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COMMENT

Diffusion coefficient for two- and three-dimensional disordered lattices

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Abstract. Using the generating function formalism, the frequency dependent diffusion coefficient is obtained for disordered lattices in two and three dimensions. Values for the lowest order constant and the first correction term are found as a power series in the cumulants of the inverse transition rates.

Calculation of the statistical properties of static, disordered lattices, described by the master equation

$$\dot{P}_l = \sum_m W_{lm}(P_m - P_l),$$

has recently received attention from a wide variety of methods. For example, the motion of an ion in a crystal can be studied using the random hopping model which is given by

$$\frac{\mathrm{d}}{\mathrm{d}t} P_l = \sum_r W_{ll+r} P_{l+r} - \sum_r W_{l+rl} P_l, \tag{1}$$

where $P_l(t)$ is the probability that the ion is located at lattice site l in time t and W_{ll+r} is the transition rate from site $l+r$ to site l. For this kind of problem, it is assumed that the transition rates are symmetric, $W_{lm} = W_{ml}$, and that only nearest-neighbour hopping is present. The transition rates are treated as random variables, with distribution $\rho(W)$, when the motion of the ion is in the presence of static disorder in the lattice (see Alexander *et al* (1981) for a review). In this comment we present a means of approaching the random barrier problem which is readily generalised to arbitrary dimensions, unlike previous methods which are limited to one-dimensional systems. Following the designation of Alexander *et al*, three types of disorder are distinguished:

Case *A*,	$\langle W^{-n} \rangle$ finite,		
Case *B*,	$\rho(W) = 1$,	$0 < W < 1$,	
Case *C*,	$\rho(W) = (1-\alpha) W^{-\alpha}$	$0 < \alpha < 1$,	$0 < W < 1$.

In this comment we consider only case *A*.

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Our starting point is similar to that used in an earlier publication by Stephen and Kariotis (1982), in that we make use of the replicated generating function

$$Z = \prod_{l,r} \int \mathrm{d}\varphi_l \, \langle \exp[-\tfrac{1}{2}\Omega\varphi_l^2 - \tfrac{1}{2} W_{ll+r}(\phi_l - \varphi_{l+r})^2] \rangle. \tag{2}$$

In this expression, Ω is the frequency variable, W_{ll+r} is the transition rate, and the field variables φ_l are n-component vectors which are used to represent the probability variables, P_l. The angular brackets denote averaging over the random variables W_{ll+r}. Equation (2) is readily generalised to higher dimensions with the addition of extra indices. The Green function, or propagator, in coordinate space is

$$G(m, \Omega) = \prod_l \int \mathrm{d}\varphi_l \, \tfrac{1}{2}\varphi^2(m) \langle \mathrm{e}^{-\mathscr{H}} \rangle. \tag{3}$$

n represents the number of replicated copies of the system; at the end of the calculation, the $n \to 0$ limit is taken. $\mathscr{H}$ simply represents the exponent given in equation (2). In the following calculations, we use a finite lattice, N sites in all. When $n \to 0$ it is found that no terms of order N remain, unlike the problems that arise when the replica trick is used to calculate thermodynamic quantities. We conclude from this that the $n \to 0$ limit will not create difficulties for finite systems.

The propagator, as a function of wave number and frequency is

$$G(k, \Omega) = [\Omega + D(\Omega, 1)]^{-1},$$

and the generalised diffusion coefficient may be expressed in the form

$$D(\Omega, k) = D_2(\Omega)k^2 + D_4(\Omega)k^4 + \ldots.$$

It is our intent in this paper to investigate the frequency dependence of D_2. The transformation from coordinate to wave number representation is obtained by performing the integrals in equation (3) in terms of new field variables

$$\psi(k) = \frac{1}{\sqrt{N}} \sum_l \exp(\mathrm{i}k \cdot l)\varphi_l.$$

Using the method which will be described in the following paragraphs, we find the small frequency behaviour of D_2 to be

$$d = 1, \qquad D_2(\Omega) = D_0 + D_1\sqrt{\omega}, \tag{4a}$$

$$d = 2, \qquad = D_0 + (1/2\pi)D_1\omega|\ln(\omega)|, \tag{4b}$$

$$d = 3, \qquad = D_0 + (1/2\pi^3)D_1\omega, \tag{4c}$$

where

$$D_0 = \langle 1/w \rangle^{-1}, \qquad D_1 = D_0^3[\langle 1/w^2 \rangle - \langle 1/w \rangle^2], \qquad \omega = \Omega/4D_0.$$

In $d = 1$, the result reproduces those of Machta (1981) and Zwanzig (1982). As will be discussed shortly, there are corrections to these expressions which are higher order in powers of the fluctuations, and in powers of the frequency variable. To begin, we write the Green function in the form

$$G(k, \Omega) = \prod_q \int \mathrm{d}\psi(q) \, \mathrm{e}^{-\mathscr{H}[\psi]} \psi^2(k)/n, \tag{5}$$

where it is assumed that we look for all contributions of order n. This averaging is taken with respect to the function $\mathscr{H}[\psi(q)]$ which is obtained from the Fourier transformed generating function

$$\begin{aligned} Z &= \int \prod_{l,r} \mathrm{d}\varphi_l \, \langle \exp[-\tfrac{1}{2}\Omega\varphi_l^2 - \tfrac{1}{2}W_{ll+r}(\varphi_l - \varphi_{l+r})^2] \rangle \\ &= \int \prod_{l,r} \mathrm{d}\varphi_l \exp[-\tfrac{1}{2}\Omega\varphi_l^2] \langle \exp[-\tfrac{1}{2}W_{ll+r}(\varphi_l - \varphi_{l+r})^2] \rangle. \end{aligned} \tag{6}$$

Since we claim that the following manipulations are valid in arbitrary dimensions, the site index l must contain d labels. From here on, consider a particular bond, denoted $W_l \equiv W_{ll+r}$ which is rewritten

$$\Phi(\Delta_l) = \langle \exp[-\tfrac{1}{2}W_l\Delta_l^2] \rangle = \int \mathrm{d}\zeta_l \, \langle \exp[-\tfrac{1}{2}(\zeta_l^2/W_l) + \mathrm{i}\zeta_l \cdot \Delta_l] \rangle, \tag{7}$$

where

$$\Delta_l = \varphi_l - \varphi_{l+r}$$

The integration varible ζ_l is also replicated so that

$$\zeta_l^2 \equiv \sum_{\alpha=1}^{n} \zeta_\alpha^2(l).$$

Lower case n denotes n replicas, lower case greek letters are replica sums. In addition, there is a normalisation factor in front of the integral proportional to $(W_l)^{n/2}$; this can be neglected in the $n \to 0$ limit. Taking the cumulant average of the Gaussian we find

$$\Phi(\Delta_l) = \int \mathrm{d}\zeta_l \exp(\mathrm{i}\zeta_l\Delta_l) \exp[-\tfrac{1}{2}(1/D_0)\zeta_l^2 + \tfrac{1}{4}c_2\zeta_l^4 - \tfrac{1}{8}c_3\zeta_l^6 + \ldots]$$

where

$$D_0 = \langle 1/w \rangle^{-1}, \qquad c_2 = [\tfrac{1}{2}\langle 1/w^2 \rangle - \langle 1/w \rangle^2]$$
$$c_3 = (1/3!)[\langle 1/w^3 \rangle - 3\langle 1/w^2 \rangle\langle 1/w \rangle + 2\langle 1/w \rangle^3]$$

and

$$\zeta_l^4 = \sum_{\alpha,\beta}^{n} \zeta_\alpha^2(l)\zeta_\beta^2(l).$$

Then this is re-inverted

$$\Phi(\Delta_l) = \exp[-\tfrac{1}{2}D_0\Delta_l^2] \langle \exp[\tilde{\mathscr{L}}(\zeta_l)] \rangle \tag{8}$$

where now the angular brackets refer to integration of

$$\tilde{\mathscr{L}}(\zeta_l) = \tfrac{1}{4}c_2(\zeta_l^2)^2 - \tfrac{1}{8}c_3(\zeta_l^2)^3 + \ldots \tag{9}$$

taken with respect to the Gaussian

$$\exp[-(1/2D_0)(\zeta_l - \mathrm{i}\Delta_l D_0))^2].$$

The new average is expressed in terms of the cumulants of $\tilde{\mathscr{L}}$

$$\Phi(\Delta_l) = \exp[-\tfrac{1}{2}D_0\Delta_l^2] \exp[\mathscr{L}(\Delta_l)] \tag{10}$$
$$\mathscr{L}(\Delta_l) \equiv \langle \tilde{\mathscr{L}}(\zeta_l) \rangle + \tfrac{1}{2}[\langle \tilde{\mathscr{L}}^2(\zeta_l) \rangle - \langle \tilde{\mathscr{L}}(\zeta_l) \rangle^2] + \ldots.$$

In order to obtain the low-frequency correction to the diffusion coefficient, we need to keep only the term linear in c_2. All higher cumulants and products of cumulants will contribute corrections only to terms beyond the first-order result.

The effective 'Hamiltonian' that we will use appears in the expression

$$Z = \int \prod_l d\varphi_l \exp[-\tfrac{1}{2}\Omega\varphi_l^2 - \tfrac{1}{2}D_0\Delta_l^2 + \tfrac{1}{4}c_2\langle\zeta_l^4\rangle], \tag{11}$$

$$\langle\zeta_l^4\rangle = D_0^4\Delta_l^4 - 4D_0^3\Delta_l^2 + O(n).$$

The generating function is now translationally invariant and may be expressed in terms of the Fourier variables; the Green function is

$$G(k,\Omega) = \int \prod_q d\psi(q) \exp(-\mathcal{H}_0[\psi]) \exp(\tfrac{1}{4}c_2\mathcal{H}_I^a + \tfrac{1}{4}c_2\mathcal{H}_I^b)\psi^2(k)/n \tag{12}$$

where

$$\mathcal{H}_0[\psi] = \tfrac{1}{2}\sum_q [\Omega + D(q)]\psi^2(q),$$

$$\mathcal{H}_I^a[\psi] = -\frac{1}{N}4D_0^3\sum_q \psi^2(q)D(q),$$

$$\mathcal{H}_I^b[\psi] = \frac{1}{N}D_0^4\sum_{\substack{\{q\}\\ \alpha\beta}} \psi_\alpha(q_1)\psi_\alpha(q_2)\psi_\beta(q_3)\psi_\beta(q_4)\prod_{i=1}^4 P(q_i).$$

Also, we have made use of the following abbreviations

$$D(q) = 4D_0\sum_{j=1}^d \sin^2(q_j/2),$$

$$P(q) = \sum_{j=1}^d (1 - e^{iq_j}).$$

In all of these expressions, the lattice spacing has been set equal to one.

Before continuing, several remarks are required. First, the sign of the 'interaction' term is wrong for doing perturbation theory. This is normally explained by pointing out that the higher cumulants act to regulate the large $\psi(q)$ behaviour of the exponent. Even so, technically speaking, perturbation theory is not valid, however, a large-order type analysis of this series is not of interest at the moment; such considerations will require attention at a later date.

Second, had we taken the cumulant series with respect to W rather than W^{-1}, everything would follow through as it has in the above manipulations. However, the Δ_l^2 contribution to $\mathcal{H}_I$ would be missing and without this term, the cancellation of the Ω-independent part of Δ_l^4 would not take place. It may be possible to associate $\mathcal{H}_I$ with a diagrammatic formalism, say, treating the C_m cumulant as a vertex interaction of order $2m$. This has already been accomplished by Denteneer and Ernst (1984) for the one-dimensional case. In the above approach, however, the presence of these extraneous terms generated by the choice of $\langle W^{-n}\rangle$ as the expansion coefficients makes the diagrammatic formalism less attractive.

With these remarks out of the way, the calculation is readily completed by considering the required integrals in perturbation theory

$$G(k,\Omega)=\prod_q \int \mathrm{d}\psi(q)\,\frac{\psi^2(k)}{n}\,\mathrm{e}^{-\mathscr{H}_0}[1+\tfrac{1}{4}c_2\mathscr{H}_I],$$

$$= G_0(k,\Omega)+2C_2D_0^3G_0^2(k)[D(k)/D_0]Q_d(\Omega)+\mathrm{O}(Nn),$$

where

$$G_0^{-1}(k,\Omega)=\Omega+D(k),$$

which for small wave number is

$$G_0^{-1}(k,\Omega)=\Omega+D_0k^2,$$

and the frequency-dependent correction term contains the function

$$Q_d(\Omega)=-\frac{\omega}{\pi^d}\int_0^\pi \mathrm{d}x_1\int_0^\pi \mathrm{d}x_2\ldots\int_0^\pi \mathrm{d}x_d\frac{1}{\omega+\sin^2 x_1+\ldots+\sin^2 x_d} \qquad (13)$$

$$\omega\equiv\Omega/4D_0.$$

$Q_d(\Omega)$ can be evaluated exactly for two and three dimensions, however, for the sake of explicit expressions, we used the small-q approximation in $d=2$ and 3. These results appear in equation (4). Denteneer and Ernst (1984) give explicit forms for Q_d.

In summary, we have presented a method for calculating the frequency dependent diffusion coefficient in terms of the cumulants of the inverse transition rates. The method employs the replica trick to put the problem into the form of a classical field theory. In one dimension, the coefficients can be obtained exactly. In higher dimensions, the coefficients can be obtained as power series in the cumulants of the disorder.

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