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LETTER TO THE EDITOR

A lattice model for x-ray emission and absorption: the edge singularity

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Abstract. The model for x-ray scattering known as the Mahan–Nozières–De Dominicis model is extended to a finite concentration of randomly distributed core electrons. A systematic, renormalized expansion for the phase shift of the imaginary-time Green function of the deep-level electrons is derived in the limit of high dimensions, i.e. within a dynamical mean-field theory. A global analytic expression interpolating between short- and long-time asymptotics is obtained. An algebraic singularity in the zero-temperature Green function for long times is revealed. The critical exponent is estimated and compared with that of Nozières and De Dominicis.

An intensive theoretical investigation of x-ray absorption and emission spectra was launched after the discovery of edge anomalies in the soft x-ray region of photoemission spectra of metals [1]. The essence of this phenomenon can be summarized by a process where a core electron is excited into the conduction band whereby a transient electron–hole pair is created. This pair causes a collective rearrangement of the ground state of the conduction electrons on a long time scale. The simplest model for the description of the edge anomaly in the x-ray spectra was proposed by Mahan [2] and is now often called the Mahan–Nozières–De Dominicis (MND) model. It describes a system of a single localized (infinitely heavy) electron interacting with a Fermi sea of conduction electrons. The Hamiltonian of the MND model is

$$\hat{H}_{\text{MND}} = \sum_{\mathbf{k}} \epsilon(\mathbf{k}) \hat{c}^\dagger(\mathbf{k}) \hat{c}(\mathbf{k}) + E_0 \hat{d}^\dagger \hat{d} + \sum_{\mathbf{k}, \mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} \hat{c}^\dagger(\mathbf{k}) \hat{c}(\mathbf{k}') \hat{d}^\dagger \hat{d} \quad (1)$$

where $\hat{c}^\dagger(\mathbf{k})$ ($\hat{c}(\mathbf{k})$) are creation (destruction) operators, respectively, for the conduction electrons with momentum \mathbf{k} and kinetic energy $\epsilon(\mathbf{k})$. E_0 is the atomic energy of a localized electron created (annihilated) by \hat{d}^\dagger (\hat{d}), respectively. The potential $V_{\mathbf{k}\mathbf{k}'}$ describes the screened Coulomb interaction between the localized and the conduction electrons. The spin of the electron is unimportant here and can be neglected. The x-ray transition rate is a function of the time-dependent Green function of the core d electron which shows an algebraic singularity in the MND model (1). There are several approaches to derive this ‘edge singularity’. One can either use a many-body perturbation theory where the conduction electrons are scattered by a time-dependent potential due to the excited electron–hole pair [2, 3], or one can separate the dynamics of the conduction electrons from that of the core electron [4]. In the first case the singularity is connected with the Anderson orthogonality catastrophe [5] and in the second case a singular integral equation determines the edge

behaviour of the propagator of the core quasiparticle [4]. In both derivations the edge singularity is tightly linked to the discontinuity of the electron distribution at the Fermi level.

The validity of the MND model is restricted to very low concentrations of core electrons ($n_d \simeq 0$) or core holes ($n_d \simeq 1$), where the localized quasiparticles do not influence the equilibrium ground state of the conduction electrons. This is no longer the case if we increase the concentration of the heavy particles, e.g. by doping the system with randomly distributed impurities. A finite concentration of the deep-level quasiparticles significantly changes the properties of the conduction electrons in the MND model. To be able to describe the effects of different macroscopic configurations of the core electrons on both the *ground state of the conduction electrons* and the *x-ray spectra* it is necessary to extend the MND Hamiltonian (1), which explicitly treats the only core particle participating in the x-ray scattering process, to a model explicitly dealing with an arbitrary macroscopic distribution of the core electrons. If we approximate the screened Coulomb interaction V by a contact Hubbard term U we obtain the spinless Falicov–Kimball model [6] with the local d electrons as the simplest lattice extension of the MND model. A natural question arises: does the edge singularity from the MND model also survive for this model with an arbitrary macroscopic concentration of core electrons, especially if the core electrons may be randomly distributed on diluted impurities? In the Falicov–Kimball model the quasiparticle pole of the conduction electrons at the Fermi energy is smeared out and the *correlated conduction electrons* have a finite lifetime. Hence none of the standard techniques from the MND problem can be used here.

The aim of this paper is to answer the question about the existence of the MND-type singularity in a model with a macroscopic concentration of localized electrons. To this end we investigate the imaginary-time Green function of the local electrons of the spinless Falicov–Kimball model with randomly distributed local electrons in the limit of *high dimensions*. We develop a new method yielding the *long-time asymptotics without any particular assumption* about the propagator of the conduction electrons. Furthermore we reveal the edge singularity in both the thermal and the spectral Green functions of the local electrons.

The model to be investigated can be defined through a tight-binding Hamiltonian [6]:

$$\hat{H}_{\text{FK}} = -t \sum_{\langle ij \rangle} \hat{c}_i^\dagger \hat{c}_j + \sum_i \varepsilon_i^d \hat{d}_i^\dagger \hat{d}_i + U \sum_i \hat{c}_i^\dagger \hat{c}_i \hat{d}_i^\dagger \hat{d}_i. \quad (2)$$

We choose the energies of the localized electrons $\varepsilon_i^d = \varepsilon^d$ with probability $1-x$ and $\varepsilon_i^d = \infty$ with probability x , to simulate dilution of the core electrons. That is, only a portion $(1-x)L$ of the total number L of the lattice sites can be occupied by the local d electrons. This randomness in the energies ε_i^d causes no substantial complications in comparison with the pure Falicov–Kimball model. In the limit of infinite dimensions ($d \rightarrow \infty$) at least, the disordered model can be solved in the same way as the non-random model [7]. The limit of high spatial dimensions is, in analogy to classical statistical mechanics, introduced to identify the exact solution of the model in $d = \infty$ with a comprehensive mean-field theory [8]. This limit simplifies the calculation by the suppression of spatial correlations due to the presence of infinitely many neighbours; accordingly the hopping amplitude must be scaled as $t \rightarrow t^*/\sqrt{2d}$ with t^* fixed ($t^* \equiv 1$). In this way the average kinetic energy remains finite in high dimensions [9]. The infinite-dimensional model with Hamiltonian (2) can be reduced to a problem of a single site embedded in a medium described by a homogeneous dynamical potential $\tilde{\Sigma}_c(\omega)$, the self-energy of the conduction electrons. This potential as

well as the the configurationally averaged free energy can be calculated exactly for the model (2) in infinite dimensions (i.e. on a sophisticated mean-field level) [7]. However, the exact analytic form of the Green function of the local electrons, needed for the κ -ray spectra, is not known. It can be formally represented by an infinite determinant [10, 11] and for finite temperatures can be evaluated numerically [11]. We need, however, an *analytic* expression for the Green function of the local electrons to be able to decide about the edge singularity. To obtain it, we construct the imaginary-time Green function in a formalism similar to the method of Nozières and De Dominicis [4].

The configurationally averaged Green function of a local d electron can be written as a renormalized atomic propagator [10, 11]

$$G_d(\tau, \beta; U) = -\theta(\tau) \langle n_i^d \exp[(\beta - \tau)(\varepsilon_i^d - \mu) - \beta \mathcal{E}_\beta(\beta; U) + \tau \mathcal{E}_\beta(\tau; U)] \rangle_{av} \quad (3)$$

where $\beta = 1/k_B T$, $k_B = 1$, $\tau \in (0, \beta)$ is the imaginary time, $n_i^d = \llbracket 1 + \exp\{-\beta[\mu - \varepsilon_i^d + \mathcal{E}_\beta(\beta, U)]\} \rrbracket^{-1}$ is the configuration-dependent density of the d electrons, μ is the chemical potential and

$$\begin{aligned} \mathcal{E}_\beta(\tau, U) &= \frac{1}{\tau} \text{tr} \ln \left(\hat{1} - U \hat{C}(\tau) \hat{G}_\beta \right) \\ &\equiv \frac{1}{\tau} \int_0^\tau dt \left[\ln \left(\hat{1} - U \hat{C}(\tau) \hat{G}_\beta \right) \right] (t, t) \end{aligned} \quad (4)$$

is the time-dependent phase shift. Operators

$$[\hat{C}(\tau)](t, t') = \delta(t - t') \chi_{(0, \tau)}(t)$$

where $\chi_{(0, \tau)}(t)$ is the characteristic function on the interval $(0, \tau)$ and

$$[\hat{G}_\beta](t, t') = [\hat{G}_c^{-1} + \hat{\Sigma}_c]^{-1}(t - t')$$

is an effective local, imaginary-time propagator of the conduction electrons, with Σ_c the self-energy and G_c the averaged, site-diagonal part of the propagator of the conduction electrons. They are determined exactly from the averaged free energy [7]. Note that the interaction-induced energy shift $\mathcal{E}_\beta(\tau, U)$ depends only on the averaged quantities G_c and Σ_c and hence is the same for all random configurations of the d electrons.

The main difficulty in the evaluation of the function $G_d(\tau, \beta)$ from (3) lies in the integral (4). Nozières and De Dominicis [4] introduced a new function $\Gamma_\beta(\lambda, \tau; t, t')$ satisfying an integral equation

$$\Gamma_\beta(\lambda, \tau; t, t') = \mathcal{G}_\beta(t - t') + \lambda \int_0^\tau dt'' \mathcal{G}_\beta(t - t'') \Gamma_\beta(\lambda, \tau; t'', t'). \quad (5)$$

From $\Gamma_\beta(\lambda, \tau; t, t')$ the phase shift $\mathcal{E}_\beta(\tau, U)$ is defined as an integral over the interaction strength λ :

$$\mathcal{E}_\beta(\tau, U) = -\frac{1}{\tau} \int_0^\tau dt \int_0^U d\lambda \Gamma_\beta(\lambda, \tau; t, t). \quad (6)$$

They further converted (5), for real times at zero temperature, to a singular integral equation with a known solution by replacing the actual real-time propagator $\mathcal{G}_\infty(it - it')$ by its long-time asymptotics $(it - it')^{-1}$ [4]. This approach cannot be applied here, since the imaginary part of the self-energy $\tilde{\Sigma}_c$ does not vanish at the Fermi level and the conduction electrons do not form a Fermi liquid. The tilde generally denotes the frequency representation.

Hence we must proceed differently here to obtain the long-time asymptotics of \mathcal{E}_β from (6). We first project the functions $\mathcal{G}_\beta(t)$ and $\Gamma_\beta(\lambda, \tau, t, t')$ onto the interval $(-\tau, \tau)$ and then extend them periodically on $(-\infty, \infty)$ so that the Fourier transformation on the interval $(-\tau, \tau)$ can be applied to (5). This new periodicity does not influence the result, for only the values of $\Gamma_\beta(\lambda, \tau; t, t')$ on the interval $(0, \tau)$ are relevant. Two important observations are worth noting. First, although the effective local propagator of the conduction electrons $\mathcal{G}_\beta(t)$ has fermionic character on the interval $(-\beta, \beta)$, i.e. $\mathcal{G}_\beta(t + \beta) = -\mathcal{G}_\beta(t)$, its projection on $(-\tau, \tau)$, the function $\tilde{\mathcal{G}}_\beta(\tau, t)$, has no specific symmetry and contains contributions from both the fermionic and the bosonic Matsubara frequencies, $\omega_n = \pi n / \tau$. Second, the Fourier representation does not diagonalize integral equation (5), unless $\tau = \beta$. The integral in (5) mixes the fermionic and the bosonic degrees of freedom and hence (5) remains a matrix (integral) equation even in the Fourier representation. Nevertheless, it is more convenient to work in the frequency representation than in the time representation.

The Fourier transform of (5) on the interval $(-\tau, \tau)$ reads

$$\tilde{\Gamma}_{f,\nu} = \tau \delta_{f,\nu} \tilde{\mathcal{G}}_f + \lambda \tilde{\mathcal{G}}_f \left(\tilde{\Gamma}_{f,\nu} - \frac{2}{\tau} \sum_b H_{f,b} \tilde{\Gamma}_{b,\nu} \right) \quad (7a)$$

$$\tilde{\Gamma}_{b,\nu} = \tau \delta_{b,\nu} \tilde{\mathcal{G}}_b + \lambda \tilde{\mathcal{G}}_b \left(\tilde{\Gamma}_{b,\nu} - \frac{2}{\tau} \sum_f H_{b,f} \tilde{\Gamma}_{f,\nu} \right) \quad (7b)$$

where

$$f := (2n_f + 1)\pi / \tau \quad b := 2n_b\pi / \tau$$

are fermionic and bosonic Matsubara frequencies, respectively, on the interval $(-\tau, \tau)$. The frequency $\nu = \pi n / \tau$ is an inactive variable,

$$\tilde{\mathcal{G}}_f := \frac{1}{2} \int_{-\tau}^{\tau} dt \exp\{if t\} \mathcal{G}_\beta(t)$$

$$\tilde{\Gamma}_{f,\nu} := \frac{1}{4} \int_{-\tau}^{\tau} dt dt' \exp\{if t - i\nu t'\} \Gamma_\beta(\lambda, \tau; t, t')$$

and analogously for the bosonic frequencies. The kernel

$$-2H_{f,b} := -2(if - ib)^{-1}$$

is the Fourier transform of the function $\text{sign}(t)$ on $(-\tau, \tau)$. In the case $\tau = \beta$, we obtain $\tilde{\mathcal{G}}_b = 0$ and (7) reduces to a set of decoupled algebraic equations.

We transform (7) into two Fredholm integral equations by separating $\tilde{\Gamma}_f$ from $\tilde{\Gamma}_b$. A formal solution of these Fredholm equations is

$$\tilde{\Gamma}_{f,\nu} = \frac{1}{\tau} \sum_{f'} \left[\hat{X}_{(f)}^{-1} \right]_{f,f'} \left[\tau \delta_{f',\nu} \tilde{\mathcal{G}}_{f'}(\lambda) - 2\lambda \delta_{\nu,b} \tilde{\mathcal{G}}_{f'}(\lambda) H_{f',b} \tilde{\mathcal{G}}_b(\lambda) \right] \quad (8a)$$

$$\tilde{\Gamma}_{b,\nu} = \frac{1}{\tau} \sum_{b'} \left[\hat{X}_{(b)}^{-1} \right]_{b,b'} \left[\tau \delta_{b',\nu} \tilde{\mathcal{G}}_{b'}(\lambda) - 2\lambda \delta_{\nu,f} \tilde{\mathcal{G}}_{b'}(\lambda) H_{b',f} \tilde{\mathcal{G}}_f(\lambda) \right] \quad (8b)$$

where

$$[\hat{X}_{(f)}]_{f,f'} := \tau \delta_{f,f'} - \lambda^2 \bar{G}_f(\lambda) 4/\tau \sum_b H_{f,b} \bar{G}_b(\lambda) H_{b,f}$$

and

$$\bar{G}_f(\lambda) := \bar{G}_f / (1 - \lambda \bar{G}_f).$$

Analogous equations hold for the bosonic functions. The inversion of the matrices $\hat{X}_{(f)}$ and $\hat{X}_{(b)}$ is calculated with respect to $\hat{1}_{\mu,\nu} := \tau \delta_{\mu,\nu}$ so that the continuum limit $\tau \rightarrow \infty$ is well defined. Only a special combination of the full two-frequency functions $\bar{\Gamma}_{f,\nu}$ and $\bar{\Gamma}_{b,\nu}$ contributes to the phase shift $\mathcal{E}_\beta(\tau, U)$. It is obtained from the Fourier transform of (6) as

$$\mathcal{E}_\beta(\tau, U) = -\frac{1}{\tau} \int_0^U d\lambda \left(\frac{1}{\tau} \sum_f \bar{\Gamma}_{f,f} + \frac{1}{\tau} \sum_b \bar{\Gamma}_{b,b} - \frac{2}{\tau^2} \sum_{f,b} (\bar{\Gamma}_{f,b} - \bar{\Gamma}_{b,f}) H_{b,f} \right). \tag{9}$$

Since the operators $\hat{X}_{(f)}$ and $\hat{X}_{(b)}$ cannot be diagonalized, it is not possible to find the full solution to (8) and (9). However, we can systematically expand $\hat{X}_{(f)}^{-1}$ and $\hat{X}_{(b)}^{-1}$ in powers of the matrix

$$\lambda^2 \bar{G}_f(\lambda) H_{f,b} \bar{G}_b(\lambda)$$

which is bounded for all values of λ . In this way we define a renormalized expansion for $\mathcal{E}_\beta(\tau, U)$ where the interaction strength U is no longer a small parameter. Already the first few terms of the expansion exactly reproduce the asymptotics of $\mathcal{E}_\beta(\tau, U)$ for short and long imaginary times $\tau \leq \beta$. The asymptotics for short times are rather simple, since this corresponds to the weak-coupling limit. The dominant contribution in the long-imaginary-time limit generates the δ function in the operators $\hat{X}_{(f)}$ and $\hat{X}_{(b)}$. It is proportional to τ , while the other terms are of the order of unity. However, the matrix $H_{f,b}$ becomes singular in the limit $\tau \rightarrow \infty$, and diverges linearly along the diagonal. The singular integrals are then treated as principal value integrals and they may cause logarithmically singular corrections to $\mathcal{E}_\infty(\tau, U)$. They are not the most dominant in the limit $\tau \rightarrow \infty$, since the terms proportional to $H_{f,b}^2$ can diverge linearly in τ . Analysing (8) and (9) we find that only two terms, proportional to λ and λ^2 , in the expansion of the integrand in (9) contain $H_{f,b}^2$. The most dominant contribution in the large- τ limit is then given by

$$\begin{aligned} \mathcal{E}_\beta(\tau, U) = & - \int_0^U d\lambda \left(\frac{1}{\tau} \sum_f \bar{G}_f(\lambda) + \frac{1}{\tau} \sum_b \bar{G}_b(\lambda) \right. \\ & \left. - \frac{4\lambda}{\tau^3} \sum_{f,b} H_{f,b}^2 \bar{G}_f(\lambda) \bar{G}_b(\lambda) [2 + \lambda \bar{G}_f(\lambda) + \lambda \bar{G}_b(\lambda)] \right). \end{aligned} \tag{10}$$

The λ integration in the RHS of (10) can be performed explicitly and the sums over Matsubara fermionic and bosonic frequencies can be transformed through contour integration

to integrals over real frequencies. We finally obtain the principal result of the paper:

$$\begin{aligned} \mathcal{E}_\beta(\tau, U) = & 2 \operatorname{Re} I(i0_+) + \frac{8}{\pi\tau} P \int_{-\infty}^{\infty} \frac{dx}{1 + \exp(x\tau)} \frac{1}{x^2} \operatorname{Im} I_+(x + i0_+) \\ & - \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{dx}{1 + \exp(x\tau)} \operatorname{Im} \ln [1 - U\mathcal{G}_f(x + i0_+)] \\ & - \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{dx}{1 - \exp(x\tau)} \operatorname{Im} \ln [1 - U\mathcal{G}_b(x + i0_+)] \end{aligned} \quad (11)$$

where

$$I_+(x + i\eta) := I(x + i\eta) - I(0 + i\eta)$$

and

$$\begin{aligned} I(x + i0_+) = & \frac{1}{2\pi i} P \int_{-\infty}^{\infty} \frac{dx'}{1 - \exp(x'\tau)} \sum_{\sigma} \left\{ \frac{\sigma}{\mathcal{G}_b(x' + i\sigma 0_+) - \mathcal{G}_f(x + x' + i0_+)} \right. \\ & \times \left[4 \left\{ \mathcal{G}_b(x' + i\sigma 0_+) \ln [1 - U\mathcal{G}_f(x + x' + i0_+)] \right. \right. \\ & \left. \left. - \mathcal{G}_f(x + x' + i0_+) \ln [1 - U\mathcal{G}_b(x' + i\sigma 0_+)] \right\} \right. \\ & \left. + U\mathcal{G}_b(x' + i\sigma 0_+) \mathcal{G}_f(x + x' + i0_+) \right. \\ & \left. \times \left(\frac{1}{1 - U\mathcal{G}_f(x + x' + i0_+)} - \frac{1}{1 - U\mathcal{G}_b(x' + i\sigma 0_+)} \right) \right] \Bigg\} \end{aligned} \quad (12)$$

with $\sigma = \pm 1$. The analytically continued fermionic and bosonic functions $\mathcal{G}_f(z)$ and $\mathcal{G}_b(z)$ are defined as

$$\mathcal{G}_f(z) = \frac{1}{2} \left(\tilde{\mathcal{G}}(z) + \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega X(\omega\tau, \omega\beta) \frac{\operatorname{Im} \tilde{\mathcal{G}}(\omega + i0_+)}{\omega - z} \right) \quad (13a)$$

$$\mathcal{G}_b(z) = \frac{1}{2} \left(\tilde{\mathcal{G}}(z) - \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega X(\omega\tau, \omega\beta) \frac{\operatorname{Im} \tilde{\mathcal{G}}(\omega + i0_+)}{\omega - z} \right) \quad (13b)$$

where

$$X(\omega\tau, \omega\beta) := \exp(\omega\tau) / [1 + \exp(\omega\beta)] + \exp(-\omega\tau) / [1 + \exp(-\omega\beta)]$$

and

$$\tilde{\mathcal{G}}(z) := \frac{1}{2} \int_{-\infty}^{\infty} dt \exp(izt) \mathcal{G}_{\infty}(t)$$

is the zero-temperature Green function. Equations (11)–(13) determine the phase shift of the thermal Green function of the local electrons in the Falicov–Kimball model in infinite dimensions. Equation (11) is an approximate solution to (8) and (9) that correctly reproduces opposite asymptotics of short and long imaginary times. Apart from this, it is exact up to U^3 for any τ and β ($\tau \leq \beta$).

We can now analyse the long-time asymptotics of the energy shift $\mathcal{E}_\beta(\tau, U)$. We put $\beta = \infty$ and take the limit $\tau \rightarrow \infty$. This order of limits causes the effective interaction strength U to be reduced by a factor of two ($\mathcal{G}_f, \mathcal{G}_b \rightarrow \bar{\mathcal{G}}/2$). In this long-time limit the first and the last two terms of (11) are of the order of unity and the second term is of the order of τ^{-1} . However, the integral itself diverges logarithmically in the limit $\tau \rightarrow \infty$. We hence have a non-analyticity in the next-to-leading order in the limit of large times. This is precisely the *edge singularity of the MND model* [4]. If we introduce a cut-off ξ in the first integral in the RHS of (10) we obtain an explicit expression for the logarithmically divergent term

$$\begin{aligned} \mathcal{E}^s(\tau, U) = & -(4/\pi^2) \left[\left(U \operatorname{Re}\{\bar{\mathcal{G}}(-i0_+)/[1 - \frac{1}{2}U\bar{\mathcal{G}}(i0_+)]\} \right. \right. \\ & + 2 \operatorname{Re} \bar{\mathcal{G}}(i0_+) \operatorname{Im}\{\ln[1 - \frac{1}{2}U\bar{\mathcal{G}}(i0_+)]\}/\operatorname{Im}[\bar{\mathcal{G}}(i0_+)] \\ & \left. \left. - (U^2/4) \left[\operatorname{Im}\{\bar{\mathcal{G}}(i0_+)/[1 - \frac{1}{2}U\bar{\mathcal{G}}(i0_+)]\} \right]^2 \right) \right] \tau \ln \xi \tau. \end{aligned} \quad (14)$$

Equation (14) determines the logarithmic correction in the limit of large imaginary times. For the x-ray spectra, however, the *real-time* asymptotics are relevant. We cannot directly apply our method to the real-time Green function, since the Fourier coefficients of the function Γ from (5) may not be well defined. Real times can, nevertheless, be reached through an analytic continuation (Wick rotation). Continuing (10) to real times, we obtain for the logarithmic correction for real times $\tau \rightarrow it$. If we put $\bar{\Sigma}_c(\omega) = 0$, we reduce the Falicov–Kimball model to the MND model. Expression (14) differs from the result of Nozières and De Dominicis in all orders of the expansion in U , except for the lowest one, i.e. U^2 . This can be explained by the fact that (14) is not exact, since the logarithmic corrections are only of the next-to-leading order in τ , which is not exactly contained in the solution (11). A separate treatment of the case $\tau = \infty$ is necessary to derive the exact critical exponent. Such an investigation is presently in progress [12].

To conclude, we have presented a new scheme yielding an analytic form for the Green function of the local electrons in the diluted Falicov–Kimball model, the simplest model for the deep-level x-ray spectra with a macroscopic concentration of core electrons. We have proposed a renormalized, systematic expansion for the phase shift of this Green function and constructed a global, approximate formula (11) interpolating between short and long times. We have derived, contrary to the other theories, the edge singularity of the x-ray spectra without any assumption about the form of the propagator of the conduction electrons. Although the critical exponent for the edge singularity did not come out exactly here, the proposed construction enables one to understand the edge singularity in a more general context going beyond the MND model with a single core electron. Especially, in conjunction with the method of Anderson and co-workers [13], it can be used to investigate the existence of the Kondo effect in lattice models.

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References

- [1] Ohtaka K and Tanabe Y 1990 *Rev. Mod. Phys.* **62** 929
- [2] Mahan G D 1967 *Phys. Rev.* **163** 612
- [3] Roulet B, Gavoret J and Nozières P 1969 *Phys. Rev.* **178** 1072
Nozières P, Gavoret J and Roulet B 1969 *Phys. Rev.* **178** 1084
- [4] Nozières P and De Dominicis C 1969 *Phys. Rev.* **178** 1097
- [5] Anderson P W 1967 *Phys. Rev.* **164** 352; *Phys. Rev. Lett.* **18** 1048
- [6] Falicov L M and Kimball J C 1969 *Phys. Rev. Lett.* **22** 997
- [7] Janiš V and Vollhardt D 1992 *Phys. Rev. B* **46** 15712
- [8] See, e.g., Vollhardt D 1993 *Correlated Electron Systems* ed V J Emery (Singapore: World Scientific)
- [9] Metzner W and Vollhardt D 1989 *Phys. Rev. Lett.* **62** 324
- [10] Janiš V 1991 *Z. Phys. B* **83** 227
- [11] Brandt U and Urbanek M P 1992 *Z. Phys. B* **89** 297
- [12] At criticality, $\tau = \infty$, (8) becomes a singular integral equation of the type investigated by Nozières and De Dominicis in [4]. However, the former shows a logarithmic singularity in the frequency representation and the latter in the time representation.
- [13] Anderson P W and Yuval G 1969 *Phys. Rev. Lett.* **23** 89
Yuval G and Anderson P W 1970 *Phys. Rev. B* **1** 1522
Anderson P W, Yuval G and Hamann D R 1970 *Phys. Rev. B* **1** 4464