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Effective-Medium Approximation for Energy-Dependent Hopping on a Lattice

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We have generalised the standard lattice Coherent-Potential-Approximation (CPA)/Effective-Medium-Approximation (EMA) scheme to include the case of energy dependent hopping. This case is complicated by the fact that, due to the detailed-balance condition, the hopping rates w_{ij} are non-symmetric, i. e. $w_{ij} \neq w_{ji}$. Results for the frequency dependent diffusion coefficient are compared with Monte-Carlo simulations for a uniform and bimodal site energy distribution.

Introduction The effective-medium approximation (EMA) is a simple and powerful method for describing hopping dynamics in disordered systems [1]. The lattice version [2], also called coherent-potential approximation, compares quite well with numerical simulations and takes into account the percolative aspects of hopping transport [1,3] in a qualitative manner. Most of the EMA versions proposed so far deal with the case of symmetric hopping rates. This excludes hopping in a disordered energy landscape, in which, due to the detailed-balance condition, the hopping rates are asymmetric, i.e. $w_{ij} \neq w_{ji}$. For the case of electron hopping in semiconductors a version of the EMA for asymmetric hopping rates has been formulated some time ago [5] (for more recent developments, see also [6]). Less attention has been paid to the case of classical hopping processes, and we will focus on this situation in the present article following an approach discussed in detail elsewhere [4]. After summarizing the derivation of the self-consistency equation for the effective hopping rate, we test the EMA scheme by comparing results for the frequency dependent diffusion coefficient with data obtained from Monte-Carlo simulations.

Effective Medium Approximation

Self consistency equation We consider one particle that can perfom jumps among nearest neighbor sites of a hypercubic lattice in d dimensions with lattice spacing $a \equiv 1$. To each lattice site i there is assigned a random energy E_i drawn from a distribution $\psi(E)$. The jump rates $w_{ij} = w(E_i, E_j)\,\Delta_{ij}$ (where $\Delta_{ij} = 1$, if site i and j are nearest neighbors and 0 otherwise) are supposed to fulfil the detailed balance condition. The master equation for the probability $g_{ij}(t)$ to find the particle on site j at time t, when it started on site i reads

$$\frac{\mathrm{d}g_{ij}(t)}{\mathrm{d}t} = \sum_k \left[w_{ik}g_{kj}(t) - w_{ki}g_{ij}(t)\right], \tag{1}$$

which is supplemented by the initial condition $g_{ij}(t=0) = \delta_{ij}$.

After introducing symmetrised jump rates, $v_{ij} = v(E_i, E_j)\,\Delta_{ij} = v_{ji}$ with $v(E_i, E_j) = w(E_i, E_j)\exp(-\beta E_j) = v(E_j, E_i)$, and after rescaling the Green function $h_{ij}(t) = \exp(\beta E_i)\,g_{ij}(t)$, we obtain from (1) ($z_{E_i} \equiv z\exp(-\beta E_i)$)

$$z_{E_i} H_{ij}(z) - \delta_{ij} = \sum_k v_{ik}\big[H_{kj}(z) - H_{ij}(z)\big]\,, \tag{2}$$

where we have denoted the Laplace transform of $h_{ij}(t)$ by $H_{ij}(z)$. Analogous to the usual EMA [2], we now introduce an ordered effective medium for each class of random walks constrained to the same energy E. In this medium the effects of the random transition rates v_{ij} are approximated by a frequency dependent hopping rate $\Gamma(z, E)$. The corresponding master equation is

$$z_E F_{ij}(z) - \delta_{ij} = \sum_k \Gamma(z, E)\,\big[F_{kj}(z) - F_{ij}(z)\big]\,, \tag{3}$$

where $F_{ij}(z, E) = (2\pi)^{-d}\int_{-\pi}^{\pi} \mathrm{d}^d k (z_E + \Gamma(z, E)\,\chi(\mathbf{k}))^{-1}\exp(i\,\mathbf{k}\cdot(\mathbf{R}_j - \mathbf{R}_k))$ is the Green function of the effective medium associated with the energy E; $\chi(\mathbf{k}) = 2[d - \sum_{\mu=1}^{d}\cos k_\mu]$, and $\mathbf{R}_j$ denotes the position of site j.

The effective jump rate $\Gamma(z, E)$ is determined by the basic idea of the EMA: For one bond in the effective medium the quantity $\Gamma(z, E)$ is substituted by a rate $v(E, E')$ of the disordered system. Requiring that $F_{ij}(z, E)$ does not change on the average, yields the equation [2]

$$\left\langle \frac{\Gamma(z, E) - v(E, E')}{d\Gamma(z, E) - [\Gamma(z, E) - v(E, E')]\,[1 - z\,\mathrm{e}^{-\beta E}F_{00}(z, E)]} \right\rangle_{E'} = 0\,, \tag{4}$$

where $\langle\ldots\rangle_{E'} = \int \mathrm{d}E'\psi(E')\ldots$ denotes an average over the distribution $\psi(E')$ of site energies E'.

Frequency dependent diffusion coefficient The frequency dependent diffusion coefficient (dynamic diffusivity) in the EMA can be expressed as [4]

$$\begin{aligned} D^{\mathrm{EMA}}(z, E) &= \frac{z^2\mathrm{e}^{-\beta E}}{2dZ}\ \sum_j \mathrm{e}^{-\beta E_j}\sum_i F_{ij}(z, E)\,(\mathbf{R}_i - \mathbf{R}_j)^2 \\ &= \frac{z^2\mathrm{e}^{-\beta E}}{2d}\ (-\nabla_k^2)_{k=0}\hat{F}_{\mathbf{k}}(z, E) = \mathrm{e}^{\beta E}\,\Gamma(z, E)\,. \end{aligned} \tag{5}$$

Averaging over E yields

$$D^{\mathrm{EMA}}(z) \equiv \frac{\langle \mathrm{e}^{-\beta E}\,D^{\mathrm{EMA}}(z, E)\rangle_E}{\langle \mathrm{e}^{-\beta E}\rangle_E} = \frac{\langle\Gamma(z, E)\rangle_E}{\langle \mathrm{e}^{-\beta E}\rangle_E}\,. \tag{6}$$

We included the Boltzmann factor with respect to E into the averaging for the following reason: When all possible diffusion paths (for a given time $t \simeq 2\pi/\omega = -2\pi/\mathrm{Im}\,z$) are classified into different sets according to their final site energy E, then a particular member (path) of a set will occur in the true system with a probability proportional to $\exp(-\beta E)$. Equation (6) is our final result for the frequency-dependent diffusion coefficient in the EMA.

For $\omega \to \infty$ we obtain $\Gamma(z, E) = v(E, E')$ and thus the correct high-frequency limit (mean jump rate) $D^{\mathrm{EMA}}(\omega \to \infty) = \big\langle \mathrm{e}^{-\beta E'} w(E, E')\big\rangle_{E', E}/\langle \mathrm{e}^{-\beta E}\rangle_E$. As already known from

the EMA for symmetric rates, it turns out that the low-frequency limit $D(\omega \to 0)$ resulting from the EMA is too large in comparison with the true value. If we consider the long-time diffusion coefficient D_1 to be derived from theories more appropriate for long times (in $d = 1$ there exists an exact expression [7], and in $d > 1$ one may at least calculate the activation energy by a critical percolation path analysis [3]), we can include the correct low-frequency limit into the EMA by rescaling the temperature of the EMA. To this end, we choose a temperature $\beta_{\mathrm{EMA}}^{-1}$ so that the difference between the high-frequency and low-frequency limits in the EMA solution equals the corresponding difference in the real system for the true temperature β^{-1}. This method will be referred to as "temperature rescaled EMA".

Results In order to test the EMA, we compare the frequency dependent diffusion coefficient $D(\omega)$ in the EMA with that obtained from Monte-Carlo (MC) simulations. We choose jump rates $w(E, E') = \nu_0 \exp\left[-\frac{\beta}{2}(E - E')\right]$ (ν_0: attempt frequency), and consider (i) a uniform site energy distribution

$$\psi(E) = 1/E_0, \qquad 0 < E \leq E_0 \tag{7}$$

and (ii) a bimodal distribution

$$\psi(E) = p\,\delta(E) + (1 - p)\,\delta(E - E_0) \tag{8}$$

with $p = 0.7$ and $E_0 \equiv 1$.

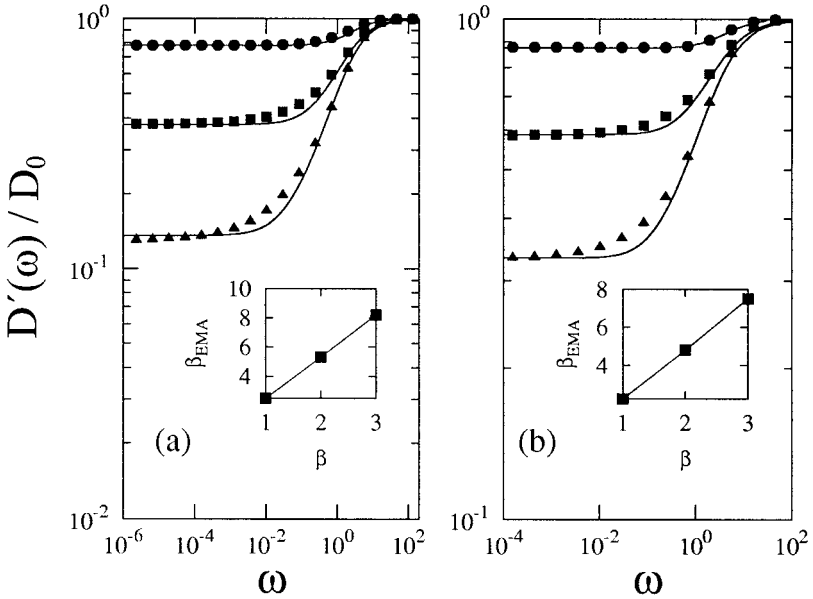

Fig. 1. Real part of the diffusion coefficient as a function of frequency for the uniform energy distribution and three inverse temperatures $\beta = 1$ (●), 2 (■), 3 (▲). The solid lines correspond to the temperature rescaled EMA, in (a) for $d = 2$ and in (b) for $d = 3$. The dependence of β_{EMA} on β is shown in the inset. The dispersion exponents (see text) are $n = 0.07, 0.20, 0.33$ and $n_{\mathrm{EMA}} = 0.07, 0.23, 0.37$ in $d = 2$, and $n = 0.05, 0.13, 0.24$ and $n_{\mathrm{EMA}} = 0.05, 0.14, 0.25$ in $d = 3$ for $\beta = 1, 2, 3$, respectively

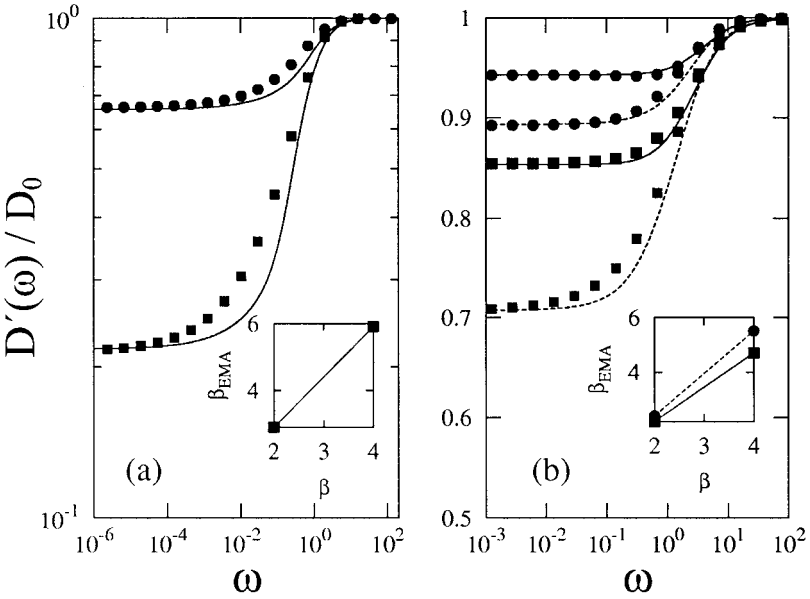

Fig. 2. Real part of the diffusion coefficient as a function of frequency for the bimodal distribution and $\beta = 2$ (●) and 4 (■), in (a) for $d = 1$ and in (b) for $d = 2, 3$. The lines correspond to the EMA results; in (b) solid lines refer to $d = 3$ and dashed lines to $d = 2$

The results for the real part $D'(\omega)$ obtained for the uniform energy distribution (7) are shown in Fig. 1. The symbols correspond to the MC simulations, while the lines correspond to the temperature rescaled EMA. Part (a) of the figure shows the results for $d = 2$, and part (b) the results for $d = 3$ (redrawn from [4]). The inset shows the relation between β and β_{EMA}. As can been seen from the figure, the agreement between simulation and approximation is rather good.

Figure 2 displays $D'(\omega)$ for the bimodal distribution (8) for $\beta = 2, 4$ in (a) for $d = 1$, and in (b) for $d = 2$ and 3. For $d > 1$, sites with $E = 0$ percolate (since p is larger than the percolation threshold) and accordingly there exists a lower bound for $D'(\omega \to 0)$ when $\beta \to \infty$. Since this lower bound is not much different from the high frequency limit, the dispersion is weak in $d > 1$. We therefore have used a linear diffusivity scale in Fig. 2b.

As commonly found in disordered hopping systems, the spectra exhibit a dc plateau at low frequencies $\omega \ll \omega_{\mathrm{lf}}$, show dispersion in an intermediate frequency regime $\omega_{\mathrm{lf}} \ll \omega \ll \omega_{\mathrm{hf}}$, and become constant again at high frequencies $\omega \gg \omega_{\mathrm{hf}}$. The crossover frequency ω_{hf} is almost independent of temperature, while ω_{lf} decreases with increasing β. The dispersive part can be characterised by an effective exponent n, $D'(\omega) \sim \omega^n$ for $\omega_{\mathrm{lf}} \ll \omega \ll \omega_{\mathrm{hf}}$ (values for n in Fig. 1 are given in the figure caption). The crossover frequencies predicted by the EMA compare remarkably well with those obtained from the MC simulations. Also the exponents n are reproduced to a good approximation by the EMA (the agreement is particularly good for the uniform site energy distribution, while for the bimodal distribution the deviations are more pronounced).

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