Available online at www.sciencedirect.com
SCIENCE DIRECT®
Physica B 359–361 (2005) 684–686
PHYSICA B
www.elsevier.com/locate/physb

f-Electron spectral function near a quantum critical point

J.K. Freericks[a,*], V.M. Turkowski[a], V. Zlatić[b]

[a]Department of Physics, Georgetown University, Washington, DC 20057, USA
[b]Institute of Physics, Bijenicka c. 46, POB 304 10000 Zagreb, Croatia

Abstract

We calculate the f-electron spectral function using a Keldysh formalism for the Falicov–Kimball model in infinite dimensions. We study the region close to the quantum critical point on both the hypercubic and Bethe lattices.

PACS: 71.10.−w; 71.27.+a; 71.30.+h

Keywords: f-Electron; Spectral function; Falicov–Kimball model

The Falicov–Kimball model [1] involves conduction electrons, which are free to move through the lattice, and f-electrons which are immobile. The two electrons interact with each other by a Coulomb interaction (of strength U) when they are located at the same lattice site. The Hamiltonian is (at half-filling)

$$\mathscr{H} = -\frac{t^*}{\sqrt{Z}}\sum_{\langle ij\rangle}(c_i^\dagger c_j + c_j^\dagger c_i) + U\sum_i c_i^\dagger c_i f_i^\dagger f_i - \frac{U}{2}\sum_i (c_i^\dagger c_i + f_i^\dagger f_i), \quad (1)$$

where $c_i^\dagger$ (c_i) creates (destroys) a conduction electron at site i, $f_i^\dagger$ (f_i) creates (destroys) a localized electron at site i, and t^* is the hopping integral [2]. The symbol Z represents the number of nearest neighbors, and $\langle ij\rangle$ denotes a sum over all nearest neighbor pairs. The formalism for solving the conduction-electron Green's function was worked out by Brandt and Mielsch [3].

Brandt and Urbanek [4] describe how to calculate the f-electron spectral function using the Keldysh technique to directly determine the greater Green's function (along the Keldysh contour) and then Fourier transforming to real frequency (see also Ref. [5] for a review of the formalism). The greater Green's function is defined to be

$$G_f^>(t) = -\mathrm{Tr}\langle e^{-\beta\mathscr{H}_{\mathrm{imp}}} S_c(\lambda) f(t) f^\dagger(0)\rangle / \mathscr{Z}_{\mathrm{imp}} \quad (2)$$

*Corresponding author. Tel.: +1 202 687 6159; fax: +1 202 687 2087.
E-mail address: freericks@physics.georgetown.edu (J.K. Freericks).

0921-4526/$ - see front matter
doi:10.1016/j.physb.2005.01.192

with $f(t) = \exp(\mathrm{i}t\mathscr{H}_{\mathrm{imp}})f\exp(-\mathrm{i}t\mathscr{H}_{\mathrm{imp}})$ and the evolution operator is given by

$$S_c(\lambda) = \mathscr{T}_c \exp\left[\int_c \mathrm{d}\bar{t}\int_c \mathrm{d}\bar{t}'\, c^\dagger(\bar{t})\lambda_c(\bar{t},\bar{t}')c(\bar{t}')\right]. \quad (3)$$

The subscript imp denotes the use of the impurity Hamiltonian (no hopping) with the evolution operator corresponding to the dynamical mean field [3] $\lambda(\omega)$ (the dynamical mean field mimics the hopping of conduction electrons onto and off a given site; it is adjusted so that the impurity conduction-electron Green's function equals the local lattice Green's function). The time ordering is along the Keldysh contour (see Fig. 1), and the contour-ordered dynamical mean field is found from a Fourier transform of $\lambda(\omega)$

$$\lambda_c(\bar{t},\bar{t}') = -\frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega\,\mathrm{Im}\,\lambda(\omega)\exp[-\mathrm{i}\omega(\bar{t}-\bar{t}')] \times [f_{\mathrm{FD}}(\omega) - \theta_c(\bar{t}-\bar{t}')], \quad (4)$$

where $f_{\mathrm{FD}}(\omega) = 1/[1+\exp(\beta\omega)]$ is the Fermi–Dirac distribution and $\theta_c(\bar{t}-\bar{t}') = 0$ if $\bar{t}'$ is in front of $\bar{t}$ on the contour c and 1 if it is behind. Green's function can be solved by directly evaluating the Feynman path integral over the contour, which reduces to calculating the determinant of a continuous matrix operator. This operator is discretized, and a conventional determinant is evaluated when we compute results numerically. Once $G^>(t)$ is found, then the DOS (at half-filling) is determined by

$$A_f(\omega) = -\frac{2}{\pi}\int_0^\infty \mathrm{d}t\,\mathrm{Re}\{G_f^>(t)\}\cos(\omega t). \quad (5)$$

We work with two different infinite coordination number lattices here: (i) the Bethe lattice, which has a noninteracting DOS that is a semicircle $\rho_{\mathrm{B}}(\omega) = \sqrt{4t^{*2}-\omega^2}/2\pi t^{*2}$ and (ii) the hypercubic lattice, which has a noninteracting DOS that is a Gaussian $\rho_{\mathrm{H}}(\omega) = \exp(-\omega^2/t^{*2})/\sqrt{\pi}t^*$. All energies are measured in units of t^*.

In Fig. 2, we plot the DOS at the critical value of U for the Mott transition on the Bethe lattice ($U = 2$), and in Fig. 3, just on the insulating side of the transition on the hypercubic lattice ($U = 1.5$). Also included is a plot of the conduction-electron DOS, which is independent of temperature [6]. Note how the f-electron spectral function has an interesting temperature evolution, where it develops a pseudogap as T is reduced. Calculations become more difficult at lower temperatures [7] (because of discretization errors along the Keldysh contour), and rapidly exhaust our computational resources. As a check on the accuracy, we use the DOS to calculate the Matsubara-frequency Green's functions and compare them to results calculated directly on the imaginary axis, and we

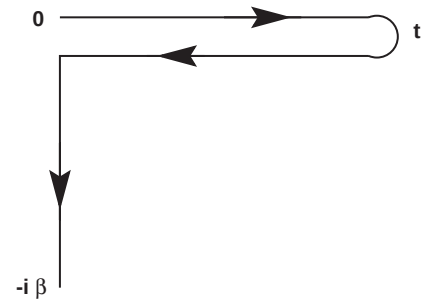

Fig. 1. Keldysh contour for evaluating the f-electron Green's function at time t. The contour runs from 0 to t, then back from t to 0 and finally goes along the imaginary axis down to $-\mathrm{i}\beta$. When we discretize the matrix operator over the Keldysh contour, we evaluate the integrals via a rectangular (midpoint) summation. We typically use no more than 2500 time steps on the contour.

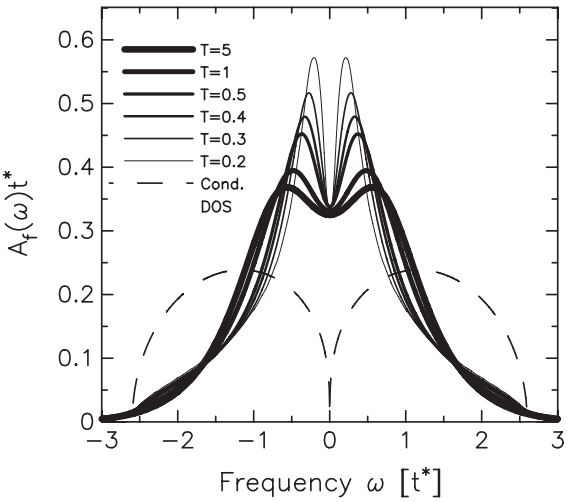

Fig. 2. f-Electron DOS for the Bethe lattice. The different thickness lines correspond to different temperatures. The conduction electron DOS is the dashed line.

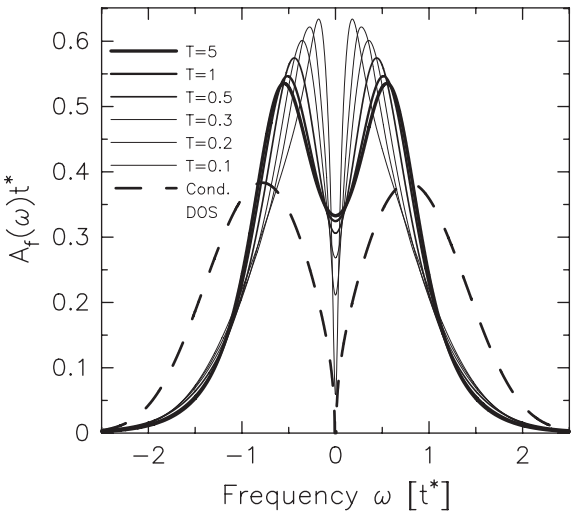

Fig. 3. Similar plot of the f-electron DOS for the hypercubic lattice.

compare the first three moments to the exact results for those moments. In general, we need to extrapolate the discretization size to zero to get accurate results, and most reported DOS here are accurate to at least 1% in all of the moments and 0.1% for all Matsubara-frequency Green's functions. A long paper evaluating other values of U has appeared in [7].

We acknowledge support of the Office of Naval Research (N00014-99-1-0328) and the National Science Foundation (DMR-0210717). Supercomputer resources were provided by the Arctic Region Supercomputer Center and the Engineering Research and Development Center.

References

[1] L.M. Falicov, J.C. Kimball, Phys. Rev. Lett. 22 (1969) 997.
[2] W. Metzner, D. Vollhardt, Phys. Rev. Lett. 62 (1989) 324.
[3] U. Brandt, C. Mielsch, Z. Phys. B 75 (1989) 365;
U. Brandt, C. Mielsch, Z. Phys. B 79 (1990) 295;
U. Brandt, C. Mielsch, Z. Phys. B 82 (1991) 37.
[4] U. Brandt, M.P. Urbanek, Z. Phys. B 89 (1992) 297.
[5] J.K. Freericks, V. Zlatić, Rev. Mod. Phys. 75 (2003) 1333.
[6] P.G.J. Van Dongen, Phys. Rev. B 45 (1992) 2267.
[7] J.K. Freericks, V.M. Turkowski, V. Zlatić, Phys. Rev. B 71 (2005) 078507.