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The one-dimensional Coulomb glass within the Bethe–Peierls–Weiss approximation

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Abstract. We present a new analytical approach to the Coulomb glass problem in one dimension, using the Bethe–Peierls–Weiss (BPW) approximation. The single-particle density of states (DOS) at zero temperature is calculated analytically; it has a soft Coulomb gap at the Fermi energy. The self-consistency condition used within the BPW scheme influences the calculated DOS. We discuss the two possible limiting cases for the self-consistency condition which give an upper and a lower bound of the DOS. The upper limit yields a DOS similar to that following from the self-consistent equation of Efros ($g(\epsilon) \sim 1/\ln(\epsilon_0/\epsilon)$); the lower limit gives a power-law Coulomb gap near the Fermi energy ($g(\epsilon) \sim \epsilon^{\kappa}$, where κ is proportional to the relative interaction strength). The results are compared with numerical simulation data and with the results of the self-consistent equation of Efros.

1. Introduction

The role of the Coulomb interaction in disordered systems with strongly localized electronic states has been investigated for about 20 years (Pollak 1970, Srinivasan 1971). Although there has been much controversy about this problem, today it is generally accepted that the long-range unscreened Coulomb repulsion between the electrons in localized states reduces the single-particle density of states (DOS) near the chemical potential μ (Efros and Shklovskii 1985, Pollak and Ortuno 1985, Pollak 1992). At zero temperature it is expected that the DOS is zero at the Fermi energy; however, it is finite at every energy different from the Fermi energy. This soft gap is called Coulomb gap. The depletion of single-particle excitations near the Fermi energy certainly influences the transport properties of the of the systems under consideration. Much experimental work (for instance on the hopping conductivity of amorphous or doped semiconductors) deals with this question. However, the results of these investigations are far from providing a coherent picture (Redfield 1973, Tokumoto *et al* 1982, Benzaquen and Walsh 1984, Timp *et al* 1986, White *et al* 1986, Tremblay *et al* 1989, Zhang 1990, Zhang *et al* 1990).

In 1975 Efros and Shklovskii proposed a simple model, the Coulomb glass (or Efros model) which has been the basis for theoretical investigations of the Coulomb

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gap problem until now (Efros and Shklovskii 1975, Efros 1976). It consists of localized electrons at the sites of a lattice which interact via an unscreened Coulomb interaction. Hopping terms between different sites are neglected. The disorder of the system is described by a fluctuating potential at the lattice sites. The Coulomb glass is equivalent to an Ising model with long-range antiferromagnetic interactions in a fluctuating magnetic field (Davies *et al* 1982, 1984). In principle, all eigenstates of the system are known for a fixed configuration of the random potentials. They are characterized by the occupation of the lattice sites. Owing to the interplay between the unscreened Coulomb interaction and disorder, the search for the ground state is a difficult many-particle problem; however, standard many-body methods are not suitable for this problem.

If the Coulomb interaction U_0 between neighbouring sites is large in comparison with the strength W_0 of the fluctuating potential, the ground state is completely 'antiferromagnetic'. However, we are even interested in the opposite situation $W_0 \gg U_0$. In this case the occupation of a site with a small potential depends very sensitively on the configuration of all other sites. Because of the competition between interaction and disorder, frustration occurs.

Efros and Shklovskii used the stability condition of the ground state against single-particle hops to derive a self-consistent equation (SCE) for the single-particle DOS at zero temperature (strictly speaking an equation for an upper bound of the DOS). The equation can be solved analytically close to the Fermi energy. The calculated DOS behaves as $|\epsilon - \mu|^{d-1}$ for the d-dimensional system ($d = 2, 3$). Later the stability of the ground state against many-particle hops was included in the derivation of the SCE (Baranovskii *et al* 1980). Raikh and Efros (1987) applied this equation to the one-dimensional system. The DOS behaves as

$$1/\ln[\epsilon_0/(\epsilon - \mu)].$$

Besides this analytical approach there are several numerical simulations of the Coulomb glass based on the stability of the ground state against single-particle hops (Baranovskii *et al* 1979, Davies *et al* 1982, 1984, Möbius and Richter 1987a, b, Möbius *et al* 1992) or based on the numerical solution of local mean-field equations (Grünewald *et al* 1982, 1983). The numerical simulations confirm the idea of a Coulomb gap in the single-particle DOS but the quantitative results differ from each other.

In this paper we investigate the Coulomb glass within the Bethe–Peierls–Weiss (BPW) approximation (Bethe 1935, Peierls 1936, Domb 1960). This method is a generalization of the mean-field approximation and it is suitable for treating the long-range Coulomb interaction. The Coulomb glass model is introduced in section 2. The BPW approximation scheme is discussed in section 3; the results for the single-particle DOS are presented in section 4. The analytical results are compared with numerical simulation data in section 5. The calculated DOS, the validity of the approximation scheme and possible generalizations are discussed in section 6.

2. The Coulomb glass model

We consider a one-dimensional lattice with a lattice constant a and $\frac{1}{2}$ electron with the charge $-e$ per site. To preserve charge neutrality, each site has a compensating charge $\frac{1}{2}e$.

The Hamiltonian of the one-dimensional Coulomb glass is given by

$$H = \sum_i \varphi_i S_i + \tfrac{1}{2} \sum_{i \neq j} U_{ij} S_i S_j \qquad U_{ij} = \frac{U_0}{|i-j|} \tag{1}$$

where the spin variable $S_i = \pm\frac{1}{2}$ describes the occupation of the site i (with a charge of $\pm\frac{1}{2}e$). The random potentials φ_i are independent of each other; they fluctuate owing to a probability distribution $W(\varphi_i)$. The properties of the Coulomb gap do not depend on the exact form of the distribution, provided that it is only slowly varying near the chemical potential μ (which is zero in our model because it is particle–hole symmetric). We use the probability distribution

$$W(\varphi_i) = \begin{cases} 1/2W_0 & |\varphi_i| < W_0 \\ 0 & |\varphi_i| > W_0. \end{cases} \tag{2}$$

The width W_0 of the distribution is assumed to be large compared with the interaction energy $U_0 = e^2/a$ of nearest neighbours. The single-particle excitation energies ϵ_i are defined by

$$\epsilon_i = \varphi_i + \sum_j U_{ij} S. \tag{3}$$

Because of the interaction terms in equation (3) the excitation energy depends on the occupation of all sites of the system.

The DOS for the single-particle excitations

$$g(\epsilon) = \left(\int \prod_j W(\varphi_j)\, \mathrm{d}\varphi_j \right) \frac{1}{N} \sum_i \langle \delta(\epsilon - \epsilon_i) \rangle \tag{4}$$

is the quantity under consideration in this paper. $\langle \cdot \rangle$ denotes the thermodynamic average for a given configuration of the random potentials. $g(\epsilon)$ is symmetric with respect to the Fermi energy $\epsilon_F = 0$ because the model is particle–hole symmetric.

3. The Bethe–Peierls–Weiss approximation

The BPW approximation (Bethe 1935, Peierls 1936, Domb 1960) is an improvement of the simple mean-field approximation. First it was applied to spin models with short-range interactions and without disorder. In recent years it has also been used to study disordered models with short- and long-range interactions such as spin glasses (Klein *et al* 1979, Schowalter and Klein 1979).

One obtains the BPW Hamiltonian by exactly taking into account the interactions of a spin S_0 (central spin) with all other spins S_i (boundary spins). The boundary spins interact only with an effective mean field. An additional self-consistency procedure for the effective mean fields must ensure that all sites are physically equivalent. The BPW Hamiltonian of the one-dimensional Coulomb glass is given by

$$H_{\mathrm{BPW}} = \varphi_0 S_0 + \sum_{i \neq 0} U_{0i} S_0 S_i + \sum_{i \neq 0} \xi_i S_i \tag{5}$$

with

$$\xi_i = \varphi_i + \sum_{j \neq 0,i} U_{ij} \langle S_j \rangle_i . \tag{6}$$

Now the partition function Z_{S_0} and the conditional thermodynamic means $\langle S_i \rangle_{S_0}$ for a fixed central spin S_0 and for $\mu = 0$ can be calculated exactly by means of the stochastic map method (Rujan 1978, Bruinsma 1983) as a function of the effective fields ξ_i. Within this method, one carries out the sums over the boundary spins (arising in the partition function and the thermodynamic means) and rewrites the cosh terms obtained as exponentials. For the partition function Z_{S_0} we obtain

$$Z_{S_0} = \exp\left\{ -\beta \left[\left(\varphi_0 + \sum_{i \neq 0} A(\xi_i, U_{0i}) \right) S_0 + \sum_i B(\xi_i, U_{0i}) \right] \right\} \tag{7}$$

where the functions A and B are given by

$$\begin{aligned} A(\xi, U) &= (1/\beta) \ln \left\{ \cosh \left[\tfrac{1}{2}\beta(\xi - \tfrac{1}{2}U) \right] / \cosh \left[\tfrac{1}{2}\beta(\xi + \tfrac{1}{2}U) \right] \right\} \\ B(\xi, U) &= -(1/2\beta) \ln \left\{ 4 \cosh \left[\tfrac{1}{2}\beta(\xi - \tfrac{1}{2}U) \right] \cosh \left[\tfrac{1}{2}\beta(\xi + \tfrac{1}{2}U) \right] \right\} . \end{aligned} \tag{8}$$

From (7) it follows that the quantities $A(\xi_i, U_{0i})$ describe the contribution of the boundary sites to the thermodynamic field h_0 of the central spin S_0. Using the definition

$$\langle S_0 \rangle = -\tfrac{1}{2} \tanh \left(\tfrac{1}{2}\beta h_0 \right) \tag{9}$$

we obtain the following equation for h_0:

$$h_0 = \varphi_0 + \sum_{i \neq 0} A(\xi_i, U_{0i}) . \tag{10}$$

We note here that the thermodynamic local field h_0 is different from the single-particle energy ϵ_0. While ϵ_0 describes the change in the system energy if S_0 is flipped and the other spins are fixed, h_0 includes relaxation effects of the other spins if S_0 is flipped.

The probability distribution g_{th} of h_0 may be written as a convolution integral:

$$g_{\mathrm{th}}(h_0) = \int \mathrm{d}\varphi_0 \, W(\varphi_0) \int \prod \mathrm{d}\xi_i \, P(\xi_1, \ldots, \xi_N) \delta \left(h_0 - \varphi_0 - \sum_j A(\xi_j, U_{0j}) \right) \tag{11}$$

where $P(\xi_1, \ldots, \xi_N)$ is the distribution of the effective fields. The conditional thermodynamic means $\langle S_i \rangle_{S_0}$ are given by

$$\langle S_i \rangle_{S_0} = -\tfrac{1}{2} \tanh \left[\tfrac{1}{2}\beta \left(\xi_i + \tfrac{1}{2} U_{0i} \operatorname{sgn} S_0 \right) \right] . \tag{12}$$

In the following we restrict our calculations to the zero-temperature limit. Then the thermodynamic mean (12) becomes the ground-state value of S_i:

$$S_i = -\tfrac{1}{2} \operatorname{sgn} \left[\tfrac{1}{2} \left(\xi_i + \tfrac{1}{2} U_{0i} \operatorname{sgn} S_0 \right) \right] . \tag{13}$$

Using equations (3) and (10) and the definitions

$$\begin{aligned} C(\xi_i, U_{0i}, S_0) &= U_{0i} S_i - A(\xi_i, U_{0i}) \\ C(\xi_i, U_{0i}) &= C\left(\xi_i, U_{0i}, -\tfrac{1}{2}\right) \end{aligned} \tag{14}$$

the single-particle energy ϵ_i may be written in terms of the quantities h_0 and ξ_i:

$$\epsilon_0 = h_0 + \sum_{i \neq 0} C(\xi_i, U_{0i}, S_0). \tag{15}$$

The physical meaning of this equation is as follows. The difference between the single-particle excitation energy and the thermodynamic local field of the site 0—which is the reason for the Coulomb gap—is caused by the spins S_i, which flip when the spin S_0 is flipped. These spins are always antiparallel to S_0, which means that they do not contribute to the thermodynamic field h_0; however, they do contribute to the single-particle excitation energy ϵ_0.

The DOS (4) may be written in the form of a convolution integral:

$$g(\epsilon) = g_{\mathrm{th}}(0) \int_0^{|\epsilon|} \mathrm{d}x \prod_i \left(\int \mathrm{d}\xi_i \right) P(\xi_1, \ldots, \xi_N) \delta\left(x - \sum_i C(\xi_i, U_{0i}) \right). \tag{16}$$

In the following we study the form of the Coulomb gap for $|\epsilon| \ll U_0$. In order to do this we need the probability distribution function $P(\xi_1, \ldots, \xi_N)$ of the effective fields. Within the BPW scheme there is no direct way to derive this distribution function. The only condition which has to be fulfilled by the distribution function $P(\xi_1, \ldots, \xi_N)$ is that the central site and the boundary sites have to be equivalent. Comparing the equations for the single-particle energy ϵ, (equation (4)) and for the effective fields (equation (6)), one may identify ξ with the single-particle excitation energies. On the other hand a comparison of equations (9) and (12) for the thermodynamic mean values of S_0 and S_i shows an equivalence of the effective fields and the thermodynamic field h_0. Within the BPW approximation, one cannot resolve this question; it is typical of mean-field equations (6) that they do not allow one to distinguish between single-particle excitation energies and thermodynamic local fields.

Another important question is whether correlations between the effective fields ξ_i at different sites play an essential role in the calculations. Certainly the assumption that the ξ_i are statistically independent of each other is not strictly valid. The long-range Coulomb interaction prefers antiparallel nearest-neighbour spins and causes correlations between the ξ_i. The contribution of the boundary sites to the thermodynamic field h_0 (equation (10)) is therefore limited to a value of the order of the Madelung energy. Thus the distribution of the thermodynamic field h_0 differs only at the edges from the distribution function of the random potentials, provided that we are in the limit of weak interaction $U_0 \ll W_0$. In particular, $g_{\mathrm{th}}(h_0)$ has no gap and varies only slowly near the Fermi energy $\epsilon_{\mathrm{F}} = 0$. To calculate the asymptotic behaviour of the DOS for $\epsilon \to 0$ we need only the value $g_{\mathrm{th}}(0)$ at the Fermi energy.

How do the correlations influence the calculation of $g(\epsilon)$? Because $C(\xi, U)$ is always positive, correlations cannot strongly influence the results. That is why we assume the ξ_i to be independent of each other in the following calculations of $g(\epsilon)$:

$$P(\xi_1, \ldots, \xi_N) = \prod P(\xi_i). \tag{17}$$

The two possible self-consistency conditions discussed above may be written as $P(\xi) = g_{\mathrm{th}}(\xi)$ (if one identifies the effective fields ξ with the thermodynamic fields h) and $P(\xi) = g(\xi)$ (if one identifies ξ with the single-particle energy ϵ).

4. Single-particle density of states

We have to calculate $g(\epsilon)$ from the convolution integral (16) and equation (17):

$$g(\epsilon) = g_{\mathrm{th}}(0) \int_0^{|\epsilon|} \mathrm{d}x \prod_i \left(\int \mathrm{d}\xi_i \, P(\xi_i) \right) \delta\left(x - \sum_i C(\xi_i, U_{0i}) \right). \tag{18}$$

Because of the symmetry of the problem we restrict the following calculations to the case $\epsilon \geqslant 0$. The function $C(\xi, U)$ is approximately given by

$$C(\xi, U) = \begin{cases} U/2 & |\xi| < U/2 \\ 0 & |\xi| > U/2. \end{cases} \tag{19}$$

Therefore the sites i with $U_{0i} > 2\epsilon$ contribute to $g(\epsilon)$ only if $C = 0$; this means if $2|\xi_i| > U_{0i}$. Thus $g(\epsilon)$ may be written as

$$g(\epsilon) = g_{\mathrm{th}}(0) \prod_{U_{0i} > 2\epsilon} \left(1 - \int_{-U_{0i}/2}^{U_{0i}/2} \mathrm{d}\xi \, P(\xi) \right) \times \int_0^{\epsilon} \mathrm{d}x \prod_{U_{0i} < 2\epsilon} \left(\int \mathrm{d}\xi_i \, P(\xi_i) \right) \delta\left(x - \sum_{U_{0i} < 2\epsilon} C(\xi_i, U_{0i}) \right). \tag{20}$$

The value of the second integral may be estimated by calculating the mean value and the mean square deviation of the integrand. Provided that $P(\xi)$ is constant near the Fermi energy or decreases for $\epsilon \to 0$, the mean is of the order of $\epsilon U_0 P(0)$ or smaller; the mean square deviation is of the order of $\epsilon^2 U_0 P(0)$ or smaller. In the limit of small interaction strength $U_0 P(0) \ll 1$ the second integral therefore yields the value 1. The DOS is now given by

$$g(\epsilon) = g_{\mathrm{th}}(0) \exp\left(\sum_{U_{0i} < 2\epsilon} \int_{-U_{0i}/2}^{U_{0i}/2} \mathrm{d}\xi \, P(\xi) \right). \tag{21}$$

In the following we want to give the results for the single-particle DOS $g(\epsilon)$ for the two possible choices for $P(\xi)$.

If one identifies the distribution $P(\xi)$ with the distribution of the thermodynamic field $g_{\mathrm{th}}(h_0)$ the ξ-integrals may be calculated in a straightforward manner. This yields

$$g(\epsilon) = g_{\mathrm{th}}(0) \exp\left(- \sum_{U_{0i} < 2\epsilon} U_{0i} g_{\mathrm{th}}(0) \right). \tag{22}$$

The sum in equation (22) is essentially a sum $\sum 1/i$ and can be easily calculated. One obtains a power-law Coulomb gap of the single-particle DOS:

$$g(\epsilon) = g_{\mathrm{th}}(0)(2|\epsilon|/U_0)^{\kappa} \qquad (\kappa = 2 g_{\mathrm{th}}(0) U_0, \epsilon \ll U_0). \tag{23}$$

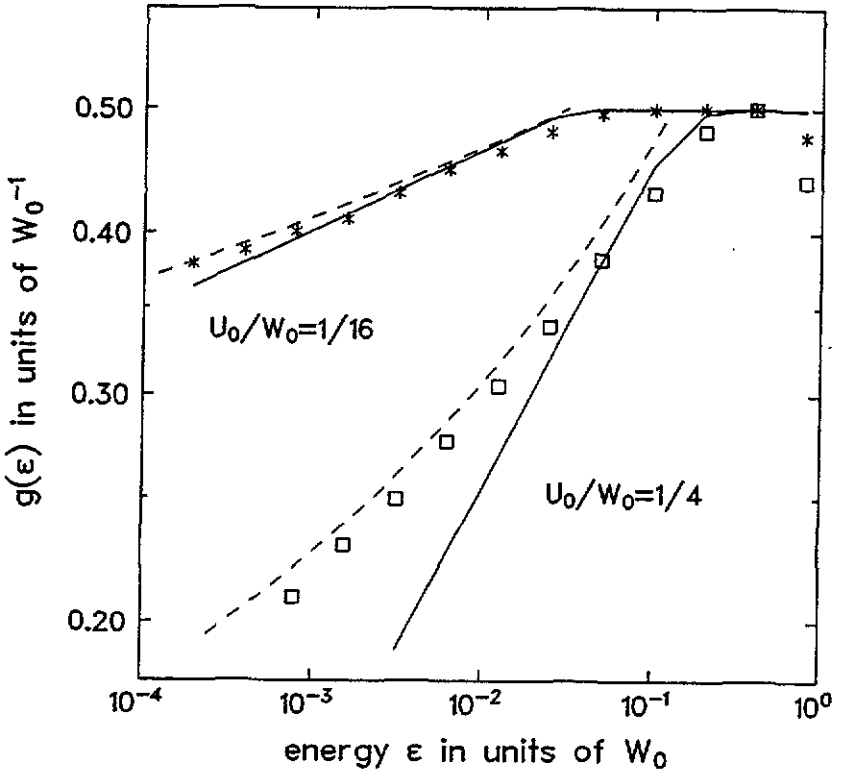

Figure 1. Log–log plot of the single-particle DOS for $U_0/W_0 = \frac{1}{4}$ and $U_0/W_0 = \frac{1}{16}$: ——, power-law Coulomb gap from $P(\xi) = g_{th}(\xi)$; ----, logarithmic gap from $P(\xi) = g(\xi)$; □, *, simulation results.

The other self-consistency condition, which means the identification of P with the single-particle DOS, leads to an integral equation for the DOS:

$$g(\epsilon) = g_{th}(0) \exp\left(- \sum_{U_{0i} < 2\epsilon} \int_{-U_{0i}/2}^{U_{0i}/2} d\epsilon' \, g(\epsilon') \right). \tag{24}$$

Now the sum may be transformed into an integral and the two integrations in the resulting equation are interchanged. Taking the logarithmic derivative with respect to ϵ, one obtains a simple differential equation in the asymptotic case $\epsilon \to 0$:

$$g'(\epsilon)/g(\epsilon) = 2(U_0/\epsilon)g(\epsilon). \tag{25}$$

The DOS has a logarithmic Coulomb gap:

$$g(\epsilon) = (1/2U_0)\,[1/\ln(U_0/2|\epsilon|)] \qquad (\epsilon \ll U_0). \tag{26}$$

Obviously this logarithmic gap is narrower than the power-law gap from above, because a smaller number of boundary spins have effective fields between $-U/2$ and $U/2$ ($P(\xi)$ has a gap near the Fermi energy in this case) and therefore fewer boundary spins contribute to the difference between h_0 and ϵ_0.

The resulting curves are presented in figure 1 for different values of U_0/W_0 together with the results of a numerical simulation of the one-dimensional model. For a detailed discussion of these two results see section 6.

5. Numerical simulation

There are very few numerical simulation data for the one-dimensional lattice model (Möbius and Richter 1987b). Besides that, these simulations are in a parameter region of $U_0/W_0 \sim 1$, where our BPW approximation is not valid. That is why we performed an numerical simulation of the one-dimensional model in the parameter region $U_0/W_0 \ll 1$ by the method first used by Baranovskii *et al* (1979) and recently by Möbius and Richter (1987a, b) and Möbius *et al* (1992).

We use a one-dimensional system with 2500 lattice sites and periodic boundary conditions. The random potentials are chosen independently from the rectangle distribution (2). We start with a random occupation of the lattice sites and then stabilize the system against excitations up to single-particle hops. The single-particle density is calculated from the metastable 'pseudo-ground state' reached in this way. In order to minimize the statistical error, we performed the calculations for 5000 different realizations of the random potentials and averaged the resulting DOSs.

The resulting curves are shown in figure 1. The simulation confirms our analytical calculation; the simulation data are between the two possible analytical results; however, it cannot be decided whether $g(\epsilon)$ follows a power law or a logarithmic law (Möbius and Richter found a logarithmic law in their parameter region).

6. Discussion

We have calculated the single-particle DOS of the one-dimensional Coulomb glass within the BPW approximation scheme. Depending on the self-consistency condition for the effective fields ξ_i we obtain a power-law Coulomb gap $g(\epsilon) \sim \epsilon^{\kappa}$ or a logarithmic gap $g(\epsilon) \sim 1/\ln(U_0/2|\epsilon|)$. It seems that the BPW approximation with the self-consistency condition $P(\xi) = g(\xi)$ is equivalent to the SCE of Efros (1976) and Raikh and Efros (1987), which gives an upper bound of the DOS. Equation (21) allows the same interpretation as the SCE of Efros: the DOS of the 'central' site is reduced if one of the other sites has a small effective field ξ_i. The SCE and our equation (21) yield the same behaviour of the DOS.

The main problem of the BPW scheme used in this paper as well as the SCE of Efros is that correlations between the 'boundary' sites are neglected, because the Coulomb gap is produced by the boundary spins, which flip, when the spin S_0 is flipped. Within our approximation of independent 'boundary fields' ξ_i, these are the spins S_i with $|\xi_i| < \frac{1}{2}U_{0i}$. These spins are always antiparallel to S_0; on the average each of them contributes $\frac{1}{2}U_{0i}$ to the difference between h_0 and ϵ_0. If the interaction between the boundary spins is considered, however, a flip of the central spin S_0 from $-\frac{1}{2}$ to $+\frac{1}{2}$ causes a very complicated relaxation process. Some boundary spins flip from $+\frac{1}{2}$ to $-\frac{1}{2}$; this reduces the effective field of the other boundary spins. That is why some of them flip from $-\frac{1}{2}$ to $+\frac{1}{2}$. Because the several contributions to ϵ_0 may have different signs, this effect should reduce the difference between ϵ_0 and h_0 and

therefore reduce the gap width. However, within the BPW scheme it is impossible to describe such a relaxation process.

Obviously the BPW approximation with the self-consistency condition $P(\xi) = g_{\rm th}(\xi)$ gives a lower approximation of the DOS near the Fermi energy, because on the one hand the distribution of the effective fields has no gap, and therefore many sites have small effective fields and contribute to the difference $\epsilon_0 - h_0$ and because on the other hand the BPW scheme does not account for the correlations that reduce the gap width. These results are confirmed by the numerical simulation of the one-dimensional lattice model. The simulation results for the single-particle DOS are between the two BPW results. It seems that the real physics is between the two limiting cases of the BPW scheme, although the BPW scheme cannot describe the complicated relaxation process discussed above. Discussing this process remains a task for the future.

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