

**Behavior of the thermopower in amorphous materials at the metal-insulator transition**

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We study the behavior of the thermal transport properties in three-dimensional disordered systems close to the metal-insulator transition within linear response. Using a suitable form for the energy-dependent conductivity  $\sigma$ , we show that the value of the dynamical scaling exponent for noninteracting disordered systems such as the Anderson model of localization can be reproduced. Furthermore, the values of the thermopower  $S$  have the right order of magnitude close to the transition as compared to the experimental results. A sign change in the thermoelectric power  $S$  — as is often observed in experiments — can also be modeled within the linear response formulation using modified experimental  $\sigma$  data as input.

**I. INTRODUCTION**

Transport phenomena in disordered quantum systems have been studied for many years,<sup>1,2</sup> yet many open problems remain. One focus of these investigations is the metal-insulator transition (MIT). This quantum phase transition from a good conducting material to an insulator may be induced by disorder due to localization<sup>1</sup> or by interactions such as electron-electron interactions and electron-lattice coupling.<sup>2,3</sup> In three-dimensional (3D) amorphous materials the MIT is mainly attributed to disorder.<sup>1</sup> For example, in heavily doped semiconductors the disorder is brought about by the random distribution of dopant atoms in the crystalline host. However, indications of electron-electron interactions have also been found, e.g., in the dc conductivity  $\sigma$  (or resistivity  $\rho=1/\sigma$ ) in doped semiconductors in both metallic<sup>4</sup> and insulating regimes.<sup>5</sup>

A further open problem is the behavior of the thermoelectric power  $S$  or the Seebeck coefficient of disordered materials near the MIT. In many amorphous alloys and both compensated Si:(P,B) and uncompensated Si:P,  $S$  continuously changes from negative to positive values or vice versa at low temperature  $T$ . This corresponds to a change of thermal conductors from electrons to holes or conversely and has been attributed to the electron-phonon interaction in amorphous alloys.<sup>6,7</sup> On the other hand, in heavily doped semiconductors the sign change is believed to be caused by electron-electron interactions (in uncompensated Si:P in the insulating regime<sup>5</sup>) or attributed to the existence of local magnetic moments and their interactions with electrons.<sup>8,9</sup> This conclusion is based on the suppression of the anomalous behavior by a magnetic field.<sup>8,9</sup> We note that the sign change in  $S$  is also observed in metals, high- $T_c$  materials, and quasicrystals.<sup>10–12</sup> Analytical treatments of metals as a degenerate free-electron gas taking into account inelastic scattering with phonons<sup>13–15</sup> as well as numerical considerations incorporating electronic correlations in superconductors<sup>16</sup> have also been shown to generate a sign change in  $S$ . But in these systems the sign change occurs at a  $T$  value that is 2 orders of magnitude higher than that in disordered systems.

Note that  $S$  is mainly due to two distinct effects: (i) the diffusion of the charge carriers and (ii) the net momentum transfer from phonons to carriers.<sup>17</sup> But for  $T<0.3$  K as considered in this work, the diffusive part of the thermopower dominates that of the phonon-drag contribution.<sup>17,18</sup> Hence, from this point on in this paper  $S$  denotes only the diffusion thermopower.

The prototype for a theoretical description of 3D disordered systems is the Anderson model of localization.<sup>19</sup> Near the MIT at  $T=0$ ,  $\sigma$  behaves as<sup>20</sup>

$$\sigma_c \propto \begin{cases} \sigma_0 \left| 1 - \frac{E_F}{E_c} \right|^\nu, & |E_F| \leq E_c, \\ 0, & |E_F| > E_c, \end{cases} \quad (1)$$

where  $E_F$  is the Fermi energy,  $E_c$  is the mobility edge that separates the extended conducting states from localized insulating states,  $\sigma$  is a constant and  $\nu$  is a universal critical exponent.<sup>1</sup> By using Eq. (1) for  $\sigma$  in a linear response formulation the behavior of the thermoelectric transport properties such as  $S$  (Refs. 21–24), the thermal conductivity  $K$  (Refs. 22–24), and the Lorenz number  $L_0$  (Refs. 23 and 24) at the MIT have been computed. Moreover, similar to  $\sigma$ , the quantities  $S$ ,  $K$ , and  $L_0$  have also been found to obey scaling.<sup>25</sup> The scaling form of the dynamical conductivity  $\sigma$  close to the MIT in 3D is given as<sup>2,26–28</sup>

$$\frac{\sigma(t, T)}{T^{1/z}} = \mathcal{F}\left(\frac{t}{T^{1/\nu z}}\right). \quad (2)$$

Here  $t$  measures a dimensionless distance from the critical point, such as  $t=(E_F-E_c)/E_c$ , the correlation-length exponent  $\nu$  in 3D is equivalent to the conductivity exponent as given in Eq. (1), and  $z$  is the dynamical exponent.<sup>2</sup> For a noninteracting system such as the Anderson model, one expects  $z=d$  in  $d$  dimensions.<sup>2</sup> But, instead of obtaining  $z=3$  in the scaling form of  $\sigma$ , one finds  $z\nu=1$ .<sup>21,24,25</sup> In addition to this discrepancy,  $S$  turns out to be at least one order of magnitude larger<sup>23,24</sup> than the experimental results in doped semiconductors<sup>9</sup> and in amorphous alloys.<sup>6,7</sup> Furthermore, the sign change in  $S$  cannot be explained using the Anderson

model and Eq. (1). One may argue that the discrepancies between the transport calculations and the experimental measurements are due to the absence of interactions in the Anderson model. Indeed, interactions may influence the behavior of the thermoelectric transport properties. Yet we emphasize that the neglect of interactions in the Anderson model is not entirely inconsistent with the experimental situation in 3D amorphous materials.<sup>29</sup> For example, recent measurements in Si:P yield  $\sigma$  scaling with  $z \approx 3$  and  $\nu \approx 1$ .<sup>30</sup> This agrees with  $z = d$  as predicted by the scaling arguments<sup>2,26</sup> for noninteracting systems.

The goal of this paper is to show that the correct value of  $z$ , the right order of magnitude of  $S$  at the MIT, and perhaps even the sign change in  $S$  at low  $T$  can be described within a linear response formulation using the noninteracting Anderson model of localization. However, in order to do so, we have to use a more suitably chosen energy-dependent  $\sigma_c$  instead of Eq. (1). After a brief review of linear transport theory, we construct a new form for  $\sigma_c$  as a function of energy  $E$  and  $T$  from experimental data. By using this model data as input for the linear response formulation, we compute the temperature dependence of  $S$ ,  $K$ ,  $L_0$ , and also  $\sigma$  and show that they have the expected qualitative and quantitative behavior close to the MIT. Finally, we show that a small variation in  $\sigma_c(E, T)$  can change the sign of  $S$ . This effect cannot be produced simply by varying the density of states  $\varrho$  or the chemical potential  $\mu(T)$ .

## II. LINEAR THERMOELECTRIC TRANSPORT THEORY

In the presence of a small temperature gradient  $\nabla T$ , the electric current density  $\langle \mathbf{j}_1 \rangle$  and the heat current density  $\langle \mathbf{j}_2 \rangle$  induced in a system are given (to linear order) as

$$\langle \mathbf{j}_i \rangle = |e|^{-i} (|e| L_{i1} \mathbf{E} - L_{i2} T^{-1} \nabla T), \quad (3)$$

where  $e$  is the electron charge and  $\mathbf{E}$  is the induced electric field.  $L_{ij}$  are the kinetic coefficients. Since we do not consider the presence of a magnetic field in this work, the Onsager relation  $L_{ij} = L_{ji}$  holds.<sup>31</sup> Ohm's law,  $\langle \mathbf{j}_1 \rangle = \sigma \mathbf{E}$ , implies  $\sigma = L_{11}$  in Eq. (3).

The flow of thermal conductors due to  $\nabla T$  is counteracted by an electric force arising from  $\mathbf{E}$  making  $\langle \mathbf{j}_1 \rangle = \mathbf{0}$ . Equation (3) then yields the thermoelectric power  $S = L_{12}/|e|TL_{11}$ , which relates  $\nabla T$  to  $\mathbf{E}$ . The sign of  $S$  determines whether the thermal carriers are electrons or holes. Using the Sommerfeld expansion for  $|E_F - E_c| > k_B T$ ,  $S$  is given by the Mott formula<sup>32</sup> as  $S = -\pi^2 k_B^2 T \sigma'(E_F)/3|e|\sigma(E_F)$ , where  $k_B$  is Boltzmann's constant,  $\sigma'$  is the derivative of  $\sigma$  with respect to  $E$ , and  $\sigma(E)$  is assumed to be a slowly varying function on the scale of  $k_B T$ .<sup>21,22,24,33,34</sup>

The thermal conductivity  $K$  determines the contribution to  $\langle \mathbf{j}_2 \rangle$  stemming from  $\nabla T$ . Using  $\sigma$  and  $S$  in  $\langle \mathbf{j}_2 \rangle$  we obtain  $K$  in terms of the kinetic coefficient as<sup>23,24</sup>

$$K = \frac{L_{22}L_{11} - L_{21}L_{12}}{|e|^2 TL_{11}}. \quad (4)$$

For the definition of the Lorenz number follows  $L_0 \equiv e^2 K/k_B^2 \sigma T$ .<sup>23,24</sup> In metals at room  $T$ ,  $L_0 = \pi^2/3$ .<sup>34</sup> It also

takes on the same value at  $T \lesssim 10$  K in metals where the electrons suffer no inelastic scattering processes.<sup>34</sup>

The primary consideration then in determining  $\sigma$ ,  $S$ ,  $K$ , and  $L_0$  is to calculate  $L_{ij}$ . Under the assumptions that the system is noninteracting and inelastic scattering processes are absent,  $L_{ij}$  are given in the Chester-Thellung-Kubo-Greenwood formulation<sup>35-37</sup> as

$$L_{ij} = \int_{-\infty}^{\infty} A(E) [E - \mu(T)]^{i+j-2} \left[ -\frac{\partial f(E, \mu, T)}{\partial E} \right] dE, \quad (5)$$

for  $i, j = 1, 2$ , where  $\mu(T)$  is the chemical potential,  $f(E, \mu, T)$  is the Fermi distribution function, and  $A(E)$  contains all the system-dependent features.

Last, we note that the  $T$  dependence of  $\mu$  can be obtained for noninteracting systems from

$$n(\mu, T) = \int_{-\infty}^{\infty} dE \varrho(E) f(E, \mu, T) \quad (6)$$

where  $n$  is the number density of electrons and  $\varrho$  is the density of states.<sup>34</sup> In the 3D Anderson model of localization,  $\varrho$  has been computed previously.<sup>24</sup> Thus keeping  $n$  constant, we find numerically<sup>24</sup> that  $\mu(T) \sim T^2$  with an increased effective mass due to the disorder as expected for noninteracting Fermi systems.<sup>34</sup>

## III. A PHENOMENOLOGICAL APPROACH

There are only two parameters that are model dependent in the transport theory discussed in Sec. II. These are  $A(E)$  and  $\mu(T)$ . In order to determine the behavior of the thermoelectric transport properties close to the Anderson MIT,  $A(E)$  in Eq. (5) has usually been set<sup>21-24,33</sup> equal to the critical behavior of  $\sigma$  given by Eq. (1). As mentioned in the Introduction, this leads to the unphysical value for  $z = 1/\nu$  and therefore an unphysical frequency and  $T$  dependence of  $\sigma$ . The main reason for this behavior is easily understood: there is no  $T$  dependence in Eq. (1) and consequently all  $T$  dependence in  $\sigma$  is due to the broadening of the Fermi function in Eq. (5) with increasing  $T$ . Thus in order to model the correct  $T$  dependence, we should add to Eq. (1), valid at  $T = 0$ , the desired  $T$  dependencies such as  $\sigma \propto T^{1/z}$  in the metallic and  $\sigma \propto \exp(-T)$  in the insulating (say, variable-range-hopping) regimes.<sup>38,39</sup> Such a purely theoretical model for  $\sigma_c(E, T)$  will then incorporate a multitude of constants that can be adjusted to fit the experimental results. Of course this is of limited practical use since the validity of these fitting parameters is hard to justify.

Here we will instead use as input for  $\sigma_c(E, T)$  recent *experimental* data obtained by Waffenschmidt *et al.*,<sup>30</sup> who measured  $\sigma$  in Si:P at the MIT under uniaxial stress. Their data yield good scaling of  $\sigma$  according to Eq. (2) with a dynamical exponent  $z = 2.94 \pm 0.3$  and  $\nu = 1 \pm 0.1$ . These values agree with the scaling arguments<sup>2,26</sup> and reasonably well with the numerical results<sup>40-42</sup> for noninteracting systems. We emphasize that it is—in principle—unimportant whether the scaling has been achieved by stress-tuning or other variations of the effective disorder content in the material. Indeed, theoretical studies in anisotropic Anderson models have shown<sup>41,42</sup> that the critical properties remain unaffected by the anisotropy (or stress). Therefore, we expect that while nonuniversal properties such as the numerical values of  $\sigma$ ,  $S$ , etc., may differ according to the material considered in a

particular experiment, the universal properties such as the critical exponents and the scaling behavior should be as discussed here.

In the  $\sigma(t, T)$  scaling of Ref. 30,  $t = (s - s_c)/s_c$ , where  $s$  is the stress and  $s_c$  the corresponding value at the transition. We sample those scaled data for several values of  $(t, T)$  and fit a spline curve<sup>43</sup>  $\sigma_c$  to these points in order to get a smooth functional form for  $\sigma(t, T)$ . Transforming the spline  $\sigma_c$  as a function not only of  $T$  but also of  $E$ , we set  $t = (E - E_c)/E_c$ . Finally, we substitute  $\sigma_c(E, T)$  for  $A(E)$  in Eq. (5) and compute the thermoelectric transport properties defined in Sec. II.

In this paper we consider temperatures from 0.01 K to 0.2 K. Far from the transition we could not probe lower than  $T < 0.02$  K. This is due to the limited input data and consequently a limited range of the spline function that generated  $\sigma_c(E, T)$ . The unit of  $\sigma_c$  is taken as  $\Omega^{-1} \text{ cm}^{-1}$  consistent with the experiments. The  $E$  scale is (arbitrarily) fixed at 1 meV, which is the order of magnitude of the binding energy of an isolated donor in a heavily doped semiconductor.<sup>5</sup> In order to compare with the previous results in the Anderson model<sup>24</sup> we let  $E_c = 7.5$ . We emphasize that this value is of no significance and can be assigned (nearly) arbitrarily. The important point to consider is the location of the Fermi energy  $E_F$  with respect to  $E_c$ . This distinguishes the electronic regimes. Thus, the metallic, critical, and insulating regimes are identified as  $|E_F| < E_c$ ,  $E_F = E_c$ , and  $|E_F| > E_c$ , respectively. Usually,  $\mu(T)$  is derived in Eq. (6) from  $\rho$  of the 3D Anderson model of localization. In the next section we shall also show the effect of using a different functional form of  $\mu(T)$ .

#### IV. RESULTS AND DISCUSSIONS

##### A. Temperature dependence of the thermoelectric transport properties

Consistent with the dynamics of the experiment in Ref. 30, we expect  $\sigma(T) \sim T^{1/z}$  at the critical regime with  $z \approx 3$ . This is indeed the behavior of  $\sigma(T)$  close to  $E_c$  as we show in Fig. 1. For  $|E_F - E_c| \leq 0.2$  meV we obtain  $z = 3.2 \pm 0.3$ . Note that  $\sigma(T) = L_{11}$  has been integrated according to Eq. (5) over the energy range where  $\partial f / \partial E \geq 10^{-20} \text{ meV}^{-1}$ . Thus our numerical calculation of  $\sigma$  is consistent since it reproduces closely the original result in Ref. 30. If we plot the results in Fig. 1 with respect to  $(\mu - E_c)/E_c T^{1/z}$  we obtain a rough scaling of  $\sigma$  similar to Fig. 4 of Ref. 30.

We next turn our attention to the thermoelectric power  $S$ . In the 3D Anderson model of localization, we know that when using Eq. (1) one obtains  $S \rightarrow 0$  in the metallic regime<sup>21,24,33</sup> while in the insulating regime  $S$  does not approach zero but seems to diverge as  $T \rightarrow 0$ .<sup>24,25</sup> At the MIT  $S$  is a constant<sup>21</sup> of the order of 100  $\mu\text{V/K}$ .<sup>23,24,44</sup> In Fig. 2, we show that in the present approach  $S$  in the vicinity of the MIT is two orders of magnitude smaller compared to these previous results for the Anderson model. The magnitude of  $S$  is in fact comparable to the experimental results in disordered systems.<sup>6,7,9</sup> Furthermore,  $S \rightarrow 0$  as  $T \rightarrow 0$  in the metallic, critical, and insulating cases. This behavior of  $S(T)$  in all electronic regimes was observed<sup>6,45</sup> in amorphous  $\text{Au}_x\text{Sb}_{1-x}$  and in amorphous  $\text{Ge}_{1-x}\text{Au}_x$ . As indicated by the different

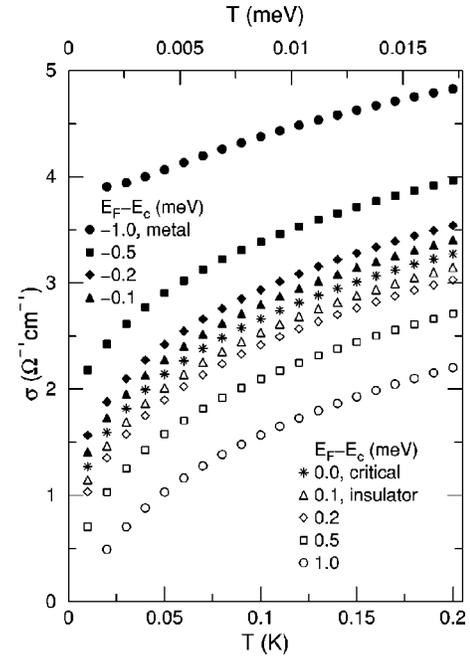


FIG. 1. Numerical calculations for the electrical conductivity  $\sigma$  as a function of temperature  $T$ . The filled symbols represent the metallic regime  $|E_F| < E_c$ , \* denotes the critical regime  $E_F = E_c$ , and the open symbols represent the insulating regime  $|E_F| > E_c$ .

lines in Fig. 2,  $S$  is in good agreement with the Mott formula since  $\sigma$  in Fig. 1 is smooth across the transition at finite  $T$ . Note that in order to evaluate the Mott formula properly for the system considered here, the  $E$  dependence of the input spline  $\sigma_c(E, T)$  was used instead of  $\sigma(T)$  from Fig. 1. We emphasize that it is no contradiction that  $S$  is positive here but mainly negative in the doped semiconductors in all electronic regimes. In the energy regions close to  $E_c > 0$  the charge carriers are holes instead of electrons as shown in

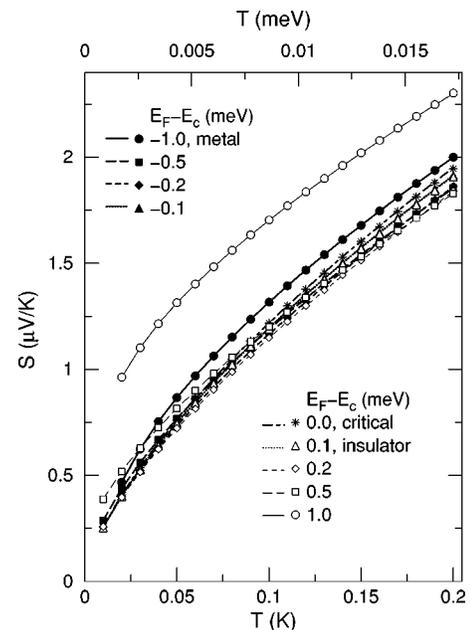


FIG. 2. The thermopower  $S$  as a function of  $T$  with the same symbols as in Fig. 1 distinguishing the metallic, critical, and insulating regimes. The lines are obtained from the Mott formula.

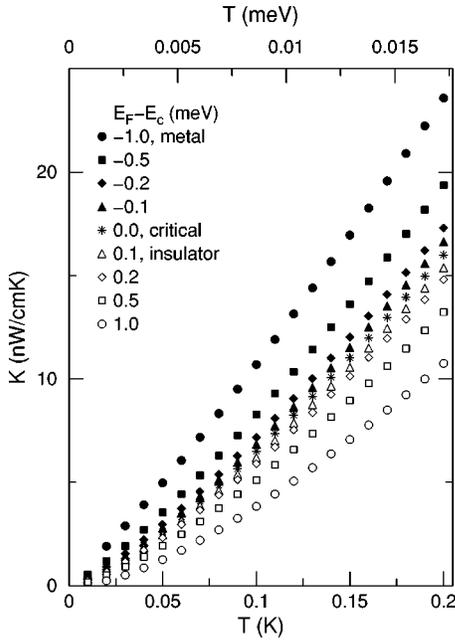


FIG. 3. The  $T$  dependence of the thermal conductivity computed with Eq. (4).

Ref. 24.  $S$  would be negative if we had chosen the left mobility edge  $E_c < 0$  for low filling.<sup>24,46</sup>

The corresponding  $T$  dependence of  $K$  is shown in Fig. 3. We find that  $K \rightarrow 0$  as  $T \rightarrow 0$  in all electronic regimes. This is also the behavior of  $K$  using  $\sigma_c$  in Eq. (1).<sup>24</sup> In the metallic regime  $K$  is larger than in the insulating regime since there are more heat carriers in the former. From the results of  $\sigma$  and  $K$  in Figs. 1 and 3, respectively, we obtain  $L_0$ . As shown in Fig. 4,  $L_0 \rightarrow \pi^2/3$  as  $T \rightarrow 0$  whether it be in the metallic, critical, or insulating regime. This is different from the results using Eq. (1) for  $\sigma$ . There one obtains an  $L_0$  that depends on the conductivity exponent in the critical and insulating regimes while it approaches the universal value<sup>34</sup>  $\pi^2/3$

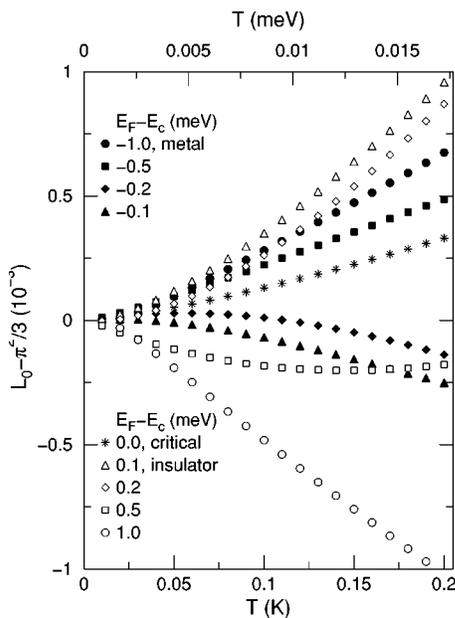


FIG. 4. The Lorenz number  $L_0$ . The results are shifted by  $\pi^2/3$ , the universal value for metals (Ref. 34).

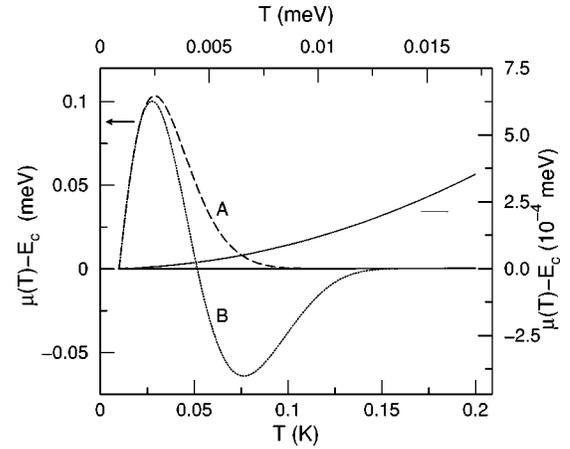


FIG. 5. Comparison between modified (dashed and dotted lines) and unmodified (solid lines) chemical potentials. The curves are shifted with respect to the mobility edge. The thin solid line is the unmodified  $\mu$  shown on a finer (right) scale.

only in the metallic regime.<sup>24</sup> Here we see no markedly distinct behavior in the metallic regime compared to the insulating regime. For  $|E_F - E_c| = 0.1, 0.2$  meV,  $L_0$  in the metallic regime is less than its corresponding value in the insulating regime. For  $|E_F - E_c| = 0.5, 1.0$  meV,  $L_0$  in the metallic regime is larger than its corresponding value in the insulating regime.

In the calculation of  $\sigma(T)$ ,  $S(T)$ ,  $K(T)$ , and  $L_0(T)$ , we used a phenomenological construction of  $\sigma_c(E, T)$ . Furthermore, we have assumed that the density of states  $\varrho$  is the same as that of the 3D Anderson model of localization given in Ref. 24. Since this  $\varrho(E)$  is a smooth and (restricted to  $E > 0$ ) monotonic function,  $\mu(T)$  obtained from Eq. (6) is also smoothly and monotonically varying with  $T$  as described in Sec. II.

### B. Effects of a structured $\varrho$

We now consider the effects of a possible structure in  $\varrho$ . We shall assume here that this structure corresponds only to variations in  $\mu(T)$  and not in  $\sigma$ . In Fig. 5 we show two examples of a modified  $\mu(T)$  in the critical regime. Example A has a pronounced maximum, while example B has both a maximum and a minimum. The height of the maximum in both examples A and B is  $\approx 0.1$  meV. Note that this is significantly larger than the half-width of the bump, which is  $\leq 0.005$  meV. This is also true for the depth of the minimum in example B. Thus a small change in  $T$  corresponds to a large change in  $\mu(T)$ . Applying these forms of  $\mu(T)$  together with Eq. (1) for  $\sigma$  reproduces the same structures in  $S$ . For example, using form B of  $\mu(T)$  we obtain an  $S$  having both a maximum and a minimum in the same  $T$  interval as  $\mu(T)$ . But  $S$  is still of the order of 100  $\mu\text{V/K}$ , while the variations are only of the order of 10  $\mu\text{V/K}$  and not large enough to cause a sign change in  $S$ . On the other hand, using the phenomenological construction of  $\sigma_c(E, T)$  yields even smaller changes. We observe variations in  $L_{11}$  and  $L_{12}$  of less than 10% from their unmodified values. Consequently, we find negligible changes in  $S$ . Figure 2 would appear unmodified. Hence we conclude that even a large change in the density of states  $\varrho$  and thus also in  $\mu(T)$  is not sufficient to

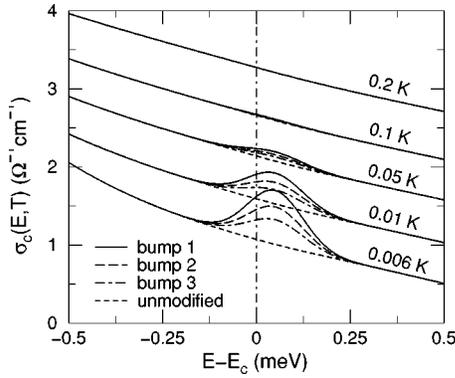


FIG. 6. The modified  $\sigma_c(E, T)$  as input having increasing bumps with decreasing  $T$  centered near at  $E - E_c = 0.05$  meV. For clarity only selected isotherms are shown. The vertical line indicates the mobility edge.

cause the change of sign for  $S$  as observed in the experiments. Nevertheless, this weak dependence of  $S$  on  $\varrho$  and  $\mu(T)$  at least justifies our use of the simple Anderson density of states in the present paper.

### C. Effects of a structured $\sigma(E)$

Let us now assume that for small  $T$  there are nonmonotonocities in  $\sigma_c(E, T)$ —although these have not been observed in the experiments.<sup>6,7,9</sup> Thus we consider the case when there is a sizable change in  $\sigma_c(E, T)$  in the region close to  $E_c$  for small  $T$ . The corresponding “bumps” in  $\sigma_c(E, T)$  are shown in Fig. 6 with different peak heights and with half-widths  $< 1$  meV. For simplicity they are essentially quadratic functions of  $E$  and have been generated such that they decay quickly as  $\exp(-T^4)$  with increasing  $T$ . The height of the bumps is  $< 1 \text{ } \Omega^{-1} \text{ cm}^{-1}$ , which is at least an order of magnitude smaller than the values observed for  $\sigma$  in the measurements.<sup>6,30</sup> The lowest temperature studied is  $T = 6$  mK and we shall only consider metallic and insulating regions with  $|E_F - E_c| \leq 0.1$  meV.

Our results in Fig. 7 using  $\sigma_c(E, T)$  with and without bumps indicate that there are only small variations in the slope of  $\log(\sigma)$  and  $\sigma \sim T^{1/3}$  remains valid within the accuracy of these estimations. We note that the lowest measured temperature in Ref. 30 is 15 mK. From Fig. 7 we see that the variations for  $T \geq 15$  mK are much smaller than those for  $T < 15$  mK. Hence, these variations in  $\sigma$  could not have been observed in the experiments.

In Fig. 8 we show how the bumps affect  $S$ . Even with the very small bump 3,  $S$  changes sign in the critical regime as  $T \rightarrow 0$ . As the bump increases this change becomes more pronounced. The temperature  $T_{S=0}$  at which the sign change occurs is 0.1 K for bump 3,  $T_{S=0} = 0.2$  K for bump 2, and  $T_{S=0} \approx 0.4$  K for bump 1. These results for  $T_{S=0}$  are still about one order of magnitude less than in semiconductors<sup>8,9</sup> and two orders of magnitude smaller than in amorphous alloys.<sup>6,7</sup> Of course, as shown in Fig. 8,  $T_{S=0}$  shifts to higher values as the bump height increases. Nevertheless, the minimum value of  $S$  for  $T < T_{S=0}$  has the same order of magnitude as the corresponding maximum value of  $S$  in Si:(P,B) and in Si:P. We emphasize that the value of  $T_{S=0}$  of course depends on the energy unit chosen and thus will vary for

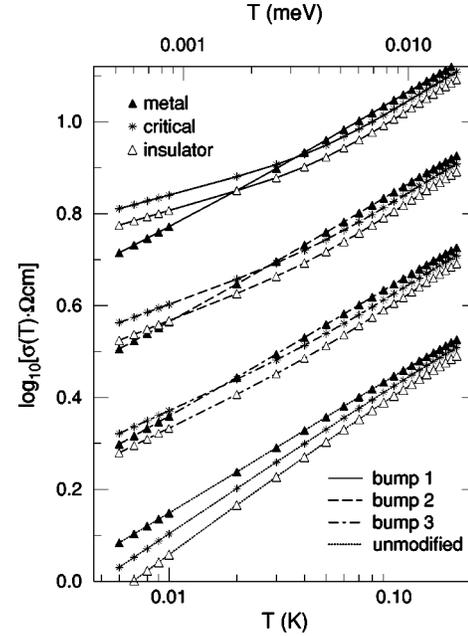


FIG. 7. Comparison between  $\sigma$  with and without bumps in the metallic, critical and insulating regimes for  $E_F - E_c = -0.1, 0.0, 0.1$  meV. For clarity each set of  $\sigma(T)$  is shifted by 0.2 along the vertical axis from each preceding set. The lines are guides for the eye only.

systems with different bandwidths, e.g., a larger bandwidth will give rise to a larger value of  $T_{S=0}$ . We observe a similar sign change in the metallic regime but the depth of the minimum is smaller than in the critical regime. The Mott formula with  $\sigma(T)$  given in Fig. 7 can readily model this behavior since  $\sigma(T)$  remains slowly varying even if  $\sigma_c(E, T)$  has a bump near  $E_c$ . In the insulating regime,  $S$  has a shallow maximum and drops back to zero as  $T \rightarrow 0$ . This is different from experiment,<sup>5</sup> where  $S$  changes sign and neither has a maximum nor minimum in the insulating regime.

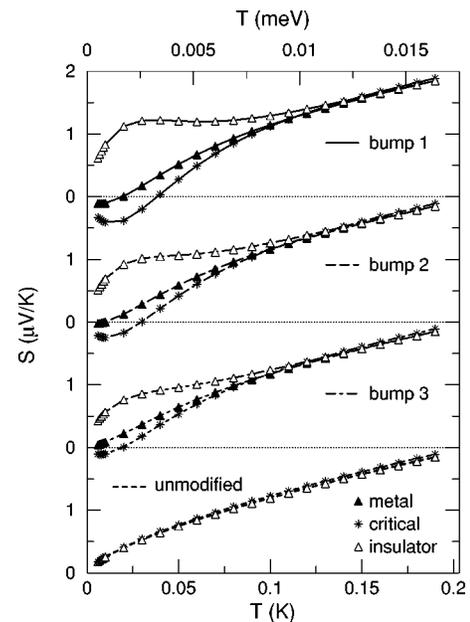


FIG. 8. The thermopower for different cases of  $\sigma_c$  input. The lines are guides for the eye only.

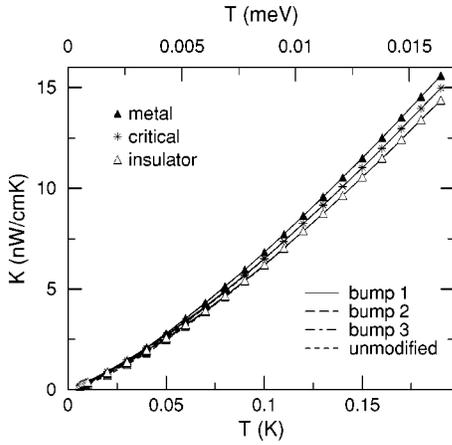


FIG. 9. The thermal conductivity remains largely unaffected by variations in  $\sigma_c(E, T)$ . The data for unmodified and modified  $\sigma_c(E, T)$  lie on top of each other. The lines are guides for the eye only.

Unlike in  $S$ , there is no dramatic change in  $K$  as can be seen in Fig. 9. We find only negligible variations at  $T < 15$  mK. This should be expected since there has also been hardly any change in the slope of  $\sigma(T)$  except for  $T < 15$  mK. However, the small increase in  $\sigma$  at  $T < 15$  mK in the metallic regime together with the minimally modified  $K$  leads to a drastic change in  $L_0$  even in the case for the smallest bump. The increase and decrease in  $\sigma$  leads to a maximum and minimum in  $L_0$ , respectively. However,  $L_0$  still approaches the universal value  $\pi^2/3$  for  $T \rightarrow 0$  as demonstrated in Fig. 10.

Let us comment on the validity of the bumps. As reviewed in the Introduction, one commonly observes a sign change in  $S$  for small  $T$ . As shown here, we can only extract such a sign change within the noninteracting Anderson model of localization by introducing an artificial bumplike structure in  $\sigma_c$ . We interpret this as evidence that the sign change is more likely due to physical processes not present in the Anderson description of disordered systems.

## V. CONCLUSIONS

In this paper, we have shown that the anticipated value of the dynamical scaling exponent  $z \approx 3$  as well as the right order of magnitude for the thermopower  $S \approx 1 \mu\text{V/K}$  at the MIT can be obtained when taking into account the expected  $T$  dependencies in addition to the simple scaling behavior of Eq. (2). Our approach is phenomenological in the sense that we have refrained from using fitting parameters and have rather taken experimental data as input. Using these data, we can explain the large deviations from experimental results as reported in the theoretical studies of Refs. 21–25 and 33. We have shown that our results for  $S$  agree with those predicted by the Mott formula since we have used a  $\sigma$  slowly varying on the scale of  $k_B T$  near the MIT. We emphasize, however, that for a disordered system where interactions are negligible, we should still expect the Anderson-type transition as given in Eq. (1) at  $T=0$ . Consequently,  $S \approx 100 \mu\text{V/K}$  at the MIT<sup>21–24</sup> should again be expected and one should observe a large increase of  $|S|$  at very low  $T$ . However, such temperatures appear presently inaccessible by experiment.

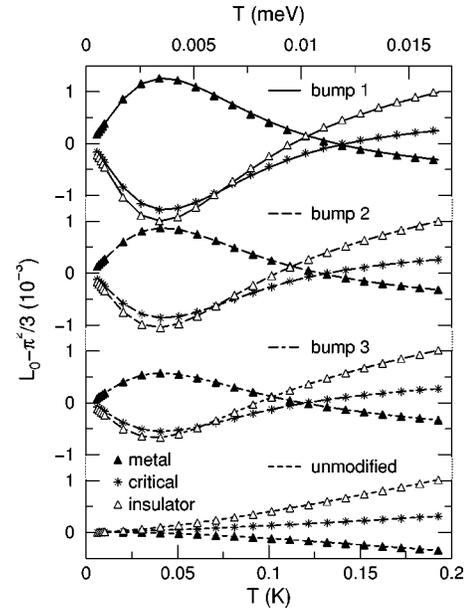


FIG. 10. The variation of the Lorenz number with  $T$  shifted by  $\pi^2/3$  for different cases of  $\sigma_c$  input. The lines are guides for the eye only.

We also note that the finite- $T$  scaling of  $\sigma$ ,  $S$ ,  $K$ , and  $L_0$  according to Eq. (2) can be performed with good accuracy for  $z \approx 3$ ,  $\nu \approx 1$ .<sup>47</sup>

As a further challenge, we considered the sign changes observed in  $S$  at low  $T$ . We found that even large variations in the chemical potential  $\mu(T)$  do not lead to a sign change in  $S$ . On the other hand, a variation in the input  $\sigma_c(E, T)$  data can give rise to such a sign change in  $S$ , while at the same time resulting in only small changes in the conductivity  $\sigma$ . Hence we have effectively modeled the underlying physical reasons for the sign change—which have been attributed to electron-electron interactions<sup>5</sup> or to the existence of local magnetic moments and their interactions with electrons<sup>8,9</sup> or to inelastic scattering with phonons<sup>13–15</sup>—by simply changing the input  $\sigma_c(E, T)$ . Regarding a possible test for the existence of such a structured  $\sigma_c(E, T)$ , we have shown that the  $T$  variation of  $L_0$  is much more sensitive to the bumps than  $\sigma$ . Thus we have been able to describe the main features of the critical behavior of  $S(T)$  although it remains unclear what might cause bumps in  $\sigma_c(E, T)$  close to  $E_c$ . A microscopic and possible system-dependent approach to the problem may eventually account for these abrupt changes in  $\sigma_c$ . Of course, if many-particle interactions and electron-phonon coupling are important, we no longer expect the feasibility of the Chester-Thellung-Kubo-Greenwood formulation<sup>35–37</sup> used here.

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