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1990 J. Phys.: Condens. Matter 2 6395

(http://iopscience.iop.org/0953-8984/2/30/005)

J. Phys.: Condens. Matter 2 (1990) 6395–6402. Printed in the UK

The effect of correlation on the mobility edge in random Heisenberg ferromagnets

Jie Yang†, Jue-lian Shen†, Lin Quan†‡ and Pu Fu-Cho†‡
† Institute of Physics, Chinese Academy of Sciences, Beijing, People's Republic of China
‡ Center of Theoretical Physics, CCAST (World Laboratory), Beijing, People's Republic of China

Received 22 August 1989, in final form 5 March 1990

Abstract. The localisation properties of spin waves for Heisenberg ferromagnets with random uniaxial anisotropy energy and random exchange interaction is studied in the framework of the weak localisation theory. The correlation effect is found to influence the phase diagrams near the band edge region strongly.

1. Introduction

The problem of Anderson localisation has received considerable attention in recent years. Important progress has been obtained in understanding the localisation properties of independent electrons in a random potential (Lee and Ramakrishnan 1985). The main features of the electron spectrum in a disordered system is the existence of a mobility edge E_c, which separates extended and localised states. The phase diagrams of the Anderson transition have been studied by various methods. Most researchers have considered the disordered potentials to be completely random at different lattice sites or, equivalently, have assumed the scattering centres to be point like in a disordered impurity model.

Recently, Zhang and Chu (1988) have considered the correlation effect on the Anderson localisation in the vicinity of the band edge. They showed that the direct effects of the correlation on the conductivity and mobility edge are to modify the two-particle vertices and to play an important role in determining the phase diagrams.

In contrast with the large amount of work done on electrons, phonons and photons (see, e.g., Kotov and Sadovskii 1983, Akkermans and Maynard 1984, Golubentsev 1984), little work has been done on the localisation of spin waves. In recent work, Bruinsma and Coppersmith (1986) have studied random Heisenberg ferromagnets within the harmonic approximation. Igarashi (1986) has considered the antiferromagnet case. They have both shown that the localisation problem of a system with a random uniaxial anisotropy energy could be related to the Anderson model for electron localisation and have found that spin waves are localised in the long-wavelength limit, as in the electronic case, in the presence of anisotropy energy, while the random exchange energy does not give rise to the localisation of spin waves in the long-wavelength limit in the absence of anisotropy energy.

0953-8984/90/306395 + 08 $03.50

In this work, we have studied the random Heisenberg model with the consideration of the correlation effect. The correlation enhances the back-scattering effect and results in a variation in the mobility edge. The longitudinal structure factor which changes its form at the mobility edge can be measured via the spin-polarised neutron scattering (Bruinsma and Coppersmith 1986, Serota 1988). The article is organised into two main sections. In section 2 we shall give the model Hamiltonian and the self-consistent equation determining the mobility edge. Results and discussion will be given in section 3.

2. The self-consistent equation

The uniaxial anisotropy Heisenberg model is given by the Hamiltonian

$$H = -\tfrac{1}{2}\sum_{\langle ij\rangle} J_{ij}\boldsymbol{S}_i \cdot \boldsymbol{S}_j - \sum_i D_i(S_i^z)^2 \tag{1}$$

where $\langle ij\rangle$ indicates a sum over pairs of nearest neighbours. The J_{ij} $(=J_0 + \delta J_{ij})$ and D_i $(=D_0 + \delta D_i)$ are random variables, with configurational averages

$$\begin{aligned} &\langle D_i\rangle_{\text{imp}} = D_0 \qquad && \langle \delta D_i \delta D_j\rangle_{\text{imp}} = [\Delta_a/(2S)^2]K(\boldsymbol{R}_i - \boldsymbol{R}_j) \\ &\langle J_{ij}\rangle_{\text{imp}} = J_0 && \langle \delta J_{ij}\delta J_{lm}\rangle_{\text{imp}} = [\Delta_{ex}/(2S)^2]\delta_{il}\delta_{jm} \end{aligned} \tag{2}$$

where S denotes the magnitude of spin and $K(\boldsymbol{R}_i - \boldsymbol{R}_j)$ is the correlation function. It gives a finite value for $\boldsymbol{R}_i \neq \boldsymbol{R}_j$ and becomes a δ-function in the absence of correlations. It corresponds to a structure factor. We exclude negative values of J and D so that the ground state is uniformly ferromagnetically ordered along the z axis at low temperatures.

Using the Holstein–Primakov transformation as

$$\begin{aligned} S_i^z &= S - a_i^+ a_i \\ S_i^+ &= (2S)^{1/2}(1 - a_i^+ a_i/4S)a_i \\ S_i^- &= (2S)^{1/2} a_i^+ (1 - a_i^+ a_i/4S) \end{aligned} \tag{3}$$

and the Fourier transforms of the boson operator a_i defined by

$$a_i = N^{-1/2}\sum_k a_k \exp(\mathrm{i}kR_i)$$

then we get the following expression for the Hamiltonian apart from a constant term:

$$H = H_0 + H_{\text{imp}} = \sum_k \varepsilon_k a_k^+ a_k + \sum_{kk'} V_{kk'} a_k^+ a_{k'} \tag{4}$$

where we have neglected the interaction term and the terms with non-conserving wave-number, and

$$\varepsilon_k = SJ_0 z(1 - \gamma_k) + 2SD_0$$

$$\gamma_k = z^{-1}\sum_\rho \exp(\mathrm{i}k\rho)$$

$$V_{kk'} = 2S[\delta D(k-k') + \delta J(k-k', 0) + \delta J(0, k'-k) - \delta J(k, k') - \delta J(-k', -k)]$$

where z and ρ denote the number of nearest-neighbour sites and the vector for the nearest neighbours; $\delta D(k)$ and $\delta J(k, k')$ are given by

$$\delta D(k) = \frac{1}{N}\sum_i \delta D_i \exp(-ikR_i)$$

$$\delta J(k, k') = \frac{1}{N}\sum_{ij} \exp(-ikR_i)\, \delta J_{ij} \exp(ik'R_j).$$

H_{imp} describes the scattering of spin waves due to the random anisotropy energy and random exchange interaction. In the long-wavelength limit, we get

$$\langle |V_{kk'}|^2 \rangle_{\text{imp}} = (\Delta_a/N)S(k-k') + (\Delta_{ex}/N)T(k, k') \to (\Delta_a/N)S(k') \tag{5}$$

with

$$S(k-k') = \sum_i K(\boldsymbol{R}_i) \exp(-i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}_i)$$

$$T(k, k') = \sum_{\rho} 4[1-\cos(\boldsymbol{k}\cdot\boldsymbol{\rho})][1-\cos(\boldsymbol{k}'\cdot\boldsymbol{\rho})].$$

So the scattering due to random exchange interaction vanishes in the long-wavelength limit. This is also one of the reasons why, in the absence of anisotropy energy, spin waves will be not localised in the long-wavelength limit.

The single-particle quantities are smoothly varying functions of disorder; so the low-order perturbation expression will be used to calculate the single-particle Green function. Within the Born approximation, the self-energy is given by

$$\Sigma^R(k, \varepsilon) = \sum_{k'} \langle |V_{kk'}|^2 \rangle_{\text{imp}} \frac{1}{\varepsilon - \varepsilon_{k'} + i\delta} \simeq \frac{\Delta_a}{N}\sum_{k'} \frac{S(k')}{\varepsilon - \varepsilon_{k'} + i\delta} \tag{6}$$

so that

$$\text{Re}\,\Sigma^R = \Gamma = PV \int \frac{\Delta_a}{N}\frac{S(k')}{\varepsilon - \varepsilon_{k'}} d^3k'$$

$$-\text{Im}\,\Sigma^R = \gamma \simeq \pi(\Delta_a/N)S(0)\rho(\varepsilon) = 1/2\tau.$$

The inclusion of the real part of the self-energy, defined in the simplest approximation as above, will lead to a shift of the band edge due to the interaction with random field. Now we can introduce the averaged single-particle Green function:

$$G(z) = \langle (z - H)^{-1} \rangle_{\text{imp}} = 1/[z - \varepsilon_k - \Sigma_k(z)]$$

with ε_k and $\Sigma_k(z)$ the energy spectrum and the self-energy correction, respectively.

To study the transport properties and localisation problem, our model Hamiltonian can be mapped onto the localisation theory of the electron system of Volhart and Wolfle (1980). Following them, we first consider the Bethe–Salpeter equation for the response function $\varphi^E_{pp'}(\boldsymbol{q}, \omega)$:

$$\varphi^E_{pp'}(\boldsymbol{q}, \omega) = G^R(\boldsymbol{p}+\boldsymbol{q}, E+\omega)G^A(\boldsymbol{p}, E)\left(-\frac{1}{2\pi i}\delta_{pp'} + \sum_{p''}\Gamma^{(i)}_{pp''}\varphi^E_{p''p'}(\boldsymbol{q}, \omega)\right) \tag{7}$$

with $\Gamma^{(i)}_{pp''}$ the irreducible vertex term, and

$$\varphi^E_{pp'}(\boldsymbol{q}, \omega) = -(1/2\pi i)\langle G^R(\boldsymbol{p}_+\boldsymbol{p}'_+, E+\omega)G^A(\boldsymbol{p}'_-\boldsymbol{p}_-, E)\rangle.$$

As shown by Vollhardt and Wolfle (1980), two classes of diagrams are important to

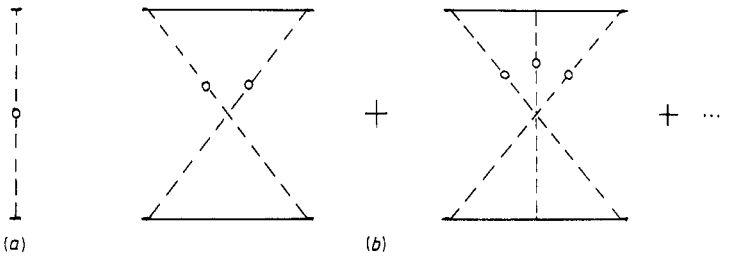

Figure 1. The irreducible vertex diagrams in the momentum representation: (*a*) the Born approximation term; (*b*) the maximally crossed diagrams.

the problem. Figure 1(*a*) comes from the Born approximation. Figure 1(*b*) is the so-called maximally crossed diagrams which are important to the localisation. In the presence of correlation, each interaction line will be attached to a structure factor $S(q)$. To lowest order in the random field, we can consider first the contribution of figure 1(*a*) to the irreducible vertex. In the long-wavelength limit, it becomes

$$\Gamma^{(i)}_{pp'}(\boldsymbol{q}, \omega) \simeq \Gamma_0 = (\Delta_a/N)S(0).$$

By summing the ladder diagrams, we get

$$\sum_{pp'} \varphi^E_{pp'}(\boldsymbol{q}, \omega) = -\frac{1}{2\pi i}\sum_p G^R(\boldsymbol{p}+\boldsymbol{q}, E+\omega)G^A(\boldsymbol{p}, E) \times \left(1 - \Gamma_0 \sum_p G^R(\boldsymbol{p}+\boldsymbol{q}, E+\omega)G^A(\boldsymbol{p}, E)\right)^{-1} = \frac{i\rho(E)}{-i\omega + D_0(E)q^2} \tag{8}$$

where the diffusion constant is given by $D_0(E) = \bar{v}_E^2 \tau(E)$.

For higher-order corrections, the diffusive form of equation (8) still holds just with a change in the diffusion constant $D_0(E)$ by the renormalised $D(\omega, E)$:

$$D^{-1}(\omega, E) = D_0^{-1}(E)\left(1 + \frac{1}{4\pi\rho(E)\gamma(E)\bar{v}_E^2}\sum_{pp'}(\boldsymbol{v}_p \cdot \boldsymbol{q})\,\Delta G_p\,\Gamma^{(i)}_{pp'}\,\Delta G_{p'}\,(\boldsymbol{v}_{p'} \cdot \boldsymbol{q})\right). \tag{9}$$

The main steps of the derivation of equation (9) is given as follows (Vollhardt and Wolfle 1980).

Defining $\Delta G_p = G^R(\boldsymbol{p}+\boldsymbol{k}, E+\omega) - G^A(\boldsymbol{p}, E)$, we obtain

$$[\omega - v_p \cdot q - \Sigma^R_{p_+}(E+\omega) + \Sigma^A_{p_-}(E)]\varphi^E_{pp'}(\boldsymbol{q}, \omega) = \Delta G_p\left(\frac{1}{2\pi i}\delta_{pp'} - \sum_{p''}\Gamma^{(i)}_{pp''}\varphi^E_{p''p'}(\boldsymbol{q}, \omega)\right). \tag{10}$$

Using the Ward identity and summing over p and p' we get the following equation:

$$\omega\varphi^E(\boldsymbol{q}, \omega) - q\varphi^E_j(\boldsymbol{q}, \omega) = -\rho(E) \tag{11}$$

where

$$\varphi^E(\boldsymbol{q}, \omega) = \sum_{pp'}\varphi^E_{pp'}(\boldsymbol{q}, \omega)$$
$$\varphi^E_j(\boldsymbol{q}, \omega) = \sum_{p'}(\boldsymbol{v}_p \cdot \boldsymbol{q})\varphi^E_{pp'}(\boldsymbol{q}, \omega). \tag{12}$$

Expanding $\Sigma_{p'}\varphi_{pp'}$ with respect to the angle of $\boldsymbol{p}$, we get the relation

$$\sum_{p'} \varphi_{pp'}(\boldsymbol{q}, \omega) = [-2\pi i\rho(E)]^{-1}\, \Delta G_p \sum_{p'p''} \left(1 + \frac{(\boldsymbol{v}_p \cdot \boldsymbol{q})(\boldsymbol{v}_{p''} \cdot \boldsymbol{q})}{v_E^2(\boldsymbol{q})}\right) \varphi_{p''p'}(\boldsymbol{q}, \omega) \tag{13}$$

where

$$v_E^2(\boldsymbol{q}) = -\frac{1}{2\pi i\rho(E)} \sum_p (\boldsymbol{v}_p \cdot \boldsymbol{q})^2\, \Delta G_p.$$

By multiplying $\boldsymbol{v}_p \cdot \boldsymbol{q}$ in equation (10) and summing over p and p', we get

$$[\omega + M_E(\boldsymbol{q}, \omega)]\varphi_j^E - (1/d)v_E^2 q \varphi^E = 0 \tag{14}$$

with

$$M_E(\boldsymbol{q}, \omega) = 2i\gamma(E) - \frac{1}{2\pi i\rho(E)\bar{v}_E^2} \sum_{pp'} (\boldsymbol{v}_p \cdot \boldsymbol{q})\, \Delta G_p\, \Gamma_{pp'}^{(i)}(\boldsymbol{q}, \omega)\, \Delta G_{p'}\, (\boldsymbol{v}_{p'} \cdot \boldsymbol{q}) \tag{15}$$

where d is the dimension of the system. By solving equations (11) and (14), we obtain

$$\varphi^E = i\rho(E)/[-i\omega + D(\omega, E)q^2] \tag{16}$$

with $D(\omega, E)$ given by equation (9). In equation (16), E acts as the Fermi energy in the corresponding electron problem.

Near the mobility edge region, one has to consider the back-scattering effect expressed by the maximally crossed diagrams. Summing these diagrams using the time-reversal symmetry, we have

$$\begin{aligned}
\Gamma_{pp'}^{(MCD)}(0, \omega) &= \sum_{p_1 p_2} \left(\frac{\Delta_a}{N} S(p - p_1) + \frac{\Delta_{ex}}{N} T'(p, p', p_1)\right) \\
&\quad \times \left(\frac{\Delta_a}{N} S(p_2 - p') + \frac{\Delta_{ex}}{N} T'(p, p', p_2)\right)(-2\pi i)\varphi_{p_1 p_2}^{(BA)} \\
&\simeq \sum_{p_1} \left(\frac{\Delta_a}{N} S(p - p_1) + \frac{\Delta_{ex}}{N} T'(p, p', p_1)\right) \\
&\quad \times \left(\frac{\Delta_a}{N} S(p_1 - p') + \frac{\Delta_{ex}}{N} T'(p, p', p_1)\right) \sum_{p_2} (-2\pi i)\varphi_{p_1 p_2}^{(BA)}.
\end{aligned} \tag{17}$$

The approximation is made because of the peaked character of the function $\varphi_{p_1 p_2}^{(BA)}$, and

$$T'(p, p', p_1) = \sum_{\rho} [1 - \exp(ip\rho)][1 - \exp(ip'\rho)][1 - \exp(-ip_1\rho)][1 - \exp(ip_1\rho)].$$

It can be shown that this term is much smaller than the first term in the problem of long-wavelength localisation; so we shall neglect this term hereafter. Inserting $\Gamma_{pp'}^{(MCD)}$ into equation (9) and considering the limit $|p + p'| \sim 0$, we have

$$\begin{aligned}
\frac{D}{D_0} &= 1 - \frac{1}{2\pi i\rho(E)\bar{v}_E^4} \sum_{pp'} \left(\frac{\Delta_a}{N}\right)^2 S(p - p')S(p + p')(\boldsymbol{v}_p \cdot \boldsymbol{q})^2 \\
&\quad \times (\Delta G_p)^2(\Delta G_{p'}) \sum_q \frac{1}{(-i\omega/D) + q^2}
\end{aligned} \tag{18}$$

where the sum over q is restricted within $q \leqslant \pi/l_E$. $l_E = \bar{v}_E\tau(E)$, the mean free path.

3. Results and discussion

The actual calculation of localisation properties requires knowledge of spectrum ε_k. In the case of long-wavelength localisation, the mobility edge will be near the bottom of the band. So the effective-mass approximation will be employed to calculate all the integrals. Near the left band edge, the spectrum is given by

$$\varepsilon_k = \varepsilon_0 + k^2/2m^*$$

where $\varepsilon_0 = 2SD_0$ is the gap introduced by anisotropy and $m^* = 1/2SJ_0a^2$, the effective mass. The corresponding momentum cut-off p_c of the integrals is taken as $p_c = \sqrt{3}\pi/2$.

The correlation function $K(\boldsymbol{R}_i - \boldsymbol{R}_j)$ will be considered to be short ranged:

$$K(\boldsymbol{R}_i - \boldsymbol{R}_j) = \exp(-|\boldsymbol{I} - \boldsymbol{R}_j|/\alpha a).$$

Then the structure factor $S(\boldsymbol{q})$ can be approximately divided into two parts:

$$S(\boldsymbol{q}) \simeq 1 + \frac{1}{a^3}\int_{R_0}^{+\infty} \mathrm{d}R \int \mathrm{d}\boldsymbol{R} \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R})\, K(\boldsymbol{R}).$$

The correlation term vanishes when α goes to zero.

To simplify the problem, we treat the density of states approximately in the vicinity of the band edge:

$$\rho(E) = -\frac{1}{\pi}\sum_p \operatorname{Im} G_p^{\mathrm{R}} \simeq \frac{1}{2\pi^2}\int 2m(\varepsilon_p - \varepsilon_0)\delta(E - \varepsilon_p - \Gamma)$$

$$\times \frac{m\mathrm{d}\varepsilon_p}{\sqrt{2m\varepsilon_p}} = \frac{(2m)^{3/2}}{4\pi^2}(E - \varepsilon_0 - \Gamma)^{1/2}. \tag{19}$$

In this way the effect of the real part of the self-energy can be involved from the very beginning. On the other hand, only the weak-scattering limit will be considered here: for $\gamma \ll E$, it is expected that γ smoothly varies near the band edge and is exactly equal to zero at band edge. Hence our approximation is reasonable near the band edge region.

The phase diagrams near the band edge region are given numerically as shown in figure 2 for $\alpha = 0$, 0.3, 0.5, 0.7 and 1.0; the energy scale and the length scale will be taken as $SJ_0 = a = 1$, and the randomness is expressed as $W^2 = \Delta_a$.

We see that direct consideration of the correlation effect has a strong influence on the mobility edge near the band edge region, and the mobility edge deviates from the curve of $\alpha = 0$ (no correlation) further with the increase in correlation. In physics, this means for any given path the coherent back-scattering effect is not limited to the time-reversed path only. All other paths within the correlation region will also contribute to the effect of coherent back-scattering.

The band edge shifted when we considered the self-energy correction Re Σ^{R}, and the mobility edge shifted with the same tendency in small randomness. This is similar to the situation for electrons although the spin waves excited are Goldstone's bosons. Here the random anisotropy energy broke down the rotational symmetry. It is very clear that in the long-wavelength limit the renormalisation effect of the spectrum caused by δJ_{ij} should be zero, and this is just the requirement of Goldstone's theorem. The real contribution to the renormalisation of the spectrum comes only from the random anisotropy energy; it is equivalent to the variation in the gap, and not only is it not equal

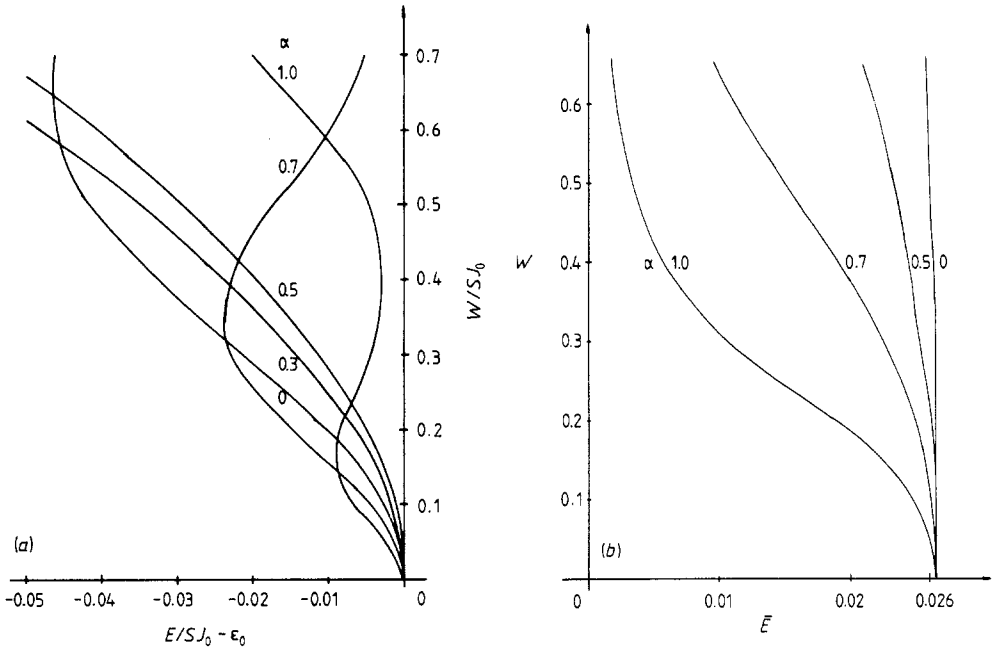

Figure 2. (*a*) Mobility edge curves for $\alpha = 0, 0.3, 0.5, 0.7$ and 1.0. The localisation region is at the left region of the curves. (*b*) The curves are replotted using the shifted and renormalised energy $\bar{E}$; the constant universal value is at $\bar{E}_c = 0.0265$.

to zero in the long-wavelength limit, but also it is W and E dependent. Then the spectrum may have values in the region of $E \leqslant \varepsilon_0$; it can have a 'tail' at the band edge.

The most important contribution of the correlation function $S(p-p')S(p+p')$ comes from the region near the peak position of $(\Delta G_p)^2(\Delta G_{p'})$, which is W and α dependent. When W and α becomes larger, $S(p-p')S(p+p')$ deviates from $S^2(0)$ further, and then it makes the coefficient of W^4 smaller. The trend of the mobility edge is influenced by this effect in some regions; for example, it causes the curve ($\alpha = 1.0$) to bend again in the negative direction on increase in the randomness.

In the 'one-loop' approximation, Kotov and Sadovskii (1984) have considered the effect of Re Σ and Im Σ and have given the variation in band edge due to the real part of the self-energy. We have checked our numerical results based upon the method given by them and find that at small $W(<0.5)$ the two methods give almost the same results.

We have also studied the scaling behaviour of the system in the vicinity of the band edge. Cohen *et al* (1985) have shown that the electronic properties have some universal features in disordered systems near the band edge despite the complexity of real disordered materials. As shown by Zhang and Chu (1988), when the characteristic length, which is about the reciprocal of a typical p, is much greater than the correlation length αa, the problem can be mapped onto the white-noise model (WNM) with $WS(0)$ as the effective disorder strength. So the results can be checked by the WNM. We can express E_c by $\bar{E}_c = (E_c - E_b)/\varepsilon_{03}$, where E_b is the band edge and $\varepsilon_{03} = W^4S^2(0)/(SJ_0)^2$, the energy scale. The curve of the mobility edge E_c can also be replotted using $\bar{E}_c$ as shown in figure 2(*b*), which is consistent with the prediction of the WNM. The universal feature is very marked in small W and α; on increases in W and α, the typical wavelength is no

longer much greater than the correlation length (or the atomic spacing a), and the mobility edge should be described by both W^2 and α independently.

Acknowledgments

The authors express sincere thanks to Professor Zhao-Qing Zhang and Dr Qian-Jin Chu for valuable discussions.

References

Akkermans E and Maynard R 1984 *Phys. Rev.* B **32** 7850–62
Bruinsma R and Coppersmith S N 1986 *Phys. Rev.* B **33** 6541–4
Cohen M H, Economou E N and Soukoulis C M 1985 *Phys. Rev.* B **32** 8268–77
Golubentsev A A 1984 *Zh. Eksp. Teor. Fiz.* **86** 47 (Engl. Transl. 1984 *Sov. Phys.–JETP* **59** 26)
Igarashi Jun-Ichi 1986 *Phys. Rev.* B **35** 5151–63
Kotov E A and Sadovskii M V 1983 *Z. Phys.* B **51** 17–23
Lee P A and Ramakrishnan T V 1985 *Rev. Mod. Phys.* **57** 287–337
Serota R A 1988 *Phys. Rev.* B **37** 9901–3
Vollhardt D and Wolfle P 1980 *Phys. Rev.* B **22** 4666–79; 1982 *Phys. Rev. Lett.* **48** 699–702
Zhang Zhao-Qing and Chu Qian-Jin 1988 *Phys. Lett.* **31A** 517–23