Quantum cluster decimation

1991 J. Phys. A: Math. Gen. 24 4599

(http://iopscience.iop.org/0305-4470/24/19/023)

J. Phys. A: Math. Gen. 24 (1991) 4599-4618. Printed in the UK

Quantum cluster decimation

Takeo Matsubara†, Chieko Totsuji† and Colin J Thompson‡

† Department of Applied Physics, Okayama University of Science, 1-1 Ridaicho, Okayama 700, Japan

‡ Mathematics Department, University of Melbourne, Parkville, Victoria 3052, Australia

Received 12 February 1991

Abstract. An exact quantum decimation is performed on an extended Hubbard model for a three-site cluster by taking the partial trace of the Boltzmann factor over states of the central site. The resulting temperature-dependent Hamiltonian for the outer two sites of the cluster contains higher order three- and four-particle interactions, $t-J$ model, pairing and superexchange interactions, and two-particle interactions which are predominantly attractive. Possible implications for high-temperature superconductivity are briefly discussed.

1. Introduction

Transformations in classical statistical mechanics involving selected summation over states in the partition function were introduced and studied in the 1940s and 1950s as a means for obtaining new exact results from known solutions of model systems such as the Ising model.

Onsager [1] for example, discussed the 'star-triangle' transformation in which a 'star' consisting of a central Ising spin $\mu_0 = \pm 1$ coupled to three neighbouring spins, is transformed, by summing the Boltzmann factor in the partition function over the central spin μ_0, into a 'triangle' consisting of the three outer spins with modified nearest-neighbour coupling. This transformation relates Ising models on the honeycomb and triangular lattices and was used, among other things, to evaluate their respective critical points exactly.

Another purely algebraic transformation introduced by Syozi [2] and known as the decoration-iteration transformation, replaces a decorated bond consisting of three spins, by a single bond consisting of the two outer spins, by summing the Boltzmann factor for the decorated bond over the states of the central spin. This transformation, illustrated in figure 1, also holds in a magnetic field and was used by numerous people to obtain a variety of new exact results for two-dimensional lattice models. A comprehensive review of results obtained by the above-mentioned methods and their generalizations has been given by Syozi [3].

In more recent times, selective summation over states in the partition function, known commonly now as decimation, has been used to generate approximate renormalization group transformations [4] and the star-triangle relation has been superseded by the so-called Yang-Baxter equations [5] which form the basis of exact solubility or integrability of two-dimensional lattice models in statistical mechanics and lattice gauge theory [6].

0305-4470/91/194599+20$03.50

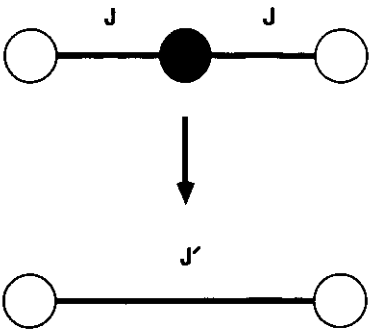

Figure 1. The decoration-iteration transformation.

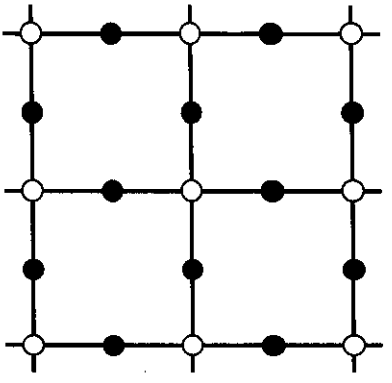

Figure 2. A Cu-O_2 plane with open circles corresponding to Cu and full circles corresponding to O_2.

Interest in the decoration-iteration or decimation transformation has recently been revived with the discovery of the high-T_c superconductors which have Cu-O_2 planes, shown in figure 2, as a common feature. Many models and pairing mechanisms have been proposed for the Cu-O_2 planes including the extended Hubbard model with on-site and nearest-neighbour repulsion between fermionic holes on the Cu and O_2 sites [7]. In formulating a statistical mechanical treatment of such models it is natural to consider a quantum mechanical analogue of decimation involving a partial trace over O_2 sites in say an extended Hubbard model of a Cu-O_2 plane.

Unlike classical decimation however, in which one can factorize individual Boltzmann factors for decorated bonds and rigorously perform the partial sum over states of the central or decorated site, the non-commutability of terms in the extended Hubbard model Hamiltonian corresponding to decorated bonds, makes rigorous decimation in the quantum case a virtually impossible task. One can, nevertheless, as a first approximation, consider quantum decimation of Boltzmann factors corresponding to simple fermion clusters, as a means for gaining some understanding of the nature of the effective couplings that can be mediated in such clusters. We have in fact performed such a calculation rigorously for the elementary cluster, shown in figure 1,

consisting of spinless fermions on three sites with on-site and nearest-neighbour repulsion [8]. In this case we found by the decimation process that the effective coupling between the outer sites was attractive for a wide range of temperatures and densities and on this basis suggested oxygen-mediated attraction between holes on Cu-sites as a possible pairing mechanism for high-T_c superconductivity.

In reality of course, the holes in extended Hubbard models of $Cu-O_2$ planes are not spinless and in fact it is commonly believed that 'spin' also plays an essential role in high-T_c.

Our purpose here is to report on a quantum cluster decimation (QCD) calculation for the elementary cluster of fermions with spin on three sites with on-site and nearest-neighbour interactions.

In the spinless case there are two states per site (unoccupied or occupied by a particle) so in the number representation we have to manipulate $2^3 = 8$-dimensional matrices in the decimation process. With the inclusion of spin, however, there are four states per site (unoccupied, occupied by a spin-up or a spin-down particle, and occupied by a spin-up and a spin-down particle) so the decimation process now involves manipulation of $4^3 = 64$-dimensional matrices. We were, nevertheless, able to perform the decimation process exactly in this case and found that the original on-site and nearest-neighbour interactions gave rise to complicated temperature and density dependent three- and four-particle interactions as well as effective spin-dependent pair interactions of the superexchange form, and renormalized single and pair hopping terms. In other words, all of the effective couplings obtained by the more conventional perturbative [9] and canonical transformation [10] methods can also be obtained by our QCD method with the added feature that our effective couplings are dependent on the temperature and the density.

The earlier perturbative methods [9] can be criticized on the grounds that they are based on perturbations from the ground state and therefore may only be relevant at very low temperatures. Similarly, the canonical transformation method [10] is simply an exponential unitary transformation on the Hamiltonian in which all but the lowest-order terms are discarded in a somewhat *ad hoc* fashion. Both the perturbative and canonical transformation methods do not involve the temperature in any essential way so their relevance to statistical mechanical calculations is not at all clear.

Our QCD method is strongly based in statistical mechanics and involves the temperature and density in an essential way. The obvious drawback of the method, however, is that it ignores the non-commutability problem mentioned previously and can only be feasibly carried out on small elementary clusters. Nevertheless, we see our calculations to date as a first step in a systematic development of an alternative approach in quantum statistical mechanics involving a selective summation or 'tracing-out' of states in the partition function. It is clear, however, that we need to incorporate ideas of self-consistency and renormalization into our method before it can become a viable and practical tool. Work along these lines is currently in progress.

In outline this paper is arranged as follows. In section 2, we present the classical decimation transformation for a lattice gas cluster of three sites and review some of our previous results. In section 3, we derive a 64×64 representation of the three-site cluster Hamiltonian and the associated Boltzmann factor for fermions with spin and perform a partial trace over states of the central site. In section 4, we derive and discuss the form of the effective cluster Hamiltonion for the two outer sites of the original cluster. Technical details are relegated to appendices and our results are discussed in section 5.

2. Classical lattice gas decimation

In order to get some idea of what is involved in the decimation process, we first consider the simplest case of classical decimation of a three-site lattice gas cluster with Hamiltonian

$$\mathcal{H}_{\rm cl} = Jn(n_1 + n_2) \tag{2.1}$$

where $n = 0, 1$ is the occupation number of the central site of the cluster and $n_i = 0, 1$ for $i = 1, 2$ are the occupation numbers of the outer two sites of the cluster.

The contribution to the grand canonical partition function obtained from the cluster by summing over the states of the central site is given by

$$\sum_{n=0,1} \exp[-\beta Jn(n_1+n_2)] \exp(\beta\mu n) = 1 + z \exp[-\beta J(n_1+n_2)] \tag{2.2}$$

where μ is the chemical potential and $z = \exp(\beta\mu)$ is the activity.

We now define the effective cluster Hamiltonian $\mathcal{H}_{\rm cl}^{\rm eff}$ and effective chemical potential $\tilde{\mu}$ by

$$1 + z \exp[-\beta J(n_1+n_2)] = C \exp(-\beta\mathcal{H}_{\rm cl}^{\rm eff}) \exp[\beta\tilde{\mu}(n_1+n_2)] \tag{2.3}$$

and make the ansatz

$$\mathcal{H}_{\rm cl}^{\rm eff} = \tilde{J} n_1 n_2. \tag{2.4}$$

Since $n_i = 0, 1$ for $i = 1, 2$ we see that (2.3) with $\mathcal{H}_{\rm cl}^{\rm eff}$ given by (2.4) is satisfied identically provided

$$C = 1 + z \tag{2.5}$$

$$\exp(\beta\tilde{\mu}) = (1+zx)(1+z)^{-1} \tag{2.6}$$

and

$$\exp(-\beta\tilde{J}) = 1 + z(1-x)^2(1+zx)^{-2} \tag{2.7}$$

where

$$x = \exp(-\beta J) \tag{2.8}$$

The important point to notice from (2.7) is that $\tilde{J} < 0$, i.e. *the effective coupling is always attractive* regardless of the sign of the original coupling J.

For the classical lattice gas, where Boltzmann factors for clusters commute, we deduce from the above simple decimation calculation that the grand canonical partition function for the decorated square lattice gas with N bonds for example (i.e. the classical $Cu\text{-}O_2$ plane shown in figure 2) is in fact equal to $(1+z)^N$ times the grand canonical partition function for the usual square lattice gas but with effective nearest-neighbour (attractive) coupling J and effective chemical potential $\mu + 4\tilde{\mu}$.

The above results are, of course, well known but are usually expressed in Ising spin language.

In a previous article [8], we generalized the above cluster Hamiltonian (2.1) to include particles with spin so that in place of (2.1) we considered the three-site cluster Hamiltonian

$$\mathcal{H}_{\rm cl} = J(n_\uparrow + n_\downarrow)(n_{1\uparrow} + n_{2\uparrow} + n_{1\downarrow} + n_{2\downarrow}) + U_0 n_\uparrow n_\downarrow \tag{2.9}$$

where n_{σ}, $\sigma = \uparrow, \downarrow$, denotes the occupation number of the central cluster site by a particle with spin σ, and $n_{i\sigma}$, $\sigma = \uparrow, \downarrow$ and $i = 1, 2$, denotes the occupation numbers of the outer sites of the cluster by particles with spin σ.

It will be noted that (2.9) is in fact the Hamiltonian for an extended Hubbard model of a three-site cluster with zero hopping integral t, on-site repulsion U_0 and nearest-neighbour interaction J. Our task in the following sections will be to perform the decimation with hopping included in (2.9).

In the classical case (2.9) decimation proceeds as before by summing the Boltzmann factor for the cluster states $n_\sigma = 0, 1$, $\sigma = \uparrow, \downarrow$ of the central site and seeking an effective chemical potential $\tilde{\mu}$ and cluster Hamiltonian $\mathscr{H}_{\rm cl}^{\rm eff}$ for the outer sites, such that

$$\sum_{\{n_\sigma = 0,1\}} \exp(-\beta \mathscr{H}_{\rm cl}) \exp[\beta\mu(n_\uparrow + n_\downarrow)]$$

$$= C \exp(-\beta \mathscr{H}_{\rm cl}^{\rm eff}) \exp\left\{\beta\tilde{\mu}\left[\sum_\sigma (n_{1\sigma} + n_{2\sigma})\right]\right\}. \tag{2.10}$$

In this case a simple pair interaction ansatz such as (2.4) for $\mathscr{H}_{\rm cl}^{\rm eff}$ is inadequate and in order for (2.10) to be satisfied identically for all possible states of the outer sites we must postulate effective three- and four-particle interactions in addition to an effective two particle interaction. We refer the interested reader to our previous article [8] for details and merely note here that again the effective pair interaction is always attractive regardless of the sign of the original coupling J. The weaker three- and four-particle interactions on the other hand show mixtures of attraction and repulsion in the temperature-density plane.

3. The 64×64 representation of the quantum cluster Hamiltonian and the partial trace decimation

We consider the three-site cluster Hamiltonian

$$\mathscr{H}_{\rm cl} = -t \sum_{\sigma=\uparrow,\downarrow} [a_\sigma^\dagger(a_{1\sigma} + a_{2\sigma}) + (a_{1\sigma}^\dagger + a_{2\sigma}^\dagger)a_\sigma]$$

$$+ U_0 n_\uparrow n_\downarrow + J(n_\uparrow + n_\downarrow)(n_{1\uparrow} + n_{2\uparrow} + n_{1\downarrow} + n_{2\downarrow}) \tag{3.1}$$

where $a_{i\sigma}(a_{i\sigma}^\dagger)$ is the usual fermi destruction (creation) operator for a particle with spin σ on the outer sites $i = 1, 2$, $a_\sigma(a_\sigma^\dagger)$ the corresponding operators for the central site of the cluster and $n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma}$, $n_\sigma = a_\sigma^\dagger a_\sigma$ the respective number operators for the three sites.

Our problem is to take the partial trace over states $\{a_\sigma, a_\sigma^\dagger\}$ corresponding to the central site such that

$$\mathrm{Tr}_{\{a_\sigma, a_\sigma^\dagger\}}\{\exp(-\beta\mathscr{H}_{\rm cl}) \exp[\beta\mu(n_\uparrow + n_\downarrow)]\}$$

$$= C \exp(-\beta \mathscr{H}_{\rm cl}^{\rm eff}) \exp[\beta\tilde{\mu}(n_{1\uparrow} + n_{2\uparrow} + n_{1\downarrow} + n_{2\downarrow})] \tag{3.2}$$

and to find appropriate expressions for the effective cluster Hamiltonian $\mathscr{H}_{\rm cl}^{\rm eff}$ and effective chemical potential $\tilde{\mu}$.

At this stage it is convenient to introduce the canonical transformation

$$a_{+\sigma} = \frac{1}{\sqrt{2}}(a_{1\sigma} + a_{2\sigma})$$

$$a_{-\sigma} = \frac{1}{\sqrt{2}}(a_{1\sigma} - a_{2\sigma}) \tag{3.3}$$

and to express (3.1) in the form

$$\mathcal{H}_{\rm cl} = -t\sqrt{2}\sum_{\sigma}(a_{\sigma}^{\dagger}a_{+\sigma} + a_{+\sigma}^{\dagger}a_{\sigma}) + U_0 n_{\uparrow}n_{\downarrow} + J\sum_{\sigma}(n_{\uparrow}+n_{\downarrow})(n_{+\sigma}+n_{-\sigma}) \quad (3.4)$$

where

$$n_{\pm\sigma} = a_{\pm\sigma}^{\dagger}a_{\pm\sigma} \quad (3.5)$$

are modified number operators.

We now adopt the number representation for (3.4) in which all operators are represented by 64×64 matrices with row and column indices specified by the set of states or 'numbers' $\{n_{\uparrow}, n_{\downarrow}, n_{+\uparrow}, n_{+\downarrow}, n_{-\uparrow}, n_{-\downarrow}\}$. In this way $\mathcal{H}_{\rm cl}$ can be expressed in the following hierarchical block form

$$\mathcal{H}_{\rm cl} = \begin{matrix}(n_{\uparrow}n_{\downarrow})\\(11)\\(10)\\(01)\\(00)\end{matrix}\begin{matrix}\begin{matrix}(11) & (10) & (01) & (00)\end{matrix}\\\begin{pmatrix}H_{11} & H_{12} & H_{13} & H_{14}\\ H_{21} & H_{22} & H_{23} & H_{24}\\ H_{31} & H_{32} & H_{33} & H_{34}\\ H_{41} & H_{42} & H_{43} & H_{44}\end{pmatrix}\end{matrix} \quad (3.6a)$$

where the H_{ij} are 16×16 matrices and also have the block form

$$H_{ij} = \begin{matrix}(n_{+\uparrow}n_{+\downarrow})\\(11)\\(10)\\(01)\\(00)\end{matrix}\begin{matrix}\begin{matrix}(11) & (10) & (01) & (00)\end{matrix}\\\begin{pmatrix}h_{11}^{ij} & h_{12}^{ij} & h_{13}^{ij} & h_{14}^{ij}\\ h_{21}^{ij} & h_{22}^{ij} & h_{23}^{ij} & h_{24}^{ij}\\ h_{31}^{ij} & h_{32}^{ij} & h_{33}^{ij} & h_{34}^{ij}\\ h_{41}^{ij} & h_{42}^{ij} & h_{43}^{ij} & h_{44}^{ij}\end{pmatrix}\end{matrix} \quad (3.6b)$$

with the h_{kl}^{ij} 4×4 matrices of the same form with rows and columns arranged in the order (11) (10) (01) (00) corresponding to $(n_{-\uparrow}n_{-\downarrow})$.

We note that the interaction part of $\mathcal{H}_{\rm cl}$:

$$U_0 n_{\uparrow}n_{\downarrow} + J\sum_{\sigma}(n_{\uparrow}+n_{\downarrow})(n_{+\sigma}+n_{-\sigma}) \quad (3.7a)$$

is diagonal in this representation whereas the kinetic energy part of $\mathcal{H}_{\rm cl}$:

$$-t\sqrt{2}\sum_{\sigma}(a_{\sigma}^{\dagger}a_{+\sigma} + a_{+\sigma}^{\dagger}a_{\sigma}) \quad (3.7b)$$

is diagonal with respect to the subspace specified by $(n_{-\uparrow}n_{-\downarrow})$ but non-diagonal with respect to the subspace specified by $(n_{\uparrow}n_{\downarrow}n_{+\uparrow}n_{+\downarrow})$.

Using (3.7*a*), we easily see that the non-zero diagonal blocks of $\mathcal{H}_{\rm cl}$ are given in terms of

$$h_{11}^{(11)} = \begin{pmatrix}U_0+8J & 0 & 0 & 0\\ 0 & U_0+6J & 0 & 0\\ 0 & 0 & U_0+6J & 0\\ 0 & 0 & 0 & U_0+4J\end{pmatrix} \equiv \boldsymbol{D}_0 \quad (3.8a)$$

$$h_{22}^{(11)} = h_{33}^{(11)} = \begin{pmatrix}U_0+6J & 0 & 0 & 0\\ 0 & U_0+4J & 0 & 0\\ 0 & 0 & U_0+4J & 0\\ 0 & 0 & 0 & U_0+2J\end{pmatrix} \equiv \boldsymbol{D}_1 \quad (3.8b)$$

$$h_{44}^{(11)} = \begin{pmatrix} U_0+4J & 0 & 0 & 0 \\ 0 & U_0+2J & 0 & 0 \\ 0 & 0 & U_0+2J & 0 \\ 0 & 0 & 0 & U_0 \end{pmatrix} \equiv \boldsymbol{D}_2 \tag{3.8c}$$

$$h_{11}^{(22)} = h_{11}^{(33)} = \begin{pmatrix} 4J & 0 & 0 & 0 \\ 0 & 3J & 0 & 0 \\ 0 & 0 & 3J & 0 \\ 0 & 0 & 0 & 2J \end{pmatrix} \equiv \boldsymbol{D}_3 \tag{3.8d}$$

$$h_{33}^{(22)} = h_{22}^{(22)} = h_{22}^{(33)} = h_{33}^{(33)} = \begin{pmatrix} 3J & 0 & 0 & 0 \\ 0 & 2J & 0 & 0 \\ 0 & 0 & 2J & 0 \\ 0 & 0 & 0 & J \end{pmatrix} \equiv \boldsymbol{D}_4 \tag{3.8e}$$

and

$$h_{44}^{(22)} = h_{44}^{(33)} = \begin{pmatrix} 2J & 0 & 0 & 0 \\ 0 & J & 0 & 0 \\ 0 & 0 & J & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \equiv \boldsymbol{D}_5 \tag{3.8f}$$

while the remaining diagonal blocks are equal to the 4×4 null matrix O_4, i.e.,

$$h_{kl}^{(44)} = O_4 \qquad k, l = 1, 2, 3, 4. \tag{3.8g}$$

The non-diagonal part of $\mathscr{H}_{\mathrm{cl}}$, (3.7*b*), has non-zero matrix elements $-t\sqrt{2}$ connecting states and in blocks given by

$$a_{\uparrow}^{\dagger}a_{+\uparrow}\begin{cases}(01\,11\,pq)\to(11\,01\,pq) & h_{13}^{(31)}\\ (01\,10\,pq)\to(11\,00\,pq) & h_{(24)}^{(31)}\\ (00\,11\,pq)\to(10\,01\,pq) & h_{13}^{(42)}\\ (00\,10\,pq)\to(10\,00\,pq) & h_{24}^{(42)}\end{cases}$$

$$a_{\downarrow}^{\dagger}a_{+\downarrow}\begin{cases}(10\,11\,pq)\to(11\,10\,pq) & h_{12}^{(21)}\\ (10\,01\,pq)\to(11\,00\,pq) & h_{34}^{(21)}\\ (00\,11\,pq)\to(01\,10\,pq) & h_{12}^{(43)}\\ (00\,01\,pq)\to(01\,00\,pq) & h_{34}^{(43)}\end{cases}$$

$$a_{+\uparrow}^{\dagger}a_{\downarrow}\begin{cases}(11\,01\,pq)\to(01\,11\,pq) & h_{31}^{(13)}\\ (11\,00\,pq)\to(01\,10\,pq) & h_{42}^{(13)}\\ (10\,01\,pq)\to(00\,11\,pq) & h_{31}^{(24)}\\ (10\,00\,pq)\to(00\,10\,pq) & h_{42}^{(24)}\end{cases} \tag{3.8h}$$

$$a_{+\downarrow}^{\dagger}a_{\downarrow}\begin{cases}(11\,10\,pq)\to(10\,11\,pq) & h_{21}^{(12)}\\ (11\,00\,pq)\to(10\,01\,pq) & h_{43}^{(12)}\\ (01\,10\,pq)\to(00\,11\,pq) & h_{21}^{(34)}\\ (01\,00\,pq)\to(00\,01\,pq) & h_{43}^{(34)}\end{cases}$$

and all other matrix elements are zero.

It then follows that $\mathscr{H}_{\rm cl}$ can be expressed as a 64×64 matrix composed of several diagonal 4×4 submatrices with the following structure

$$\mathscr{H}_{\rm cl}=\begin{pmatrix}
\boldsymbol{D}_0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & & & \\
0 & \boldsymbol{D}_1 & 0 & 0 & \boldsymbol{T} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & & & \\
0 & 0 & \boldsymbol{D}_1 & 0 & 0 & 0 & 0 & 0 & \boldsymbol{T} & 0 & 0 & 0 & & O_{16} & & \\
0 & 0 & 0 & \boldsymbol{D}_2 & 0 & 0 & \boldsymbol{T} & 0 & 0 & \boldsymbol{T} & 0 & 0 & & & & \\
0 & \boldsymbol{T} & 0 & 0 & \boldsymbol{D}_3 & 0 & 0 & 0 & & & & & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \boldsymbol{D}_4 & 0 & 0 & & & & & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \boldsymbol{T} & 0 & 0 & \boldsymbol{D}_4 & 0 & & O_{16} & & & \boldsymbol{T} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \boldsymbol{D}_5 & & & & & 0 & \boldsymbol{T} & 0 & 0 \\
0 & 0 & \boldsymbol{T} & 0 & & & & & \boldsymbol{D}_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \boldsymbol{T} & & & & & 0 & \boldsymbol{D}_4 & 0 & 0 & \boldsymbol{T} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & & O_{16} & & & 0 & 0 & \boldsymbol{D}_4 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & & & & & 0 & 0 & 0 & \boldsymbol{D}_5 & 0 & 0 & \boldsymbol{T} & 0 \\
 & & & & 0 & 0 & \boldsymbol{T} & 0 & 0 & \boldsymbol{T} & 0 & 0 & & & & \\
 & & & & 0 & 0 & 0 & \boldsymbol{T} & 0 & 0 & 0 & 0 & & & & \\
 & O_{16} & & & & & & & & & & & & O_{16} & & \\
 & & & & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \boldsymbol{T} & & & & \\
 & & & & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & & & &
\end{pmatrix} \tag{3.9}$$

where

$$\boldsymbol{T}=\begin{pmatrix} -t\sqrt{2} & 0 & 0 & 0 \\ 0 & -t\sqrt{2} & 0 & 0 \\ 0 & 0 & -t\sqrt{2} & 0 \\ 0 & 0 & 0 & -t\sqrt{2} \end{pmatrix}$$

and O_n denotes the $n\times n$ null matrix.

We are now in a position to construct the matrix

$$\exp(-\beta\mathscr{H}_{\rm cl})\exp[\beta\mu(n_\uparrow+n_\downarrow)].$$

In view of the special form of $\mathscr{H}_{\rm cl}$ given in (3.9), we only need to construct the following three types of exponential functions of the matrices:

$$\exp\left[-\beta\begin{pmatrix}\boldsymbol{D}_1 & \boldsymbol{T}\\ \boldsymbol{T} & \boldsymbol{D}_3\end{pmatrix}\right]\equiv \boldsymbol{K}=\begin{pmatrix}K^{(1)} & K_{12}\\ K_{21} & K^{(2)}\end{pmatrix} \tag{3.10}$$

$$\exp\left[-\beta\begin{pmatrix}\boldsymbol{D}_5 & \boldsymbol{T}\\ \boldsymbol{T} & O_3\end{pmatrix}\right]\equiv L=\begin{pmatrix}L^{(1)} & L_{12}\\ L_{21} & L^{(2)}\end{pmatrix} \tag{3.11}$$

and

$$\exp\left[-\beta\begin{pmatrix}\boldsymbol{D}_2 & \boldsymbol{T} & \boldsymbol{T} & O_4\\ \boldsymbol{T} & \boldsymbol{D}_4 & O_4 & \boldsymbol{T}\\ \boldsymbol{T} & O_4 & \boldsymbol{D}_4 & \boldsymbol{T}\\ O_4 & \boldsymbol{T} & \boldsymbol{T} & O_4\end{pmatrix}\right]\equiv M=\begin{pmatrix}M^{(1)} & M_{12} & M_{13} & M_{14}\\ M_{21} & M^{(2)} & M_{23} & M_{24}\\ M_{31} & M_{32} & M^{(2)} & M_{34}\\ M_{41} & M_{42} & M_{43} & M^{(4)}\end{pmatrix}. \tag{3.12}$$

Given K, L and M, we have

$$\exp(-\beta\mathscr{H}_{\mathrm{cl}}) = \left(\begin{array}{cccc|cccc|cccc|cccc}
e^{-\beta D_0} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & K^{(1)} & 0 & 0 & K_{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & K^{(1)} & 0 & 0 & 0 & 0 & 0 & K_{12} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & M^{(1)} & 0 & 0 & M_{12} & 0 & 0 & M_{13} & 0 & 0 & M_{14} & 0 & 0 & 0 \\
\hline
0 & K_{21} & 0 & 0 & K^{(2)} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & e^{-\beta D_4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & M_{21} & 0 & 0 & M^{(2)} & 0 & 0 & M_{23} & 0 & 0 & M_{24} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & L^{(1)} & 0 & 0 & 0 & 0 & 0 & L_{12} & 0 & 0 \\
\hline
0 & 0 & K_{21} & 0 & 0 & 0 & 0 & 0 & K^{(2)} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & M_{31} & 0 & 0 & M_{32} & 0 & 0 & M^{(2)} & 0 & 0 & M_{34} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & e^{-\beta D_4} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & L^{(1)} & 0 & 0 & L_{12} & 0 \\
\hline
0 & 0 & 0 & M_{41} & 0 & 0 & M_{42} & 0 & 0 & M_{43} & 0 & 0 & M^{(4)} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & L_{21} & 0 & 0 & 0 & 0 & 0 & L^{(2)} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & L_{21} & 0 & 0 & L^{(2)} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & I
\end{array}\right). \tag{3.13}$$

The 16×16 reduced matrix

$$Z=\mathrm{Tr}_{\{a_\sigma,a_\sigma^\dagger\}}[\exp(-\beta\mathscr{H}_{\mathrm{cl}})\exp\{\beta\mu(n_\uparrow+n_\downarrow)\}] \tag{3.14}$$

obtained by taking the partial trace over $\{a_\sigma, a_\sigma^\dagger\}$ states is now easily obtained from (3.13) by adding the 16×16 diagonal block matrices enclosed in solid lines, multiplied by their appropriate, respective, powers of the fugacity

$$z=\mathrm{e}^{\beta\mu}. \tag{3.15}$$

Thus from (3.13) and (3.14), we have

$$Z=\begin{bmatrix} z^2\,\mathrm{e}^{-\beta D_0}+2zK^{(2)}+M^{(4)} & 0 & 0 & 0 \\ 0 & z^2K^{(1)}+z\{\mathrm{e}^{-\beta D_4}+M^{(2)}\}+L^{(2)} & 0 & 0 \\ 0 & 0 & z^2K^{(1)}+z\{\mathrm{e}^{-\beta D_4}+M^{(2)}\}+L^{(2)} & 0 \\ 0 & 0 & 0 & z^2M^{(1)}+2zL^{(1)}+1 \end{bmatrix}. \tag{3.16}$$

The problem now is to represent Z in the form (3.2) and to find appropriate expressions for the effective Hamiltonian $\mathscr{H}_{\mathrm{cl}}^{\mathrm{eff}}$ and effective chemical potential $\tilde{\mu}$.

4. The effective cluster Hamiltonian

In the number representation (3.13) of $\exp(-\beta\mathscr{H}_{\mathrm{cl}})$, the partial trace (3.14) over $\{a_\sigma, a_\sigma^\dagger\}$-states results in the diagonal 16×16 matrix Z given by (3.16). It is readily confirmed, however, that of the sixteen diagonal elements of Z only nine are independent. In order to represent Z in the form (3.2) therefore, we need an effective Hamiltonian $\mathscr{H}_{\mathrm{cl}}^{\mathrm{eff}}$ with seven independent parameters, which together with C and $\tilde{\mu}$ give the required nine unknowns.

Motivated by our previous classical treatment, we include three-particle and four-particle interactions, as well as pair interactions and an effective hopping term, in $\mathscr{H}_{\mathrm{cl}}^{\mathrm{eff}}$. This gives a total of six obvious parameters. The required additional parameters, $J_e^\pm$, and $J_3^\pm$ in place of J_3, in (4.1), which distinguish $n_{+\sigma}$ and $n_{-\sigma}$ states, are included in the expectation that superexchange-type interactions should play an important role when quantum effects, arising from fermions with spin, are taken into account.

We are thus led to the ansatz

$$\mathscr{H}_{\mathrm{cl}}^{\mathrm{eff}}=-\tilde{t}\sum_\sigma(a_{1\sigma}^\dagger a_{2\sigma}+a_{2\sigma}^\dagger a_{1\sigma})+J_2(n_{1\uparrow}+n_{1\downarrow})(n_{2\uparrow}+n_{2\downarrow})+J_e^+n_{+\uparrow}n_{+\downarrow}+J_e^-n_{-\uparrow}n_{-\downarrow}$$
$$+J_3^+n_{+\uparrow}n_{+\downarrow}(n_{-\uparrow}+n_{-\downarrow})+J_3^-n_{-\uparrow}n_{-\downarrow}(n_{+\uparrow}+n_{+\downarrow})+J_4n_{+\uparrow}n_{+\downarrow}n_{-\uparrow}n_{-\downarrow}. \tag{4.1}$$

In view of the fact that

$$\sum_\sigma(a_{1\sigma}^\dagger a_{2\sigma}+a_{2\sigma}^\dagger a_{1\sigma})=n_{+\uparrow}+n_{+\downarrow}-n_{-\uparrow}-n_{-\downarrow} \tag{4.2}$$

the effective Hamiltonian (4.1) is diagonal in the number representation in which Z is diagonal. We are thus led, by direct computation, to the results given in table 1.

Table 1. The nine independent diagonal elements of Z and corresponding expressions for $C\exp(-\beta\mathscr{H}_{\rm cl}^{\rm eff})\exp[\beta\tilde{\mu}(n_{1\uparrow}+n_{2\uparrow}+n_{1\downarrow}+n_{2\downarrow})]$.

$n_{+\uparrow}n_{+\downarrow}n_{-\uparrow}n_{-\downarrow}$	$Z(n_{+\uparrow}n_{+\downarrow}n_{-\uparrow}n_{-\downarrow})$	$C\exp\left[\beta\tilde{\mu}\sum_{\sigma}(n_{1\sigma}+n_{2\sigma})\right]\exp[-\beta\mathscr{H}_{\rm cl}^{\rm eff}]$
1111	$z^2\,e^{-\beta(U_0+8J)}+2zK_{11}^{(2)}+M_{11}^{(4)}$	$C\exp[4\beta\tilde{\mu}-\beta(4J_2+J_e^{+}+J_e^{-}+2J_3^{+}+2J_3^{-}+J_4)]$
1110	$z^2\,e^{-\beta(U_0+6J)}+2zK_{22}^{(2)}+M_{22}^{(4)}$	$C\exp[3\beta\tilde{\mu}-\beta(-\tilde{t}+2J_2+J_e^{+}+J_3^{+})]$
1100	$z^2\,e^{-\beta(U_0+4J)}+2zK_{44}^{(2)}+M_{44}^{(4)}$	$C\exp[2\beta\tilde{\mu}-\beta(-2\tilde{t}+J_e^{+})]$
1011	$z^2K_{11}^{(1)}+z\{e^{-3\beta J}+M_{11}^{(2)}\}+L_{11}^{(2)}$	$C\exp[3\beta\tilde{\mu}-\beta(\tilde{t}+2J_2+2J_e^{-}+J_3^{-})]$
1010	$z^2K_{22}^{(1)}+z\{e^{-2\beta J}+M_{22}^{(2)}\}+L_{22}^{(2)}$	$C\exp[2\beta\tilde{\mu}-\beta J_2]$
1000	$z^2K_{44}^{(1)}+z\{e^{-\beta J}+M_{44}^{(2)}\}+L_{44}^{(2)}$	$C\exp[\beta\tilde{\mu}-\beta\tilde{t}]$
0011	$z^2M_{11}^{(1)}+2zL_{11}^{(1)}+1$	$C\exp[2\beta\tilde{\mu}-\beta(2\tilde{t}+J_e^{-})]$
0010	$z^2M_{22}^{(1)}+2zL_{22}^{(1)}+1$	$C\exp[\beta\tilde{\mu}-\beta\tilde{t}]$
0000	$z^2M_{44}^{(1)}+2zL_{44}^{(1)}+1$	C

Successive elimination of variables starting with C in table 1 gives the explicit expressions in table 2 for the parameters in (4.1), in terms of the diagonal components of the matrices K, L and M defined in (3.10)–(3.13), which in turn depend on the original parameters in $\mathscr{H}_{\rm cl}$ (2.1).

Explicit expressions for the diagonal elements of K and L are derived in appendix A and listed in table 3. Similar expressions are derived for the diagonal elements of M in appendix B for the special case $U_0=2J$. In the extreme case of infinite on-site

Table 2. Explicit expressions for the nine parameters in terms of the components of Z given in table 1.

$$C = Z(0000)$$

$$\exp(\beta\tilde{\mu}) = \frac{[Z(0010)Z(1000)]^{1/2}}{Z(0000)}$$

$$\exp(\beta\tilde{t}) = \left[\frac{Z(1000)}{Z(0010)}\right]^{1/2}$$

$$\exp(-\beta J_e^{+}) = \frac{Z(1100)Z(0000)}{[Z(1000)]^2}$$

$$\exp(-\beta J_e^{-}) = \frac{Z(0011)Z(0000)}{[Z(0010)]^2}$$

$$\exp(-\beta J_2) = \frac{Z(1010)Z(0000)}{Z(0010)Z(1000)}$$

$$\exp(-\beta J_3^{+}) = \frac{Z(1110)Z(0010)[Z(1000)]^2}{Z(0000)Z(1100)[Z(1010)]^2}$$

$$\exp(-\beta J_3^{-}) = \frac{Z(1011)Z(1000)[Z(0010)]^2}{Z(0000)Z(0011)[Z(1010)]^2}$$

$$\exp(-\beta J_4) = \frac{Z(1111)Z(1100)Z(0011)[Z(1010)]^4Z(0000)}{[Z(1000)Z(0010)Z(1110)Z(1011)]^2}$$

Table 3. Parameter values determining the diagonal elements of K and L from (A4).

Element	$-a/\beta$	$-b/\beta$
$K_{11}^{(1)}, K_{11}^{(2)}$	U_0+6J	$4J$
$K_{22}^{(1)}, K_{22}^{(2)}$ $K_{33}^{(1)}, K_{33}^{(2)}$	U_0+4J	$3J$
$K_{44}^{(1)}, K_{44}^{(2)}$	U_0+2J	$2J$
$L_{11}^{(1)}, L_{11}^{(2)}$	$2J$	0
$L_{22}^{(1)}, L_{22}^{(2)}$ $L_{33}^{(1)}, L_{33}^{(2)}$	J	0
$L_{44}^{(1)}, L_{44}^{(2)}$	0	0

repulsion ($U_0 \to \infty$), the problem, as shown in appendix C, simplifies and we are again able to obtain explicit expressions for the effective coupling parameters. In all other cases, however, we must resort to numerical methods.

Numerical results for the effective coupling parameters J_2 and $J_e^{\pm}$ are shown in figures 3 and 4 for combinations of $U_0 = 2J$, $U_0 = \infty$, $t/|J| = 1.0$ and $t/|J| = 10.0$ and as functions of the variables $x = e^{-\beta J}$ and $z = e^{\beta\mu}$. Results for intermediate values of U_0 show similar behaviour.

We note that J_2 is very similar in form to the spinless analogue derived previously and that for attractive $J(x > 1)$, J_2 becomes repulsive for large $t/|J|$. Otherwise J_2 is predominantly attractive and essentially independent of μ for the physically interesting region $\mu > 0 (z > 1)$ and $J > 0 (0 < x < 1)$.

The effective exchange couplings $J_e^{\pm}$ are comparable with $J_e^{+} \gtrsim J_e^{-}$ for small to moderate U_0, especially in the region of interest $(0 < x < 1, z > 1)$. For very large U_0 and $t/|J|$, however, $J_e^{+} \gg J_e^{-}$ for small x. Similarly, as seen in figure 4, $\frac{1}{2}(J_e^{+} + J_e^{-}) - J_2$ is small for most parameter values except for large U_0 and $t/|J|$ and small x.

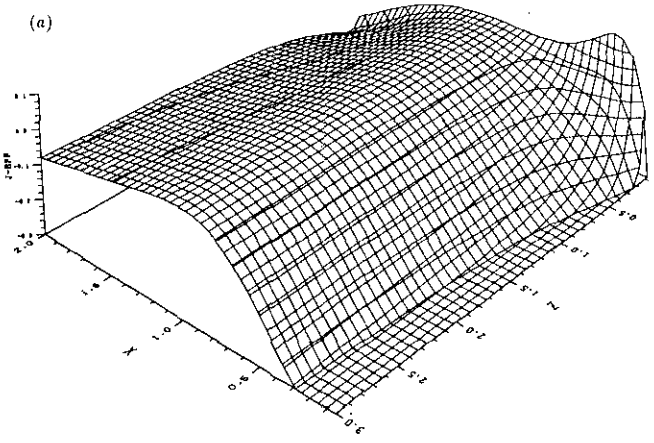

Figure 3. J_2 as a function of $x = e^{-\beta J}$ and $z = e^{\beta\mu}$ for (*a*) $U_0 = 2J$, $t = |J|$; (*b*) $U_0 = 2J$, $t = 10|J|$; (*c*) $U_0 = \infty$, $t = |J|$; and (*d*) $U_0 = \infty$, $t = 10|J|$.

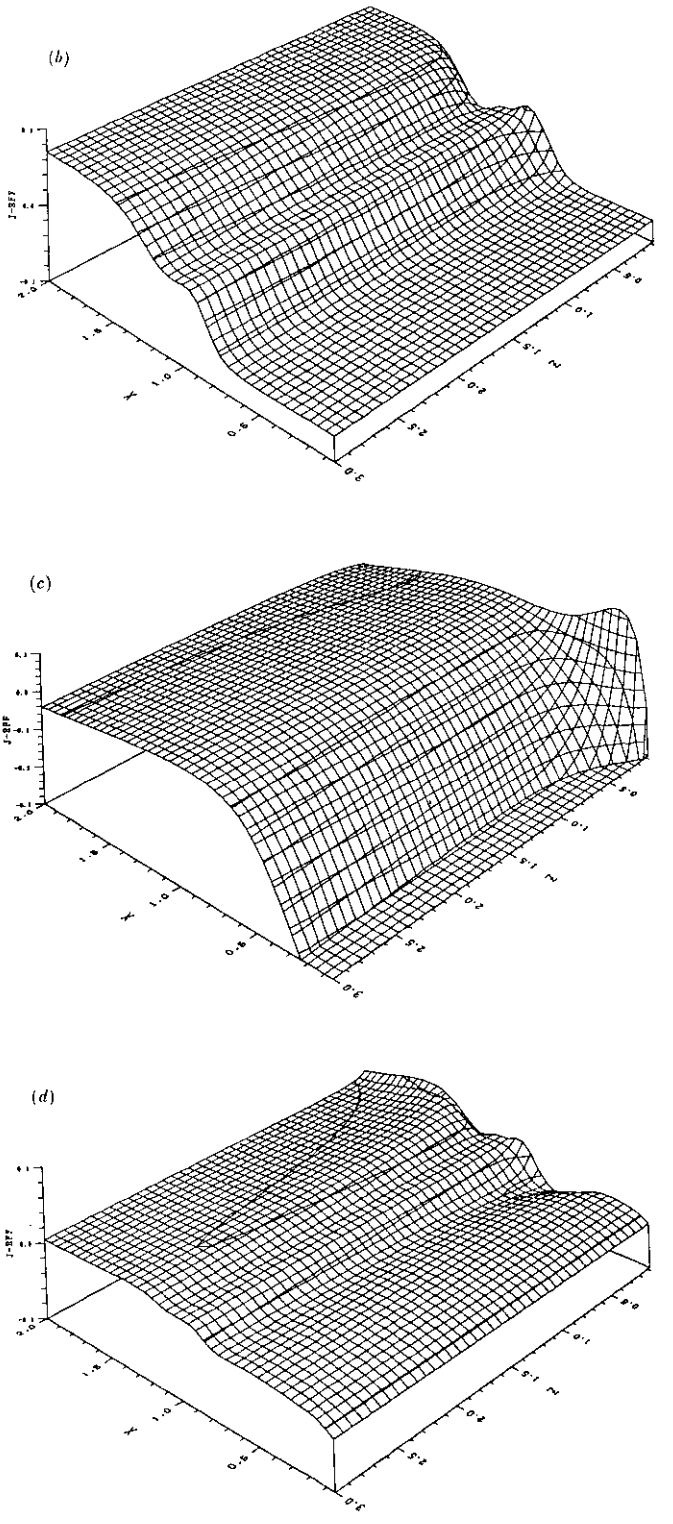

Figure 3. (continued)

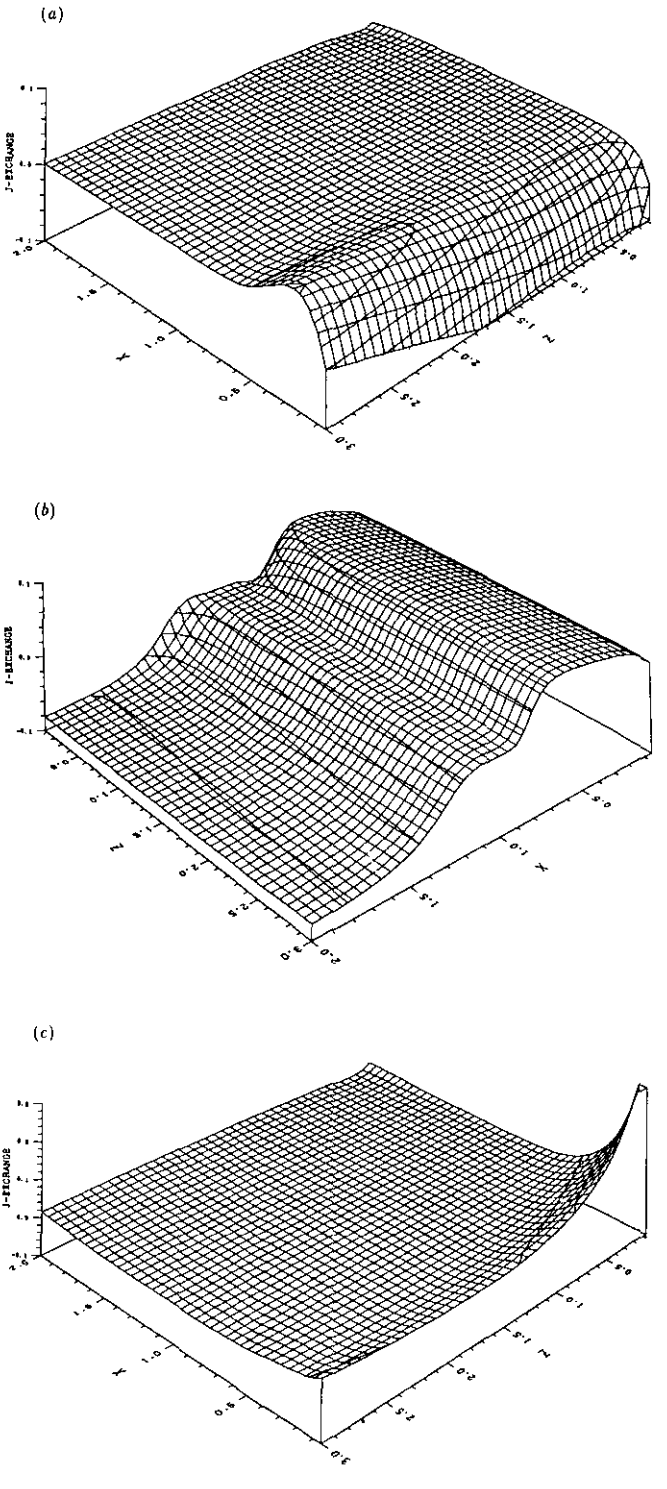

Figure 4. $\frac{1}{2}(J_2^+ + J_c^-) - J_2$ as a function of $x = e^{-\beta J}$ and $z = e^{\beta\mu}$ for (*a*) $U_0 = 2J$, $t = |J|$; (*b*) $U_0 = 2J$, $t = 10|J|$; (*c*) $U_0 = \infty$, $t = |J|$; and (*d*) $U_0 = \infty$, $t = 10|J|$.

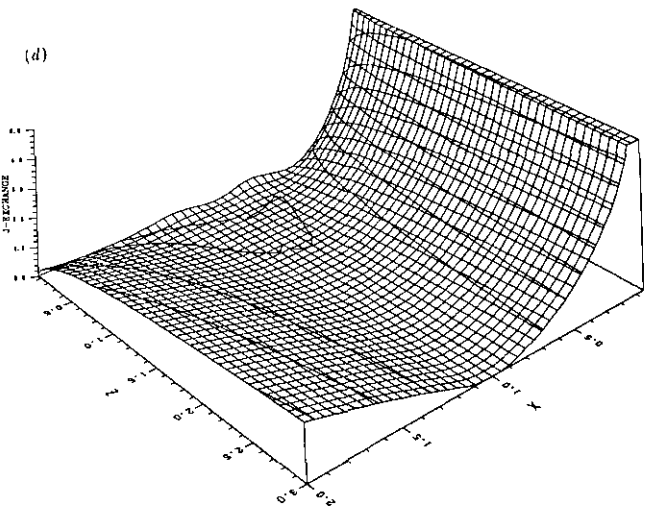

Figure 4. (continued)

Perturbation calculations given in appendix D confirm the above results and show that quantum hopping and spin effects in our QCD procedure gives rise to the usual superexchange interactions.

Further discussion of the superexchange terms and the relation between our $\mathcal{H}_{cl}^{eff}$ Hamiltonian and that of the so-called $t-J$ model is given in the following section.

5. Discussion

In this paper we have applied our quantum cluster decimation (QCD) method to a three-site extended Hubbard model for fermions with spin which includes hopping, on-site and nearest-neighbour interactions.

By taking a partial trace over state of the central site of the cluster, we derived an effective cluster Hamiltonian for the two outer sites which includes effective temperature and density dependent hopping integral, chemical potential, pair-, three- and four-particle interactions.

Of particular interest are the effective superexchange terms in (4.1):

$$J_e^+ n_{+\uparrow} n_{+\downarrow} + J_e^- n_{-\uparrow} n_{-\downarrow} = \tfrac{1}{4}(J_e^+ + J_e^-)(N_\uparrow N_\downarrow + Q_\uparrow Q_\downarrow) + \tfrac{1}{4}(J_e^+ - J_e^-)(N_\uparrow Q_\downarrow + N_\downarrow Q_\uparrow) \tag{5.1}$$

where in terms of the original number operators $n_{i\sigma}$,

$$N_\sigma = n_{1\sigma} + n_{2\sigma} \tag{5.2}$$

and

$$Q_\sigma = a_{1\sigma}^\dagger a_{2\sigma} + a_{2\sigma}^\dagger a_{1\sigma}. \tag{5.3}$$

The second term in (5.1) involving products of N_σ and Q_σ operators can be interpreted as a renormalized effective hopping term while the first term in (5.1) can be transformed into the familiar superexchange form by defining the usual spin

operators

$$\begin{aligned} S_i^x + iS_i^y &= a_{i\uparrow}^\dagger a_{i\downarrow} \\ S_i^x - iS_i^y &= a_{i\downarrow}^\dagger a_{i\uparrow} \qquad i = 1, 2 \\ S_i^z &= \tfrac{1}{2}(n_{i\uparrow} - n_{i\downarrow}) \end{aligned} \tag{5.4}$$

and noting, after some elementary manipulation, that

$$N_\uparrow N_\downarrow + Q_\uparrow Q_\downarrow = (d_1^\dagger + d_2^\dagger)(d_1 + d_2) + \tfrac{1}{2} n_1 n_2 - 2(\boldsymbol{S}_1 \cdot \boldsymbol{S}_2) \tag{5.5}$$

where

$$\begin{aligned} d_i &= a_{i\downarrow} a_{i\uparrow} \\ n_i &= n_{i\uparrow} + n_{i\downarrow} \end{aligned} \qquad i = 1, 2. \tag{5.6}$$

The first term in (5.5) represents a 'pair density' operator and the remaining terms form the familiar combination that appears in the t-J model [11] which has traditionally been derived by perturbation or canonical transformation methods.

Acknowledgments

This work has been supported in part by a Grant-in-Aid for Fundamental Science Research from the Ministry of Education, Science and Culture of Japan under Grant No 63540282. One of the authors (CT) is grateful to the Hayashi Memorial Foundation for Female Scientists for financial support.

Appendix A. Diagonal elements of the matrices K (3.10) and L (3.11)

In order to find the elements of the exponential of a symmetric 2×2 matrix

$$A = \begin{pmatrix} a & c \\ c & b \end{pmatrix} \tag{A1}$$

we diagonalize A by the orthogonal matrix S of eigenvectors of A and write

$$\exp(A) = \exp(S^{-1} D S) = S^{-1} \exp(D) S = S^{-1} \begin{pmatrix} \exp \lambda_1 & 0 \\ 0 & \exp \lambda_2 \end{pmatrix} S \tag{A2}$$

where

$$D = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \tag{A3}$$

and λ_1, λ_2 are the eigenvalues of A.

An elementary calculation then shows, in particular, that the diagonal elements of $\exp(A)$ are given by

$$\exp([a+b]/2) \left\{ \cosh(\tfrac{1}{2}\sqrt{(a-b)^2 + 4c^2}) \pm \frac{(a-b)}{\sqrt{(a-b)^2 + 4c^2}} \sinh(\tfrac{1}{2}\sqrt{(a-b)^2 + 4c^2}) \right\}. \tag{A4}$$

The diagonal elements of the block matrices K and L defined by (3.10) and (3.11) are then easily obtained from (A4) by setting a and b equal to the quantities specified in table 3, and c equal to $\sqrt{2}\beta t$.

Appendix B. Diagonal elements of the matrix M (3.12)

In order to find the diagonal elements of the matrix M defined by (3.12), we need to diagonalize a matrix of the form

$$A=\begin{pmatrix} a & c & c & 0 \\ c & b & 0 & c \\ c & 0 & b & c \\ 0 & c & c & 0 \end{pmatrix}. \tag{B1}$$

The required results then follow from straightforward generalizations of (A2) and (A4).

For the special case $a=2b$, corresponding from (3.12), (3.8c) and (3.8e) to $U_0=2J$, the eigenvalues of A are given by

$$b,\ b,\ \text{and}\ d=b\pm\sqrt{b^2+4c^2} \tag{B2}$$

and the diagonal elements of

$$M=\exp(-\beta A) \tag{B3}$$

are found by the method outlined in appendix A to be

$$\begin{aligned} M^{(1)} &= \mathrm{e}^{-\beta b}\left[\frac{2c^2}{d^2}+\left(\frac{b^2+2c^2}{d^2}\right)\cosh\beta d-\frac{b}{d}\sinh\beta d\right] \\ M^{(2)} &= M^{(3)}=\mathrm{e}^{-\beta b}\left[\tfrac{1}{2}\left(1+\frac{b^2}{d^2}\right)+\frac{2c^2}{d^2}\cosh\beta d\right] \\ M^{(4)} &= \mathrm{e}^{-\beta b}\left[\frac{2c^2}{d^2}+\left(\frac{d^2+b^2}{2d^2}\right)\cosh\beta d+\frac{b}{d}\sinh\beta d\right]. \end{aligned} \tag{B4}$$

In (3.12), the $M^{(i)}$ are block matrices with diagonal elements, from (3.8c) and (3.8e) given by (B4) with $b=3J$ for $M^{(i)}_{11}$, $b=2J$ for $M^{(i)}_{22}=M^{(i)}_{33}$ and $b=J$ for $M^{(i)}_{44}$ with i respectively 1, 2 and 4 in (B4) and $c=-\sqrt{2}t$.

For $U_0\neq 2J$, one must resort to numerical methods to evaluate the required matrix elements in (3.12). The limit $U_0\to\infty$, however, affords another special case which can, as shown in appendix C, be treated analytically.

Appendix C. The strong-coupling limit $U_0\to\infty$

In the strong-coupling limit ($U_0\to\infty$), double occupancy of the central site of the cluster by particles of either spin is prohibited. This means that in the number representation, all of the elements of $\mathscr{H}_{\mathrm{cl}}$ associated with the (11) component of $(n_\uparrow n_\downarrow)$, corresponding to the first 16 rows and columns of (3.9), can be discarded, leaving the lower 48×48 matrix representation for $\mathscr{H}_{\mathrm{cl}}$.

The matrix K defined in (3.10) is now irrelevant, L defined in (3.11) remains relevant and (3.12) is replaced by the evaluation of the exponential matrix $\tilde{M}$ defined

by

$$\exp\left[-\beta\begin{pmatrix} \boldsymbol{D}_4 & \boldsymbol{O}_4 & \boldsymbol{T} \\ \boldsymbol{O}_4 & \boldsymbol{D}_4 & \boldsymbol{T} \\ \boldsymbol{T} & \boldsymbol{T} & \boldsymbol{O}_4 \end{pmatrix}\right] \equiv \tilde{M} = \begin{pmatrix} \tilde{M}^{(1)} & \tilde{M}_{12} & \tilde{M}_{13} \\ \tilde{M}_{21} & \tilde{M}^{(1)} & \tilde{M}_{23} \\ \tilde{M}_{31} & \tilde{M}_{32} & \tilde{M}^{(3)} \end{pmatrix}. \tag{C1}$$

Similar reductions occur in (3.13) and (3.16) with the nine independent diagonal elements of Z in table 1 replaced by

$$\begin{aligned} Z(1111) &= 2z\,\mathrm{e}^{-4\beta J} + \tilde{M}_{11}^{(3)} \\ Z(1110) &= 2z\,\mathrm{e}^{-3\beta J} + \tilde{M}_{22}^{(3)} \\ Z(1100) &= 2z\,\mathrm{e}^{-2\beta J} + \tilde{M}_{44}^{(3)} \\ Z(1011) &= z(\mathrm{e}^{-3\beta J} + \tilde{M}_{11}^{(1)}) + L_{11}^{(2)} \\ Z(1010) &= z(\mathrm{e}^{-2\beta J} + \tilde{M}_{22}^{(1)}) + L_{22}^{(2)} \\ Z(1000) &= z(\mathrm{e}^{-\beta J} + \tilde{M}_{44}^{(1)}) + L_{44}^{(2)} \\ Z(0011) &= 2zL_{11}^{(1)} + 1 \\ Z(0010) &= 2zL_{22}^{(1)} + 1 \\ Z(0000) &= 2zL_{44}^{(1)} + 1. \end{aligned} \tag{C2}$$

In order to evaluate the diagonal elements of $\tilde{M}$, we first note that the eigenvalues of the matrix

$$A = \begin{pmatrix} b & 0 & c \\ 0 & b & c \\ c & c & 0 \end{pmatrix} \tag{C3}$$

are given by

$$b, \tfrac{1}{2}(b \pm \sqrt{b^2 + 8c^2}) \equiv \tfrac{1}{2}(b \pm d). \tag{C4}$$

Repeating the arguments in appendices A and B then shows that the diagonal elements of

$$\tilde{M} = \exp(-\beta A) \tag{C5}$$

are given by

$$\begin{aligned} \tilde{M}^{(1)} = \tilde{M}^{(2)} &= \frac{1}{2}\left\{\mathrm{e}^{-\beta b} + \mathrm{e}^{-\beta b/2}\left[\cosh(\beta d/2) - \frac{b}{d}\sinh(\beta d/2)\right]\right\} \\ \tilde{M}^{(3)} &= \mathrm{e}^{-\beta b/2}\left[\cosh(\beta d/2) + \frac{b}{d}\sinh(\beta d/2)\right]. \end{aligned} \tag{C6}$$

In (C1) the $\tilde{M}^{(i)}$ are again block diagonal matrices with elements from (3.8e) given by (C6) with $b = 3J$ for $\tilde{M}_{11}^{(i)}$, $b = 2J$ for $\tilde{M}_{22}^{(i)} = \tilde{M}_{33}^{(i)}$ and $b = J$ for $\tilde{M}_{44}^{(i)}$ with i respectively 1 and 3 and $c = -\sqrt{2}t$.

Appendix D. Perturbation expansions for K, L and M for small t

Using the well known formula

$$\exp[-\beta(\mathscr{H}_0+\mathscr{H}_1)] = \exp(-\beta\mathscr{H}_0)\left[1-\int_0^\beta \mathscr{H}_1(s)\,ds+\int_0^\beta\int_0^s \mathscr{H}_1(s)\mathscr{H}_1(s')\,ds'\,ds\ldots\right] \tag{D1}$$

where

$$\mathscr{H}_1(s)=\exp(s\mathscr{H}_0)\mathscr{H}_1\exp(-s\mathscr{H}_0) \tag{D2}$$

the matrix K defined by (3.10) can be written as

$$K=\begin{pmatrix} e^{-\beta D_1} & 0 \\ 0 & e^{-\beta D_3}\end{pmatrix}+\frac{T^2}{(D_1-D_3)^2} \times\begin{pmatrix} e^{-\beta D_3}-e^{-\beta D_1}\{1+\beta(D_1-D_3)\} & 0 \\ 0 & e^{-\beta D_1}-e^{-\beta D_3}\{1+\beta(D_3-D_1)\}\end{pmatrix} +\ldots \tag{D3}$$

from which one easily obtains

$$K_{11}^{(1)}=e^{-\beta(U_0+6J)}+\frac{2t^2}{(U_0+2J)^2}\{e^{-4\beta J}-e^{-\beta(U_0+6J)}[1+\beta(U_0+2J)]\}+\ldots \tag{D4}$$

with similar expressions for the remaining diagonal elements.

Similarly from (3.11) and (3.12), and (D1), we have

$$L^{(1)}=e^{-\beta D_5}+\frac{T^2}{D_5^2}[1-e^{-\beta D_5}(1+\beta D_5)]+\ldots$$

$$L^{(2)}=I+\frac{T^2}{D_5^2}[e^{-\beta D_5}-(1-\beta D_5)]+\ldots$$

$$M^{(1)}=e^{-\beta D_2}+\frac{2T^2}{(D_2-D_4)^2}[e^{-\beta D_4}-e^{-\beta D_2}\{1+\beta(D_2-D_4)\}]+\ldots \tag{D5}$$

$$M^{(2)}=e^{-\beta D_4}+\frac{T^2}{(D_2-D_4)^2}[e^{-\beta D_2}-e^{-\beta D_4}\{1-\beta(D_2-D_4)\}] +\frac{T^2}{D_4^2}\{1-e^{-\beta D_4}(1+\beta D_4)\}+\ldots=M^{(3)}$$

$$M^{(4)}=I+\frac{2T^2}{D_4^2}[e^{-\beta D_4}-\{1-\beta D_4\}]+\ldots$$

from which perturbation expansions for the diagonal elements of L and M easily

follow. For example,

$$L_{11}^{(1)} = e^{-2\beta J} + \frac{2t^2}{(2J)^2}[1 - e^{-2\beta J}\{1 + 2\beta J\}] + \ldots$$

$$M_{11}^{(1)} = e^{-\beta(U_0+4J)} + \frac{4t^2}{(U_0+J)^2}[e^{-3\beta J} - e^{-\beta(U_0+4J)}\{1 + \beta(U_0+J)\}] + \ldots$$

and so forth.

References

[1] Onsager L 1944 *Phys. Rev.* **65** 117
[2] Syozi I 1951 *Prog. Theor. Phys.* **6** 306
[3] Syozi I 1972 *Phase Transitions and Critical Phenomena* vol 1 ed C Domb and M S Green (New York: Academic)
[4] Wilson K G 1975 *Rev. Mod. Phys.* **47** 773
[5] Baxter R J 1982 *Exactly Solved Models in Statistical Mechanics* (London: Academic)
[6] Barber M N and Pearce P A (eds) 1990 *Yang–Baxter Equations, Conformal Invariance and Integrability in Statistical Mechanics and Field Theory* (Singapore: World Scientific)
[7] Emery V J 1987 *Phys. Rev. Lett.* **58** 2794
[8] Thompson C J and Matsubara T 1991 A Unified Statistical Mechanical Approach to High-Temperature Superconductivity *Studies in High-Temperature Superconductors* vol 7 ed A V Narlikar (New York: Nova Science Publishers)
[9] Emery V J 1976 *Phys. Rev.* B **14** 2989
[10] MacDonald A H, Girvin S M and Yoshioka D 1988 *Phys. Rev.* B **37** 9735; 1990 *Phys. Rev.* B **41** 2565 Oles A M 1990 *Phys. Rev.* B **41** 2562
[11] Hirsch J E 1985 *Phys. Rev. Lett.* **54** 1317