Low-frequency conductivity of one-dimensional disordered systems

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A simple method is presented to calculate the low-frequency conductivity for one-dimensional disordered diffusive systems with nonsingular distributions of the transfer rates.

The dynamics of a variety of one-dimensional (1D) disordered system can be described by a model which consists of an infinite set of coupled rate equations, connecting nearest-neighbor sites by random independent transfer rates:[1]

$$\dot{P}_n = W_n(P_{n+1}-P_n) + W_{n-1}(P_{n-1}-P_n) \ . \tag{1}$$

Here, using the picture of diffusing particles, P_n is the particle density at site n, and W_n is the conductivity between sites n and $n+1$.

Particularly, the model successfully describes diffusion processes in 1D superionic conductors[2] and quasi-1D electronic systems.[3,4]

For systems with existing inverse moments of the transfer rates, a variety of methods have been presented to calculate the low-frequency diffusion coefficient.[1,4–8] All of these papers are based on effective medium type or related arguments. The only exact method so far has been presented by Zwanzig.[9]

In this Brief Report I demonstrate a simple method for a straightforward calculation of the low- (and high-) frequency conductivity of systems, which are characterized by Eq. (1). This method is mathematically equivalent to Zwanzig's work,[9] but, I believe, can be understood more intuitively and therefore may be applied more easily to other situations.

To start, let us rewrite Eq. (1) as a continuity equation for the particle current

$$\dot{P}_n + (j_n - j_{n-1}) = 0 \tag{2}$$

and assume a linear law for the current:

$$j_n = -W_n(P_{n+1}-P_n-E_n) \ . \tag{3}$$

Here I have inserted an external field $E_n(t)$ explicitly (factors, like inverse temperature, are already included in E_n). The W_n are assumed to be randomly distributed, with existing inverse moments, and uncorrelated in space, e.g.,

$$\left\langle \frac{1}{W_n}\frac{1}{W_m}\right\rangle = \left\langle \frac{1}{W^2}\right\rangle \delta_{n,m} + \left\langle \frac{1}{W}\right\rangle (1-\delta_{n,m}) \ . \tag{4}$$

We seek the linear response of the current to the external field E_n. (Because the fluctuation dissipation theorem holds for this system, the calculation of the conductivity is equivalent to the determination of the diffusion coefficient.)

To proceed, let us consider the following equation:

$$\dot{\psi}_n - W_n(\psi_{n+1} - 2\psi_n + \psi_{n-1} - E_n) = c \ . \tag{5}$$

Upon taking the difference of this equation between site n and $n-1$ we immediately recover Eq. (2) by setting

$$P_n = \psi_n - \psi_{n-1} \ .$$

It can be shown that the constant c added to the right side of Eq. (5) does not play any role for the current in this model.[10] Therefore, we will set $c=0$ from now on. Using Eq. (3), Eq. (5) may be rewritten:

$$j_n(t) = -\dot{\psi}_n(t) \ . \tag{6}$$

What is left to be done is the solution of Eq. (5), which turns out to be simpler than the solution of Eq. (2) in the low-frequency limit, and has the advantage of being directly connected with the current. The high-frequency results may be derived from Eq. (5) too, but they are well known,[1] so I shall not reproduce them here.

Taking the Laplace transform of Eq. (5) and dividing by W_n, we have ($c=0$)

$$\left[\frac{s}{W_n} - \Delta_n^2\right]\psi_n = -E_n(s) \ , \tag{7}$$

where

$$\Delta_n^2\psi_n = \psi_{n+1} - 2\psi_n + \psi_{n-1} \ .$$

The Green's function $g_{n,m}(s)$ of this equation is defined by

$$\left[\frac{s}{W_n} - \Delta_n^2\right] g_{n,m}(s) = \delta_{n,m} \ . \tag{8}$$

Inserting the formal solution of Eq. (7) into the Laplace transform of Eq. (6) we have

$$j_n(s) = s \sum_m g_{n,m}(s) E_m(s) \ . \tag{9}$$

Because the averaged Green's function is translationally invariant, we see from the definition of the conductivity that

$$\sigma_{\text{av}}(s) = s \sum_n \langle g_{n,m}(s)\rangle \ . \tag{10}$$

We now define a Green's function g^0 by

$$\left[\left\langle \frac{s}{W}\right\rangle - \Delta_n^2\right] g^0_{n,m} = \delta_{n,m} \ . \tag{11}$$

This equation is easily solved. We have in Fourier space

$$g^0(k,s) = \frac{1}{\left\langle \frac{s}{W}\right\rangle + 2(1-\cos k)} \tag{12}$$

and[11]

$$g_m^0(s)=\frac{1}{u}V^{|m|} \tag{13}$$

with

$$u=\left[4\left\langle\frac{s}{W}\right\rangle+\left\langle\frac{s}{W}\right\rangle^2\right]^{1/2},\quad V=\frac{2}{2+\left\langle\frac{s}{W}\right\rangle+u}\ .$$

Rearranging Eq. (8) with the help of Eq. (11), we obtain the following relation:

$$g_{n,m}(s)=g_{n-m}^0(s)+\sum_l g_{n-l}^0(s)O_l(s)g_{l,m}(s)\ , \tag{14}$$

where

$$O_l(s)=s\left[\left\langle\frac{1}{W}\right\rangle-\frac{1}{W_l}\right]\ .$$

This equation may be solved iteratively and then averaged, producing the same expansion for the conductivity as in Ref. 9:

$$\begin{aligned}\sigma_{\mathrm{av}}(s)&=s\sum_n\langle g_{n,m}(s)\rangle\\ &=sg^0(k=0,\ s)\left[1+\sum_l\langle O_l(s)g_{l,m}(s)\rangle\right]\ .\end{aligned} \tag{15}$$

Although this is not an expansion in the frequency but rather in inverse moments, one may check[9] that, given a power of frequency, there is only a finite number of different contributions from this expansion. Using Eqs. (12) and (13) in (15) and checking the frequency dependence of the various terms, one obtains in the low-frequency limit

$$\begin{aligned}\sigma_{\mathrm{av}}(s)=\left\langle\frac{1}{W}\right\rangle^{-1}\Bigg[1&+\tfrac{1}{2}m_{-2}\left\langle\frac{s}{W}\right\rangle^{1/2}-\tfrac{1}{4}m_{-3}\left\langle\frac{s}{W}\right\rangle\\ &+\tfrac{11}{24}m_{-2}^2\left\langle\frac{s}{W}\right\rangle+O\left[\left\langle\frac{s}{W}\right\rangle^{3/2}\right]\Bigg]\end{aligned} \tag{16}$$

with

$$m_{-l}=\left\langle\left[\frac{1}{W}-\left\langle\frac{1}{W}\right\rangle\right]^l\right\rangle\Big/\left\langle\frac{1}{W}\right\rangle^l\ .$$

The term proportional to $s^{1/2}$ was found by all authors,[4–9] whereas for the linear term in s, so far only one calculation exists,[7] which, however, does not reproduce our result. The deviation from the correct result in Ref. 7 is due to the fact that the effective medium approximation fails to reproduce all contributions linear in s.[12] An exact evaluation of the T-matrix expansion in Ref. 7 should, however, give our result again.

Note that the step from Eq. (5) to Eq. (7) is only allowed for $W_n\neq 0$. Thus an interesting class of systems [class c of Ref. 1] has to be excluded here.

It should be pointed out that our method is restricted to one dimension. In higher dimensions one cannot simply extract the low-frequency conductivity from an expansion in inverse moments of the distribution of the transfer rates.

In conclusion, I have presented a simple and direct method to calculate the low-frequency conductivity for one-dimensional disordered systems. Approximate methods were shown to be correct to leading order in the frequency, whereas deviations may arise in higher-order terms.

Due to a relation which connects the Laplace transform of Eq. (1) and our Green's function, Eq. (8), one may use this method to determine a variety of additional quantities (e.g., the autocorrelation function) in the low-frequency limit. In addition, our method seems to be helpful for systems with asymmetric hopping.

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[10]In systems with asymmetric hopping [cf., e.g., B. Derrida and R. Orbach, Phys. Rev. B 27, 4694 (1983)] c plays the role of $j_{\mathrm{drift}}^{\mathrm{av}}$.
[11]$g_m^0(s)$ may be obtained by using Eq. (7.4) of Ref. 1 with $\omega\rightarrow\langle s/W\rangle$ and $W\rightarrow 1$.
[12]The missing contribution is due to the term proportional to δ_{q_1,q_2-q_3} in Eq. (39) of Ref. 9.