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Density of states in the band tails and random multiplication in a diffusive medium

A. M. Jayannavar and J. Köhler
Abteilung Theoretische Physik, Universität Ulm, Albert-Einstein-Allee 11, 7900 Ulm, West Germany
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We have considered the problem of random multiplication of particles or fields in a diffusive medium. Both the short-time and asymptotic behavior is evaluated. We have used already known results on the density of states in disordered systems and on transverse spin depolarization in a medium with random magnetic fields. We have treated both bounded and unbounded random potentials. We reaffirm certain recent results and also point out some differences.

In recent years the subject of random multiplication of diffusing particles has attracted much attention. More recently several contradictory results have been reported in the literature.[1-3] The basic equation governing this process in d dimensions can be written as[1-3]

$$\frac{\partial P(x,t)}{\partial t} = D\nabla_d^2 P(x,t) + V(x)P(x,t)\,, \tag{1}$$

where $P(x,t)$ is the particle (or field) density, ∇_d^2 the d-dimensional Laplacian, D the diffusion constant, and $V(x)$ the random potential (or field) with given statistics. The above Eq. (1) appears in diverse fields such as physics, chemistry, and biology. For $V(x)$ being a strictly negative random variable (bounded from above by zero) the problem reduces to that of a random walk in a random trapping medium. These models have been used successfully in studying several physical situations[4-14] such as trapping of excitons, diffusion controlled reactions, dielectric relaxation, self-attracting polymer chains, and chemical binding of interstitial hydrogen in metals by impurities, etc. When the random potential $V(x)$ is replaced by an imaginary random potential $[iV(x)]$, the problem reduces to that of transverse spin depolarization of a diffusing particle in an environment with random magnetic fields.[15-20]

The problem we address in this paper is when the random potential $V(x)$ takes both positive and negative values, and for this case contradictory results have been reported in recent literature.[1-3] This model is related to the evolution of biological species[21] which move in a space via diffusion and $V(x)$ taking positive and negative values at different spatial points representing the distribution of nutrients and inhibitors, respectively. Another physical realization is the chain reaction with random fissile distributions. Such a model has been studied[22] for a given single realization of the random potential and the asymptotic behavior has been shown to be equivalent to that of a quantum localization problem, in particular to the hopping process from one localized center to another. In such a case for a given single realization of random potential the growth of $P(x,t)$ is characterized by strong intermittency in that the asymptotic behavior is concentrated in several peaks which grow exponentially.[3] The peak positions are situated at the space points where $V(x)$ takes on large positive values. Such a sensitive functional dependence of $P(x,t)$ on the realizations of the random potential lead to non-self-averaging behavior (namely fluctuations dominating the mean values[2,3]).

In this work we calculate the ensemble- and spatial-averaged[2] behavior of $P(x,t)$ for both short- and long-time (asymptotic) domains. Our treatment is simple and we make use of already known rigorous asymptotic results on electronic density of states in disordered systems and on spin-polarization decay. We have considered both Gaussian and bounded random potentials. First, we reaffirm the asymptotic results due to Rosenbluth[2] for Gaussian potentials and give an expression for short-time evolution. We then consider the case of bounded potentials where certain differences with the known results[3] are pointed out.

One can readily notice that Eq. (1) is similar to the quantum problem of electrons moving in a random potential. In particular, if we replace the time t by imaginary time $(-it)$, $(1/2m)$ by D, and $V(x)$ by $-V(x)$ in the Schrödinger equation (by setting $\hbar$ equal to unity) we get Eq. (1). The attractive potential in Eq. (1) corresponds to a repulsive potential for the corresponding Schrödinger equation. If we assume the initial condition for $P(x,t=0)=n_0$ to be space independent, then the asymptotic expression $\langle\langle P(x,t)\rangle\rangle$ (two angular brackets denote the ensemble average over all realizations of the random potential and spatial average over entire volume) is given

by, apart from preexponential factors[5]

$$\langle\langle P(x,t)\rangle\rangle = n_0 \int dE\, e^{-Et}\rho(E)\,, \tag{2}$$

where $\rho(E)$ is the averaged density of states for the corresponding Schrödinger equation. A similar expression can be found for the probability that the particle is found at the origin at time t given that it starts at the same space point at $t=0$.[13] It can be clearly seen from Eq. (2) that the long-time behavior is dominated by the negative-energy tail in the density of states.

The nature of the density of states in disordered condensed-matter systems has been studied over several decades.[13,23–38] The analytical treatments are based on different techniques such as node-counting methods,[26,27] semiclassical methods,[29] wave mechanical calculations,[28] Feynman's path-integral formulations,[35] field-theoretic instanton approach,[13,37] functional space,[30] and by replica-functional integral representation of one-particle Green's function.[32–34] For the case of Gaussian white-noise random potentials, i.e., $\langle V(x)\rangle = 0$ and $\langle V(x)V(x')\rangle = \sigma^2\delta(x-x')$, the density of states in the tail region is given by[28,32,33]

$$\rho(E) = |E|^{d(5-d)/4}\exp(-c_d|E|^{2-d/2})\,,$$

where d is the dimensionality of the medium and $c_1 = 8\sqrt{D}/(3\sigma^2)$.[28] Now keeping the leading exponential term in the density of states, using Eq. (2) and carrying out the integral by the saddle-point approximation we get immediately for one dimension $\langle\langle P(x,t)\rangle\rangle = \exp[\sigma^4 t^3/(48D)]$. The coefficient in the exponent is exactly the same as that obtained by Rosenbluth. For two and three dimensions the long-time behavior of $\langle\langle P(x,t)\rangle\rangle$ is divergent. For the case of Gaussian-correlated potentials $\langle V(x)V(x')\rangle = g(|x-x'|)$ [where $g(x)$ is an arbitrary decaying function of x, provided it can be expanded in the form of a Taylor series at $x=0$], the asymptotic result for the density of states in the negative-energy tail is given by[32,34,35]

$$\rho(E) = |E|^{d}\exp[-|E|^2/2g(0)]\,,$$

which in turn implies $\langle\langle P(x,t)\rangle\rangle = \exp[g(0)t^2/2]$. These results confirm the recent results due to Rosenbluth.[2] Usually, for correlated Gaussian disorder, the density of states in the negative-energy spectrum cross over to asymptotic Gaussian form (as mentioned above) from the Urbach regime (namely the pure exponential dependence on the energy). This Urbach regime spans several orders of magnitude in the energy spectrum depending on short-range correlations of random potentials and provided that the correlation function $g(x)$ is integrable, i.e., $\int g(x)d^dx$ exists.[34] This is suggestive of the fact that the asymptotic behavior $\exp(at^2)$ is reached through a crossover from the $\exp(ct)$ dependence [even though strictly speaking Eq. (2) is valid for the asymptotic regime].

Now we will turn to the short-time behavior of $\langle\langle P(x,t)\rangle\rangle$. To this end we use the approach due to Zeldovich *et al.*[3] and due to Czech and Kehr[15,16] for the spin-depolarization problem. We first discretize Eq. (1). In this case the particle hops randomly with hopping rate $\gamma(=D/a^2)$ on a lattice with spacing a (taken to be unity). The discretization procedure itself amounts to introduce a correlation in the random potential of the order of a and random potentials at different points are assumed to be uncorrelated Gaussian variables with variance σ. For simplicity we assume that the particle starts at the origin, then the solution for $\langle\langle P(x,t)\rangle\rangle$ is given by[3,16]

$$\langle\langle P(x,t)\rangle\rangle = \left\langle\left\langle \exp\left[\sum_r V_r t_r(t)\right]\right\rangle_{\{V_r\}}\right\rangle_{\mathrm{RW}}\,, \tag{3}$$

where $t_r(t)$ is the total time that the particle has spent on the particular site r in time t and $\langle\cdots\rangle_{\mathrm{RW}}$ and $\langle\cdots\rangle_{\{V_r\}}$ represent the average over different realizations of the random walk and different configurations of V_r, respectively. First, we can readily perform the average over $\{V_r\}$ and at once we get

$$\langle\langle P(x,t)\rangle\rangle = \left\langle \exp\left[\frac{\sigma^2}{2}\sum_r t_r^2(t)\right]\right\rangle_{\mathrm{RW}}\,. \tag{4}$$

Now the problem has reduced to that of a spin-depolarization problem with the replacement of σ^2 by $-\sigma^2$ [see Eq. (2.5) in Ref. 16]. Having established the one-to-one correspondence with spin-depolarization problem we state the final results (for details see Ref. 16). Using Jensen's inequality for convex functions one easily obtains a lower bound for $\langle\langle P(x,t)\rangle\rangle$ given by

$$\langle\langle P(x,t)\rangle\rangle \geq \exp\left[\frac{\sigma^2}{2}\left\langle\sum_r t_r^2(t)\right\rangle_{\mathrm{RW}}\right]\,. \tag{5}$$

The expression (5) is nothing but the first cumulant expansion of (4) and the equality is valid in the short-time domain (until the terms in the exponent become of the order of unity[16]). The right-hand side of Eq. (5) can be written as

$$\exp\left[\sigma^2\int_0^t d\tau(t-\tau)\tilde{P}(0,\tau)\right]\,,$$

where $\tilde{P}(0,t)$ is the probability of finding the particle at the origin at time t, being started at the same point at time $t=0$. For pure random walks[16] for time $t<(1/\gamma)$, $\tilde{P}(0,t)$ is of the order of unity and for time $t>(1/\gamma)$, $\tilde{P}(0,t)\sim t^{-d/2}$. Hence in the region $0<t<(1/\gamma)$, we have for all dimensions d that $\langle\langle P(x,t)\rangle\rangle$ grows as $\exp(\sigma^2t^2/2)$ and in the region $t>1/\gamma$ it grows as $\exp(c\sigma^2t^{3/2})$, $\exp(c\sigma^2t\ln t)$, and $\exp(a_0\sigma^2t)$ in one, two, and three dimensions, respectively.[16]

Finally, we turn to the problem of when the random potential V_r is bounded. For simplicity we consider the case where the potentials are binary in nature; i.e., it takes only two values $+V$ and $-V$ randomly with probability p and $(1-p)$, respectively. In the corresponding quantum problem the energy spectrum is bounded from below at energy $(-V)$. At this boundary the density of states shows an essential singular behavior (namely Lifshitz singularity) and is given by[13,14,36–38]

$$\rho(E)\sim\exp(-\mathrm{const}\lambda|E+V|^{-d/2})\,,$$

where λ is given by $\lambda = -\ln(1-p)$. Substituting this expression into Eq. (2) and defining the new variable $x=E+V$ and further carrying out the integral by saddle-

point approximation, we get

$$\langle\langle P(x,t)\rangle\rangle \sim \exp(Vt)\exp[-a_d(\lambda^{2/d}t)^{d/(d+2)}] .$$

In particular, we note that the correction to the leading exponential $\exp(Vt)$ is dimensionality dependent and is quite different from that suggested by Zeldovich *et al.*[3] for bounded potentials [which is independent of dimensionality and is given by $\exp(Vt-bt/\ln t)$]. We would also like to point out that if the potential $V(x)$ in Eq. (1) is bounded from above by a positive value of, for instance, $V_{\max}$, then by defining $P(x,t)=f(x,t)\exp(V_{\max}t)$ it is clear from Eq. (1) that $f(x,t)$ is nothing but the survival probability for the pure trapping model with effective potential $V_{\text{eff}}(x)=[V(x)-V_{\max}]$, which is negative and bounded by zero from above. Hence it is clear that the leading correction to our original problem [$\exp(V_{\max}t)$] is nothing but the leading term for the total survival probability in the corresponding trapping problem which is known for various forms of continuous random potentials (see Refs. 14 and 37).

We have calculated the asymptotic behavior based on our existing knowledge about the density of states. Alternatively, in one dimension one can solve this problem by knowing the span distribution of a random walk. In this procedure one first performs the average over the random potential realizations in Eq. (3). The remaining average $\langle f(\{t_r\})\rangle_{\text{RW}}$, with respect to all the realizations of the random walks, is performed as follows. For a given time t which corresponds to n random steps we consider those realizations where the particle visits s distinct sites. $W_n(s)$ is the probability that the random walk visits s distinct sites (s is bounded from above by n). If site r is visited among s then $t_r(n)$ in Eq. (3) is taken to be n/s; i.e, one assumes all the s sites are visited with equal probability and then one performs the average with respect to $W_n(s)$ (for details see Ref. 16). Consider, for example, when the random potentials at different sites are uncorrelated and take on the values $+V$ and $-V$ randomly with equal probability. Then one can easily perform the average over random potentials in Eq. (3) and the remaining average over random walks can be written as

$$\langle\langle P(x,t)\rangle\rangle = \sum_s W_n(s)[(e^{Vn/s}+e^{-Vn/s})/2]^s , \qquad (6)$$

where the expression for $W_n(s)$ in one dimension is given by[39]

$$W_n(s) = \frac{8n}{s^3}\sum_{j=1}^{\infty}\left[\frac{(2j+1)^2\pi^2 n}{s^2}-1\right] \times \exp\left[-\frac{\pi^2(2j+1)^2 n}{2s^2}\right] . \qquad (7)$$

Now it is sufficient to keep the first term in Eq. (7) (for the asymptotic regime) and, substituting back into Eq. (6), replace the summation by an integral, and with the saddle-point approximation we obtain

$$\langle\langle P(x,t)\rangle\rangle = \exp(Vn - An^{1/3}) .$$

This has exactly the same time dependence as mentioned above. This procedure can be easily carried out for other forms of random potentials. For the case of rectangularly distributed (uniformly distributed) continuous potentials between $+V$ and $-V$, we obtain the asymptotic result

$$\langle\langle P(x,t)\rangle\rangle = \exp(Vt)\exp[-ct^{1/3}(\ln t)^{2/3}] .$$

Our results for rectangular distributions should be compared with the known[14,40] singular behavior of density of states near the band edge, namely $\rho(E)=\exp(c\ln|E+V|/|E+V|^{1/2})$. Alternatively, this method of span distribution of random walks can be used to calculate the asymptotic behavior of density of states for various forms of random potentials.[41]

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