Anisotropic tight-binding model for localization

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The anisotropic tight-binding model, which is defined by a disordered tight-binding Hamiltonian with a transfer-energy-matrix element in the z direction, t, different than the one in the x-y plane is studied using finite-size scaling methods. The dependence of the mobility edge on the strength of anisotropy t ($0 \le t \le 1$) is obtained for the center of the band, $E=0$. Even for very low-t values an appreciable amount of disorder is needed to localize the $E=0$ state. These results are found to be in satisfactory agreement with the predictions of the potential-well analogy, coupled with the coherent-potential approximation.

I. INTRODUCTION

Much of the work on disordered systems has been concentrated on isotropic systems.[1,2] Developments based on the analogy of the localization problem with that of a bound state in a potential well[3] allows us to calculate transport or localization properties[3] such as the position of the mobility edge, localization length, etc., from quantities that can be obtained from mean-field theories such as the Soven-Taylor coherent-potential approximation[4] (CPA). These results, which are based on the approximate scheme of the CPA and the potential-well analogy (PWA), were successfully checked with the most reliable numerical technique based on the transfer-matrix or strip method.[5–10] Impressive agreement has been found for tight-binding disordered systems in two and three dimensions for a rectangular,[3,7,8] Gaussian,[9] and binary[10] probability distribution of the site energy.

Recently, the effects of anisotropy in disordered systems have received considerable attention. This is due to the fact that the newly discovered high-T_c superconductors are highly anisotropic. There is a very strong coupling between the atoms in the plane and very weak coupling t between planes. It is, therefore, appropriate to study the localization behavior of disordered anisotropic systems; in particular, how the mobility-edge trajectory and how different transport or localization properties depend on the strength of the anisotropy t. It is also important to determine whether the scaling theory of localization[11,12] is valid for highly anisotropic systems.

The purpose of the present paper is to make a detailed numerical study of the localization behavior of the disordered anisotropic tight-binding model based on the finite-size scaling methods using the very reliable transfer-matrix finite-scaling technique. We calculate for the center of the band, $E=0$, the mobility-edge trajectory in the W-t plane, where W is strength of disorder and t the anisotropy coupling. For $t=0$ and $t=1$, we obtain the two- and three-dimensional cases, respectively, in agreement with previous results. This trajectory is in excellent agreement with the predictions of the newly developed PWA based on the CPA of the anisotropic tight-binding model.

In Secs. II and III we describe the formalism and the methods of calculation, and in Sec. IV we present and discuss the results. In the final section we summarize the conclusions of this work.

II. MODEL AND POTENTIAL-WELL ANALOGY FOR ANISOTROPIC SYSTEMS

We restrict our attention to a system which can be described with a tight-binding Hamiltonian with only diagonal disorder

$$H=\sum_n |n\rangle \varepsilon_n \langle n| + \sum_{n,m} t_{nm} |n\rangle\langle m| , \tag{2.1}$$

where the sites $\{n\}$ form a regular cubic lattice. The off-diagonal matrix elements $t_{nm} \neq 0$ only for nearest-neighbor sites. We also choose $t_{nm}=t_x=t_y=1$ when both sites n and m lie in the same plane z, and $t_{nm}=t_z=t \le 1$ when both sites n and m lie in the z direction. Thus our system consists of planes weakly coupled in the z direction. Disorder is introduced by choosing random site energies ε_n from a random rectangular probability distribution of width W.

The potential-well analogy[3] is based on the striking analogy in the equations for obtaining localized states in disordered systems and bound states in local potential wells. The mathematical proof of a real mapping of the one problem on the other is still lacking and would be an extraordinary discovery. Based on this analogy, one can immediately infer some of the basic results[1,3] of localization theory of disordered systems such as the fact that for

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$d \leq 2$ all states are localized[11] while for $d > 2$ a mobility edge which separates extended from localized states exists. The PWA coupled with the CPA has been proven[7–10] to be very successful in obtaining the mobility-edge trajectory and localization properties around the metal to insulator (M-I) transition for a number of cases. In the following, we will develop the PWA for anisotropic tight-binding system and establish the criteria for obtaining localized states.

The first-order approximation of the zero-temperature ($T=0$) configurationally averaged conductivity[4] σ_{i0} is given by

$$\sigma_{i0}=\frac{2e^2\hbar}{\pi\Omega}\sum_{\mathbf{k}} v_i^2(\mathbf{k})\langle G_2(E,\mathbf{k})\rangle^2 , \tag{2.2}$$

where $G_2(E)$ is the imaginary part of the Green's function $G(E)=(E-H)^{-1}$, $v_i(\mathbf{k})$ is the ith component of the velocity $\mathbf{v}(\mathbf{k})=dE(\mathbf{k})/\hbar d\mathbf{k}$, and Ω is the volume of the specimen. The maximally crossed diagrams produce a correction to σ_0 of the following form:[4]

$$\frac{\delta\sigma_i}{\sigma_{i0}}=\frac{\sigma_i-\sigma_{i0}}{\sigma_{i0}}=\frac{e^2}{\pi\hbar}\frac{2}{(2\pi)^3}\int d\mathbf{k}\frac{1}{-i\omega(2e^2\rho)+\sum_{i=1}^{3}\sigma_{i0}k_i^2}, \tag{2.3a}$$

where ρ is the density of states per unit cell per spin and the limit $\omega\rightarrow 0$ must be taken. Equation (2.3a) can also be written as

$$\frac{\delta\sigma_i}{\sigma_{i0}}=-\frac{\Omega}{(2\pi)^3}\int d\mathbf{k}\frac{1}{-i\pi\hbar\omega\Omega\rho+\sum_{i=1}^{3}\frac{\pi\hbar\Omega}{e^2}\frac{\sigma_{i0}}{\alpha_i^2}[1-\cos(k_i\alpha_i)]}, \tag{2.3b}$$

where α_i is the effective lattice constant in the i direction and $\Omega=\prod_{i=1}^{3}\alpha_i$. Since our tight-binding model was taken cubic, it is reasonable to assume that our effective lattice is cubic as well so that $\alpha_i=\alpha$, $i=x,y,z$. The quantity α^{-1} introduced through the effective lattice serves as an upper cutoff in the integral of Eq. (2.3a). It was found[3] that α is proportional to the mean free path l:

$$\alpha=C_1 l=C_1\langle v\rangle\tau , \tag{2.4}$$

where τ is the relaxation time, $\langle v\rangle$ is the velocity averaged over the surface $E(\mathbf{k})=\text{const}$ (zero in the present case), and C_1 is a constant equal to 6.70 for the 3D cubic case and 7.07 for the 2D square case.

At the critical value of the disorder that localization first occurs, one has that $\sigma_i(\omega\rightarrow 0)=0$. Therefore, from Eq. (2.3b) we get that

$$1=\frac{\Omega}{(2\pi)^3}\int d\mathbf{k}\frac{1}{\sum_{i=1}^{3}\frac{\pi\hbar\Omega}{e^2}\frac{\sigma_{i0}}{\alpha_i^2}[1-\cos(k_i\alpha_i)]} . \tag{2.5}$$

This expression of the localization condition has exactly the same structure as the equation which determines the critical potential depth ε_c for the appearance of a bound state in a potential well in a tight-binding model defined in the effective lattice with hopping matrix elements $t_i^e=(1,1,t_e)$. For this potential-well problem,[4] we have a bound state when the potential-well depth ε_c satisfies the following equation:

$$1=\frac{\Omega}{(2\pi)^3}\int d\mathbf{k}\frac{1}{2\sum_{i=1}^{3}\left|\frac{t_i^e}{\varepsilon_c}\right|[1-\cos(k_i\alpha_i)]} . \tag{2.6}$$

From Eqs. (2.5) and (2.6), a correspondence can be formally established,

$$\frac{\pi\hbar\Omega\sigma_{i0}}{e^2\alpha_i^2}=2\left|\frac{t_i^e}{\varepsilon_c}\right|=t_i^e C(t_c) , \tag{2.7}$$

where

$$C(t_e)=\left|\frac{2}{\varepsilon_c}\right|=\frac{\Omega}{(2\pi)^3}\int d\mathbf{k}\frac{1}{[1-\cos(k_1\alpha_1)]+[1-\cos(k_2\alpha_2)]+t_e[1-\cos(k_3\alpha_3)]} . \tag{2.8}$$

Taking into account that $\alpha_i=\alpha$ $(i=x,y,z)$ and $t_i^e=(1,1,t_e)$, we obtain from (2.6)

$$\frac{\pi\hbar}{e^2}\alpha\sigma_{x0}=C(t_e) , \tag{2.9}$$

$$t_e=\frac{\sigma_{z0}}{\sigma_{x0}}=\frac{\sigma_{z0}}{\sigma_{y0}} . \tag{2.10}$$

From Eqs. (2.4), (2.9), and (2.10), one can obtain the mobility edge assuming that one can calculate τ, σ_{x0}, σ_{z0}.

III. CPA TREATMENT FOR THE CONDUCTIVITY σ_{i0}

In the weak scattering limit, the static conductivity σ_{i0} is given[3,4] by

$$\sigma_{i0}(E)=\frac{e^2}{\hbar}\frac{1}{4\pi^3}S(E)\left\langle\frac{v_i^2}{v}\right\rangle\tau , \tag{3.1}$$

where $i=x$, y, and z, $S(E)$ is the area of the surface $E(\mathbf{k})=E$, and the average is taken over this surface. Normally $S(E)$ is tedious to calculate, even for the iso-

tropic case of $t=1$. The limiting values of $S(E)$ at the band center $E=0$ are

$$S(E=0)=\begin{cases}92.64 & \text{for } t=1\ ,\\ 111.66 & \text{for } t=0\ .\end{cases} \tag{3.2}$$

However,

$$S(E)\left\langle\frac{v_i^2}{v}\right\rangle$$

can be expressed in terms of the lattice Green's functions. In particular, choosing the lattice constant α_0 as the unit of length, we have

$$S\left\langle\frac{v_x^2}{v}\right\rangle=S\left\langle\frac{v_y^2}{v}\right\rangle =\frac{4(2\pi)^2}{\hbar}[\mathrm{Im}G(E;0,0,0)-\mathrm{Im}G(E;2,0,0)]\ , \tag{3.3a}$$

and

$$S\left\langle\frac{v_z^2}{v}\right\rangle=\frac{4(2\pi)^2}{\hbar}t^2[\mathrm{Im}G(E;0,0,0)-\mathrm{Im}G(E;0,0,2)]\ , \tag{3.3b}$$

where $G(E;l-\mathbf{m})$ is Green's function of the periodic anisotropic tight-binding system. From Eqs. (3.1) and (3.3), we have that

$$t_e=\frac{\sigma_{z0}}{\sigma_{x0}}=t^2\frac{[\mathrm{Im}G(E;0,0,0)-\mathrm{Im}G(E;0,0,2)]}{[\mathrm{Im}G(E;0,0,0)-\mathrm{Im}G(E;2,0,0)]}\ , \tag{3.4}$$

and

$$\langle v\rangle\equiv\left\langle\frac{v_x^2}{v}\right\rangle+\left\langle\frac{v_y^2}{v}\right\rangle+\left\langle\frac{v_z^2}{v}\right\rangle=\left\langle\frac{v_x^2}{v}\right\rangle(2+t_e)\ . \tag{3.5}$$

By combining Eqs. (2.4), (2.9), (3.1), (3.3), and (3.4), we can rewrite the localization criterion in (2.9) in terms of a critical relaxation time τ_c, i.e.,

$$\tau_c^2=\frac{1}{64\pi^2}\frac{S(E)}{C_1}\times\frac{C(t_e)}{(2+t_e)[\mathrm{Im}G(E;0,0,0)-\mathrm{Im}G(E;2,0,0)]^2}\ . \tag{3.6}$$

The relaxation time τ can be calculated through the CPA by utilizing the relation $\tau=0.5\hbar/(\mathrm{Im}\Sigma)$, where Σ is the CPA self-energy obtained by solving the following self-consistent equation:

$$\Sigma=\left\langle\frac{\varepsilon_n}{1-(\varepsilon_n-\Sigma)G(E-\Sigma)}\right\rangle\ . \tag{3.7}$$

For $E=0$, the solution Σ of this equation has no real part. Hence, no shift in energy is taking place. For simplicity, we will concentrate on the band center $E=0$.

When the anisotropy coupling t equals zero, the system is two dimensional and all the states are exponentially localized,[1–4] even for small amounts of disorder.[11] Hence, the critical strength of disorder W_c^* in 2D is equal 0^+. For $t=1$, the numerical techniques as well as the CPA give that $W_c=16.5$ at the center of the band[3], $E=0$. We are interested in finding the behavior of the W_c versus t.

Green's function $G(Z,l-\mathbf{m})$ is explicitly written[4] as

$$G(Z,l-\mathbf{m})=\frac{1}{(2\pi)^3}\int\int\int\frac{\cos[(l_1-m_1)\phi_1]\cos[(l_2-m_2)\phi_2]\cos[(l_3-m_3)\phi_3]}{Z-2\cos\phi_1-2\cos\phi_2-2t\cos\phi_3}d\phi_1 d\phi_2 d\phi_3\ . \tag{3.8}$$

It can be easily shown that

$$\mathrm{Im}G(0;0,0,0)=\frac{1}{2\pi^2}\int_0^\pi K(k)d\phi_3\ , \tag{3.9a}$$

$$\mathrm{Im}G(0;0,0,2)=\frac{1}{2\pi^2}\int_0^\pi\cos(2\phi_3)K(k)d\phi_3\ , \tag{3.9b}$$

$$\mathrm{Im}G(0;2,0,0)=\frac{1}{\pi^2}\int_0^{\pi/2}[-4E(k)+(1+t^2\cos^2\phi_3)K(k)]d\phi_3\ , \tag{3.9c}$$

and

$$C(t_e)=\frac{1}{\pi^2}\int_0^\pi k'K(k')d\phi_3\ , \tag{3.9d}$$

where $k^2=1-t^2\cos^2\phi_3/4$ and $k'=2/(2+t_e-t_e\cos\phi_3)$, and K and E are the complete elliptic integrals of first and second kind, respectively.

In the limit of small coupling $t\to 0$, we obtain the following expressions:

$$\mathrm{Im}G(0;0,0,0)\simeq\frac{2}{\pi}\ln 2-\frac{1}{2\pi}\ln t\ , \tag{3.10a}$$

$$\mathrm{Im}G(0;0,0,2)\simeq-\frac{1}{4\pi}\ , \tag{3.10b}$$

$$\mathrm{Im}G(0;2,0,0)\simeq\frac{2}{\pi}(\ln 2-1)-\frac{1}{2\pi}\ln t\ , \tag{3.10c}$$

$$C(t_e)\simeq\frac{1}{2\pi}\ln\frac{32}{t_e}\ , \tag{3.10d}$$

and

$$t_e\simeq t^2(\ln 2+\tfrac{1}{8}-\tfrac{1}{4}\ln t)\ . \tag{3.10e}$$

Hence in the $t\to 0$ limit, the localization criterion given by Eq. (3.6) becomes

$$\tau_c^2=\frac{S_{2D}(E=0)}{2^{10}C_1\pi}\ln\frac{32}{t_e}\ . \tag{3.11}$$

This is a very interesting result. It shows that the critical relaxation time τ_c and therefore the critical disorder W_c

depend very weakly on the anisotropy coupling t. In other words, even for very small coupling t, i.e., for a quasi-two-dimensional system, a considerable amount of disorder is needed to have all states localized.

IV. NUMERICAL RESULTS

In Fig. 1 we plot the density of states (DOS), of the ordered anisotropic tight-binding model. Notice that as the anisotropy coupling t decreases from its isotropic value of $t=1$, the DOS approaches its 2D value. For $t=1$ the 3D DOS has two Van Hove singularities[4] at $E=2$ and $E=6$, while for $t=0$ the 2D DOS has a square-root singularity at the band edge $E=4$, and a logarithmic singularity at $E=0$. As t decreases from its isotropic value $t=1$, the band edge decreases from its $E=6$ value for $t=1$ to its $E=4$ value for $t=0$, being equal to $4+2t$ for intermediate values. In addition, the Van Hove singularity at $E=2$ for $t=1$ splits into two square-root singularities, one below and one above the $E=2$ value. The singularity below the $E=2$ value eventually becomes, for $t=0$, the logarithmic singularity at $E=0$, while the singularity above the $E=2$ value becomes the square-root singularity at $E=4$. In particular, the singularities are given by $E=2t$, $4-2t$, and $4+2t$.

In Fig. 2, we plot the behavior of the critical relaxation time τ_c as a function of t. τ_c is calculated by using Eq. (3.6). To obtain τ_c, we must know how $S(E=0)/C_1$ changes for different values of t. This is not easy, due to uncertainties in the value of C_1. However, since $S(E=0)/C_1$ equals 13.83 for $t=1$ and 15.79 for $t=0$, we can approximate it by its value for $t=1$ (3D). The limiting behavior of τ_c, for small t, agrees very well with the results obtained from Eq. (3.11).

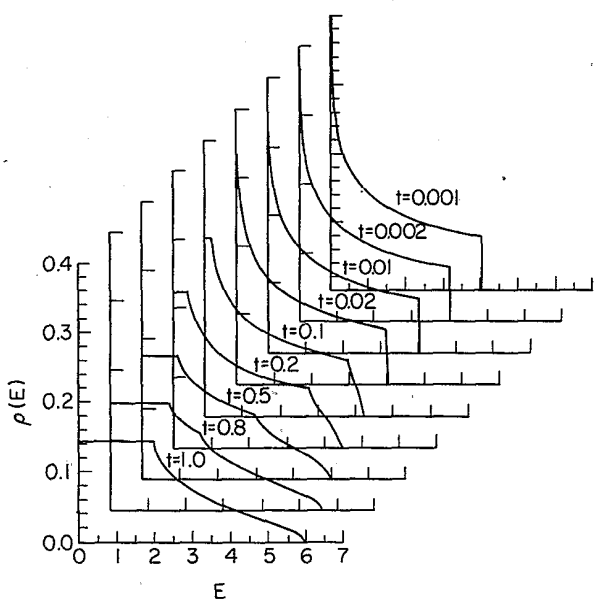

FIG. 1. The density of states $\rho(E)$ vs energy E for different anisotropies t. $t=1$ is the case of a 3D simple-cubic lattice, while $t=0$ is the 2D square lattice case.

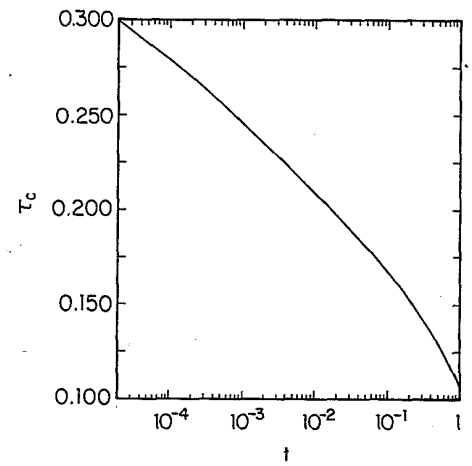

FIG. 2. The critical relaxation time τ_c vs the anisotropy t.

Using the CPA, Eq. (3.7), we numerically calculated the imaginary part Σ_2 of the self-energy at $E=0$ for different values of disorder W. Then the mean lifetime τ is given by $0.5\hbar\Sigma_2^{-1}$. The critical τ_c and thus the critical disorder W_c is obtained by using Eq. (3.6). In Fig. 3, we plot W_c as a function of anisotropy t. Notice that the predictions of our anisotropic CPA together with the PWA, shown as solid triangles, are in excellent agreement with the reliable numerical results, shown as open triangles, of the transfer-matrix finite-scaling method.[5–7]

To treat the anisotropic tight-binding model, using our transfer-matrix method we choose the direction of the longest length N to be along the y direction, while the z axis, with off-diagonal coupling t, is along one of the short directions. Thus, for a given t and for $E=0$, we calculate the largest localization length λ_M of a wire of

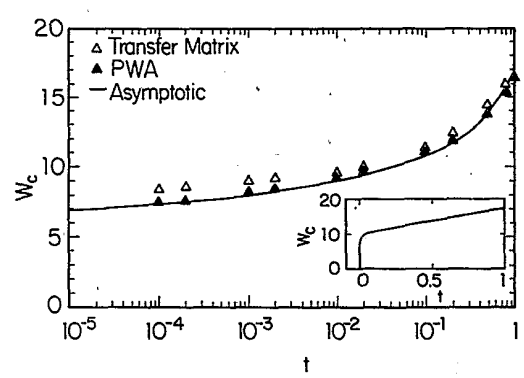

FIG. 3. The critical disorder W_c for obtaining localized states at $E=0$ vs the anisotropy t. Open and solid triangles are the numerical and PWA with the CPA results, respectively. Thick solid line shows the predictions of our asymptotic theory [Eqs. (3.10) and (3.11)]. In the inset, W_c vs t is plotted on a linear scale.

square cross section M^2 and length N as $N \to \infty$. Then from a plot of λ_M versus M, one can determine the localization properties of the system.[5–10] In particular, by studying λ_M/M versus M, one obtains a reasonable estimate of the mobility-edge trajectory shown in Fig. 3. At exactly the mobility edge for $t=1$, $\lambda_M/M=0.6$, while for extended and localized states, we have λ_M/M versus M increases or decreases, respectively. This criterion has been checked by us[8–10] for disordered tight-binding models in isotropic 3D disordered tight-binding models with a rectangular, Gaussian, and binary probability distribution for the site energies. In our study here, we have used $M=2-9$ and $N=6000$.

Plotted also in Fig. 3, as a solid line, is an expression of W_c derived from Eq. (3.6) by further approximations. We have noticed that the expression $(2+t_e)[\mathrm{Im}G(0;0,0,0)-\mathrm{Im}G(0,2,0,0)]^2$ varies less than 2% in the range of $0 \le t \le 1$. We, therefore, can take it as a constant equal to $8/\pi^2$. This approximation has been used in deriving Eq. (3.11). Therefore, using Eq. (3.11) we derive the imaginary part of the critical self-energy, Σ_{2c}. On the other hand, for small t, we expect small W_c and in this case the CPA equation is given by its weak scattering limit

$$i\Sigma_{2c}=\frac{W_c^2}{12}G_0(-i\Sigma_{2c}) , \tag{4.1}$$

where G_0 is the unperturbed Green's function for the two-dimensional square lattice. By this choice, we can fit the numerical data, as well as the more complete form of the anisotropies CPA with PWA. As $t \to 0$, W_c behaves as $|\ln t|^{-1/4}/|\ln|\ln t|^{1/2}|$.

In Fig. 4, we plot the conductivity σ_x versus the strength of the disorder W for three values of t. The conductivity in the other direction is given by $\sigma_z=t_e\sigma_x$. The conductivity σ_x can be calculated[13] from

$$\sigma_i=\frac{\sigma_{i0}}{f(\phi)} , \tag{4.2}$$

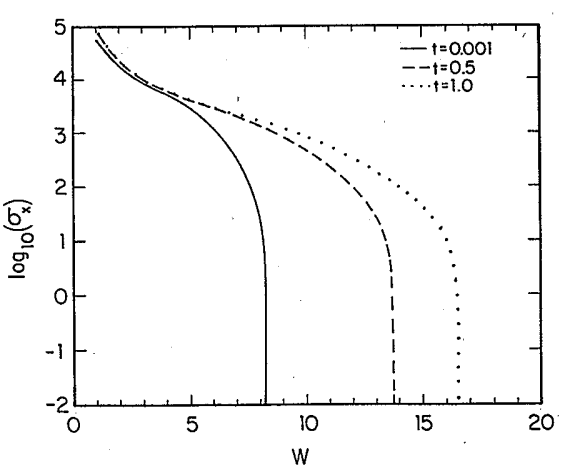

FIG. 4. Conductivity σ_x (in units of $10^{-4}e^2/\hbar a$, where a is the lattice spacing) vs strength of disorder W for the center of the band $E=0$ for different amount of anisotropies t.

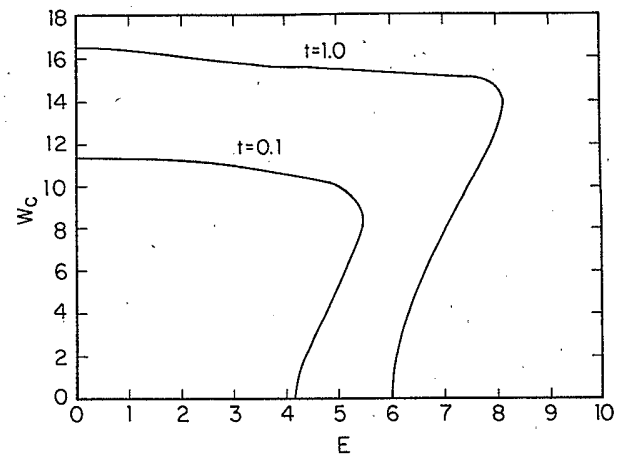

FIG. 5. Dependence of the mobility edge of the strength of the diagonal disorder W_c for two values of the anisotropy t.

for $i=x$, y, and z, where $\phi=\tau^2/\tau_c^2$ and $f(\phi)=1+6/\phi(\phi-1)$. Of course, $\sigma_x=\sigma_y$ and $\sigma_z=t_e\sigma_x$. From Fig. 4, notice that $\sigma_x=0$ if $W \ge W_c(t)$. The results for $t=1$ agree reasonably well with those presented in Fig. 4 of Ref. 13.

Finally, we used the transfer-matrix and finite-scaling method to obtain the mobility-edge trajectory for $t=0.1$ and for all values of E. This is shown in Fig. 5, where the strength of the critical disorder W_c versus E is shown for $t=0.1$. Notice that the shape of the mobility-edge trajectory is similar to that for $t=1$ shown in Fig. 4 of Ref. 8, which has been redrawn in Fig. 5. The $t=0.1$ trajectory is shifted to lower W and E values. For $E=0$, $W_c=11.5$, while for $W \le 1$, $E_c \simeq 4.2$.

V. CONCLUSIONS

This paper demonstrates that the anisotropic PWA developed here, coupled with the CPA, is capable of producing results for quantities such as the conductivity and the mobility-edge trajectory not only in qualitative but in quantitative agreement with independent numerical data. The most striking result of the present study is summarized in Fig. 3, where the dependence of W_c on t is presented. Notice that even for very small anisotropic coupling, $t \simeq 0.001$, the critical disorder W_c needed to localize the $E=0$ state is close to $W \simeq 7$. This is simply due to the fact that the two-dimensional character is very unstable, being approached (as $t \to 0$) very slowly as $|\ln t|^{-1/4}$. In other words, even a very small off-the-plane coupling is enough to destroy the two-dimensional character of the localization.

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