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The trapping problem and Anderson localization

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Abstract

The equivalence between the trapping problem for randomly moving objects and the time evolution of a quantum mechanical particle in disordered media is sketched. For static traps, the spectral properties of the corresponding Hamiltonian are shown to determine the survival probability of the reactants. Effects of an external drift are considered using the non-Hermitian generalization of the localization problem. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

For more than 80 years, there is an interest in the kinetics of reactions on fluctuating manifolds. See the review article of den Hollander and Weiss [1]. One of the most commonly studied models is the trapping problem, in which an A-type reactant diffuses around until it hits a (randomly located) B-type object. The reaction between the species A and B is $A + B \to B$, i.e., when A and B molecules react, A is annihilated while B remains intact. If $[A(\boldsymbol{x})]$ and $[B(\boldsymbol{x})]$ denote the concentrations of species A and B, respectively, at the spatial point $\boldsymbol{x}$, the kinetic equation for the disappearance of the A's is

$$\frac{\mathrm{d}[A(\boldsymbol{x})]}{\mathrm{d}t} = -k[A(\boldsymbol{x})][B(\boldsymbol{x})], \qquad (1)$$

where k is the reaction rate constant. We assume no repulsion between the diffusing molecules; each reactant may be considered as an independent random walker.

In general, one may define the quantity $c(\boldsymbol{x})$, which is the average probability to find an A particle at the point $\boldsymbol{x}$. Neglecting the fluctuations induced by the discrete nature of the A's, the dynamics of c is determined by

$$\frac{\partial c(\boldsymbol{x},t)}{\partial t} = D\nabla^2 c(\boldsymbol{x},t) - U(\boldsymbol{x})c(\boldsymbol{x},t), \qquad (2)$$

where $U(\boldsymbol{x})$ is proportional to the concentration of the B molecules at $\boldsymbol{x}$ and D is the diffusivity of the A particles.

The linear nature of Eq. (2) implies that the time evolution of c is uniquely determined by the spectral properties of the evolution (Liouville) operator $\mathscr{L} \equiv D\nabla^2 - U(\boldsymbol{x})$. If $\phi_n(\boldsymbol{x})$ and ε_n represent the nth

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eigenstate and eigenvalue of the Liouville operator, the time evolution of c is given by

$$c(\boldsymbol{x},t) = \sum_n c_n \phi_n(\boldsymbol{x}) \mathrm{e}^{\varepsilon_n t}, \tag{3}$$

where the coefficients $\{c_n\}$ are determined by the initial condition,

$$c_n = \int \mathrm{d}^d\boldsymbol{x}\ \phi_n(\boldsymbol{x}) c(\boldsymbol{x}, t=0). \tag{4}$$

Although $c(\boldsymbol{x})$ is a positive definite probability function, the eigenfunctions of the Hermitian matrix $\mathscr{L}$ may take negative and even complex values. However, the positive definiteness of c is preserved by the dynamics determined by (2). The fact that $\mathscr{L}$ is diagonalized above the complex field implies only that the initial condition could not be chosen to be identical with any arbitrary eigenfunction of the Liouville operator.

Let us illustrate the equivalence between this trapping problem and the dynamics of a quantum particle in disordered potential (Anderson localization) [2]. Consider the Schroedinger equation for a particle (say, an electron) in random potential (e.g., a bulk of doped silicon),

$$-\mathrm{i}\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(x)\psi. \tag{5}$$

Eq. (2) for c may be mapped into Eq. (5) for the imaginary time evolution of the electron's wavefunction where D plays the role of Planck constant divided by $2m$, and the traps concentration in the chemical reaction corresponds to the random potential normalized by $-\hbar$. Accordingly, $\varepsilon \equiv -E/\hbar$, where E is the energy of the quantum particle. In the trapping problem the "potential", $U(\boldsymbol{x})$, is negative definite, i.e., there is only annihilation of A type reactants. The corresponding Anderson problem is characterized by positive definite potential, so that the spectrum of the Hamiltonian is bounded from below by zero. As a result, the spectrum of the Liouville operator $\mathscr{L}$ is bounded from above by zero and all its eigenstates decay exponentially.

The correspondence between the various trapping problem and quantum mechanical quantities is summarized in Table 1.

Table 1

Trapping problem	Quantum particle
D	$-\hbar/2m$
$U(\boldsymbol{x})$	$-V(\boldsymbol{x})/\hbar$
t	it
$c(\boldsymbol{x},t)$	ψ

While a quantum mechanical eigenstate acquire a phase, $\mathrm{e}^{-\mathrm{i}Et/\hbar}$, during its time evolution, the corresponding eigenstate of the trapping problem is suppressed by the factor $\mathrm{e}^{\varepsilon t}$ (note that ε is negative). The dynamics of both systems is determined only by the initial condition and the spectrum of the evolution operator, so one may use known results and derive physical intuition from one field to the other. In the next section, the knowledge about the spectral properties of Anderson problem is used to derive some results for the trapping problem. In Section 3, the recent progress in the field of non-Hermitian delocalization is implemented to the trapping problem in the presence of drift.

2. Density of states and survival probability

The survival probability of an A particle at time t is defined as

$$S(t) \equiv \int \mathrm{d}^d\boldsymbol{x}\, c(\boldsymbol{x},t) \propto \int_{\varepsilon_d}^{0} g(\varepsilon)\,\mathrm{e}^{\varepsilon t}\,\mathrm{d}\varepsilon, \tag{6}$$

where $g(\varepsilon)$ is the density of states and ε_d is the lower bound of the spectrum. Although $g(\varepsilon)$ is a non-universal quantity, it is known that, for most of the physical cases, where the disorder is taken from some kind of bounded distribution, the density of states is almost constant at the middle of the band, while at the tails [3,4,8]

$$g(\varepsilon) \propto g_0 \exp[-|\varepsilon_0/\Delta\varepsilon|^{d/2}], \tag{7}$$

where $\Delta\varepsilon$ measures the distance of the relevant eigenvalue from the end of the tail, i.e., in our case, from zero or from ε_d. $\varepsilon_0 \sim D/l_0^2$, where l_0 is the typical length between two sites. This, together with Eq. (3), enables us to determine the survival probability at different time domains:

Short times – the decay comes only from these eigenvalues which satisfy $\varepsilon_\mathrm{c} > 1/t$. If ε_c is in the tail of the density of states, the decay rate is given by

$$S(t) \sim \mathrm{e}^{(\mathrm{D}t/l_0^2)^{d/2}}. \tag{8}$$

This expression is in agreement with the one-dimensional result presented in Ref. [1]. It should be noted that, for a model with no lower bound to the spectrum (such as a model with Gaussian or other unbounded disorder distribution, or a continuum model) the "short time" limit is not well defined.

Long times – as $t \to \infty$, the behavior of the total number of surviving particles is dominated by energies near the top of the band. A saddle point evaluation of Eq. (6) in d dimensions then leads to

$$S(t) \propto \exp[-(t/t_0)^{d/(d+2)}], \tag{9}$$

with $t_0 = l_0^2/D$, in agreement with [3–6].

Intermediate times – At intermediate times the density of states is almost constant and the decay of $S(t)$ is exponential. The range of times in which one may see the stretched exponential behavior is determined, accordingly, by the width of the density of states tails. This, in turn, could be estimated by looking for the range of energies (eigenvalues of the Liouville operator) which are correlated with rare events, i.e., large spatial regions with high/low potential energy. In particular, if the disorder is weak, this range of "tail" states is out of the free particle spectrum, and its width is proportional to the strength of the disorder, while for strong disorder the tail width is determined by the diffusion constant.

Another implementation of the trapping – localization correspondence is to the transport properties of the A's in such a hostile environment. Let us assume that the A reactants are deposited at the center of the sample and are detected at its edge. (In photoconduction experiment, e.g., electrons are excited to the conduction band of a semiconductor by a pulse of light, and the traps are recombination centers [5,6]. The DC conductivity is then affected only by the electrons which arrive at the surface before recombination takes place.) This feature is strongly related to the localization properties of the eigenfunction of the Liouville operator. In particular, (4) implies that the contribution of localized states ($\phi_n(x) \sim \exp(-\kappa|\boldsymbol{x} - \boldsymbol{x_0}|)$, where κ is the inverse localization length) to the edge density falls exponentially with L, the linear size of the sample, while for extended states the coefficients c_n are proportional to L^{-d}. For strong disorder or low dimensionality ($d \leqslant 2$) one may expect all the states to be localized, while at higher dimensions the sample conductivity is determined by the extended states at the middle of the band.

3. Effects of drift

Let us discuss now the situation of random walk with drift, i.e., asymmetric walk, where some direction in space is preferred. In this case Eq. (2) is modified:

$$\frac{\partial c(\boldsymbol{x},t)}{\partial t} - \boldsymbol{v} \cdot \nabla c = D\nabla^2 c(\boldsymbol{x},t) - U(\boldsymbol{x})c(\boldsymbol{x},t) \tag{10}$$

where $\boldsymbol{v}$ is the (constant) drift velocity. The relevant Liouville operator,

$$\mathscr{L} = D\nabla^2 + \boldsymbol{v} \cdot \nabla - U(\boldsymbol{x}) \tag{11}$$

is no longer Hermitian. However, one may still diagonalize this operator using a complete set of left and right eigenfunctions [7]. If such set exists, the time evolution of c is given by

$$c(\boldsymbol{x},t) = \sum_n c_n \phi_n^{\mathrm{R}}(\boldsymbol{x}) \mathrm{e}^{\varepsilon_n t}, \tag{12}$$

where

$$c_n = \int \mathrm{d}^d \boldsymbol{x}\, \phi_n^{\mathrm{L}}(\boldsymbol{x}) c(\boldsymbol{x}, t=0), \tag{13}$$

and $\phi_n^{\mathrm{R}}(\boldsymbol{x})$, $\phi_n^{\mathrm{L}}(\boldsymbol{x})$ are the left and right eigenfunctions which correspond to the ε_n eigenvalue. In the special case of (10) it is possible to complete the square to obtain,

$$\mathscr{L} = D\left(\nabla + \frac{\boldsymbol{v}}{2D}\right)^2 - U(\boldsymbol{x}) - \frac{v^2}{4D}. \tag{14}$$

Thus, the effect of the drift is splitted into global shift of the energy levels by $-v^2/4D$, accompanied by a "gauge transformation" $\nabla \to \nabla + \boldsymbol{v}/2D$. Following [7] we note that the imaginary gauge field may be eliminated using the transformation

$$\phi_n(\boldsymbol{x},t) \to \mathrm{e}^{\pm \boldsymbol{v}\cdot\boldsymbol{x}/2D} \phi_n(\boldsymbol{x},t) \tag{15}$$

(the ± correspond to the left and right eigenfunctions). This transformation takes the Liouville operator to its original form shifted by the factor $v^2/4D$, and its spectrum is related to the driftless case by $\varepsilon_n \to \varepsilon_n - v^2/4D$. The above stretched exponential behavior of the long time tail is now superimposed on the simple exponential decay from the drift, i.e.,

$$S(t) \propto \exp\left[-\frac{v^2 t}{4D}\right] \exp[-(t/t_0)^{d/(d+2)}]. \tag{16}$$

What are the conditions for Eq. (15) to be applicable? The exponential factor diverges as $\boldsymbol{v} \cdot \boldsymbol{x} \to \infty$, so

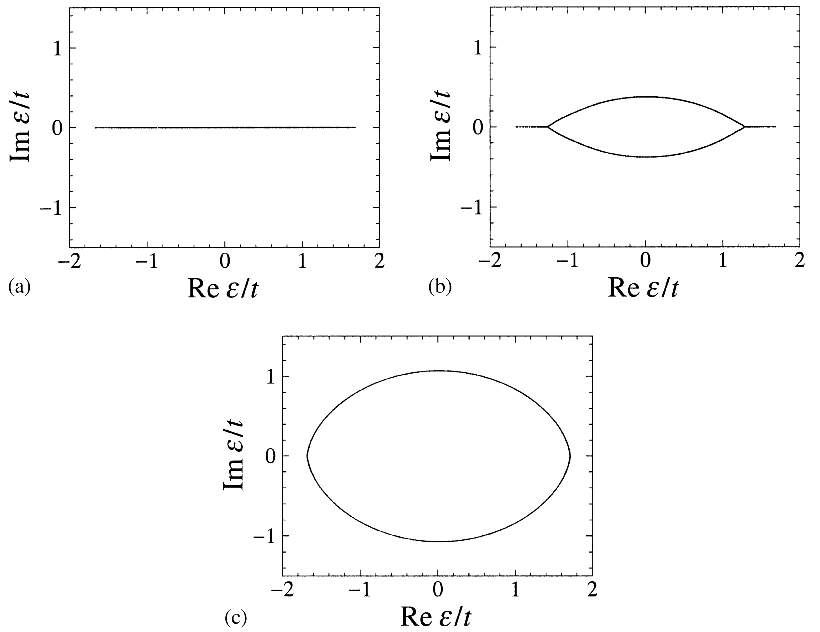

Fig. 1. Energy spectra of one-dimensional 1000-site lattice model with random on site potential and drift, where t is the hopping rate (D/l_0^2) and ε is the eigenvalue of Liouville operator. The resulting spectrum for the same realization of the random potential is plotted here for three different values of v. (a) Case of small v; all eigenstates are localized (top) (b) intermediate v; bubble of complex eigenvalues indicating extended states appears near the center of the band (middle) (c) large v; all the eigenstates are extended (bottom).

that the corresponding wavefunction is not square integrable, unless the "original" eigenfunction is localized, $\phi \sim \mathrm{e}^{-\kappa|x|}$, with Liapunov exponent $\kappa > v/2D$. As the drift grows, transformation (15) interfere with the boundary conditions for any finite sample. In this case the eigenvalues become *complex* [7]. The localization length is known to be maximal at the center of the band and minimal at the tails. As a result, a "bubble" of complex eigenvalues is formed at the center of the band and spread to its edges, as shown in Fig. 1 for a one-dimensional lattice realization of this system.

Since the dynamics at long times is determined by the tail of the spectrum, the effect of the drift on the stretched exponent for $S(t \to \infty)$ is important only if the drift is strong enough to delocalize the tail states. The density of states in one dimension is then [8]

$$g(\Delta\varepsilon) \propto 1/(\Delta\varepsilon)^{1/2}, \qquad (17)$$

which gives only logarithmic corrections to the exponential decay of the survival probability, in qualitative agreement with the transition as a function of the bias found by Movaghar et al. [5,6]. In higher dimension, it is also true that the density of states at the tail diverges according to a power law [8] and the corrections to the exponential decay of $S(t)$ are only logarithmic.

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