A recursive formulation of thermoelectric transport in disordered systems

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Until recently, the available predictions for the behavior of the thermoelectric power S close to the disorder-induced metal-insulator (Anderson) transition (MIT) ranged from constant to diverging behaviour using various approximation schemes. Using directly the Chester-Thellung-Kubo-Greenwood formulation of linear response together with averaged density-of-states and conductivity data, we obtain the behavior of S at low temperature and show that S does not diverge at the MIT. However, within this formulation, the scaling yields unphysical values for the critical exponents. In order to circumvent this problem and to study the critical behavior of the thermopower at the MIT in an experimentally relevant systems, we next take the d.c. conductivity data from [Waffenschmidt et al., PRL 1999] on stress-tuned Si:P as input for our calculations. Now scaling is recovered and the values of S have the right order of magnitude close to the transition. Last, in order to overcome the need for an input conductivity, we microscopically calculate all thermoelectric transport properties in a disordered wire using the recursive Green's function method (RGFM). From the kinetic coefficients, we can compute, for example, the Peltier coefficient in the limit as the temperature T goes to zero. Our numerical results for a 1D chain obeying an Anderson-type tight-binding model yield that the distribution over a large number of configurations of the Peltier coefficient is Lorentzian. Classically, we should expect a Gaussian distributed Peltier coefficient. We are also able to simulate inelastic scattering processes and the effects of a finite T.