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Exact solution of the extended Falicov–Kimball model in the limit of zero conduction band width

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Abstract. A method for solving exactly the Falicov–Kimball model in the limit of vanishing conduction band is proposed. By means of the path integral formalism, a general procedure for the evaluation of the exact n-point Green functions at a finite temperature is developed. The results obtained here represent a starting point for a perturbation expansion in the conduction electron band width.

1. Introduction

The electronic properties of rare-earth and transition-metal compounds have been intensively studied for a long time. When the external conditions (temperature, pressure, composition) are varied, compounds of this type often undergo phase transitions involving variation in the filling of the electron levels. In most cases, these transitions are of the insulator-to-metal or semiconductor-to-metal type. Also there is often a change in magnetic properties due to the vanishing of localised magnetic moments, so that these transitions can be of the magnetic-to-non-magnetic state type.

One of the most striking examples of such a behaviour is provided by the samarium chalcogenides. The compound SmS is a semiconductor which exhibits a sharp transition (first order) to a metallic state when the pressure is raised to 6.5 kbar [1]. On the contrary, in the compounds SmSe and SmTe, which at normal pressure have crystal structures and electric and magnetic properties very similar to those of SmS, the same kind of transition takes place continuously (second-order transition) over a broad pressure range from 0 to 50–60 kbar [2].

Several theoretical models start from the idea that these phenomena are due to the delocalisation of f electrons into d-conduction band states. Among them, the model proposed by Falicov and Kimball (FK) [3] provides a natural interpretation of the above-mentioned transitions. In order to explain also the existence in rare-earth compounds of non-integral valence states, an extended FK (EFK) model has subsequently been introduced [4], including the possibility of hybridisation between localised and itinerant states.

In the EFK model the Hamiltonian is given by the periodic Anderson [5] Hamiltonian with an extra term corresponding to the Coulomb interaction between localised and conduction electrons. This term is known to be responsible for an abrupt transition

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between two valence states and then it is crucial in the explanation of the behaviour of those compounds which exhibit first-order metal-to-insulator transitions [6].

Since an exact determination of eigenfunctions and eigenvalues of this Hamiltonian presents insurmountable difficulties, many approximate theoretical approaches have been proposed in order to provide a qualitative understanding of the model, at least for special ranges of values of the parameters involved. Among them, we recall, for example, approaches which treat the hybridisation perturbatively [6], mean-field theories based on the Hartree–Fock approximation [4, 7], and theories exploiting the so-called alloy analogue approximation [8].

In this paper, by making use of the path integral method developed in [9], we shall derive an exact solution of the EFK model in the limit of zero-width conduction band. In a future paper, we shall introduce perturbatively the kinetic term for the conduction electrons.

This approach is motivated by the fact that many interesting features of the model seem to be related to a simultaneous non-perturbative treatment of the on-site Coulomb interaction between localised electrons and between localised and conduction electrons and the hybridisation between conduction band and localised electron states.

We wish to stress that the limit of infinitely narrow conduction band width does not affect the metal-to-insulator transition, as pointed out for example in [5]. Also, in the approximate form the model still retains the essential features of the mixed valence properties of some real systems [10], and for a special range of values of the parameters involved it is equivalent to the narrow-band version of the Kondo Hamiltonian [11].

2. The model

Let us consider the EFK model for zero-width conduction band:

$$H = H_{\mathrm{FK}} + H_{\mathrm{A}} \tag{1}$$

where

$$H_{\mathrm{FK}} = G(f^{\dagger}f)(c^{\dagger}c)$$

is the so-called FK term,

$$H_{\mathrm{A}} = \varepsilon f^{\dagger}f + V(f^{\dagger}c + c^{\dagger}f) + Uf^{\dagger}_{\uparrow}f_{\uparrow}f^{\dagger}_{\downarrow}f_{\downarrow} \tag{2}$$

is the Anderson Hamiltonian where the kinetic energy of conduction electrons is put equal to zero and

$$f = \begin{pmatrix} f_{\uparrow} \\ f_{\downarrow} \end{pmatrix} \qquad c = \begin{pmatrix} c_{\uparrow} \\ c_{\downarrow} \end{pmatrix}.$$

Here $c_s^{\dagger}$, c_s ($f_s^{\dagger}$, f_s) are the creation and annihilation operators for conduction (localised) electrons with spin s; ε is the f-electron energy; V and U are the hybridisation and the on-site Coulomb repulsion energies, respectively.

Since different sites are decoupled, it is sufficient to consider one-impurity case. The model has finite degrees of freedom and can be solved completely in terms of 16×16 matrices by diagonalising the Hamiltonian (1).

Indeed, noting that the total number of particles

$$N = f^{\dagger}f + c^{\dagger}c$$

Table 1. Eigenstates of H.

Eigenstate	Energy	Number of electrons	Total spin
$\|0\rangle$	$E_{16} = 0$	0	0
$\|f_s\rangle \equiv \cos\varphi\, f_s^\dagger \|0\rangle + \sin\varphi\, c_s^\dagger \|0\rangle$	$E_{14} = E_{15} = \frac{1}{2}(\varepsilon - \Delta_2)$	1	$\pm\frac{1}{2}$
$\|c_s\rangle \equiv -\sin\varphi\, f_s^\dagger \|0\rangle + \cos\varphi\, c_s^\dagger \|0\rangle$	$E_8 = E_{12} = \frac{1}{2}(\varepsilon + \Delta_2)$	1	$\pm\frac{1}{2}$
$\|S_s\rangle \equiv f_s^\dagger c_s^\dagger \|0\rangle$	$E_6 = E_{11} = \varepsilon + G$	2	± 1
$\|S_0\rangle \equiv (2)^{-1/2}(f_\uparrow^\dagger c_\downarrow^\dagger + f_\downarrow^\dagger c_\uparrow^\dagger)\|0\rangle$	$E_4 = \varepsilon + G$	2	0
$\|T_-\rangle \equiv [x_7 f_\uparrow^\dagger f_\downarrow^\dagger + z_7 c_\uparrow^\dagger c_\downarrow^\dagger - y_7(f_\uparrow^\dagger c_\downarrow^\dagger - f_\downarrow^\dagger c_\uparrow^\dagger)]\|0\rangle$	$E_7 = z_1$	2	0
$\|T_0\rangle \equiv [x_{10} f_\uparrow^\dagger f_\downarrow^\dagger + z_{10} c_\uparrow^\dagger c_\downarrow^\dagger - y_{10}(f_\uparrow^\dagger c_\downarrow^\dagger - f_\downarrow^\dagger c_\uparrow^\dagger)]\|0\rangle$	$E_{10} = z_2$	2	0
$\|T_-\rangle \equiv [x_{13} f_\uparrow^\dagger f_\downarrow^\dagger + z_{13} c_\uparrow^\dagger c_\downarrow^\dagger - y_{13}(f_\uparrow^\dagger c_\downarrow^\dagger - f_\downarrow^\dagger c_\uparrow^\dagger)]\|0\rangle$	$E_{13} = z_3$	2	0
$\|F_s\rangle \equiv [\cos\theta f_s^\dagger c_s^\dagger f_{-s}^\dagger + \sin\theta f_s^\dagger c_s^\dagger c_{-s}^\dagger]\|0\rangle$	$E_5 = E_9 = \frac{1}{2}[(3\varepsilon + U + \Delta_1) + 4G]$	3	$\pm\frac{1}{2}$
$\|C_s\rangle \equiv [-\sin\theta f_s^\dagger c_s^\dagger f_{-s}^\dagger + \cos\theta f_s^\dagger c_s^\dagger c_{-s}^\dagger]\|0\rangle$	$E_2 = E_3 = \frac{1}{2}[(3\varepsilon + U - \Delta_1) + 4G]$	3	$\pm\frac{1}{2}$
$\|FC\rangle \equiv f_\uparrow^\dagger c_\uparrow^\dagger f_\downarrow^\dagger c_\downarrow^\dagger \|0\rangle$	$E_1 = 2\varepsilon + U + 4G$	4	0

$\Delta_1 = [(\varepsilon + U)^2 + 4V^2]^{1/2}$, $\Delta_2 = (\varepsilon^2 + 4V^2)^{1/2}$, and x_a, y_a, z_a ($a = 7, 10, 13$) are given by equations (11).

and the total spin

$$\boldsymbol{S} = f^\dagger(\boldsymbol{\sigma}/2)f + c^\dagger(\boldsymbol{\sigma}/2)c$$

are conserved quantities, the eigenstates of H can be classified as shown in table 1. The quantities z_1, z_2, z_3 appearing there are the solutions of the equation

$$z^3 - (3\varepsilon + G + U)z^2 + [(2\varepsilon + U)(\varepsilon + G) - 4V^2]z + 2V^2(2\varepsilon + U) = 0. \tag{3}$$

Knowledge of the energy levels allows us to determine the partition function and then all the thermodynamics quantities can be easily computed. Also, the thermal Green functions can be calculated by the standard method implying the computation of eight 16×16 matrices. In this paper, we present a solution of the model in more compact form by using the path integral formalism and we give the explicit expression for the two-point Green function for localised electrons. Let us consider the generating functional for temperature Green functions:

$$Z[J, K] = \mathrm{Tr}\left[\exp(-\beta H)\, T \exp\left(\int_0^\beta \mathrm{d}\tau\, [J^\dagger(\tau)f(\tau) + f^\dagger(\tau)J(\tau) + c^\dagger(\tau)K(\tau) + K^\dagger(\tau)c(\tau)]\right)\right].$$

Here T orders the operators according to their value of τ, with the smallest at right, and

$$J = \begin{pmatrix} J_\uparrow \\ J_\downarrow \end{pmatrix} \qquad K = \begin{pmatrix} K_\uparrow \\ K_\downarrow \end{pmatrix}$$

are the sources associated with f and c, respectively.

If we divide the interval $0 \leqslant \tau \leqslant \beta$ into N parts, it is possible to show that $Z[J, K]$ can

be written as

$$Z[J,K] = \lim_{N\to\infty} (Z^{(N)}[J,K]) \tag{4}$$

where

$$Z^{(N)}[J,K] = \exp\left(\sum_{k=1}^{N} \frac{\partial}{\partial J_k}\frac{\partial}{\partial J^*_{k+1}} + \frac{\partial}{\partial K_k}\frac{\partial}{\partial K^*_{k+1}}\right)$$
$$\times \exp\left(\sum_{m=1}^{N} \frac{\beta V}{N}\frac{\partial}{\partial J_m}\frac{\partial}{\partial K^*_m} + \frac{\partial}{\partial K_m}\frac{\partial}{\partial J^*_m}\right)$$
$$\times \exp\left(-\sum_{i=1}^{N} \frac{\beta G}{N}\frac{\partial}{\partial J_i}\frac{\partial}{\partial J^*_i}\frac{\partial}{\partial K_i}\frac{\partial}{\partial K^*_i}\right) \Omega^N \prod_{j=1}^{N} Z_s^{(N)}[J_j, K_j] \tag{5}$$

with

$$\Omega = (1-\beta\varepsilon/N)^2 - \beta U/N$$
$$J_j \equiv J(\tau_j) \qquad K_j \equiv K(\tau_j) \qquad (\tau_j = j\beta/N)$$

and

$$Z_s^{(N)}[J,K] = (1+K^\dagger_\uparrow K_\uparrow)(1+K^\dagger_\downarrow K_\downarrow)[1+\Omega^{-1}(1-\beta\varepsilon/N)(J_\uparrow J^*_\uparrow + J_\downarrow J^*_\downarrow)$$
$$+ \Omega^{-1} J_\uparrow J_\uparrow J^*_\downarrow J^*_\downarrow].$$

In writing equation (5), we have assumed that

$$\partial/\partial J^*_{N+1} = -\partial/\partial J^*_1 \qquad \partial/\partial K^*_{N+1} = -\partial/\partial K^*_1 .$$

Following the same procedure outlined in [9], we can rewrite $Z^{(N)}[J,K]$ in the form

$$Z^{(N)}[J,K] = \Omega^N \prod_{i=1}^{N} F^i \Gamma^i \Delta^{i,i+1} \hat{\Delta}^{i,i+1} \prod_{j=1}^{N} R^j \hat{R}^j \tag{6}$$

where

$$F^j = [1-(\beta G/N)(\partial/\partial J_{\uparrow j})(\partial/\partial J^*_{\uparrow j})(\partial/\partial K_{\uparrow j})(\partial/\partial K^*_{\uparrow j})]$$
$$\times [1-(\beta G/N)(\partial/\partial J_{\downarrow j})(\partial/\partial J^*_{\downarrow j})(\partial/\partial K_{\downarrow j})(\partial/\partial K^*_{\downarrow j})]$$
$$\Gamma^j = [1+(\beta V/N)(\partial/\partial J_{\uparrow j})(\partial/\partial K^*_{\uparrow j})][1+(\beta V/N)(\partial/\partial J_{\downarrow j})(\partial/\partial K^*_{\downarrow j})]$$
$$\times [1+(\beta V/N)(\partial/\partial J^*_{\uparrow j})(\partial/\partial K_{\uparrow j})][1+(\beta V/N)(\partial/\partial J^*_{\downarrow j})(\partial/\partial K_{\downarrow j})]$$
$$\Delta^{j,j+1} = [1+(\partial/\partial J_{\uparrow j})(\partial/\partial J^*_{\uparrow j+1})][1+(\partial/\partial J_{\downarrow j})(\partial/\partial J^*_{\downarrow i+1})]$$
$$\hat{\Delta}^{j,j+1} = [1+(\partial/\partial K_{\uparrow j})(\partial/\partial K^*_{\uparrow j+1})][1+(\partial/\partial K_{\downarrow j})(\partial/\partial K^*_{\downarrow j+1})]$$
$$R^j = 1+[(1-\beta\varepsilon/N)/\Omega](J_{\uparrow j}J^*_{\uparrow j} + J_{\downarrow j}J^*_{\downarrow j}) + (J_{\uparrow j}J^*_{\uparrow j}J_{\downarrow j}J^*_{\downarrow j})/\Omega$$
$$\hat{R}^j = (1+K_{\uparrow j}K^*_{\uparrow j})(1+K_{\downarrow j}K^*_{\downarrow j}).$$

After some algebra it can be shown that equation (6) leads to

$$Z^{(N)}[J,K] = \Omega^N \operatorname{Tr}(\mathbf{S}^1\mathbf{S}^2 \ldots \mathbf{S}^N) \tag{7}$$

where the 16×16 matrices $\mathbf{S}^j[J,K]$ are given by

$$\mathbf{S}^j[J,K] = F^j \mathbf{M}^j[J,K]$$

the matrices $\mathbf{M}^j[j, K]$ being defined as in [9]. In the limit $J = K = 0$ the matrices $\mathbf{M}^j$ and $\mathbf{S}^j$ do not depend on j and the only elements of $\mathbf{S}$ different from the corresponding ones in $\mathbf{M}$ are

$$S_{11} = M_{11} - 4ag + 2g^2b$$
$$S_{kk} = M_{kk} - ag \qquad k = 2, 3$$
$$S_{kk} = M_{kk} - bg \qquad k = 5, 6, 7, 9, 10, 11$$
$$S_{25} = S_{52} = M_{25} - bgu$$
$$S_{39} = S_{93} = M_{39} - bgu$$

with

$$g = \beta G/N \qquad u = \beta V/N \qquad a = (1 - \beta\varepsilon/N)/\Omega \qquad b = 1/\Omega.$$

The non-vanishing elements of the matrix $\mathbf{M}[0, 0]$ are reported in the Appendix.

Let us define

$$\mathbf{O} = \mathbf{PS}[0, 0]\mathbf{P}^{-1}$$

where the matrix $\mathbf{P}$ is such that $\mathbf{O}$ is diagonal. From equation (7), we have

$$Z^{[N]}[0, 0] = \Omega^N \operatorname{Tr}\{(\mathbf{S}[0, 0])^N\} = \Omega^N \sum_{a=1}^{16} [O_{aa}]^N \tag{8}$$

so that, once the diagonalisation of $\mathbf{S}[0, 0]$ is performed, the partition function $Z[0, 0]$ is derived from equation (4).

Since $\mathbf{S}[0, 0]$ is real and symmetric, the eigenvalues $O_{aa} \equiv O^a$ are real and the 16×16 matrix $\mathbf{P}$ is orthogonal. Referring to the eigenvalues N^a of $\mathbf{M}[0, 0]$, which we report in the appendix A2, we have

$$O^a = N^a \qquad a = 1, 6, 8, 11, 12, 14, 15, 16$$
$$O^4 = a - bg - u^2b$$
$$O^2 = O^3 = \{(S_{22} + S_{55}) + [(S_{22} - S_{55})^2 + 4S_{25}^2]^{1/2}\}/2$$
$$O^5 = O^9 = \{(S_{22} + S_{55}) - [(S_{22} - S_{55})^2 + 4S_{25}^2]^{1/2}\}/2$$

while O^7, O^{10}, O^{13} are the roots of the cubic equation

$$\begin{vmatrix} 1 - x & -2ua & u^2b \\ -ua & a - bg + u^2b - x & -ub \\ u^2b & -2ub & b - x \end{vmatrix} = 0.$$

In the limit $N \to \infty$, we can show that the solutions of this equation take the form

$$O^a = 1 + (\beta/N)(2\varepsilon + U - E_a) + O(N^{-2})$$

where the energies E_a coincide with the roots of equation (3).

The above results allow us to calculate the partition function from equation (8). We have

$$Z[0, 0] = \lim_{N \to \infty} (Z^{(N)}[0, 0]) = \sum_{a=1}^{16} \exp(-\beta E_a)$$

where the energies E_a are given in table 1.

We now pass to the evaluation of the matrix **P**, which can be shown to have the following non-vanishing elements:

$$\begin{aligned}
&P_{11} = P_{66} = P_{11,11} = P_{16,16} = 1\\
&P_{22} = P_{33} = P_{55} = P_{99} = \cos\gamma\\
&P_{25} = P_{39} = -P_{52} = -P_{93} = \sin\gamma\\
&P_{88} = P_{12,12} = P_{14,14} = P_{15,15} = \cos\varphi\\
&P_{8,14} = P_{12,15} = -P_{14,8} = -P_{15,12} = \sin\varphi\\
&P_{47} = P_{4,10} = (\tfrac{1}{2})^{1/2}\\
&P_{a4} = x_a \qquad P_{a7} = y_a \qquad P_{a,10} = -y_a \qquad P_{a,13} = z_a
\end{aligned} \tag{9}$$

where

$$\begin{aligned}
&\sin\gamma = [\![\{1-(S_{22}-S_{55})/[(S_{22}-S_{55})^2+4S_{25}^2]^{1/2}\}/2]\!]^{1/2}\\
&\sin\varphi = -[\![\{1-(S_{88}-S_{14,14})/[(S_{88}-S_{14,14})^2+4S_{8,14}^2]^{1/2}\}/2]\!]^{1/2}
\end{aligned} \tag{10}$$

and the quantities x_a, y_a, z_a ($a = 7, 10, 13$) are determined by the following equations:

$$\begin{aligned}
&(1-O^a)x_a + 2uay_a + u^2bz_a = 0\\
&uax_a + (a - bg + u^2b + O^a)y_a + ubz_a = 0\\
&u^2bx_a + 2uby_a + (b - O^a)z_a = 0
\end{aligned}$$

together with the orthogonality condition

$$x_ax_b + 2y_ay_b + z_az_b = \delta_{ab}.$$

In the limit $N \to \infty$ the solutions of this system take the form

$$\begin{aligned}
&(x_a)^2 = 4V^2E_a^2/D\\
&(y_a)^2 = E_a^2(2\varepsilon + U - E_a)^2/D\\
&(z_a)^2 = 4V^2(2\varepsilon + U - E_a)^2/D
\end{aligned} \tag{11}$$

where

$$D = 4V^2E_a^2 + 2(2V^2 + E_a^2)(2\varepsilon + U - E_a)^2$$

and the energies E_a are again the roots of equation (3). Furthermore, we have

$$\begin{aligned}
&\lim_{N\to\infty}(\sin\gamma) = [(\Delta_1 + \varepsilon + U)/2\Delta_1]^{1/2}\\
&\lim_{N\to\infty}(\sin\varphi) = -[(\Delta_2 + \varepsilon)/2\Delta_2]^{1/2}
\end{aligned} \tag{12}$$

where Δ_1 and Δ_2 are given by equations (10).

Knowledge of **P** allows us to evaluate the thermal n-point Green functions. In order to show this, we recall that their analytic expressions can be derived from the relation [9]

$$\begin{aligned}
&\langle\Psi_{m_n}(\tau_n)\Psi_{m_{n-1}}(\tau_{n-1})\ldots\Psi_{m_1}(\tau_1)\rangle\\
&\quad = \mathrm{Tr}[\exp(-\beta H)\,\Psi_{m_n}(\tau_n)\Psi_{m_{n-1}}(\tau_{n-1})\ldots\Psi_{m_1}(\tau_1)\\
&\quad = Z[0,0]^{-1}\exp[-\beta(2\varepsilon + U)]\\
&\qquad \times \mathrm{Tr}[\mathbf{X}^{m_1}(\tau_1 - \tau_n + \beta)\ldots\mathbf{X}^{m_{n-1}}(\tau_{n-1} - \tau_{n-2})\mathbf{X}^{m_n}(\tau_n - \tau_{n-1})]
\end{aligned} \tag{13}$$

where we have defined

$$\Psi_1(\tau) = f_\uparrow(\tau) \qquad \Psi_5(\tau) = c_\uparrow(\tau)$$
$$\Psi_2(\tau) = f_\uparrow^\dagger(\tau) \qquad \Psi_6(\tau) = c_\uparrow^\dagger(\tau)$$
$$\Psi_3(\tau) = f_\downarrow(\tau) \qquad \Psi_7(\tau) = c_\downarrow(\tau)$$
$$\Psi_4(\tau) = f_\downarrow^\dagger(\tau) \qquad \Psi_8(\tau) = c_\downarrow^\dagger(\tau)$$

and $\tau_k < \tau_{k+1} (k = 1, \ldots, n-1)$. The symbol $\mathbf{X}^l(\tau)$ denotes a 16×16 matrix whose elements are

$$X^l(\tau)_{nm} = \lim_{N\to\infty} \left[\sum_k A_{nk} \left(\frac{N\tau}{\beta} \right) B^l_{km} \right] \tag{14}$$

with

$$A(N\tau/\beta) = (\mathbf{S}[0,0])^{N\tau/\beta} \qquad B^l_{km} = (-)^{l+1} \partial \mathbf{S}[J,K]_{km} / \partial x_l |_{J=K=0}.$$

The quantities x_l are defined as

$$x_1 = J_\uparrow^* \qquad x_5 = K_\uparrow^*$$
$$x_2 = J_\uparrow \qquad x_6 = K_\uparrow$$
$$x_3 = J_\downarrow^* \qquad x_7 = J_\downarrow^*$$
$$x_4 = J_\downarrow \qquad x_8 = K_\downarrow .$$

It is easy to show that

$$\lim_{N\to\infty} (\mathbf{S}[0,0]^{N\tau/\beta})_{lk} = \sum_{m=1}^{16} \tilde{P}_{ml} \tilde{P}_{mk} \lim_{N\to\infty} [(\mathrm{O}^m)^{N\tau/\beta}]$$
$$= \exp[\tau(2\varepsilon + U)] \sum_{m=1}^{16} \tilde{P}_{ml} \tilde{P}_{mk} \exp(-\tau E_m) \tag{15}$$

where the energies E_m are given in table 1 and the elements of the matrix $\tilde{\mathbf{P}} = \lim_{N\to\infty} \mathbf{P}$ can be readily obtained from equations (9) and (12).

Also, the only non-vanishing elements of the matrices $\tilde{\mathbf{B}}^l = \lim_{N\to\infty} \mathbf{B}^l$ are

$$\begin{aligned}
&\tilde{B}^1_{15} = \tilde{B}^1_{28} = \tilde{B}^1_{37} = \tilde{B}^1_{48} = \tilde{B}^6_{9,13} = \tilde{B}^1_{10,14} = \tilde{B}^1_{11,15} \\
&\qquad = \tilde{B}^1_{12,16} = 1 \\
&\tilde{B}^3_{19} = \tilde{B}^3_{2,10} = \tilde{B}^3_{3,11} = \tilde{B}^3_{4,12} = -\tilde{B}^3_{5,13} = -\tilde{B}^3_{6,14} \\
&\qquad = -\tilde{B}^3_{7,15} = -\tilde{B}^3_{8,16} = 1 \\
&\tilde{B}^5_{12} = \tilde{B}^5_{34} = -\tilde{B}^5_{56} = -\tilde{B}^5_{78} = -\tilde{B}^5_{9,10} = -\tilde{B}^5_{11,12} \\
&\qquad = \tilde{B}^5_{13,14} = \tilde{B}^5_{15,16} = 1 \\
&\tilde{B}^7_{13} = -\tilde{B}^7_{24} = -\tilde{B}^7_{57} = \tilde{B}^7_{68} = -\tilde{B}^7_{8,11} = \tilde{B}^7_{10,12} \\
&\qquad = \tilde{B}^7_{13,15} = -\tilde{B}^7_{14,16} = 1.
\end{aligned} \tag{16}$$

From the relations

$$\tilde{\mathbf{B}}^1 = (\tilde{\mathbf{B}}^2)^t \qquad \tilde{\mathbf{B}}^3 = (\tilde{\mathbf{B}}^4)^t \qquad \tilde{\mathbf{B}}^5 = (\tilde{\mathbf{B}}^6)^t \qquad \tilde{\mathbf{B}}^7 = (\tilde{\mathbf{B}}^8)^t$$

one immediately obtains the non-vanishing elements of $\tilde{\mathbf{B}}^2$, $\tilde{\mathbf{B}}^4$, $\tilde{\mathbf{B}}^6$ and $\tilde{\mathbf{B}}^8$. Combining equations (13), (15) and (16), the thermal n-point Green functions can be computed. It is worth noting that all the computations are reduced to perform products of the sparse matrices (at most three elements different from zero on each line) $\tilde{\mathbf{P}}$ and $\tilde{\mathbf{B}}^l$.

3. Two-point Green function at a finite temperature

Since n-point Green functions including in a non-perturbative way the effects of G, V and U have never been calculated, as an application of our method in this section we compute explicitly the exact two-point Green function for localised electrons. Putting $n = 2$, $m_1 = 2$ and $m_2 = 1$ in equation (13), we have

$$G_>(\tau_2 - \tau_1) = \langle f_\uparrow(\tau_2) f_\uparrow^\dagger(\tau_1)\rangle$$
$$= Z[0,0]^{-1} \exp[-\beta(2\varepsilon + U)] \operatorname{Tr}[\mathbf{X}^2(\tau_1 - \tau_2 + \beta)\mathbf{X}^1(\tau_2 - \tau_1)]. \tag{17}$$

Evaluating the trace in this equation by means of equation (14), we obtain

$$\begin{aligned} G_>(\tau) = Z[0,0]^{-1} &\exp[-\beta(2\varepsilon + U)] \\ &\times \Big[\exp[-\beta(e_2 + 2G)] \sin^2\theta \exp[\tau(e_2 - 2G)] \\ &+ \exp[-\beta(e_5 + 2G)] \cos^2\theta \exp[\tau(e_5 - 2G)] \\ &+ (\tfrac{3}{2}) \exp[-\beta(e_4 + G)] \cos^2\theta \exp[\tau(e_4 - e_2 - G)] \\ &+ (\tfrac{3}{2}) \exp[-\beta(e_4 + G)] \sin^2\theta \exp[\tau(e_4 - e_5 - G)] \\ &+ \exp(-\beta e_{16}) \cos^2\varphi \exp[\tau(e_{16} - e_8)] \\ &+ \exp(-\beta e_{16}) \sin^2\varphi \exp[\tau(e_{16} - e_{14})] \\ &+ (\tfrac{3}{2}) \exp(-\beta e_8) \sin^2\varphi \exp[\tau(e_8 - e_4 - G)] \\ &+ (\tfrac{3}{2}) \exp(-\beta e_{14}) \cos^2\varphi \exp[\tau(e_{14} - e_4 - G)] \\ &+ \sum_a \exp(-\beta e_a)(y_a \cos\theta + z_a \sin\theta)^2 \exp[\tau(e_a - e_2 - 2G)] \\ &+ \sum_a \exp(-\beta e_a)(y_a \sin\theta - z_a \cos\theta)^2 \exp[\tau(e_a - e_5 - 2G)] \\ &+ \sum_a \exp(-\beta e_8)(x_a \cos\varphi - y_a \sin\varphi)^2 \exp[\tau(e_8 - e_a)] \\ &+ \sum_a \exp(-\beta e_{14})(x_a \sin\varphi + y_a \cos\varphi)^2 \exp[\tau(e_{14} - e_a)] \Big) \end{aligned} \tag{18}$$

where $\tau = \tau_2 - \tau_1$, $e_n = E_n - 2\varepsilon - U$ and $a = 7, 10, 13$. Starting from equation (18) the causal temperature Green function

$$G(\tau_2 - \tau_1) = -\langle T[f_\uparrow(\tau_2) f_\uparrow^\dagger(\tau_1)]\rangle$$

can be easily calculated by means of the formula

$$G(\tau) = -[\theta(\tau) G_>(\tau) - \theta(-\tau) G_>(\tau + \beta)].$$

Knowledge of the advanced temperature Green function (18) allows us to evaluate

the spectral density $\rho(\omega)$ from which the real-time Green functions can be easily obtained. Denoting by $\omega_n = (2n+1)\pi/\beta$ the Matsubara frequencies, the Fourier transform of equation (18) gives

$$G_>(\omega_n) = -Z[0,0]^{-1}\exp[-\beta(2\varepsilon+U)]\sum_{j=1}^{20}\frac{g_j}{\mathrm{i}\omega_n-\xi_j} \tag{19}$$

where we have defined

$$\xi_1 = -e_2 + 2G \qquad \xi_{11} = -e_{13} + e_2 + 2G$$
$$\xi_2 = -e_5 + 2G \qquad \xi_{12} = -e_7 + e_5 + 2G$$
$$\xi_3 = -e_4 + e_2 + G \qquad \xi_{13} = -e_{10} + e_5 + 2G$$
$$\xi_4 = -e_4 + e_5 + G \qquad \xi_{14} = -e_{13} + e_5 + 2G$$
$$\xi_5 = -e_{16} + e_8 \qquad \xi_{15} = -e_8 + e_7$$
$$\xi_6 = -e_{16} + e_{14} \qquad \xi_{16} = -e_8 + e_{10}$$
$$\xi_7 = -e_8 + e_4 + G \qquad \xi_{17} = -e_8 + e_{13}$$
$$\xi_8 = -e_{14} + e_4 + G \qquad \xi_{18} = -e_{14} + e_7$$
$$\xi_9 = -e_7 + e_2 + 2G \qquad \xi_{19} = -e_{14} + e_{10}$$
$$\xi_{10} = -e_{10} + e_2 + 2G \qquad \xi_{20} = -e_{14} + e_{13}$$

and

$$g_1 = \sin^2\theta\{\exp[-\beta(e_2+2G)] + \exp(-4\beta G)\}$$
$$g_2 = \cos^2\theta\{\exp[-\beta(e_5+2G)] + \exp(-4\beta G)\}$$
$$g_3 = (\tfrac{3}{2})\cos^2\theta\{\exp[-\beta(e_4+G)] + \exp[-\beta(e_2+2G)]\}$$
$$g_4 = (\tfrac{3}{2})\sin^2\theta\{\exp[-\beta(e_4+G)] + \exp[-\beta(e_5+2G)]\}$$
$$g_5 = \cos^2\varphi\,[\exp(-\beta e_{16}) + \exp(-\beta e_8)]$$
$$g_6 = \sin^2\varphi\,[\exp(-\beta e_{16}) + \exp(-\beta e_{14})]$$
$$g_7 = (\tfrac{3}{2})\sin^2\varphi\{\exp[-\beta(e_4+G)] + \exp(-\beta e_8)\}$$
$$g_8 = (\tfrac{3}{2})\cos^2\varphi\{\exp[-\beta(e_4+G)] + \exp(-\beta e_{14})\}$$
$$g_9 = (y_7\cos\theta + z_7\sin\theta)^2\{\exp[-\beta(e_2+2G)] + \exp(-\beta e_7)\}$$
$$g_{10} = (y_{10}\cos\theta + z_{10}\sin\theta)^2\{\exp[-\beta(e_2+2G)] + \exp(-\beta e_{10})\}$$
$$g_{11} = (y_{13}\cos\theta + z_{13}\sin\theta)^2\{\exp[-\beta(e_2+2G)] + \exp(-\beta e_{13})\}$$
$$g_{12} = (y_7\sin\theta - z_7\cos\theta)^2\{\exp[-\beta(e_5+2G)] + \exp(-\beta e_7)\}$$
$$g_{13} = (y_{10}\sin\theta - z_{10}\cos\theta)^2\{\exp[-\beta(e_5+2G)] + \exp(-\beta e_{10})\}$$
$$g_{14} = (y_{13}\sin\theta - z_{13}\cos\theta)^2\{\exp[-\beta(e_5+2G)] + \exp(-\beta e_{13})\}$$
$$g_{15} = (x_7\cos\varphi - y_7\sin\varphi)^2[\exp(-\beta e_8) + \exp(-\beta e_7)]$$
$$g_{16} = (x_{10}\cos\varphi - y_{10}\sin\varphi)^2[\exp(-\beta e_8) + \exp(-\beta e_{10})]$$

$$g_{17} = (x_{13}\cos\varphi - y_{13}\sin\varphi)^2[\exp(-\beta e_8) + \exp(-\beta e_{13})]$$
$$g_{18} = (x_7\sin\varphi + y_7\cos\varphi)^2[\exp(-\beta e_{14}) + \exp(-\beta e_7)]$$
$$g_{19} = (x_{10}\sin\varphi + y_{10}\cos\varphi)^2[\exp(-\beta e_{14}) + \exp(-\beta e_{10})]$$
$$g_{20} = (x_{13}\sin\varphi + y_{13}\cos\varphi)^2[\exp(-\beta e_{14}) + \exp(-\beta e_{13})].$$

From the relation

$$\rho(\omega) = -(1/\pi)\,\mathrm{Im}[G_>(\omega_n = \omega + \mathrm{i}\eta)]$$

where η is a positive infinitesimal, we have

$$\rho(\omega) = Z[0,0]^{-1}\exp[-\beta(2\varepsilon + U)]\sum_j g_j\delta(\omega - \xi_j).$$

By means of this result the Fourier transform of the retarded and the advanced real-time Green functions can be obtained using the integral representation

$$G^{R,A}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}\omega' \frac{\rho(\omega')}{\omega - \omega' \pm \mathrm{i}\eta}.$$

All these results will be used for a perturbative expansion of the conduction electron band width which will be the subject of a future paper.

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Appendix

A1. Non-vanishing elements of the matrix $\mathbf{M}[0, 0]$

$$M_{11} = 1 - 2u^2a + u^4b$$
$$M_{22} = M_{33} = 1 - u^2a$$
$$M_{25} = M_{52} = M_{39} = M_{93} = u(a - u^2b)$$
$$M_{44} = 1$$
$$M_{47} = M_{74} = -M_{4,10} = -M_{10,4} = ua$$
$$M_{4,13} = M_{13,4} = -M_{7,10} = -M_{10,7} = u^2b$$
$$M_{55} = M_{66} = M_{99} = M_{11,11} = a - u^2b$$
$$M_{77} = M_{88} = M_{10,10} = M_{12,12} = a$$
$$M_{7,13} = M_{13,7} = -M_{8,14} = -M_{14,8} = ub$$
$$M_{10,13} = M_{13,10} = M_{12,15} = M_{15,12} = -ub$$
$$M_{13,13} = M_{14,14} = M_{15,15} = M_{16,16} = b.$$

A2. Eigenvalues of the matrix $\mathbf{M}[0, 0]$

$$N^1 = 1 - 2u^2a + u^4b$$

$$N^2 = N^3 = \tfrac{1}{2}(1-u^2a+a-u^2b) + \tfrac{1}{4}[(1-u^2a-a+u^2b)^2 + 4u^2(a-u^2b)^2]^{1/2}$$

$$N^4 = N^6 = N^{11} = a - u^2b$$

$$N^5 = N^9 = \tfrac{1}{2}(1-u^2a+a-u^2b) - \tfrac{1}{4}[(1-u^2a-a+u^2b)^2 + 4u^2(a-u^2b)^2]^{1/2}$$

$$N^7 = x_1 \qquad N^{10} = x_2 \qquad N^{13} = x_3$$

$$N^8 = N^{12} = \tfrac{1}{2}(a+b) + \tfrac{1}{4}[(a-b)^2 + 4u^2b^2]^{1/2}$$

$$N^{14} = N^{15} = \tfrac{1}{2}(a+b) - \tfrac{1}{4}[(a-b)^2 + 4u^2b^2]^{1/2}$$

where x_i $(i = 1, 2, 3)$ are the solutions of the cubic equation

$$\begin{vmatrix} 1-x & -2ua & u^2b \\ -ua & a+u^2b-x & -ub \\ u^2b & -2ub & b-x \end{vmatrix} = 0.$$

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