

# Equivalence of the Falicov-Kimball and Brandt-Mielsch forms for the free energy of the infinite-dimensional Falicov-Kimball model

A. M. Shvaika\*

*Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, 1 Svientsitskii Strasse, 79011 Lviv, Ukraine*

J. K. Freericks†

*Department of Physics, Georgetown University, Washington, DC 20057*

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Falicov and Kimball proposed a real-axis form for the free energy of the Falicov-Kimball model that was modified for the coherent potential approximation by Plischke. Brandt and Mielsch proposed an imaginary-axis form for the free energy of the dynamical mean field theory solution of the Falicov-Kimball model. It has long been known that these two formulas are numerically equal to each other; an explicit derivation showing this equivalence is presented here.

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The Falicov-Kimball model<sup>1</sup> is one of the simplest many-body Hamiltonians. It was introduced in 1969 to describe metal-insulator transitions in a number of rare-earth and transition-metal compounds and was solved in the limit of infinite dimensions by Brandt and Mielsch.<sup>2-4</sup> The earlier work of Falicov's group<sup>5</sup> was modified by Plischke<sup>6</sup> for the coherent-potential approximation to give an explicit formula for the Helmholtz free energy in terms of integrals over the interacting density of states (DOS). Later, Brandt and Mielsch<sup>4</sup> derived an exact formula for the Helmholtz free energy in terms of summations over Matsubara frequencies in the infinite-dimensional limit. Numerical evaluation of these two forms for the free energy showed that they were indeed equal<sup>7,8</sup> but no explicit derivation of the equivalence has appeared.

We illustrate this equivalence here for the spinless version of the Falicov-Kimball model (generalization to higher-spin versions is simple). The spinless Falicov-Kimball Hamiltonian<sup>1</sup> is

$$\mathcal{H} = - \sum_{ij} t_{ij} c_i^\dagger c_j + E_f \sum_i f_i^\dagger f_i + U \sum_i c_i^\dagger c_i f_i^\dagger f_i, \quad (1)$$

where  $c_i^\dagger$  ( $c_i$ ) creates (destroys) an itinerant electron at site  $i$ ,  $f_i^\dagger$  ( $f_i$ ) creates (destroys) a localized electron at site  $i$ ,  $t_{ij}$  is the Hermitian hopping matrix (which is chosen to be nonzero only between nearest neighbors),  $E_f$  is the localized electron site energy, and  $U$  is the on-site Coulomb interaction between localized and itinerant electrons. Chemical potentials  $\mu$  and  $\mu_f$  are employed for the itinerant and localized electrons, respectively.

In the limit where the spatial dimension  $d$  becomes large, the many-body problem can be solved exactly when the hopping is chosen to scale<sup>9</sup> as  $t = t^*/2\sqrt{d}$ . In this case, the so-called local approximation becomes exact. We sketch the algorithm used to solve the many-body problem, in order to establish our notation.

The local Green's function  $G(z)$  can be written as the Hilbert transform of the noninteracting DOS  $\rho(\epsilon)$

$$G(z) = \int d\epsilon \rho(\epsilon) \frac{1}{z + \mu - \Sigma(z) - \epsilon} \quad (2)$$

with  $z$  in the complex plane and  $\Sigma(z)$  the local self-energy. Dyson's equation for the local self-energy reads

$$\Sigma(z) = z + \mu - \lambda(z) - G^{-1}(z) \quad (3)$$

with  $\lambda(z)$  the dynamical mean field (which must be determined self-consistently). Solving the atomic problem in a time-dependent field yields another equation for the local Green's function

$$G(z) = \frac{w_0}{z + \mu - \lambda(z)} + \frac{w_1}{z + \mu - \lambda(z) - U} \quad (4)$$

with  $w_0 = \mathcal{Z}_0 / \mathcal{Z}$ ,  $w_1 = \mathcal{Z}_1 / \mathcal{Z}$  (the localized electron density), and  $\mathcal{Z} = \mathcal{Z}_0 + \mathcal{Z}_1$  (the atomic partition function). The symbols  $\mathcal{Z}_0$  and  $\mathcal{Z}_1$  can be expressed as infinite products

$$\mathcal{Z}_0 = (1 + e^{\beta\mu}) \prod_n \left( 1 - \frac{\lambda_n}{i\omega_n + \mu} \right) \quad (5)$$

and

$$\mathcal{Z}_1 = e^{-\beta(E_f - \mu_f)} (1 + e^{\beta(\mu - U)}) \prod_n \left( 1 - \frac{\lambda_n}{i\omega_n + \mu - U} \right) \quad (6)$$

where  $\beta = 1/T$ , and we used the notation  $\lambda_n = \lambda(i\omega_n)$  with  $i\omega_n = i\pi T(2n+1)$  the fermionic Matsubara frequency.

The Brandt-Mielsch form for the Helmholtz free energy is<sup>4</sup>

$$\mathcal{F} = -T \ln \mathcal{Z} - T \int d\epsilon \rho(\epsilon) \sum_n \ln[(i\omega_n + \mu - \Sigma_n - \epsilon) G_n] + \mu_f w_1 + \mu \rho_c \quad (7)$$

with  $\rho_c$  the itinerant electron density. Our aim is to replace the Matsubara frequency summation of the logarithmic function by an integral over the real axis. To do this we use Eq. (3) to write  $G_n = 1/(i\omega_n + \mu - \lambda_n - \Sigma_n)$  and rewrite the sum in Eq. (7) as

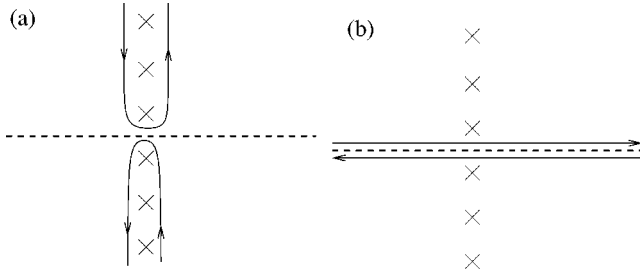


FIG. 1. Contours used in various integrals. In panel (a), we show the contour  $C$  that surrounds all of the fermionic Matsubara frequencies which are indicated by X's. The dotted line denotes the real axis. In panel (b), we show the deformed contour  $C'$  that allows one to replace the integral by one over the real axis.

$$\begin{aligned}
 & T \sum_n \ln[(i\omega_n + \mu - \Sigma_n - \epsilon)G_n] \\
 &= T \sum_n \left[ \ln \left( 1 - \frac{\epsilon}{i\omega_n + \mu - \Sigma_n} \right) \right. \\
 & \quad \left. - \ln \left( 1 - \frac{\lambda_n}{i\omega_n + \mu - \Sigma_n} \right) \right]. \quad (8)
 \end{aligned}$$

The function  $\Xi(z) = 1/[z + \mu - \Sigma(z)]$  is the irreducible part (with respect to the hopping) of the itinerant electron Green's function and it possesses the same analytic properties as do the Green's functions (a branch cut on the real axis with a change in sign of the imaginary part above or below the cut<sup>10</sup>). The dynamical mean field  $\lambda(z)$  also has the same analytic properties. As a result, the logarithmic functions in Eq. (8) are analytic functions above and below the real axis (the only branch cut lies on the real axis) and they behave as  $1/z$  for  $|z| \rightarrow \infty$ . This implies that we can express the Matsubara frequency summation as a contour integral around the contour  $C$  illustrated in Fig. 1(a) yielding

$$\begin{aligned}
 & T \sum_n \ln[(i\omega_n + \mu - \Sigma_n - \epsilon)G_n] \\
 &= \frac{1}{2\pi i} \int_C dz f(z) \left[ \ln \left( 1 - \frac{\epsilon}{z + \mu - \Sigma(z)} \right) \right. \\
 & \quad \left. - \ln \left( 1 - \frac{\lambda(z)}{z + \mu - \Sigma(z)} \right) \right] \quad (9)
 \end{aligned}$$

with  $f(z) = 1/[1 + \exp(\beta z)]$  the Fermi-Dirac distribution. The contour  $C$  is deformed to  $C'$  which runs parallel to the real axis as shown in Fig. 1(b). Since there is a branch cut on the real axis, the integral over  $C'$  becomes the imaginary part of the integral from  $-\infty$  to  $\infty$

$$\begin{aligned}
 \mathcal{F} &= -T \ln \mathcal{Z} + \mu_f w_1 + \mu \rho_c + \frac{1}{\pi} \int d\omega \int d\epsilon \rho(\epsilon) f(\omega) \\
 & \times \left[ \text{Im} \ln \left( 1 - \frac{\epsilon}{\omega + \mu - \Sigma(\omega)} \right) \right. \\
 & \quad \left. - \text{Im} \ln \left( 1 - \frac{\lambda(\omega)}{\omega + \mu - \Sigma(\omega)} \right) \right]. \quad (10)
 \end{aligned}$$

Because the sign of the imaginary part of the functions that make up the argument of the logarithms is fixed above and below the real axis, the value of the imaginary part of the logarithms is defined to lie in the range between  $-\pi$  and  $0$  or  $0$  and  $\pi$ , depending on this sign. To satisfy the analytic properties of the logarithms in Eq. (10), note that the expression in the square brackets can be rewritten as

$$\text{Im} \ln \frac{\omega + \mu - \Sigma(\omega) - \epsilon}{\omega + \mu - \Sigma(\omega) - \lambda(\omega)}, \quad (11)$$

but one must be careful not to shift the imaginary part of the logarithm by an integer multiple of  $2\pi$ , which corresponds to a different sheet of the logarithm.

Noting that

$$f(\omega) = -T \frac{d}{d\omega} \ln[1 + \exp(-\beta\omega)] \quad (12)$$

allows us to integrate by parts (since the boundary terms vanish) and gives

$$\begin{aligned}
 \mathcal{F} &= -T \ln \mathcal{Z} + \mu_f w_1 + \mu \rho_c \\
 & + \frac{T}{\pi} \int d\omega \int d\epsilon \rho(\epsilon) \ln[1 + e^{-\beta\omega}] \\
 & \times \text{Im} \left[ \frac{1 - \Sigma'(\omega)}{\omega + \mu - \Sigma(\omega) - \epsilon} - \frac{1 - \Sigma'(\omega) - \lambda'(\omega)}{\omega + \mu - \lambda(\omega) - \Sigma(\omega)} \right] \quad (13)
 \end{aligned}$$

with the prime indicating a derivative with respect to  $\omega$ . The integral over  $\epsilon$  can be performed by using Eq. (2) and the fact that the DOS has unit weight, to yield

$$\begin{aligned}
 \mathcal{F} &= -T \ln \mathcal{Z} + \mu_f w_1 + \mu \rho_c \\
 & + \frac{T}{\pi} \int d\omega \ln[1 + e^{-\beta\omega}] \text{Im}[G(\omega)\lambda'(\omega)]. \quad (14)
 \end{aligned}$$

The interacting DOS is defined to be  $A(\omega) = -\text{Im}[G(\omega)]/\pi$ . Using this fact, we can add and subtract an integral over  $A(\omega)$  to produce

$$\begin{aligned}
 \mathcal{F} &= -T \int d\omega A(\omega) \ln(1 + e^{-\beta\omega}) - T \ln \mathcal{Z} + \mu_f w_1 + \mu \rho_c \\
 & + \frac{T}{\pi} \int d\omega \ln[1 + e^{-\beta\omega}] \text{Im}[G(\omega)\{-1 + \lambda'(\omega)\}]. \quad (15)
 \end{aligned}$$

Next, we substitute in Eq. (4) for  $G(\omega)$  and add

$$\begin{aligned}
 0 &= \frac{T}{\pi} \int d\omega \ln(1 + e^{-\beta\omega}) \text{Im} \left[ \frac{w_1}{\omega + \mu - U + i0^+} \right] \\
 & + T w_1 \ln(1 + e^{\beta(\mu - U)}) \quad (16)
 \end{aligned}$$

and

$$0 = \frac{T}{\pi} \int d\omega \ln(1 + e^{-\beta\omega}) \text{Im} \left[ \frac{1 - w_1}{\omega + \mu + i0^+} \right] + T(1 - w_1) \ln(1 + e^{\beta\mu}) \quad (17)$$

to Eq. (15). Collecting terms gives

$$\begin{aligned} \mathcal{F} = & -T \int d\omega A(\omega) \ln(1 + e^{-\beta\omega}) - T \ln \mathcal{Z} + \mu_f w_1 + \mu \rho_c \\ & + \frac{T}{\pi} \int d\omega \ln[1 + e^{-\beta\omega}] \text{Im} \left\{ \frac{w_1}{\omega + \mu - U + i0^+} \right. \\ & \times \left[ 1 + \frac{(\omega + \mu - U)[-1 + \lambda'(\omega)]}{\omega + \mu - U - \lambda(\omega)} \right] + \frac{1 - w_1}{\omega + \mu + i0^+} \\ & \times \left. \left[ 1 + \frac{(\omega + \mu)[-1 + \lambda'(\omega)]}{\omega + \mu - \lambda(\omega)} \right] \right\} + T w_1 \ln(1 + e^{\beta(\mu - U)}) \\ & + T(1 - w_1) \ln(1 + e^{\beta\mu}). \end{aligned} \quad (18)$$

The terms inside  $\text{Im}\{\dots\}$  can be expressed as a derivative

$$\begin{aligned} \mathcal{F} = & -T \int d\omega A(\omega) \ln(1 + e^{-\beta\omega}) - T \ln \mathcal{Z} + \mu_f w_1 + \mu \rho_c \\ & + \frac{T}{\pi} \int d\omega \ln[1 + e^{-\beta\omega}] \frac{d}{d\omega} \text{Im} \left\{ w_1 \ln \left[ 1 - \frac{\lambda(\omega)}{\omega + \mu - U} \right] \right. \\ & + (1 - w_1) \ln \left[ 1 - \frac{\lambda(\omega)}{\omega + \mu} \right] \left. \right\} + T w_1 \ln(1 + e^{\beta(\mu - U)}) \\ & + T(1 - w_1) \ln(1 + e^{\beta\mu}). \end{aligned} \quad (19)$$

Now we integrate by parts and recall Eq. (12). Since the boundary terms vanish, we are left with an integral over the real axis, which can be reexpressed in terms of the contour  $C'$ , and then deformed into an integral over the contour  $C$ . This gives

$$\begin{aligned} \mathcal{F} = & -T \int d\omega A(\omega) \ln(1 + e^{-\beta\omega}) - T \ln \mathcal{Z} + \mu_f w_1 + \mu \rho_c \\ & - \frac{1}{2i\pi} \int_C d\omega f(\omega) \left\{ w_1 \ln \left[ 1 - \frac{\lambda(\omega)}{\omega + \mu - U} \right] \right. \\ & + (1 - w_1) \ln \left[ 1 - \frac{\lambda(\omega)}{\omega + \mu} \right] \left. \right\} + T w_1 \ln(1 + e^{\beta(\mu - U)}) \\ & + T(1 - w_1) \ln(1 + e^{\beta\mu}). \end{aligned} \quad (20)$$

The contour integral can be evaluated by residues which produces a sum over Matsubara frequencies

$$\begin{aligned} \mathcal{F} = & -T \int d\omega A(\omega) \ln(1 + e^{-\beta\omega}) - T \ln \mathcal{Z} + \mu_f w_1 + \mu \rho_c \\ & + T \sum_n \left\{ w_1 \ln \left( 1 - \frac{\lambda_n}{i\omega_n + \mu - U} \right) + (1 - w_1) \right. \\ & \times \ln \left( 1 - \frac{\lambda_n}{i\omega_n + \mu} \right) \left. \right\} + T w_1 \ln(1 + e^{\beta(\mu - U)}) \\ & + T(1 - w_1) \ln(1 + e^{\beta\mu}). \end{aligned} \quad (21)$$

The sum over Matsubara frequencies can be replaced by terms that involve  $\ln \mathcal{Z}_0$  and  $\ln \mathcal{Z}_1$  from Eqs. (5) and (6). Collecting terms gives

$$\begin{aligned} \mathcal{F} = & -T \int d\omega A(\omega) \ln(1 + e^{-\beta\omega}) + T w_1 \ln \frac{\mathcal{Z}_1}{\mathcal{Z}} \\ & + T(1 - w_1) \ln \frac{\mathcal{Z}_0}{\mathcal{Z}} + E_f w_1 + \mu \rho_c. \end{aligned} \quad (22)$$

Using the definitions for  $w_0$  and  $w_1$  in terms of the  $\mathcal{Z}$ 's, and the relation

$$\begin{aligned} \ln(1 + e^{-\beta\omega}) = & -\beta\omega f(\omega) - f(\omega) \ln f(\omega) \\ & - [1 - f(\omega)] \ln[1 - f(\omega)] \end{aligned} \quad (23)$$

gives us our final result for the Helmholtz free energy

$$\begin{aligned} \mathcal{F} = & \int d\omega A(\omega) f(\omega) (\omega + \mu) + E_f w_1 + T \int d\omega A(\omega) \\ & \times \{ f(\omega) \ln f(\omega) + [1 - f(\omega)] \ln[1 - f(\omega)] \} \\ & + T [w_1 \ln w_1 + (1 - w_1) \ln(1 - w_1)]. \end{aligned} \quad (24)$$

This is the Falicov-Kimball-Plischke form for the free energy<sup>1,5,6</sup> which completes the derivation. This form of the Helmholtz free energy is also correct for the Falicov-Kimball model with correlated hopping and it can be proved in the same way starting from the expressions of Ref. 10.

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\*Electronic address: ashv@icmp.lviv.ua; URL: <http://ph.icmp.lviv.ua/~ashv>

†Electronic address: freericks@physics.georgetown.edu; URL: <http://www.physics.georgetown.edu/~jkf>

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