 18M_{xy}^2 M_z \\
&\quad + 3K_z M_z^2 - 2M_z^3 - 18K_{xy}^2 t + 6K_z^2 t - 36K_z M_{xy} t + 36M_{xy}^2 t + 12K_z M_z t \\
&\quad + 72M_{xy} M_z t - 12M_z^2 t - 24K_z t^2 + 144M_{xy} t^2 + 48M_z t^2 + 128t^3 \\
p_2 &= F(-t) \\
q_2 &= G(-t) \qquad\qquad (18) \\
p_3 &= 12K_{xy}^2 + 3K_z^2 + 3(J_{xy} + M_{xy})^2 + (J_z + M_z - K_z)^2 \\
q_3 &= 2(9J_{xy}^2 J_z - J_z^3 - 18J_z K_{xy}^2 - 9J_{xy}^2 K_z + 3J_z^2 K_z + 72K_{xy}^2 K_z + 6J_z K_z^2 \\
&\quad - 8K_z^3 + 18J_{xy} J_z M_{xy} - 18J_{xy} K_z M_{xy} + 9J_z M_{xy}^2 - 9K_z M_{xy}^2 + 9J_{xy}^2 M_z \\
&\quad - 3J_z^2 M_z - 18K_{xy}^2 M_z + 6J_z K_z M_z + 6K_z^2 M_z + 18J_{xy} M_{xy} M_z + 9M_{xy}^2 M_z \\
&\quad - 3J_z M_z^2 + 3K_z M_z^2 - M_z^3).
\end{aligned}$$

We should note that ferromagnetism is, in a usual situation, not supposed to be compatible with superconductivity. The states $|\Psi_{\mathrm{P}}^{(\mathrm{N})}; \mathrm{ferro}\rangle$, on the contrary, manifestly realize the coexistence of ferromagnetism and superconductivity via the η-pairing mechanism.

The η-pairing states with momentum $P \neq 0, \pi$ can also be ground states of the Hamiltonian (2). In this case, however, the model should be simplified to the one with $t = X$ and $Y = V = 0$ [9], and then has a large symmetry which causes high degeneracy of the ground states. It follows that the existence of ODLRO might not guarantee superconductivity, at least in one dimension [17]. To lift the degeneracy, we need to 'perturb' the simple model which contains the parameters t, X, and U only. For instance, the pair hopping term Y explicitly breaks the degeneracy in favour of superconducting states.

Consider next briefly the CDW states with different magnetism (at half-filling):

$$|\mathrm{CDW;\ para}\rangle = \prod_{i\in\mathcal{C}} c^\dagger_{i\uparrow}c^\dagger_{i\downarrow} \prod_{j\in\mathcal{A}} f^\dagger_{j\uparrow} \prod_{l\in\mathcal{A}'} f^\dagger_{l\downarrow}|0\rangle \tag{19}$$

$$|\mathrm{CDW;\ Néel}\rangle = \prod_{i\in\mathcal{C}} c^\dagger_{i\uparrow}c^\dagger_{i\downarrow} \prod_{j\in\mathcal{B}} f^\dagger_{j\uparrow} \prod_{l\in\mathcal{B}'} f^\dagger_{l\downarrow}|0\rangle \tag{20}$$

$$|\mathrm{CDW;\ ferro}\rangle = \prod_{i\in\mathcal{C}} c^\dagger_{i\uparrow}c^\dagger_{i\downarrow} \prod_{j} f^\dagger_{j\uparrow}|0\rangle \tag{21}$$

where $\mathcal{C}$ is an even (odd) sublattice of a bipartite lattice. These states of the decoupled form can be eigenfunctions of the Hamiltonian (2), as is the case of the η-pairing states. Using again the OGS method, we can obtain the criteria for stability of the states (19)–(21).

For the CDW states to be eigenstates of the Hamiltonian (2) we primarily need the restrictions $t = X$ and $Y = 0$. One can see that $|\mathrm{CDW;\ para}\rangle$ is constructed from the local states $|2_\sigma 0_\tau\rangle$ and $|0_\sigma 2_\tau\rangle(\sigma,\tau = \uparrow,\downarrow)$, that $|\mathrm{CDW;\ Néel}\rangle$ is from the states $|2_\uparrow 0_\downarrow\rangle \pm |2_\downarrow 0_\uparrow\rangle$ and $|0_\uparrow 2_\downarrow\rangle \pm |0_\downarrow 2_\uparrow\rangle$, and that $|\mathrm{CDW;\ ferro}\rangle$ is from the states $|2_\sigma 0_\sigma\rangle$ and $|0_\sigma 2_\sigma\rangle$, respectively. We present the conditions for each of the states (19)–(21) to be an optimal ground state:

$|\mathrm{CDW;\ para}\rangle$ (local ground state energy) : $U/Z - V + 2\mu/Z$

$$\begin{aligned} V > \frac{|\mu|}{Z} \qquad M_{xy} = M_z = 0 \qquad \frac{U}{Z} < \min\bigg\{ & -2|t| + 2V + \frac{K_z}{2} - \frac{2|\mu|}{Z}, V + \frac{J_z}{4} \\ & + \frac{K_z}{4}, V + \frac{J_z}{4} - \frac{K_z}{2}, V - \frac{J_z}{4} - \frac{1}{2}\sqrt{J_{xy}^2 + K_z^2}, V - \frac{|J_{xy}|}{4} \\ & - \frac{1}{4}\sqrt{(J_z + |J_{xy}|)^2 + 4K_{xy}^2}, \frac{2t}{3} + 2V - \frac{K_z}{6} - \frac{2|\mu|}{Z} + 2\xi_1^{(1)}, \\ & - \frac{2t}{3} + 2V - \frac{K_z}{6} - \frac{2|\mu|}{Z} + 2\xi_2^{(1)}, V - \frac{J_z}{12} - \frac{K_z}{6} + \xi_3^{(1)} \bigg\} \end{aligned} \tag{22}$$

$|\mathrm{CDW;\ Néel}\rangle$ (local ground state energy) : $U/Z - V - M_z/4 + 2\mu/Z$

$$\begin{aligned} V > \frac{|\mu|}{Z} \qquad M_{xy} = 0 \qquad M_z > 0 \qquad \frac{U}{Z} < \min\bigg\{ & -2|t| + 2V + \frac{K_z}{2} + M_z \\ & - \frac{2|\mu|}{Z}, V + \frac{J_z}{4} + \frac{K_z}{4} + \frac{M_z}{2}, V + \frac{J_z}{4} - \frac{K_z}{2} + \frac{M_z}{2}, V - \frac{J_z}{4} - \frac{M_z}{2} \\ & - \frac{1}{2}\sqrt{J_{xy}^2 + K_z^2}, V - \frac{|J_{xy}|}{4} - \frac{M_z}{4} - \frac{1}{4}\sqrt{(J_z - M_z + |J_{xy}|)^2 + 4K_{xy}^2}, \\ & \frac{2t}{3} + 2V - \frac{K_z}{6} + \frac{M_z}{3} - \frac{2|\mu|}{Z} + 2\xi_1^{(2)}, -\frac{2t}{3} + 2V - \frac{K_z}{6} + \frac{M_z}{3} - \frac{2|\mu|}{Z} \\ & + 2\xi_2^{(2)}, V - \frac{J_z}{12} - \frac{K_z}{6} + \frac{M_z}{6} + \xi_3^{(2)} \bigg\} \end{aligned} \tag{23}$$

$|\mathrm{CDW;\ ferro}\rangle$ (local ground state energy) : $U/Z - V + M_z/4 + 2\mu/Z$

$$\begin{aligned} V > \frac{|\mu|}{Z} \qquad M_z < -|M_{xy}| \qquad \frac{U}{Z} < \min\bigg\{ & -2|t| + 2V + \frac{K_z}{2} - \frac{2|\mu|}{Z}, V + \frac{J_z}{4} \\ & + \frac{K_z}{4}, V + \frac{J_z}{4} - \frac{K_z}{2}, V - \frac{J_z}{4} - \frac{M_z}{2} - \frac{1}{2}\sqrt{(J_{xy} - M_{xy})^2 + K_z^2}, \\ & \times V \pm \frac{1}{4}(J_{xy} + M_{xy}) - \frac{M_z}{4} - \frac{1}{4}\sqrt{[(J_z - M_z) \mp (J_{xy} - M_{xy})]^2 + 4K_{xy}^2}, \\ & \times \frac{2t}{3} + 2V - \frac{K_z}{6} - \frac{2M_z}{3} - \frac{2|\mu|}{Z} + 2\xi_1^{(3)}, \end{aligned}$$

$$-\frac{2t}{3}+2V-\frac{K_z}{6}-\frac{2M_z}{3}-\frac{2|\mu|}{Z}+2\xi_2^{(3)},\ V-\frac{J_z}{12}-\frac{K_z}{6}-\frac{M_z}{3}+\xi_3^{(3)}\Big\} \quad (24)$$

where $\xi_i^{(1)}$, $\xi_i^{(2)}$, and $\xi_i^{(3)}$ are the same as ξ_i in (11), (15) and (17), respectively. To obtain the best bound, we may choose $\mu = 0$.

3. Bilayer generalized Hubbard model

The presence of a double CuO_2 layer in materials such as $YBa_2Cu_3O_{7-y}$ compounds is considered to play a significant role in high-T_c superconductivity. Some numerical calculations made on the bilayer Hubbard model find no evidence for superconducting ODLRO [18, 19], suggesting a need for a different mechanism (model) for superconductivity. In this section we will consider an n-layered generalized Hubbard model which is described by the following Hamiltonian defined on a d-dimensional lattice of L sites ($\langle jl\rangle$ and $\langle\lambda\nu\rangle$ denote neighbouring sites and neighbouring layers, respectively):

$$H=\sum_{\langle jl\rangle}h_{jl}=\sum_{\langle jl\rangle}\left(\sum_{\lambda}h_{jl\lambda}^{(intra)}+\sum_{\langle\lambda\nu\rangle}(h_{j\lambda\nu}^{(inter)}+h_{l\lambda\nu}^{(inter)})+\sum_{\lambda}h_{jl}^{(site)}\right) \quad (25)$$

with

$$\begin{aligned} h_{jl\lambda}^{(intra)} &= -t_{\parallel}\sum_{\sigma}(c_{j\lambda\sigma}^{\dagger}c_{l\lambda\sigma}+c_{l\lambda\sigma}^{\dagger}c_{j\lambda\sigma})+X_{\parallel}\sum_{\sigma}(c_{j\lambda\sigma}^{\dagger}c_{l\lambda\sigma}+c_{l\lambda\sigma}^{\dagger}c_{j\lambda\sigma})(n_{j\lambda-\sigma}+n_{l\lambda-\sigma}) \\ &\quad +V_{\parallel}(n_{j\lambda}-1)(n_{l\lambda}-1)+Y_{\parallel}(c_{j\lambda\uparrow}^{\dagger}c_{j\lambda\downarrow}^{\dagger}c_{l\lambda\downarrow}c_{l\lambda\uparrow}+c_{l\lambda\uparrow}^{\dagger}c_{l\lambda\downarrow}^{\dagger}c_{j\lambda\downarrow}c_{j\lambda\uparrow}) \\ &\quad +J_{xy\parallel}\left(S_{j\lambda}^{x}S_{l\lambda}^{x}+S_{j\lambda}^{y}S_{l\lambda}^{y}\right)+J_{z\parallel}S_{j\lambda m}^{z}S_{l\lambda}^{z} \qquad (26) \\ h_{j\lambda\nu}^{(inter)} &= -t_{\perp}\sum_{\sigma}(c_{j\lambda\sigma}^{\dagger}c_{j\nu\sigma}+c_{j\nu\sigma}^{\dagger}c_{j\lambda\sigma})+X_{\perp}\sum_{\sigma}(c_{j\lambda\sigma}^{\dagger}c_{j\nu\sigma}+c_{j\nu\sigma}^{\dagger}c_{j\lambda\sigma})(n_{j\lambda-\sigma}+n_{j\nu-\sigma}) \\ &\quad +V_{\perp}(n_{j\lambda}-\lambda)(n_{j\nu}-\lambda)+Y_{\perp}(c_{j\lambda\uparrow}^{\dagger}c_{j\lambda\downarrow}^{\dagger}c_{j\nu\downarrow}c_{j\nu\uparrow}+c_{j\nu\uparrow}^{\dagger}c_{j\nu\downarrow}^{\dagger}c_{j\lambda\downarrow}c_{j\lambda\uparrow}) \\ &\quad +J_{xy\perp}\left(S_{j\lambda}^{x}S_{j\nu}^{x}+S_{j\lambda}^{y}S_{j\nu}^{y}\right)+J_{z\perp}S_{j\lambda m}^{z}S_{j\nu}^{z} \end{aligned}$$

$$h_{jl}^{(site)}=\frac{U}{Z}l\left(\left(n_{j\lambda\uparrow}-\frac{1}{2}\right)\left(n_{j\lambda\downarrow}-\frac{1}{2}\right)+\left(n_{l\lambda\uparrow}-\frac{1}{2}\right)\left(n_{l\lambda\downarrow}-\frac{1}{2}\right)\right)-\frac{\mu}{Z}(n_{j\lambda}+n_{l\lambda}) \quad (27)$$

where $c_{j\lambda\sigma}^{\dagger}$ ($c_{j\lambda\sigma}$) and $\{S_{j\lambda}^{\alpha}\}$ ($\alpha = x, y, z$) are the creation (anihilation) operator and the spin-$\frac{1}{2}$ spin operators for electrons in the λth layer at site j ($\sigma = \uparrow, \downarrow$), respectively. The chemical potential and the coordination number of the d-dimensional lattice are denoted by μ and Z, respectively. We have decomposed the Hamiltonian into the three parts. The local Hamiltonians $h_{jl\lambda}^{(intra)}$ and $h_{j\lambda\nu}^{(inter)}$ represent the (nearest-neighbour) interactions between the electrons at the neighbouring sites and at the neighbouring layers, respectively. We take into consideration, in addition to the usual Hubbard interactions $t_{\parallel}$, $t_{\perp}$, and U, correlated hopping terms ($X_{\parallel}$ and $X_{\perp}$), nearest-neighbour Coulomb interactions ($V_{\parallel}$ and $V_{\perp}$), pair hopping terms ($Y_{\parallel}$ and $Y_{\perp}$), and spin interactions of XXZ type. In the present case, what we have to diagonalize in the OGS approach is the local Hamiltonian h_{jl} in (25).

For a superconducting state of layered systems, we introduce the 'multiple' η-pairing state with a set of momenta $\{P\} = \{P_1, P_2, \ldots, P_n\}$, each element of which denotes the momentum of a respective layer,

$$|\Psi_{\{P\}}^{(N_1,N_2,\ldots,N_n)}\rangle=\prod_{\lambda=1}^{n}(\eta_{P_\lambda}^{\dagger})^{N_\lambda}|0\rangle \qquad \eta_{P_\lambda}^{\dagger}=\sum_{j=1}^{L}e^{iP_\lambda j}c_{j\lambda\downarrow}^{\dagger}c_{j\lambda\uparrow}^{\dagger} \quad (28)$$

where $2N_\lambda$ is the number of the electrons in the λth layer. Note that we can assign different momenta for different layers. This situation is out of the scope of the present study, though.

In the remaining part of this section we restrict ourselves to the 'double' η-pairing states, namely, we study two-chain systems if $d = 1$, bilayer systems if $d = 2$, and so on. In the OGS approach, we have only to deal with the problem of the diagonalization of the local Hamiltonian (25). Write a local (two-site) state as $|a_\sigma b_\tau\rangle$ where a (b) denotes a single-site state of electrons in the first layer, and σ (τ) in the second layer. In the present case, the number of the possible two-site states is $4^2 \times 4^2 = 256$. One can see that the η-pairing state $|\Psi^{(N_1,N_2)}_{\{P_1,P_2\}}\rangle$ is constructed from all of (some of) the following states (among the eigenstates of h_{jl}):

$$
\begin{array}{ll}
\text{eigenstate} & \text{energy} \\
|0_0 0_0\rangle & \frac{U}{Z} + 2V_\parallel \\
|2_0 0_0\rangle \pm |0_0 2_0\rangle & \frac{U}{Z} \pm Y_\parallel + \frac{2\mu}{Z} \\
|0_2 0_0\rangle \pm |0_0 0_2\rangle & \frac{U}{Z} \pm Y_\parallel + \frac{2\mu}{Z} \\
\alpha_\pm(|0_2 2_0\rangle + |2_0 0_2\rangle) + |2_2 0_0\rangle + |0_0 2_2\rangle & \frac{U}{Z} - 2V_\parallel \pm \sqrt{Y_\parallel^2 + V_\perp^2} + \frac{4\mu}{Z} \\
|2_0 2_0\rangle & \frac{U}{Z} + 2V_\parallel - 2V_\perp + \frac{4\mu}{Z} \\
|0_2 0_2\rangle & \frac{U}{Z} + 2V_\parallel - 2V_\perp + \frac{4\mu}{Z} \\
|2_2 0_2\rangle \pm |0_2 2_2\rangle & \frac{U}{Z} \pm Y_\parallel + \frac{6\mu}{Z} \\
|2_2 2_0\rangle \pm |2_0 2_2\rangle & \frac{U}{Z} \pm Y_\parallel + \frac{6\mu}{Z} \\
|2_2 2_2\rangle & \frac{U}{Z} + 2V_\parallel + \frac{8\mu}{Z}
\end{array}
\tag{29}
$$

with

$$
\alpha_\pm = Y_\parallel \bigg/ \left(V_\perp \pm \sqrt{V_\perp^2 + Y_\parallel^2} \right) \tag{30}
$$

where we have required the restrictions $t_\parallel = X_\parallel, t_\perp = X_\perp$, and $Y_\perp = 0$ upon which all of the eigenstates (29) become eigenstates of h_{jl} in (25). (Although the conditions $t_\parallel = X_\parallel$ and $t_\perp = X_\perp$ are not necessary for η-pairing states with $\{P\} = \{\pi, \pi\}$ to be eigenstates of the Hamiltonian (25), we keep it in mind throughout this section for simplicity.)

The η-pairing states with $\{P\} = \{0, 0\}$ and $\{P\} = \{\pi, \pi\}$ are eigenstates of H with the same eigenvalue $U/Z + 2V_\parallel$ if we set $t_\parallel = X_\parallel, X_\perp = t_\perp,\ Y_\parallel = \pm 2V_\parallel$ (+ for $\{P\} = \{0, 0\}$ and − for $\{P\} = \{\pi, \pi\}$), $V_\perp = 0$, and $\mu = 0$. These states are constructed from all of the eigenstates (29) (+ for $\{P\} = \{0, 0\}$ and − for $\{P\} = \{\pi, \pi\}$). On account of the conditions $t_\parallel = X_\parallel$ and $t_\perp = X_\perp$, the model has the particle–hole symmetry which reduces the diagonalization problem in the N_e-electron sector ($N_e \geqslant 5$) to that in the sector of $8 - N_e$ electrons. We demand the η–pairing state to be the optimal ground state to obtain the restrictions on the interaction parameters. As a result, we can write the inequality which should be satisfied for the η-pairing states with $\{P\} = \{0, 0\}$,

$$
\begin{aligned}
V_\parallel < 0 \qquad \frac{U}{Z} < \min \Bigg\{ & D, \frac{1}{8}\left(-6V_\parallel + J_{z\parallel} - \sqrt{(16t_\perp)^2 + (4V_\parallel + J_{z\parallel})^2}\right), \\
& \frac{1}{8}\left(-2|J_{xy\parallel}| - J_{z\parallel} - 12V_\parallel - \sqrt{(16t_\parallel)^2 + (2|J_{xy\parallel}| + J_{z\parallel} - 4V_\parallel)^2}\right), \\
& \frac{1}{8}\left(-2J_{xy\parallel} - J_{z\parallel} - 28V_\parallel - \sqrt{(16t_\parallel)^2 + (2J_{xy\parallel} + J_{z\parallel} + 12V_\parallel)^2}\right),
\end{aligned}
$$

$$\frac{1}{12}(J_{z\|}+J_{z\perp})+\min\left(-\frac{5V_\|}{3}+\xi_1, 5V_\|+\xi_5\right),$$
$$-\frac{1}{12}(J_{z\|}+J_{z\perp})+\min\left(-\frac{5V_\|}{3}+\frac{J_{xy\|}}{6}+\xi_2, -\frac{5V_\|}{3}-\frac{J_{xy\|}}{6}+\xi_6,\right.$$
$$\left.5V_\|+\frac{J_{xy\|}}{6}+\xi_7\right),$$
$$\left.-\frac{14V_\|}{3}+\min\left(f_1(t_\|,t_\perp), f_1(-t_\|,t_\perp), f_1(t_\|,-t_\perp), f_1(-t_\|,-t_\perp)\right)\right\} \qquad (31)$$

and that for $\{P\}=\{\pi,\pi\}$,

$$V_\| < 0 \qquad \frac{U}{Z} < \min\left\{D, -6V_\| - \sqrt{3t_\perp^2+(2|t_\||+|t_\perp|-4V_\|)^2},\right.$$
$$\frac{1}{8}\left(-28V_\|+J_{z\|}-\sqrt{(16t_\perp)^2+(12V_\|-J_{z\|})^2}\right),$$
$$\frac{1}{8}\left(-2J_{xy\|}-J_{z\|}-12V_\|-\sqrt{(16t_\|)^2+(2J_{xy\|}+J_{z\|}-4V_\|)^2}\right),$$
$$\frac{1}{8}\left(+2J_{xy\|}-J_{z\|}-28V_\|-\sqrt{(16t_\|)^2+(2J_{xy\|}-J_{z\|}-12V_\|)^2}\right),$$
$$-\frac{5V_\|}{3}+\frac{1}{12}(J_{z\|}+J_{z\perp})+\xi_1,$$
$$\left.-\frac{1}{12}(J_{z\|}+J_{z\perp})+\min\left(-\frac{5V_\|}{3}+\xi_2, 5V_\|+\xi_7\right)\right\} \qquad (32)$$

where

$$D=\min\left\{-2|t_\||-2|t_\perp|-2V_\|, -2V_\|-\frac{|J_{z\perp}|}{4}, -V_\|+\frac{J_{z\|}}{4},\right.$$
$$-V_\|-\frac{|J_{xy\|}|}{2}-\frac{J_{z\|}}{4}, -2V_\|-\frac{1}{8}\left(|J_{z\perp}|+\sqrt{(16t_\|)^2+J_{z\perp}^2}\right),$$
$$-\frac{2}{3}\left(|t_\||+|t_\perp|\right)-\frac{4V_\|}{3}+\frac{1}{6}(J_{z\|}+J_{z\perp}), -V_\|-\frac{|J_{xy\|}|}{4},$$
$$-V_\|-\frac{1}{4}\left(J_{z\|}+\sqrt{4J_{xy\|}^2+J_{z\perp}^2}\right), -\frac{4V_\|}{3}-\frac{1}{18}(J_{z\|}+J_{z\perp})$$
$$\left.+\min\left(f_2(t_\|,t_\perp), f_2(-t_\|,t_\perp), f_2(t_\|,-t_\perp), f_2(-t_\|,-t_\perp)\right)\right\} \qquad (33)$$

$$f_1(t_\|,t_\perp)=\tfrac{2}{3}(t_\|-t_\perp)+2\xi_3 \qquad f_2(t_\|,t_\perp)=\tfrac{2}{9}(t_\|+t_\perp+3\xi_4) \qquad (34)$$

and

$$\xi_i = A_i\cos(\theta_i/3), A_i\cos[(\theta_i+2\pi)/3], A_i\cos[(\theta_i+4\pi)/3] \qquad A_i=\tfrac{1}{3}\sqrt{p_i}$$
$$\cos\theta_i=\tfrac{1}{54}A_i^{-3}q_i \qquad (35)$$

with

$$p_1=F_1(V_\|,J_{xy\|})\equiv 48(t_\|^2+t_\perp^2)+3J_{z\perp}^2/16+(8V_\|+2J_{z\|}-J_{z\perp})^2/16$$
$$q_1=G_1(V_\|,J_{xy\|})\equiv J_{z\perp}^3/4-3J_{z\perp}^2J_{z\|}/8-3J_{z\perp}J_{z\|}^2/8+J_{z\|}^3/4$$
$$+t_\|^2(72J_{z\perp}-144J_{z\|}-576V_\|)-3J_{z\perp}^2V_\|/2-3J_{z\perp}J_{z\|}V_\|+3J_{z\|}^2V_\|$$
$$-6J_{z\perp}V_\|^2+12J_{z\|}V_\|^2+16V_\|^3+t_\perp^2(-144J_{z\perp}+72J_{z\|}+288V_\|)$$

$$
\begin{aligned}
p_2 &= F_2(V_\parallel, J_{xy\parallel}) \equiv 48(t_\parallel^2 + t_\perp^2) + 3J_{z\perp}^2/16 + (8V_\parallel + 4J_{xy\parallel} - 2J_{z\parallel} + J_{z\perp})^2/16 \\
q_2 &= G_2(V_\parallel, J_{xy\parallel}) \equiv 2J_{xy\parallel}^3 + 3J_{xy\parallel}^2 J_{z\perp}/2 - 3J_{xy\parallel}J_{z\perp}^2/4 - J_{z\perp}^3/4 - 3J_{xy\parallel}^2 J_{z\parallel} \\
&\quad -3J_{xy\parallel}J_{z\perp}J_{z\parallel}/2 + 3J_{z\perp}^2 J_{z\parallel}/8 + 3J_{xy\parallel}J_{z\parallel}^2/2 + 3J_{z\perp}J_{z\parallel}^2/8 - J_{z\parallel}^3/4 \\
&\quad +t_\parallel^2(-288J_{xy\parallel} - 72J_{z\perp} + 144J_{z\parallel} - 576V_\parallel) + 12J_{xy\parallel}^2 V_\parallel + 6J_{xy\parallel}J_{z\perp}V_\parallel \\
&\quad -3J_{z\perp}^2 V_\parallel/2 - 12J_{xy\parallel}J_{z\parallel}V_\parallel - 3J_{z\perp}J_{z\parallel}V_\parallel + 3J_{z\parallel}^2 V_\parallel + 24J_{xy\parallel}V_\parallel^2 \\
&\quad +6J_{z\perp}V_\parallel^2 - 12J_{z\parallel}V_\parallel^2 + 16V_\parallel^3 + t_\perp^2(144J_{xy\parallel} + 144J_{z\perp} - 72J_{z\parallel} + 288V_\parallel) \\
p_3 &= 6(t_\parallel^2 + 2t_\perp^2 + 4V_\parallel^2) + (t_\parallel + 2t_\perp + 2V_\parallel)^2 + 9(t_\parallel - 2V_\parallel)^2 \qquad (36) \\
q_3 &= 128t_\perp^3 - 128t_\parallel^3 + 96t_\perp^2 V_\parallel - 192t_\perp V_\parallel^2 - 1024V_\parallel^3 \\
&\quad +t_\parallel^2(-48t_\perp + 384V_\parallel) + t_\parallel(48t_\perp^2 + 384t_\perp V_\parallel + 768V_\parallel^2) \\
p_4 &= 6t_\perp^2 + J_{z\perp}^2/2 + (3t_\perp + J_{z\perp})^2 + (2t_\parallel - t_\perp + J_{z\parallel} - J_{z\perp}/2)^2 \\
q_4 &= 9J_{xy\parallel}^2 J_{z\perp} + 2J_{z\perp}^3 - 18J_{xy\parallel}^2 J_{z\parallel} - 3J_{z\perp}^2 J_{z\parallel} - 3J_{z\perp}J_{z\parallel}^2 + 2J_{z\parallel}^3 \\
&\quad +(18J_{xy\parallel}^2 + 12J_{z\perp}^2 - 12J_{z\perp}J_{z\parallel} - 6J_{z\parallel}^2)t_\perp + (-48J_{z\perp} + 24J_{z\parallel})t_\perp^2 - 128t_\perp^3 \\
&\quad +(-36J_{xy\parallel}^2 + 36J_{xy\parallel}J_{z\perp} - 6J_{z\perp}^2 - 72J_{xy\parallel}J_{z\parallel} - 12J_{z\perp}J_{z\parallel} + 12J_{z\parallel}^2 \\
&\quad +(72J_{xy\parallel} - 24J_{z\perp} - 24J_{z\parallel})t_\perp + 48t_\perp^2)t_\parallel \\
&\quad +(-144J_{xy\parallel} + 24J_{z\perp} - 48J_{z\parallel} + 48t_\perp)t_\parallel^2 - 128t_\parallel^3 \\
p_5 &= F_1(-3V_\parallel, J_{xy\parallel}) \qquad q_5 = -G_1(-3V_\parallel, J_{xy\parallel}) \\
p_6 &= F_2(V_\parallel, -J_{xy\parallel}) \qquad q_6 = -G_2(V_\parallel, -J_{xy\parallel}) \\
p_7 &= F_2(-3V_\parallel, -J_{xy\parallel}) \qquad q_7 = -G_2(-3V_\parallel, -J_{xy\parallel}).
\end{aligned}
$$

As is the case for the model for heavy fermions, the η-pairing states with momentum $\{P\} \neq \{0, 0\}, \{\pi, \pi\}$ are ground states of the Hamiltonian (25) if we choose $t_\parallel = X_\parallel$, $t_\perp = X_\perp$, $Y_\parallel = Y_\perp = V_\parallel = V_\perp = 0$. These conditions lead to high degeneracy of the ground states of the model. When we take into consideration the pair hopping terms $Y_\parallel$ and $Y_\perp$, the degeneracy is lifted in favour of superconducting states.

Next we obtain the criteria for the stability of CDW states. The CDW states (at half filling) are defined by

$$
|\mathrm{CDW}\rangle = \prod_{i\in\mathcal{C}} c_{i1\uparrow}^\dagger c_{i1\downarrow}^\dagger \prod_{j\in\mathcal{C}'} c_{j2\uparrow}^\dagger c_{j2\downarrow}^\dagger |0\rangle \qquad (37)
$$

($\mathcal{C}$ and $\mathcal{C}'$ are even (odd) sublattices of a bipartite lattice) and are constructed from the local states $|2_0 0_2\rangle$ and $|0_2 2_0\rangle$ (or the states $|2_2 0_0\rangle$ and $|0_0 2_2\rangle$). These states become eigenstates of the local Hamiltonian h_{ij} in (25) with the same energy $E = U/Z - 2V_\parallel - 2V_\perp + 4\mu/Z$ if we choose $Y_\parallel = Y_\perp = 0$. Demand that all the remaining eigenenergies are higher than E to obtain the inequality,

$$
\begin{aligned}
&V_\parallel > 0 \qquad V_\perp > 0 \qquad V_\parallel + V_\perp > \frac{|\mu|}{Z} \\
&\frac{U}{Z} < \min\left\{ -2|t_\parallel| - 2|t_\perp| + 6(V_\parallel + V_\perp) - \frac{6|\mu|}{Z}, 2(V_\parallel + V_\perp) - \frac{2|\mu|}{Z}, \right. \\
&\qquad V_\parallel + V_\perp - \frac{|J_{xy\parallel}|}{4}, \min(V_\parallel, V_\perp) + 2(V_\parallel + V_\perp) + \frac{J_{z\perp}}{4} - \frac{2|\mu|}{Z}, \\
&\qquad 3V_\parallel + 2V_\perp - \frac{|J_{xy\parallel}|}{2} - \frac{J_{z\parallel}}{4} - \frac{2|\mu|}{Z},
\end{aligned}
$$

$$2V_\parallel + \frac{5V_\perp}{2} - \frac{1}{8}\left(|J_{z\perp}| + \sqrt{(16t_\parallel)^2 + (4V_\perp - J_{z\perp})^2}\right) - \frac{2|\mu|}{Z},$$
$$V_\parallel + 2V_\perp + \frac{J_{z\parallel}}{4}, -(V_\parallel + V_\perp) - \frac{J_{z\parallel}}{4}\left(J_{z\parallel} + \sqrt{4J_{xy\parallel}^2 + J_{z\perp}^2}\right),$$
$$\frac{3V_\parallel}{2} + 2V_\perp + \frac{1}{8}\left(J_{z\perp} - \sqrt{(16t_\perp)^2 + (4V_\parallel - J_{z\perp})^2}\right), \frac{5V_\parallel}{2}$$
$$+2V_\perp - \frac{1}{8}\left(2J_{xy\parallel} + J_{z\perp} + \sqrt{(16t_\perp)^2 + (4V_\parallel - 2J_{xy\parallel} - J_{z\parallel})^2}\right) - \frac{2|\mu|}{Z},$$
$$\frac{1}{12}(J_{z\parallel} + J_{z\perp}) - 2|\mu| + \min\left(\frac{7}{3}(V_\parallel + V_\perp) + \xi_1, -\frac{7}{3}(V_\parallel + V_\perp) + \xi_5\right),$$
$$-\frac{1}{12}(J_{z\parallel} + J_{z\perp}) - 2|\mu|$$
$$+\min\left(\frac{7V_\parallel}{3} + \frac{J_{xy\parallel}}{6} + \xi_2, -\frac{7V_\parallel}{3} + \frac{J_{xy\parallel}}{6} + \xi_6, -\frac{7V_\parallel}{3} - \frac{J_{xy\parallel}}{6} + \xi_7\right),$$
$$\frac{10V_\parallel}{3} - |\mu| + \min\left(g_1(t_\parallel, t_\perp), g_1(-t_\parallel, t_\perp), g_1(t_\parallel, -t_\perp), g_1(-t_\parallel, -t_\perp)\right),$$
$$-\frac{1}{18}(J_{z\parallel} + J_{z\perp}) - \frac{2|\mu|}{3}$$
$$+\min\left(g_2(t_\parallel, t_\perp), g_2(-t_\parallel, t_\perp), g_2(t_\parallel, -t_\perp), g_2(-t_\parallel, -t_\perp)\right)\Bigg\} \qquad (38)$$

where

$$g_1(t_\parallel, t_\perp) = \tfrac{2}{3}(-t_\parallel + t_\perp) + 2\xi_3 \qquad g_2(t_\parallel, t_\perp) = -\tfrac{2}{9}(t_\parallel + t_\perp - 3\xi_4) \qquad (39)$$

and ξ_i is defined in equations (35) with

$$p_1 = F_1(V_\parallel, V_\perp) \equiv 48(t_\parallel^2 + t_\perp^2) + 3(J_{z\perp} + 4V_\perp)^2/16 + (8V_\parallel - 4V_\perp + 2J_{z\parallel} - J_{z\perp})^2/16$$

$$\begin{aligned} q_1 = G_1(V_\parallel, V_\perp) \equiv{}& J_{z\perp}^3/4 - 3J_{z\perp}^2 J_{z\parallel}/8 - 3J_{z\perp}J_{z\parallel}^2/8 + J_{z\parallel}^3/4 \\ &+(3J_{z\perp}^2 - 3J_{z\perp}J_{z\parallel} - 3J_{z\parallel}^2/2)V_\perp + (12J_{z\perp} - 6J_{z\parallel})V_\perp^2 \\ &+16V_\perp^3 + t_\parallel^2(72J_{z\perp} - 144J_{z\parallel} + 288V_\perp - 576V_\parallel) \\ &+(-3J_{z\perp}^2/2 - 3J_{z\perp}J_{z\parallel} + 3J_{z\parallel}^2 + (-12J_{z\perp} - 12J_{z\parallel})V_\perp - 24V_\perp^2)V_\parallel \\ &+(-6J_{z\perp} + 12J_{z\parallel} - 24V_\perp)V_\parallel^2 + 16V_\parallel^3 \\ &+t_\perp^2(-144J_{z\perp} + 72J_{z\parallel} - 576V_\perp + 288V_\parallel) \end{aligned}$$

$$\begin{aligned} p_2 = F_2(V_\parallel, V_\perp, J_{xy\parallel}) \equiv{}& 48(t_\parallel^2 + t_\perp^2) + 3(4V_\perp - J_{z\perp})^2/16 \\ &+(8V_\parallel - 4V_\perp + 4J_{xy\parallel} - 2J_{z\parallel} + J_{z\perp})^2/16 \end{aligned}$$

$$\begin{aligned} q_2 = G_2(V_\parallel, V_\perp, J_{xy\parallel}) \equiv{}& 2J_{xy\parallel}^3 + 3J_{xy\parallel}^2 J_{z\perp}/2 - 3J_{xy\parallel}J_{z\perp}^2/4 - J_{z\perp}^3/4 - 3J_{xy\parallel}^2 J_{z\parallel} \\ &-3J_{xy\parallel}J_{z\perp}J_{z\parallel}/2 + 3J_{z\perp}^2 J_{z\parallel}/8 + 3J_{xy\parallel}J_{z\parallel}^2/2 + 3J_{z\perp}J_{z\parallel}^2/8 - J_{z\parallel}^3/4 \\ &+(-6J_{xy\parallel}^2 + 6J_{xy\parallel}J_{z\perp} + 3J_{z\perp}^2 + 6J_{xy\parallel}J_{z\parallel} - 3J_{z\perp}J_{z\parallel} - 3J_{z\parallel}^2/2)V_\perp \\ &+(-12J_{xy\parallel} - 12J_{z\perp} + 6J_{z\parallel})V_\perp^2 + 16V_\perp^3 \\ &+t_\parallel^2(-288J_{xy\parallel} - 72J_{z\perp} + 144J_{z\parallel} + 288V_\perp - 576V_\parallel) \\ &+(12J_{xy\parallel}^2 + 6J_{xy\parallel}J_{z\perp} - 3J_{z\perp}^2/2 - 12J_{xy\parallel}J_{z\parallel} - 3J_{z\perp}J_{z\parallel} + 3J_{z\parallel}^2 \\ &+(-24J_{xy\parallel} + 12J_{z\perp} + 12J_{z\parallel})V_\perp - 24V_\perp^2)V_\parallel \\ &+(24J_{xy\parallel} + 6J_{z\perp} - 12J_{z\parallel} - 24V_\perp)V_\parallel^2 + 16V_\parallel^3 \end{aligned}$$

$$+t_\perp^2(144J_{xy\|} + 144J_{z\perp} - 72J_{z\|} - 576V_\perp + 288V_\|) \quad (40)$$

$$p_3 = 3(3t_\|^2 + 4t_\perp^2 + 2V_\|^2) + (t_\| + 2t_\perp - 2V_\| + 4V_\perp)^2 + 6(t_\| - V_\|)^2$$

$$q_3 = 128t_\perp^3 - 128t_\|^3 - 128V_\perp^3 + t_\perp^2(192V_\perp - 96V_\|) + 192V_\perp^2 V_\| + 192V_\perp V_\|^2$$
$$-128V_\|^3 + t_\|^2(-48t_\perp - 96V_\perp + 192V_\|) + t_\perp(-192V_\perp^2 + 192V_\perp V_\| + 96V_\|^2)$$
$$+t_\|(48t_\perp^2 - 96V_\perp^2 + t_\perp(-96V_\perp - 96V_\|) - 192V_\perp V_\| + 192V_\|^2)$$

$$p_4 = 6t_\perp^2 + J_{z\perp}^2/2 + (3t_\perp - J_{z\perp})^2 + (2t_\| - t_\perp - J_{z\|} + J_{z\perp}/2)^2$$

$$q_4 = -9J_{xy\|}^2 J_{z\perp} - 2J_{z\perp}^3 + 18J_{xy\|}^2 J_{z\|} + 3J_{z\perp}^2 J_{z\|} + 3J_{z\perp} J_{z\|}^2 - 2J_{z\|}^3$$
$$+(18J_{xy\|}^2 + 12J_{z\perp}^2 - 12J_{z\perp}J_{z\|} - 6J_{z\|}^2)t_\perp + (48J_{z\perp} - 24J_{z\|})t_\perp^2 - 128t_\perp^3$$
$$+(-36J_{xy\|}^2 + 36J_{xy\|}J_{z\perp} - 6J_{z\perp}^2 - 72J_{xy\|}J_{z\|} - 12J_{z\perp}J_{z\|} + 12J_{z\|}^2$$
$$+(-72J_{xy\|} + 24J_{z\perp} + 24J_{z\|})t_\perp + 48t_\perp^2)t_\|$$
$$+(144J_{xy\|} - 24J_{z\perp} + 48J_{z\|} + 48t_\perp)t_\|^2 - 128t_\|^3$$

$$p_5 = F_1(-V_\|, -V_\perp) \qquad q_5 = G_1(-V_\|, -V_\perp)$$
$$p_6 = F_2(-V_\|, -V_\perp, J_{xy\|}) \qquad q_6 = G_2(-V_\|, -V_\perp, J_{xy\|})$$
$$p_7 = F_2(-V_\|, -V_\perp, -J_{xy\|}) \qquad q_7 = G_2(-V_\|, -V_\perp, -J_{xy\|}). \quad (41)$$

We can control the fillings by changing the chemical potential μ. To obtain the best bound, we may choose $\mu = 0$.

4. Summary

We have constructed the exact ground states of models for correlated electronic systems. We introduced generalized models for heavy-fermion/bilayer systems. By the optimal ground state approach we have determined the parameter regions where the model has the η-pairing ground states which exhibit off-diagonal long-range order, and are thus superconducting. For heavy fermions, in particular, the eigenfunctions of the model have the decoupling property via the η-pairing mechanism which allows the coexistence of superconductivity and various kinds of magnetism (paramagnetism, Néel and ferromagnetism). We have also obtained the criteria for the stability of charge-density-wave states.

Acknowledgments

We would like to thank Y Akutsu for continuous encouragement and interest in this work. Stimulating discussions with K Hirai and K Ueda on heavy-fermion systems and with A A Aligia and A Schadschneider on the η-pairing mechanism are gratefully acknowledged.

References

[1] Yang C N 1989 *Phys. Rev. Lett.* **63** 2144
Yang C N and Zhang S 1990 *Mod. Phys. Lett.* B **4** 759
[2] Yang C N 1962 *Rev. Mod. Phys.* **34** 694
[3] Sewell G L 1990 *J. Stat. Phys.* **61** 415
[4] Nieh H T, Su G and Zhao B M 1995 *Phys. Rev.* B **51** 3760
[5] Essler F H L, Korepin V E and Schoutens K 1992 *Phys. Rev. Lett.* **68** 2960
Essler F H L, Korepin V E and Schoutens K 1993 *Phys. Rev. Lett.* **70** 73
[6] Arrachea L and Aligia A A 1994 *Phys. Rev. Lett.* **73** 1994 2240
[7] de Boer J, Korepin V E and Schadschneider A 1995 *Phys. Rev. Lett.* **74** 789

[8] Schadschneider A 1995 *Phys. Rev.* B **51** 10 386
[9] de Boer J and Schadschneider A 1995 *Phys. Rev. Lett.* **75** 4298
[10] Sato R in preparation
[11] Steglich F, Geibel C, Modler R, Lang M, Hellmann P and Gegenwart P 1995 *J. Low Temp. Phys.* **99** 267
[12] Sigrist M, Tsunetsugu H and Ueda K 1991 *Phys. Rev. Lett.* **67** 221
[13] Sigrist M, Tsunetsugu H, Ueda K and Rice T M 1992 *Phys. Rev.* B **46** 13 838
[14] Ueda K, Tsunetsugu H and Sigrist M 1992 *Phys. Rev. Lett.* **68** 1030
[15] Yanagisawa T and Shimoi K 1994 *Phys. Rev.* B **50** 9577
[16] Yanagisawa T and Shimoi K 1995 *Phys. Rev. Lett.* **74** 4939
[17] Arrachea L, Aligia A A and Gagliano E 1996 *Phys. Rev. Lett.* **76** 4396
[18] dos Santos R R 1995 *Phys. Rev.* B **51** 15 540
[19] Hetzel R E, von der Linden W and Hanke W 1994 *Phys. Rev.* B **50** 4159