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Survival of classical and quantum particles in the presence of traps

P.L. Krapivsky · J.M. Luck · K. Mallick

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Abstract We present a detailed comparison of the motion of a classical and of a quantum particle in the presence of trapping sites, within the framework of continuous-time classical and quantum random walk. The main emphasis is on the qualitative differences in the temporal behavior of the survival probabilities of both kinds of particles. As a general rule, static traps are far less efficient to absorb quantum particles than classical ones. Several lattice geometries are successively considered: an infinite chain with a single trap, a finite ring with a single trap, a finite ring with several traps, and an infinite chain and a higher-dimensional lattice with a random distribution of traps with a given density. For the latter disordered systems, the classical and the quantum survival probabilities obey a stretched exponential asymptotic decay, albeit with different exponents. These results confirm earlier predictions, and the corresponding amplitudes are evaluated. In the one-dimensional geometry of the infinite chain, we obtain a full analytical prediction for the amplitude of the quantum problem, including its dependence on the trap density and strength.

Keywords Diffusion · Trapping · Quantum mechanics · Quantum walk · Survival probability · Disordered systems · Lifshitz tails

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1 Introduction

A highly important quantity in the theory of random walk is the number of distinct sites visited by the walk in a given time [1]. The distribution of this number of sites governs the behavior of many physical processes. The trapping of diffusing particles is the most famous example [2–4]. It has been shown by Donsker and Varadhan [3,4] that the survival probability $P(t)$ of a classical particle diffusing in an environment containing randomly placed static traps can be expressed in terms of the distribution of distinct sites visited by the walk in the absence of traps. Classical trapping models of this kind have been explored thoroughly [5–10]. They have received many applications, including chemical transport, electron-hole recombination, exciton trapping and annihilation (see [11–13] for reviews). The long-time asymptotics of the survival probability of a classical walker in the presence of a random distribution of traps has been established by Balagurov and Vaks [2], and more rigorously by Donsker and Varadhan [3,4]. In dimension d it displays a stretched exponential behavior of the form

$$P(t) \sim \exp\left(-A_d t^{d/(d+2)}\right), \quad (1.1)$$

where the amplitude A_d is known exactly (see (6.15), (7.10)). The above result can indeed be related to the form of the Lifshitz tail of the density of states of the appropriate random operator [14–16]. The slower-than-exponential decay of the survival probability is caused by the existence of arbitrarily large trap-free regions, where the particle can survive for an anomalously large time. At short times, the survival probability however decreases exponentially, according to the Rosenstock formula, which is the result of a mean-field analysis [17]. Although the survival probability has been studied in great detail for a whole breadth of trapping models, some problems still remain open. In particular, the crossover between the small-time (Rosenstock) and large-time (Lifshitz) regimes is not fully understood. The scaling properties in the crossover region have been investigated in detail by means of Monte-Carlo simulations [18]. On the theoretical side, a precise calculation of the survival probability throughout the Lifshitz regime is only possible in one dimension. In higher dimensions, going beyond the leading term given in (1.1) requires sophisticated field-theoretical techniques involving instantons [19–25].

At low temperatures, quantum effects eventually become relevant, overshadowing the diffusive nature of transport. In the presence of traps, the asymptotic form (1.1) of the survival probability is accordingly expected to be modified in a quantum-mechanical setup. The long-time behavior of the survival of a quantum particle in the presence of traps was first studied in a series of works by Parris [26–29]. The motivation for these investigations was to understand the low-temperature reaction dynamics and exciton quenching by isolated impurities in the coherent regime. The effective dynamics for the reduced density matrix of the exciton was shown to be given by a non-Hermitian tight-binding model, with an imaginary optical potential representing scattering, dephasing and absorption by the impurities [30–33]. The long-time

asymptotics of the survival probability $\Pi(t)$ of a quantum exciton hopping in a medium with a finite density of traps was found to be

$$\Pi(t) \sim \exp\left(-B_d t^{d/(d+3)}\right). \quad (1.2)$$

In contrast with the result (1.1) pertaining to the classical case, the dependence of the amplitude B_d on the density of traps and other parameters could only be worked out within approximations [26–29]. One of the main motivations for undertaking the present work was to obtain a better understanding of the amplitude B_d (see the results (6.49), (7.21)).

In more modern language, the motion of the exciton can be interpreted as a *quantum walk*. Quantum analogs of classical random walks have been defined in two pioneering papers [34,35] as a useful concept to implement original algorithms in quantum information theory. Due to interference effects, the properties of quantum walks can drastically differ from their classical counterparts. Clever implementations of quantum algorithms can thus lead to much faster computations [36–38] (see [39,40] for reviews). As far as experimental realizations of quantum walks are concerned, it is worth mentioning the promising area of photon propagation in waveguide lattices [41,42]. On the theoretical side, two distinct classes of quantum walks have been studied. In discrete-time quantum walks [34,43–45], in addition to its position, the particle has a discrete internal quantum degree of freedom (a ‘quantum coin’), which experiences unitary evolution at each step. In continuous-time quantum walks [35,46,47], no internal state is involved, and the role of the quantum Hamiltonian is played by some hopping matrix, such as the adjacency matrix on the underlying lattice or graph [48]. These two classes of models can be reconciled by means of a precise limiting procedure [49], which turns out to be more subtle than its classical counterpart, namely the emergence of diffusion as the continuum limit of discrete random walks (see [50] for a review).

Last but not least, there has been considerable progress lately in manipulating quantum-mechanical systems. The effect of decoherence in low-dimensional quantum systems can thus be investigated experimentally [51]. A paradigm for the loss of coherence in quantum transport is provided by quantum walks in the presence of traps. The recent years have witnessed an upsurge of interest in this kind of models [52–60].

The goal of the present work is to present a systematic comparison of the motion of a classical and of a quantum particle in the presence of traps, within the framework of the continuous-time classical and quantum random walk. The main emphasis will be put on the temporal behavior of the corresponding survival probabilities $P(t)$ and $\Pi(t)$. A common feature of all the situations to be considered in this work is that quantum particles are able to benefit from interference effects in order to efficiently avoid the traps. As a consequence, static traps are far less efficient to absorb quantum particles than classical ones. This qualitative difference will manifest itself in various settings.

The outline of this article is as follows. In section 2 we review the basic features of the classical and quantum motion of a free particle on the

one-dimensional chain, emphasizing the most salient differences between both types of dynamics. Section 3 is devoted to the situation of an infinite chain with a single trap. Whereas classical random walk is recurrent, with a survival property decaying as $P(t) \sim t^{-1/2}$, the quantum particle has a non-vanishing probability to escape ballistically to infinity, and thus to survive forever. The asymptotic survival probability Π_∞ is calculated for different initial conditions. It is shown to display generically a *non-monotonic* behavior with respect to the trapping strength. The geometry of a finite ring of N sites with a single trap is studied in Section 4. The classical survival probability decays exponentially, with the associated characteristic time scaling diffusively, i.e., as N^2 . The dynamics of the quantum particle demonstrates two main differences with respect to the classical case. The survival probability tends to a non-zero asymptotic value, which is generically $\Pi_\infty = 1/2$ in this geometry. The relaxation time characterizing the convergence toward that value grows asymptotically as N^3 [26]. This characteristic time is calculated in various regimes and is shown to exhibit again a non-monotonic dependence on the trapping strength. If several traps are present on a ring, the determination of the *avoiding modes* which are responsible for the non-vanishing of the asymptotic survival probability Π_∞ , leads to an elegant problem of combinatorics, which we solve in Section 5. The case of the chain with a fixed density of traps is studied in Section 6. In the classical situation, we review the predictions of the theory of Lifshitz tails. We thus introduce tools from the theory of one-dimensional disordered systems [61,62], which are also pertinent to the analysis of the quantum situation. In the latter case, for a large but finite system, the decay rate of the survival probability is a fluctuating quantity, whose distribution is investigated. We are thus able to determine exactly the amplitude B_1 of the stretched exponential (1.2), including its dependence on the density c of traps and on the trapping strength γ (see (6.49)). The problem of a classical and of a quantum particle diffusing on a higher-dimensional lattice with traps is considered in Section 7. Here, an exact calculation of the decay rate seems to be out of reach. We are led to make an Ansatz for its scaling behavior, and draw conclusions on the behavior of the survival probability $\Pi(t)$ (see (7.21)). The last section is devoted to concluding remarks.

2 A warming up: classical and quantum diffusion on the chain

In this section we recall the basic differences between a classical and a quantum particle diffusing on the infinite chain.

2.1 A classical particle

Consider a classical particle performing continuous-time random walk on the chain. Here and throughout the following, we use dimensionless variables, assuming that the lattice spacing and the hopping frequency are set equal to

unity. The probability $p_n(t)$ for the particle to be at site n at time t obeys the differential equation

$$\frac{dp_n(t)}{dt} = p_{n+1}(t) + p_{n-1}(t) - 2p_n(t). \quad (2.1)$$

Let us assume that the particle is launched at the origin at time $t = 0$. Introducing the momentum q conjugate to n , we readily obtain

$$\hat{p}(q, t) = \sum_n p_n(t) e^{-inq} = e^{-2(1-\cos q)t}. \quad (2.2)$$

The probabilities $p_n(t)$ therefore read

$$p_n(t) = e^{-2t} I_n(2t), \quad (2.3)$$

where the I_n are the modified Bessel functions. The bulk of the probability profile has a Gaussian form

$$p_n(t) \approx \frac{e^{-n^2/(4t)}}{\sqrt{4\pi t}}, \quad (2.4)$$

characteristic of a diffusive motion. In particular, the return probability

$$p_0(t) = e^{-2t} I_0(2t) \approx \frac{1}{\sqrt{4\pi t}} \quad (2.5)$$

decays monotonically to zero.

2.2 A quantum particle

Consider now a quantum particle propagating coherently along the chain. We again use dimensionless variables, assuming that Planck's constant, the lattice spacing and the hopping amplitude are set equal to unity. Within this framework, the wavefunction $\psi_n(t)$ of the particle at site n at time t obeys the time-dependent reduced tight-binding equation

$$i \frac{d\psi_n(t)}{dt} = \psi_{n+1}(t) + \psi_{n-1}(t). \quad (2.6)$$

Let us again assume that the particle is launched at the origin at time $t = 0$.

The dispersion law between energy ε and momentum q reads

$$\varepsilon = 2 \cos q. \quad (2.7)$$

The group velocity is therefore $v = d\varepsilon/dq = -2 \sin q$. We have

$$\hat{\psi}(q, t) = e^{-2i \cos q t}, \quad \psi_n(t) = i^{-n} J_n(2t), \quad (2.8)$$

and so the quantum probabilities read

$$|\psi_n(t)|^2 = (J_n(2t))^2, \quad (2.9)$$

where the J_n are the Bessel functions. These probabilities take appreciable values in the range $-2t < n < 2t$, which spreads ballistically with the maximal velocity $v_{\max} = 2$. The probability profile exhibits sharp ballistic fronts near $n = \pm 2t$, whose width scales as $t^{1/3}$ [46], and it decays exponentially beyond these fronts. The return probability decays as

$$|\psi_0(t)|^2 = (J_0(2t))^2 \approx \frac{\cos^2(2t - \pi/4)}{\pi t}. \quad (2.10)$$

Figures 2.1 and 2.2 illustrate the most prominent differences between classical and quantum diffusion. Figure 2.1 shows a plot of both probability profiles for $t = 50$. The classical profile $p_n(t)$ is rather narrow and approximately Gaussian, whereas the quantum profile $|\psi_n(t)|^2$ is much broader and irregular. The arrows show the nominal positions of the ballistic fronts ($n = \pm 100$). Figure 2.2 shows the return probabilities against time t . The classical probability $p_0(t)$ falls off monotonically and rather slowly, whereas the quantum one, $|\psi_0(t)|^2$, falls off faster on average and shows infinitely many oscillations.

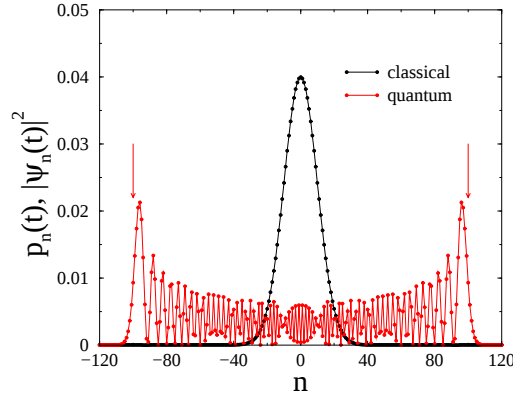


Fig. 2.1 Probability profiles $p_n(t)$ (see (2.3)) and $|\psi_n(t)|^2$ (see (2.9)) of a classical and a quantum particle launched at the origin against the particle's position n , for $t = 50$. Arrows: nominal positions of the ballistic fronts in the quantum case ($n = \pm 100$) (Color online).

3 The infinite chain with a single trap

We now study the effect of a single trap on the motion of a classical and a quantum particle on the infinite chain.

3.1 A classical particle

Consider a classical particle diffusing on the infinite chain, with a single trap at the origin. The strength γ of a classical trap is defined as its absorption

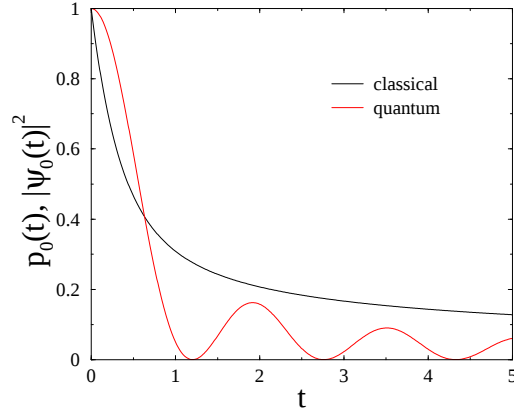


Fig. 2.2 Return probabilities $p_0(t)$ (monotonic, see (2.5)) and $|\psi_0(t)|^2$ (oscillating, see (2.10)) of a classical and a quantum particle, against time t (Color online).

rate per unit time. The differential equation (2.1) becomes

$$\frac{dp_n(t)}{dt} = p_{n+1}(t) + p_{n-1}(t) - 2p_n(t) - \gamma\delta_{n0}p_0(t). \quad (3.1)$$

Let us assume that the particle is launched at site $a \geq 0$ at time $t = 0$.

We are mostly interested in the survival probability of the particle up to time t :

$$P(t) = \sum_n p_n(t) = 1 - \gamma \int_0^t p_0(t') dt'. \quad (3.2)$$

Introducing a Laplace variable s conjugate to t and a Fourier variable (momentum) q conjugate to n , we obtain

$$\hat{p}(q, s) = \frac{e^{-iqa} - \gamma\hat{p}_0(s)}{s + 2(1 - \cos q)}. \quad (3.3)$$

The quantity $\hat{p}_0(s)$ obeys the self-consistency condition

$$\hat{p}_0(s) = \int_0^{2\pi} \frac{dq}{2\pi} \hat{p}(q, s) = \frac{z_1^a - \gamma\hat{p}_0(s)}{z_2 - z_1}, \quad (3.4)$$

where z_1 and z_2 are the zeros of the denominator of (3.3) in the variable $z = e^{-iq}$ such that $|z_1| < 1 < |z_2|$, i.e.,

$$z_{1,2} = \frac{s + 2 \mp \sqrt{s(s+4)}}{2}. \quad (3.5)$$

Hence

$$\hat{p}_0(s) = \frac{z_1^a}{\gamma + z_2 - z_1}. \quad (3.6)$$

The survival probability therefore reads in Laplace space

$$\hat{P}(s) = \hat{p}(0, s) = \frac{1}{s} \left(1 - \frac{\gamma z_1^a}{\gamma + z_2 - z_1} \right). \quad (3.7)$$

The short-time behavior of the survival probability is governed by the behavior of (3.7) as $s \rightarrow \infty$. We have

$$\hat{P}(s) = \frac{1}{s} \left(1 - \frac{\gamma}{s^{a+1}} + \dots \right), \quad (3.8)$$

and so

$$P(t) = 1 - \frac{\gamma t^{a+1}}{(a+1)!} + \dots \quad (3.9)$$

The departure of the survival probability from unity is slower when the initial distance a between the particle and the trap is larger, as could be expected.

More interesting is the asymptotic decay of the survival probability at late times, which is governed by the behavior of (3.7) as $s \rightarrow 0$. We have

$$\hat{P}(s) \approx \frac{b}{\sqrt{s}}, \quad (3.10)$$

and so

$$P(t) \approx \frac{b}{\sqrt{\pi t}}, \quad (3.11)$$

with

$$b = a + \frac{2}{\gamma}. \quad (3.12)$$

The survival probability $P(t)$ exhibits the universal decay in $1/\sqrt{t}$ of the persistence probability that a one-dimensional random walker has not returned to its starting point up to time t . The amplitude b can be interpreted as an *effective distance* between the trap and the site where the particle is launched, which is just a in the limit of a perfect trap ($\gamma \rightarrow \infty$), but gets renormalized to a larger value whenever the trap is imperfect (γ finite).

3.2 A quantum particle

Consider now a quantum particle propagating on the chain in the presence of a single trap at the origin. The strength γ of the trap is now the amplitude of an imaginary *optical potential* describing the absorbing power of the trap. The tight-binding equation (2.6) thus becomes non-Hermitian:

$$i \frac{d\psi_n(t)}{dt} = \psi_{n+1}(t) + \psi_{n-1}(t) - i\gamma\delta_{n0} \psi_0(t). \quad (3.13)$$

Complex optical potentials were introduced long ago in quantum mechanics in order to describe the inelastic scattering or the absorption of particles, in analogy with complex refraction indices in optics. In the present framework,

the effective description of the trap by an optical potential can be derived by first representing the trap as a zero-temperature phonon bath and then tracing out the degrees of freedom of the bath [27, 30–33]. A more formal approach is based on deriving a Lindblad dynamics for the particle coupled to the bath [63–65].

We again assume that the particle is launched at site $a \geq 0$ at time $t = 0$. We are again interested in the survival probability of the quantum particle up to time t . This quantity reads

$$\Pi(t) = \sum_n |\psi_n(t)|^2 = 1 - 2\gamma \int_0^t |\psi_0(t')|^2 dt'. \quad (3.14)$$

The differential equation (3.13) can be solved in the very same way as its classical analogue (3.1). We thus obtain

$$\hat{\psi}(q, s) = \frac{i(e^{-iq a} - \gamma \hat{\psi}_0(s))}{is - 2 \cos q} \quad (3.15)$$

and

$$\hat{\psi}_0(s) = \frac{1}{\gamma + \sqrt{s^2 + 4}} \left(\frac{\sqrt{s^2 + 4} - s}{2i} \right)^a. \quad (3.16)$$

There is a noticeable qualitative difference between the quantum case under study and its classical counterpart. In the present situation, the survival probability tends to a non-zero asymptotic value Π_∞ in the limit of infinitely large times:

$$\Pi_\infty = 1 - 2\gamma I, \quad I = \int_0^\infty |\psi_0(t)|^2 dt, \quad (3.17)$$

whose dependence on the trapping strength γ and on the initial distance a will now be worked out explicitly. The integral I can be evaluated directly in Laplace space, by means of the following formula:

$$\int_0^\infty f(t)g(t) e^{-\varepsilon t} dt = \int \frac{ds}{2\pi i} \hat{f}(s) \hat{g}(\varepsilon - s) \quad (0 < \text{Re } s < \varepsilon). \quad (3.18)$$

The above identity is a regularized form of the Parseval-Plancherel identity for Fourier transforms, with $\varepsilon > 0$ acting as a regulator. It holds as soon as the Laplace transforms $\hat{f}(s)$ and $\hat{g}(s)$ are analytic in the half plane $\text{Re } s > 0$. Setting $f(t) = \psi_0(t)$ and $g(t) = \bar{\psi}_0(t)$ and taking the $\varepsilon \rightarrow 0$ limit, so that $s = iy + 0$ lies to the immediate right of the imaginary axis, we obtain

$$I = I_1 + I_2(a), \quad (3.19)$$

with

$$I_1 = \frac{1}{\pi} \int_0^2 \frac{dy}{(\gamma + \sqrt{4 - y^2})^2},$$

$$I_2(a) = \frac{1}{\pi} \int_2^\infty \frac{dy}{\gamma^2 + y^2 - 4} \left(\frac{y - \sqrt{y^2 - 4}}{2} \right)^{2a}. \quad (3.20)$$

In the limit where the initial distance gets large ($a \rightarrow \infty$), $I_2(a)$ tends to zero, and so $I \rightarrow I_1$.

The explicit expressions of the above integrals depend on the position of γ with respect to 2.

- $\gamma < 2$. Setting $w = \sqrt{4 - \gamma^2}$, we obtain

$$\begin{aligned}
\pi I_1 &= -\frac{2}{w^2} + \frac{2}{w^3} \ln \frac{2+w}{2-w}, \\
\pi I_2(0) &= \frac{1}{2w} \ln \frac{2+w}{2-w}, \\
\pi I_2(1) &= -1 + \frac{\pi\gamma}{4} + \left(-\frac{1}{2w} + \frac{w}{4}\right) \ln \frac{2+w}{2-w}, \\
\pi I_2(2) &= \frac{8}{3} - w^2 - \left(\frac{1}{2} - \frac{w^2}{4}\right) \pi\gamma + \left(\frac{1}{2w} - w + \frac{w^3}{4}\right) \ln \frac{2+w}{2-w}, \\
\pi I_2(3) &= -\frac{21}{5} + \frac{14w^2}{3} - w^4 + \left(\frac{3}{4} - w^2 + \frac{w^4}{4}\right) \pi\gamma \\
&\quad + \left(-\frac{1}{2w} + \frac{9w}{4} - \frac{3w^3}{2} + \frac{w^5}{4}\right) \ln \frac{2+w}{2-w},
\end{aligned} \tag{3.21}$$

and so on.

In the weak-trapping regime ($\gamma \rightarrow 0$), the asymptotic survival probability departs from unity as

$$\Pi_\infty \approx 1 - \frac{2\gamma |\ln \gamma|}{\pi} \tag{3.22}$$

for any finite initial distance a (including $a = 0$), whereas the limiting result for $a = \infty$, i.e., $I = I_1$, yields a halved amplitude, i.e.,

$$\Pi_\infty \approx 1 - \frac{\gamma |\ln \gamma|}{\pi} \quad (a = \infty). \tag{3.23}$$

In other words, the limits $a \rightarrow \infty$ and $\gamma \rightarrow 0$ do not commute.

- $\gamma > 2$. Setting $u = \sqrt{\gamma^2 - 4}$, we now have

$$\begin{aligned}
\pi I_1 &= \frac{2}{u^2} - \frac{4}{u^3} \arctan \frac{u}{2}, \\
\pi I_2(0) &= \frac{1}{u} \arctan \frac{u}{2}, \\
\pi I_2(1) &= -1 + \frac{\pi\gamma}{4} - \left(\frac{1}{u} + \frac{u}{2}\right) \arctan \frac{u}{2}, \\
\pi I_2(2) &= \frac{8}{3} + u^2 - \left(\frac{1}{2} + \frac{u^2}{4}\right) \pi\gamma + \left(\frac{1}{u} + 2u + \frac{u^3}{2}\right) \arctan \frac{u}{2}, \\
\pi I_2(3) &= -\frac{21}{5} - \frac{14u^2}{3} - u^4 + \left(\frac{3}{4} + u^2 + \frac{u^4}{4}\right) \pi\gamma \\
&\quad - \left(\frac{1}{u} + \frac{9u}{2} + 3u^3 + \frac{u^5}{2}\right) \arctan \frac{u}{2},
\end{aligned} \tag{3.24}$$

and so on. These expressions are the analytic continuations of (3.21) as $w \rightarrow \pm iu$, as it should be.

In the strong-trapping regime ($\gamma \rightarrow \infty$), the behavior of the asymptotic survival probability depends in a crucial way on the initial distance a . If the particle is launched on the trap itself, the survival probability decays to zero as

$$\Pi_\infty \approx \frac{1}{2\gamma^2} \quad (a = 0). \quad (3.25)$$

If the particle is launched at any other site, the survival probability goes to unity as

$$\Pi_\infty \approx 1 - \frac{16a^2}{\pi(4a^2 - 1)\gamma} \quad (a > 0). \quad (3.26)$$

We have in particular

$$\Pi_\infty \approx 1 - \frac{4}{\pi\gamma} \quad (3.27)$$

in the limit of an infinitely large initial distance.

Figure 3.1 shows a plot of Π_∞ against the trapping strength γ , for several values of the initial distance a between the particle and the trap. This figure illustrates the most salient features of the asymptotic survival probability. When the quantum particle is launched on the trap itself ($a = 0$), Π_∞ decreases monotonically from unity (see (3.22)) to zero (see (3.25)). As soon as the particle is launched at a different site ($a \neq 0$), Π_∞ has a non-monotonic dependence on the trapping strength. It starts decreasing from unity for small γ (see (3.22)), reaches a non-trivial minimum $\Pi_{\infty, \min}$ for some finite trapping strength $\gamma_{\min}$, before it slowly returns to unity in the strong-trapping regime (see (3.26)).

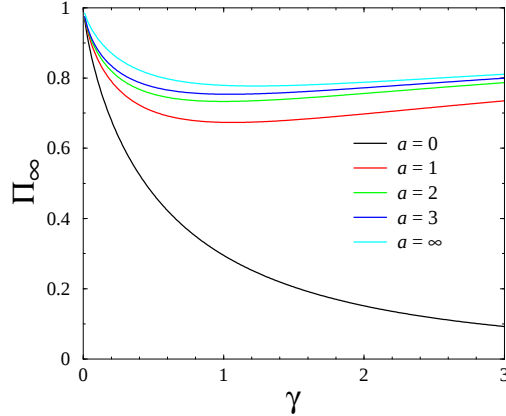


Fig. 3.1 Asymptotic survival probability Π_∞ of the quantum particle against trapping strength γ , for several values of the initial distance a between the particle and the trap. Bottom to top: $a = 0, 1, 2, 3$, and ∞ (Color online).

The values of the asymptotic survival probability Π_∞ in the borderline situation where $\gamma = 2$ can be reached by letting either $w \rightarrow 0$ in (3.21) or $u \rightarrow 0$ in (3.24). The numbers thus obtained are listed in Table 3.1 for initial distances $a = 0, 1, 2, 3$, and ∞ , as well as the coordinates $\gamma_{\min}$ and $\Pi_{\infty, \min}$ of the minimum of the curve $\Pi_\infty(\gamma)$. The quantities $\Pi_\infty(\gamma = 2)$ and $\Pi_{\infty, \min}$ show a fast convergence in $1/a^2$ toward their values in the $a = \infty$ limit. For $a = 2$, $\gamma_{\min} = 1$ exactly, while $\Pi_{\infty, \min} = 1/2 + 2/\pi - 5 \ln(2 + \sqrt{3})/(3\pi\sqrt{3})$.

a	$\Pi_\infty(\gamma = 2)$	$\gamma_{\min}$	$\Pi_{\infty, \min}$
0	$1 - 8/(3\pi) = 0.15117$	∞	0
1	$16/(3\pi) - 1 = 0.69765$	1.06254	0.67338
2	$5 - 40/(3\pi) = 0.75586$	1	0.73324
3	$272/(15\pi) - 5 = 0.77201$	1.04211	0.75369
∞	$1 - 2/(3\pi) = 0.78779$	1.22574	0.77720

Table 3.1 Values of the asymptotic survival probability Π_∞ of the quantum particle in the borderline situation $\gamma = 2$ (Column 2), and coordinates $\gamma_{\min}$ and $\Pi_{\infty, \min}$ (Columns 3 and 4) of the minimum of the curve $\Pi_\infty(\gamma)$, for several initial distances $a = 0, 1, 2, 3$, and ∞ between the particle and the trap.

The most striking feature of the above results is the non-monotonic dependence of the asymptotic survival probability Π_∞ on the trapping strength γ , which eventually returns to unity in the strong-trapping regime ($\gamma \rightarrow \infty$). The paradoxical inefficiency of a quantum trap in the nominal strong-trapping regime can be understood in the following terms. For large γ and $a > 0$, the wavefunction $\psi_0(t)$ on the trap can be expected to be proportional to $1/\gamma$, and so the integrand in (3.14), (3.17) is proportional to $1/\gamma^2$, and the differences $1 - \Pi(t)$ and $1 - \Pi_\infty$ are proportional to $1/\gamma$.

In the present situation, it can be checked explicitly that the above line of reasoning is correct. To leading order as $\gamma \rightarrow \infty$, (3.16) indeed reads

$$\gamma \hat{\psi}_0(s) \approx \left(\frac{\sqrt{s^2 + 4} - s}{2i} \right)^a, \quad (3.28)$$

and yields

$$\gamma \psi_0(t) \approx a i^{-a} \frac{J_a(2t)}{t}, \quad (3.29)$$

where J_a is again the Bessel function. Inserting the above estimate into (3.17), and using the integral [66, (6.574.2), p. 692]

$$\int_0^\infty \left(\frac{J_a(x)}{x} \right)^2 dx = \frac{4}{\pi(4a^2 - 1)}, \quad (3.30)$$

we recover (3.26).

4 A finite ring with a single trap

In this section we investigate the motion of a classical and a quantum particle on a finite ring with a single trap.

4.1 A classical particle

Consider a classical particle diffusing on a ring of N sites ($n = 0, \dots, N-1$), with periodic boundary conditions ($N \equiv 0$). In the presence of a single trap at the origin, the probability $p_n(t)$ for the particle to be at site n at time t still obeys (3.1). It will be sufficient for our purpose to look for solutions decaying as $\exp(-Et)$, i.e., for the eigenmodes of the stationary equation

$$-E p_n = p_{n+1} + p_{n-1} - 2p_n - \gamma \delta_{n0} p_0, \quad (4.1)$$

with periodic boundary conditions. Setting

$$E = 2(1 - \cos q), \quad (4.2)$$

the general solution of (4.1) reads

$$p_n = A e^{inq} + B e^{-inq} \quad (4.3)$$

for $n = 0, \dots, N$ with $N \equiv 0$. Boundary conditions yield

$$\begin{aligned} A + B &= A e^{iNq} + B e^{-iNq}, \\ \gamma(A + B) &= A e^{-iq}(e^{iNq} - 1) + B e^{iq}(e^{-iNq} - 1). \end{aligned} \quad (4.4)$$

Eigenmodes have a definite parity, i.e., they are either even (+) or odd (−) in the exchange $n \leftrightarrow N - n$.

- In the even sector, we have $p_{N-n} = p_n$, i.e., $B = A e^{iNq}$. The amplitude $p_0 = A + B$ on the trap is non-vanishing. The second line of (4.4) yields the quantization condition

$$e^{iNq} = \frac{2 \sin q + i\gamma}{2 \sin q - i\gamma}, \quad \text{i.e., } \gamma = 2 \sin q \tan \frac{Nq}{2}. \quad (4.5)$$

- In the odd sector, we have $p_{N-n} = -p_n$, i.e., $B = -A e^{iNq}$. The amplitude on the trap vanishes. This yields the quantization condition

$$e^{iNq} = 1, \quad (4.6)$$

irrespective of γ . We thus obtain the explicit momenta $q_k^{(-)} = 2\pi k/N$, i.e.,

$$E_k^{(-)} = 2 \left(1 - \cos \frac{2\pi k}{N} \right). \quad (4.7)$$

All eigenvalues are positive, and the even and odd spectra are intertwining:

- If N is odd, say $N = 2M + 1$, there are M odd and $M + 1$ even modes:

$$0 < E_1^{(+)} < E_1^{(-)} < \dots < E_M^{(+)} < E_M^{(-)} < 4 < E_{M+1}^{(+)} \quad (4.8)$$

- If N is even, say $N = 2M + 2$, there are M odd and $M + 2$ even modes:

$$0 < E_1^{(+)} < E_1^{(-)} < \dots < E_M^{(+)} < E_M^{(-)} < E_{M+1}^{(+)} < 4 < E_{M+2}^{(+)} \quad (4.9)$$

In both cases the largest eigenvalue in the even sector is larger than the band edge ($E_{\max} = 4$). It therefore corresponds to a purely imaginary momentum.

For a generic initial condition, the survival probability decays exponentially fast, as

$$P(t) \sim e^{-\lambda t}, \quad \lambda = E_1^{(+)} \quad (4.10)$$

When the ring size N is large, we have $q_1^{(+)} \approx \pi/N$, and so the decay rate λ scales as

$$\lambda \approx \frac{\pi^2}{N^2}, \quad (4.11)$$

irrespective of γ .

The decay rate however exhibits a non-trivial scaling in the regime where N is large, while the trapping strength γ is small, so that the product

$$X = N\gamma \quad (4.12)$$

is fixed. In this regime, we have $q_1^{(+)} \approx \theta/N$, and so the decay rate obeys the scaling law

$$\lambda \approx \frac{\theta^2}{N^2}, \quad (4.13)$$

where θ is an implicit function of X given by (see (4.5))

$$2\theta \tan \frac{\theta}{2} = X. \quad (4.14)$$

- For $X \ll 1$, we have $\theta^2 = X - X^2/12 + \dots$, and so

$$\lambda \approx \frac{\gamma}{N} \left(1 - \frac{N\gamma}{12} + \dots \right) \quad (N\gamma \ll 1). \quad (4.15)$$

- For $X \gg 1$, we have $\theta = \pi - 4\pi/X + \dots$, and so

$$\lambda \approx \frac{\pi^2}{N^2} \left(1 - \frac{8}{N\gamma} + \dots \right) \quad (N\gamma \gg 1), \quad (4.16)$$

in agreement with (4.11) to leading order. The scaling function $\theta(X)$ will be plotted in Figure 4.2, together with its quantum analogue (see (4.25)).

4.2 A quantum particle

Consider now a quantum particle on a finite ring of N sites, in the presence of a single trap at the origin. This problem has already been tackled in several earlier works [30,55,58].

For the present purpose, it will be sufficient to look for harmonic solutions to (3.13), proportional to $\exp(-i\epsilon t)$, i.e., for the eigenmodes of the stationary equation

$$\epsilon \psi_n = \psi_{n+1} + \psi_{n-1} - i\gamma \delta_{n0} \psi_0, \quad (4.17)$$

with periodic boundary conditions. The general solution of (4.17) is still given by (4.3), albeit with the dispersion law (2.7).

- In the even sector, the quantization condition now reads

$$e^{iNq} = \frac{2 \sin q - \gamma}{2 \sin q + \gamma}, \quad \text{i.e., } \gamma = -2i \sin q \tan \frac{Nq}{2}. \quad (4.18)$$

- In the odd sector, the quantization (4.6) still holds, irrespective of the trapping strength γ . We thus obtain the real energy eigenvalues

$$\epsilon_k^{(-)} = 2 \cos \frac{2\pi k}{N}. \quad (4.19)$$

The main qualitative difference between the quantum case and its classical counterpart is that the energy eigenvalues in the even sector are now complex numbers with negative imaginary parts, while those in the odd sector remain real. Figure 4.1 shows a plot of the energy spectrum for a ring of $N = 14$ sites with $\gamma = 1$.

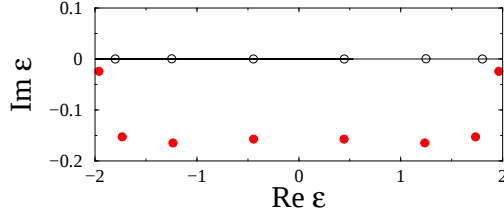


Fig. 4.1 Energy spectrum of a ring of $N = 14$ sites with $\gamma = 1$ in the complex ϵ -plane. The scale on the imaginary axis is expanded 5 times. Empty black symbols: 6 real eigenvalues of the odd sector. Full red symbols: 8 complex eigenvalues of the even sector (Color online).

Consider an arbitrary initial condition, defined by the normalized wavefunction $\psi_n(0) = \phi_n$, and introduce the projections

$$\phi_n^{(\pm)} = \frac{1}{2}(\phi_n \pm \phi_{N-n}) \quad (4.20)$$

of the initial wavefunction onto the even and odd sectors.

The projection $\phi_n^{(-)}$ undergoes a unitary evolution, i.e., it is the superposition of harmonic components in $\exp(-i\varepsilon_k^{(-)}t)$, where the energy eigenvalues $\varepsilon_k^{(-)}$ are real. The projection $\phi_n^{(+)}$ undergoes a non-unitary evolution, i.e., it is the superposition of decaying components in $\exp(-i\varepsilon_k^{(-)}t)$, where the energy eigenvalues $\varepsilon_k^{(-)}$ are complex numbers with negative imaginary parts. The survival probability $\Pi(t)$ therefore tends to a non-zero asymptotic value Π_∞ , which is nothing but the probability for the particle to be initially in the odd sector:

$$\Pi_\infty = \sum_{n=1}^{N-1} \left| \phi_n^{(-)} \right|^2. \quad (4.21)$$

In order to make the connection with the infinite chain (see Section 3), let us assume that the particle is launched at some site a on the ring. We have then generically

$$\Pi_\infty = \frac{1}{2}. \quad (4.22)$$

There are two exceptions to this rule. If $a = 0$ (the particle is launched on the trap itself), $\phi_n^{(-)}$ vanishes and we have $\Pi_\infty = 0$. More surprisingly, if N is even and $a = N/2$ (the particle is launched exactly at the antipode of the trap), $\phi_n^{(-)}$ also vanishes and we again have $\Pi_\infty = 0$. This is a mere interference phenomenon in a discrete quantum system. It is also worth noticing that (4.22) is smaller than the corresponding result on the infinite chain (see Table 3.1), where the minimum $\Pi_{\infty, \min}$ depends on the distance a , but is always larger than $1/2$. This difference can be attributed to the fact that the particle may escape to infinity on the infinite chain, whereas it is bound to make repeated returns to the trap in the ring geometry.

The excess survival probability $\Pi(t) - \Pi_\infty$ decays exponentially fast, as

$$\Pi(t) - \Pi_\infty \sim e^{-\lambda t}, \quad (4.23)$$

where the decay rate λ is dictated by the eigenvalue in the even sector whose imaginary part is the smallest, i.e.,

$$\lambda = -2 \operatorname{Im} \varepsilon_1^{(+)}. \quad (4.24)$$

The decay rate λ again exhibits a non-trivial scaling if the ring size N is large, while the trapping strength γ is small, so that their product X is kept constant (see (4.12)). We have $q_1^{(+)} \approx \zeta/N$, and so the decay rate obeys the scaling law

$$\lambda \approx \frac{2 \operatorname{Im} \zeta^2}{N^2}. \quad (4.25)$$

Using (4.18), one finds that ζ is an implicit complex function of X given by

$$2\zeta \tan \frac{\zeta}{2} = iX. \quad (4.26)$$

- For $X \ll 1$, we have $\zeta^2 = iX + X^2/12 - iX^3/180 + \dots$, and so

$$\lambda \approx \frac{2\gamma}{N} \left(1 - \frac{(N\gamma)^2}{180} + \dots \right) \quad (N\gamma \ll 1). \quad (4.27)$$

- For $X \gg 1$, we have $\zeta = \pi(1 + 4i/X - 16/X^2 - 16(12 - \pi^2)i/(3X^3) + \dots)$, and so

$$\lambda \approx \frac{16\pi^2}{N^3\gamma} \left(1 - \frac{4(24 - \pi^2)}{3(N\gamma)^2} + \dots \right) \quad (N\gamma \gg 1). \quad (4.28)$$

The decay rate λ thus shows a non-monotonic dependence on the trapping strength. It starts increasing linearly as γ/N for small γ , reaches a maximum for $X_{\max} = N\gamma_{\max} = 9.2235$, where $N^2\lambda_{\max} = 11.0846$, and then falls off as $1/(N^3\gamma)$. The power-law decay

$$\lambda \approx \frac{16\pi^2}{N^3\gamma} \quad (4.29)$$

holds more generally for N large and any finite value of γ .

Figure 4.2 shows a comparison between the scaling forms of the decay rate λ in the classical case (see (4.13)) and in the quantum one (see (4.25)).

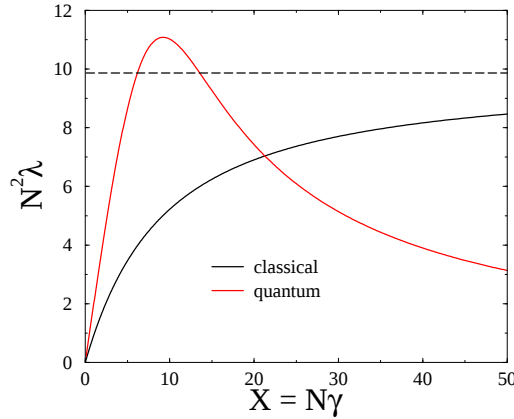


Fig. 4.2 Rescaled decay rate $N^2\lambda$ against rescaled trapping strength $X = N\gamma$ for a classical and a quantum particle on a ring with a single trap. The corresponding scaling functions are θ^2 for the classical case (monotonic, see (4.13)) and $2\text{Im}\zeta^2$ for the quantum one (non-monotonic, see (4.25)). Dashed line: asymptote at π^2 for the classical case (Color online).

5 A finite ring with several traps

We have seen in Section 4.2 that a quantum particle on a ring with a single trap survives forever with a non-zero probability Π_∞ . This is due to the existence

of *avoiding modes* which are insensitive to the presence of the trap, because their amplitude on the trap vanishes. Stated otherwise, avoiding modes are solutions of the stationary equation (4.17) whose energy eigenvalue ε is *real*. This phenomenon has no classical analogue: on a finite sample, a single trap always causes the survival probability of a classical walker to decay exponentially fast to zero.

For a single trap, avoiding modes are easy to characterize: these are the modes pertaining to the odd sector. Remarkably enough, avoiding modes can exist in the presence of more than one trap. Consider the example of a ring of N sites, in the case where $N = 2M$ is even, with two traps at the antipodal positions $n = 0$ and $n = M$. All the modes pertaining to the odd sector are still avoiding modes in the presence of these two traps.

In general, the asymptotic survival probability Π_∞ of the quantum particle is given by the square norm of the projection of its initial state $|\phi\rangle$ onto the linear subspace of avoiding modes. In other words, the result (4.21) generalizes to

$$\Pi_\infty = \sum_{|e\rangle} |\langle e|\phi\rangle|^2, \quad (5.1)$$

where $|e\rangle$ runs over a basis of avoiding modes.

The existence of avoiding modes in the presence of several traps on a ring has already been demonstrated on examples [30, 55]. Our goal is to treat the combinatorics of these modes in a systematic way. Consider the 2^N trap configurations on the ring. Each configuration is encoded in a sequence of occupation numbers $\eta_n \in \{0, 1\}$, with $\eta_n = 1$ meaning there is a trap at site n and $\eta_n = 0$ there is no trap at site n . We assume all traps have the same strength γ . For each trap configuration, we consider the stationary tight-binding equation

$$\varepsilon \psi_n = \psi_{n+1} + \psi_{n-1} - i\gamma\eta_n \psi_n, \quad (5.2)$$

with periodic boundary conditions ($N \equiv 0$), and we address the following question: *Does (5.2) have avoiding modes?*

If there is no trap, all the N eigenmodes of (5.2) are avoiding. Let us henceforth assume there is at least one trap, and proceed in two steps:

- *At the local level*, consider a cluster of consecutive sites without traps. Define the cluster length $L \geq 2$ as the number of those sites plus one, and renumber the sites as $n = 1, \dots, L-1$. This cluster supports avoiding modes of the form

$$\psi_n = \sin qn, \quad (5.3)$$

with $q = k\pi/L$ with $k = 1, \dots, L-1$.

- *At the global level*, for a given trap configuration, define ℓ as the greatest common divisor (GCD) of all the cluster lengths $L_1, L_2, \dots$. The condition for the configuration to support at least one avoiding mode simply reads $\ell \geq 2$. In the marginal situation where $\ell = 2$, one must impose the extra condition that N is a multiple of 4.

For a ring of N sites, we are thus led to define the following combinatorial numbers:

- The number $m(N, \ell)$ of non-empty trap configurations such that ℓ is the GCD of all the cluster lengths.
- The number $M(N)$ of trap configurations supporting avoiding modes.

These numbers can be calculated recursively as follows. First, $m(N, \ell)$ is non-zero only if ℓ is a divisor of N , and we have

$$m(N, \ell) = \ell \nu(N/\ell), \quad (5.4)$$

where $\nu(N)$ is a short-hand for $m(N, 1)$. Then, any non-empty configuration corresponds a unique ℓ , hence the sum rule¹

$$2^N = 1 + \sum_{\ell|N} m(N, \ell). \quad (5.5)$$

Singling out the term with $\ell = 1$, we obtain the following recursion relation:

$$\nu(N) = 2^N - 1 - \sum'_{\ell|N} \ell \nu(N/\ell), \quad (5.6)$$

where the sum runs over all the divisors ℓ of N , except $\ell = 1$. The above relation determines all the $\nu(N)$ from the initial value $\nu(1) = 1$.

The number of configurations supporting avoiding modes is

$$M(N) = 1 + \sum'_{\ell|N} \ell \nu(N/\ell), \quad (5.7)$$

where the sum runs over the divisors ℓ of N except $\ell = 1$, and $\ell = 2$ if N is not a multiple of 4. The above expression simplifies to

$$M(N) = \begin{cases} 2^N - \nu(N) - 2\nu(N/2) & (N \text{ even and } N/2 \text{ odd}), \\ 2^N - \nu(N) & (\text{else}). \end{cases} \quad (5.8)$$

The erratic dependence of $M(N)$ on the ring size N , illustrated in Table 5.1 and Figure 5.1, is reminiscent of the behavior of the classical number-theoretic functions. In particular:

N	$M(N)$	N	$M(N)$	N	$M(N)$	N	$M(N)$
1	1	6	10	11	12	16	511
2	1	7	8	12	154	17	18
3	4	8	31	13	14	18	190
4	7	9	22	14	22	19	20
5	6	10	16	15	114	20	2092

Table 5.1 Numbers $M(N)$ of trap configurations supporting avoiding modes for rings with up to $N = 20$ sites.

¹ The notation $\ell | N$ means that ℓ is a divisor of N , i.e., that N is a multiple of ℓ .

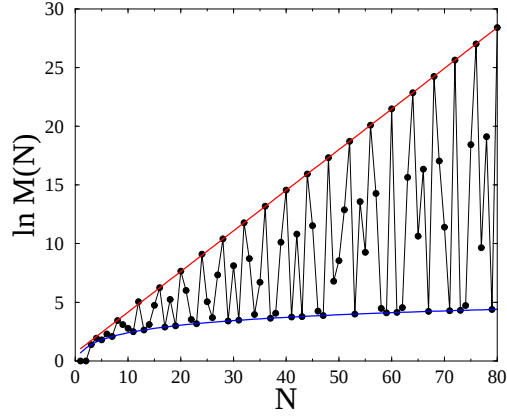


Fig. 5.1 Logarithmic plot of the number $M(N)$ of trap configurations supporting avoiding modes on a ring of N sites, against N . Symbols: exact numbers (see (5.8)). Lower blue curve: minimal values (see (5.9)), reached when N is a prime number. Upper red line: maximal values (see (5.10)), reached exactly when N is a power of 2, and approximately whenever N is a multiple of 4 (Color online).

- If N is an odd prime number, only the empty configuration and the N configurations with a single trap ($\ell = N$) support avoiding modes. We thus obtain the linear behavior

$$M(N) = N + 1. \quad (5.9)$$

- If N is a power of 2 (albeit not 2 itself), we have the exponential behavior

$$M(N) = 2^{1+N/2} - 1. \quad (5.10)$$

This number of configurations grows as the square root of the total number 2^N of trap configurations. The above growth law is approximately valid whenever N is a multiple of 4.

6 The infinite chain with a fixed density of traps

We now consider the physically more realistic situation of a classical or a quantum particle propagating on the infinite chain, with a random distribution of traps with given density. The higher-dimensional situation will be dealt with in Section 7.

6.1 A classical particle

We start with a reminder on the case of a classical particle. We assume that all traps have the same strength γ , so that we are facing a dilution disorder,

characterized by the trap density c , and encoded in the random occupation numbers:

$$\eta_n = \begin{cases} 1 & \text{with prob. } c, \\ 0 & \text{with prob. } 1 - c, \end{cases} \quad (6.1)$$

with $\eta_n = 1$ meaning there is a trap at site n , and $\eta_n = 0$ there is no trap at site n . We are led to consider the stationary equation

$$-E p_n = p_{n+1} + p_{n-1} - 2p_n - \gamma \eta_n p_n. \quad (6.2)$$

On any finite sample, the survival probability decays exponentially fast, as

$$P(t) \sim e^{-\lambda t}, \quad \lambda = E_1, \quad (6.3)$$

where E_1 is the smallest eigenvalue of (6.2).

It is known from the theory of Lifshitz tails [14–16] that the smallest eigenvalue E_1 corresponds to the lowest mode on the largest *Lifshitz region*, i.e., the largest interval which is free of traps. Let us focus on such a region of $N + 1$ consecutive sites, and renumber them as $n = 0, \dots, N$. We have therefore $\eta_n = 0$ for $n = 0, \dots, N$, whereas the configuration on the rest of the sample is left unspecified. The solution of (6.2) on the Lifshitz region reads (see (4.3))

$$p_n = A e^{inq} + B e^{-inq} \quad (n = 0, \dots, N), \quad (6.4)$$

where the wavevector q is related to E by (see (4.2))

$$E = 2(1 - \cos q). \quad (6.5)$$

Along the lines of [61], let us parametrize the boundary conditions imposed by the rest of the sample as

$$p_{-1} = Y_L p_0, \quad p_{N+1} = Y_R p_N. \quad (6.6)$$

We thus obtain the quantization condition

$$\sin(N + 2)q - (Y_L + Y_R) \sin(N + 1)q + Y_L Y_R \sin Nq = 0. \quad (6.7)$$

The wavevector corresponding to the lowest mode therefore reads

$$q_1 = \frac{\pi}{N} \left(1 + \frac{\alpha}{N} + \dots \right), \quad (6.8)$$

with

$$\alpha = \frac{1}{Y_L - 1} + \frac{1}{Y_R - 1}. \quad (6.9)$$

To leading order as the size N of the Lifshitz region is large, we therefore have the estimate

$$\lambda \approx \frac{\pi^2}{N^2}. \quad (6.10)$$

This result is formally identical to (4.11), which applies to a ring with a single trap. It holds irrespectively of the rest of the sample, which only enters

the amplitude α of the correction term through the left and right boundary parameters Y_L and Y_R .

In the limit of an infinite system, the behavior of the integrated density of states

$$H(E) = \int_0^E \rho(E') dE' \quad (6.11)$$

at low energy ($E \rightarrow 0$) can be estimated as follows: the lowest energy level E_1 is given by (6.10) with an exponentially small probability of order $(1-c)^N$ per unit length. We thus obtain the well-known Lifshitz tail [14–16]

$$H(E) \sim \exp\left(-\frac{\pi |\ln(1-c)|}{\sqrt{E}}\right). \quad (6.12)$$

Despite the rather heuristic nature of the above reasoning, the asymptotic result (6.12) is fully correct. Indeed it only misses an oscillatory prefactor of order unity. This prefactor has been shown to be a periodic function of $\pi/\sqrt{E}$ with unit period, which reflects the discrete nature of the underlying chain, and can be expressed in terms of the distribution of the boundary parameters Y_L and Y_R at $E = 0$ [61].

The asymptotic decay of the survival probability $P(t)$ can be estimated by superposing the contributions of Lifshitz regions of all sizes N , weighted by their respective probabilities $(1-c)^N$. Working with exponential accuracy and going to a continuum approximation, we get

$$P(t) \sim \int_0^\infty \exp\left(-\frac{\pi^2 t}{N^2} - |\ln(1-c)|N\right) dN. \quad (6.13)$$

Finally, evaluating the integral by the saddle-point method, we obtain

$$P(t) \sim \exp\left(-\frac{3}{2} \left(2\pi^2 |\ln(1-c)|^2 t\right)^{1/3}\right). \quad (6.14)$$

This is precisely the stretched exponential law of the survival probability announced in (1.1) for $d = 1$, with

$$A_1 = \frac{3}{2} (2\pi^2)^{1/3} |\ln(1-c)|^{2/3}. \quad (6.15)$$

6.2 A quantum particle

Turning to the case of a quantum particle, we consider the stationary non-Hermitian tight-binding equation

$$\varepsilon \psi_n = \psi_{n+1} + \psi_{n-1} - i\gamma \eta_n \psi_n, \quad (6.16)$$

where the disordered configuration of traps is given by the binary distribution (6.1).

Consider for a while a very long but finite sample. The probability that it supports avoiding modes decays exponentially with the sample length. Neglecting these very improbable events, the survival probability decays exponentially fast, as

$$\Pi(t) \sim e^{-\lambda t}, \quad (6.17)$$

where the decay rate λ is dictated by the eigenvalue whose imaginary part is the smallest, i.e.,

$$\lambda = -2 \operatorname{Im} \varepsilon_1. \quad (6.18)$$

Furthermore, ε_1 is again expected to correspond to the lowest mode on the largest Lifshitz region.

Let us therefore consider, along the lines of Section 6.1, a trap-free Lifshitz region of size N (i.e., made of $N + 1$ consecutive sites). The wavevector q_1 corresponding to the lowest mode on that region is still given by (6.8), (6.9) in terms of the left and right boundary parameters Y_L and Y_R . We therefore obtain the estimate

$$\lambda \approx 2 \operatorname{Im} q_1^2 \approx \frac{4\pi^2}{N^3} \operatorname{Im} \alpha, \quad (6.19)$$

with (see (6.9))

$$\alpha = \frac{1}{Y_L - 1} + \frac{1}{Y_R - 1}. \quad (6.20)$$

The result (6.19) has two qualitative differences with respect to its classical counterpart (6.10). First, the decay rate scales as $1/N^2$ in the classical situation, and as $1/N^3$ in the quantum one. These scaling laws already hold for a ring with a single trap (see (4.11) and (4.29)). Second, the quantum decay rate (6.19) is now a *fluctuating* quantity. Indeed it depends *to leading order* on the rest of the sample through the left and right boundary parameters Y_L and Y_R . In order to proceed, it is therefore necessary to determine the distribution of these boundary parameters. This can be done as follows, along the lines of [61]. In the theory of one-dimensional disordered systems (see e.g. [62]), it is customary to introduce Riccati variables, defined as ratios of the wavefunction amplitudes at two consecutive sites:

$$Y_n = \frac{\psi_n}{\psi_{n+1}}. \quad (6.21)$$

Right at the band edge ($q = 0$, i.e., $\varepsilon = 2$), these variables obey the recursion

$$Y_n = \frac{1}{2 + i\gamma\eta_n - Y_{n-1}} = \begin{cases} \frac{1}{2 + i\gamma - Y_{n-1}} & \text{with prob. } c, \\ \frac{1}{2 - Y_{n-1}} & \text{with prob. } 1 - c. \end{cases} \quad (6.22)$$

The Riccati variable Y_n is therefore a function of the initial value Y_0 and of the random occupation numbers $\eta_1, \dots, \eta_n$. In the $n \rightarrow \infty$ limit, Y_n has a non-trivial limit distribution in the complex Y -plane, which is invariant under the random transformation (6.22). Invariant distributions with complex support have already been met in the realm of one-dimensional disordered

systems (see e.g. [67]). In the present situation of a binary dilution disorder, the invariant distribution has a fractal support which only depends on the trapping strength γ , and not on the trap density c . This fractal set is shown in Figure 6.1 for a typical trapping strength ($\gamma = 1/2$).

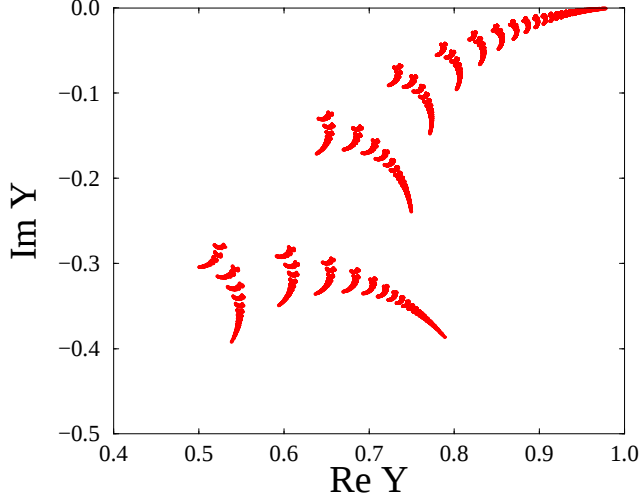


Fig. 6.1 Fractal support of the invariant distribution of the Riccati variables Y_n in the complex Y -plane for $\gamma = 1/2$ (Color online).

For the time being, let us keep considering a Lifshitz region of fixed (large) size N . If this region is embedded into an infinitely large disordered system, the left and right boundary parameters Y_L and Y_R are independent of each other, and each of them is distributed according to the above invariant distribution in the complex Y -plane. The distribution of the complex parameter α defined in (6.20) is thus determined, at least in principle. The smallest possible value $\lambda_{\min}$ of the decay rate is therefore given by the exact formula

$$\lambda_{\min} \approx \frac{8\pi^2 f}{N^3 \gamma}, \quad (6.23)$$

where the factor f reads

$$f = \min \operatorname{Re} F, \quad (6.24)$$

while the complex variables F_n are related to the Riccati variables Y_n through

$$F_n = \frac{i\gamma}{1 - Y_n}, \quad (6.25)$$

and $\min \operatorname{Re} F$ has to be understood as being the minimum of the real part of the support of the invariant distribution of the variables F_n . This support, to

be shown in Figure 6.2 below, is nothing but the image in the complex F -plane of the fractal set shown in Figure 6.1.

The expression (6.23) has the same leading scaling in $1/(N^3\gamma)$ as the result (4.29) for a ring with a single trap. The factor f only depends on the trapping strength γ , and it is normalized so that it goes to unity in the $\gamma \rightarrow \infty$ limit. In particular, f is independent of the trap density c .

In order to evaluate the factor f explicitly, let us recast the recursion (6.22) in terms of the variables F_n themselves:

$$F_n = i\gamma + \frac{F_{n-1}}{1 + \eta_n F_{n-1}} = \begin{cases} i\gamma + \frac{F_{n-1}}{1 + F_{n-1}} & \text{with prob. } c, \\ i\gamma + F_{n-1} & \text{with prob. } 1 - c. \end{cases} \quad (6.26)$$

The second line of the transformation (6.26) is a translation by the constant imaginary quantity $i\gamma$. As a consequence, the fractal support of the invariant distribution of the F_n extends up to infinity in the imaginary direction of the complex F -plane, and it consists on an infinite periodic array of identical components. Figure 6.2 shows the lower part of this fractal support in the F -plane, featuring the first component of the above mentioned periodic array, for $\gamma = 1/2$.

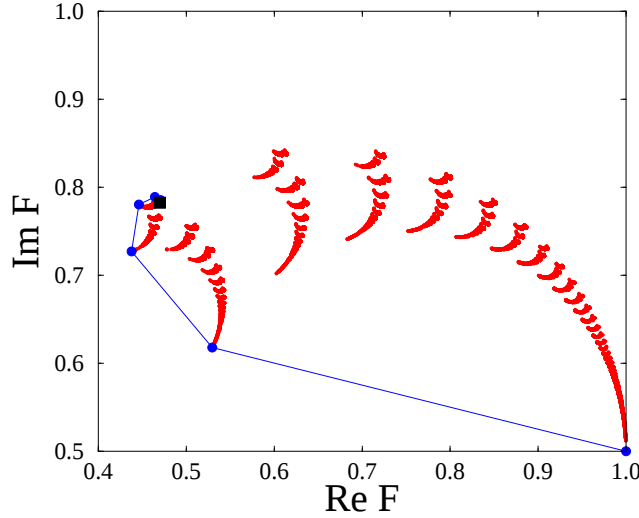


Fig. 6.2 Lower part of the fractal support of the invariant distribution of the variables F_n in the complex F -plane for $\gamma = 1/2$. Blue symbols connected by a line: sequence of extremal points F_k ($k = 1, 2, \dots$). Square: fixed point F_* (Color online).

The factor f , equal to the minimum of the real part of the fractal support, can be determined by means of the following construction. The lower right endpoint of the support is $F_1 = 1 + i\gamma$. This point is obtained by acting on

the point at infinity with the first line of (6.26). More generally, we are led to consider a discrete sequence of extremal points F_k ($k = 1, 2, \dots$), shown in Figure 6.2 as blue symbols connected by a line, defined by iterating the first line of (6.26), i.e.,

$$F_k = i\gamma + \frac{F_{k-1}}{1 + F_{k-1}}, \quad (6.27)$$

with $F_0 = \infty$. We thus obtain

$$\begin{aligned} F_1 &= 1 + i\gamma, & F_2 &= \frac{\gamma^2 + 2 + i\gamma(\gamma^2 + 5)}{\gamma^2 + 4}, \\ F_3 &= \frac{\gamma^4 + 8\gamma^2 + 3 + i\gamma(\gamma^4 + 11\gamma^2 + 14)}{(\gamma^2 + 1)(\gamma^2 + 9)}, \end{aligned} \quad (6.28)$$

and so on. These points spiral around the stable fixed point

$$F_\star = \frac{i}{2} \left(\gamma + \sqrt{\gamma(\gamma - 4i)} \right), \quad (6.29)$$

shown as a square in Figure 6.2, whose real part reads

$$f_\star = \sqrt{\frac{2\gamma}{\gamma + \sqrt{\gamma^2 + 16}}}. \quad (6.30)$$

Let us give for further use the following explicit parametrization of the extremal points. Introducing the complex variable z through

$$\sqrt{i\gamma} = 2 \sinh z \quad (0 < \text{Im } z < \pi/2), \quad (6.31)$$

we have

$$F_k = \frac{2 \sinh z \cosh(2k+1)z}{\sinh 2kz}, \quad (6.32)$$

and especially

$$F_\star = e^{2z} - 1. \quad (6.33)$$

It should now be clear from the construction shown in Figure 6.2 that the factor f is the smallest of the real parts of the extremal points F_k . In other words, we have

$$f = \text{Re } F_{k(\gamma)}, \quad (6.34)$$

where the index $k(\gamma)$ of the point with smallest real part depends on the trapping strength γ .

• $\gamma > 1$. In this first region, F_2 has the smallest real part, i.e., $k(\gamma) = 2$. We have therefore

$$f = \text{Re } F_2 = \frac{\gamma^2 + 2}{\gamma^2 + 4} \quad (\gamma > 1). \quad (6.35)$$

For large γ , this quantity departs from unity as

$$f = 1 - \frac{2}{\gamma^2} + \frac{8}{\gamma^4} + \dots, \quad (6.36)$$

while the real part of the stable fixed point departs from unity as

$$f_{\star} = 1 - \frac{2}{\gamma^2} + \frac{14}{\gamma^4} + \dots \quad (6.37)$$

- $1/\sqrt{5} < \gamma < 1$. In this second region, F_3 has the smallest real part, i.e., $k(\gamma) = 3$. We have therefore

$$f = \text{Re } F_3 = \frac{\gamma^4 + 8\gamma^2 + 3}{(\gamma^2 + 1)(\gamma^2 + 9)}, \quad (6.38)$$

and so on.

- $\gamma \rightarrow 0$. In this regime of a weak trapping strength, the extremal points come close to each other, so that it is legitimate to use a continuum approach. The variable z becomes small in this regime, scaling as

$$z \approx \frac{\sqrt{i\gamma}}{2}, \quad (6.39)$$

so that we have

$$F_{\star} \approx 2z \approx \sqrt{i\gamma} \approx (1+i)f_{\star}, \quad f_{\star} \approx \sqrt{\frac{\gamma}{2}}. \quad (6.40)$$

As a consequence of (6.32), the extremal points are given by the scaling formula

$$F_k \approx \Phi(x) f_{\star}, \quad (6.41)$$

with

$$x = k\sqrt{\frac{\gamma}{2}} = kf_{\star}, \quad (6.42)$$

while the complex function $\Phi(x) = U(x) + iV(x)$ reads

$$U(x) = \frac{\sinh 2x + \sin 2x}{\cosh 2x - \cos 2x}, \quad V(x) = \frac{\sinh 2x - \sin 2x}{\cosh 2x - \cos 2x}. \quad (6.43)$$

The function $\Phi(x)$ describes the spiral formed by the extremal points in the continuum limit. We have $U(\infty) = V(\infty) = 1$, and so $\Phi(\infty) = 1 + i$.

The function $U(x)$, describing the real parts of the extremal points, reaches its smallest minimum for $x = \pi/2$. We thus obtain the following predictions in the regime of a weak trapping strength: the index $k(\gamma)$ diverges as

$$k(\gamma) \approx \frac{\pi}{\sqrt{2\gamma}}, \quad (6.44)$$

while the factor f scales as

$$f \approx \tau\sqrt{\frac{\gamma}{2}} \approx \tau f_{\star}, \quad (6.45)$$

with

$$\tau = U\left(\frac{\pi}{2}\right) = \tanh \frac{\pi}{2} \approx 0.917152. \quad (6.46)$$

Figure 6.3 shows a plot of f and f_* against γ . Both quantities are close to each other, with f being slightly smaller than f_* . They exhibit the same overall monotonous dependence on γ , starting as $\sqrt{\gamma}$ (see (6.40) and (6.45)), and converging to unity with $1/\gamma^2$ corrections (see (6.36) and (6.37)). Figure 6.4 shows a plot of the ratio f/f_* against γ . This ratio is slightly smaller than unity, and it varies between its $\gamma \rightarrow 0$ and $\gamma \rightarrow \infty$ limits, i.e., respectively, $\tau = 0.917152$ and unity. The cusps, corresponding to the points where the integer $k(\gamma)$ jumps by one unit, are more clearly visible than in Figure 6.3. The first few regions where the integer $k(\gamma)$ is constant are labelled by the corresponding values of this integer.

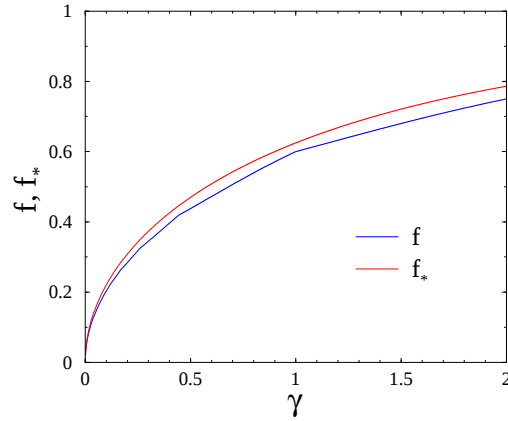


Fig. 6.3 Plot of the factor f (see (6.24)) (lower blue curve) and of the real part f_* of the stable fixed point F_* (see (6.30)) (upper red curve), against γ (Color online).

In the limit of an infinite system, the asymptotic decay of the survival probability $\Pi(t)$ of the quantum particle can be estimated by superposing the contributions of Lifshitz regions of all sizes. For a given (large) size N , the lowest decay rate $\lambda_{\min}$ is given by (6.23). Working with exponential accuracy and going to a continuum approximation, we get

$$\Pi(t) \sim \int_0^\infty \exp\left(-\frac{8\pi^2 f t}{N^3 \gamma} - |\ln(1-c)|N\right) dN. \quad (6.47)$$

Finally, evaluating the integral by the saddle-point method, we obtain

$$\Pi(t) \sim \exp\left(-\frac{4}{3} \left(\frac{24\pi^2 f t}{\gamma}\right)^{1/4} |\ln(1-c)|^{3/4}\right). \quad (6.48)$$

We have thus derived the stretched exponential law of the survival probability announced in (1.2) for $d = 1$, with

$$B_1 = \frac{4}{3} \left(\frac{24\pi^2 f}{\gamma}\right)^{1/4} |\ln(1-c)|^{3/4}. \quad (6.49)$$

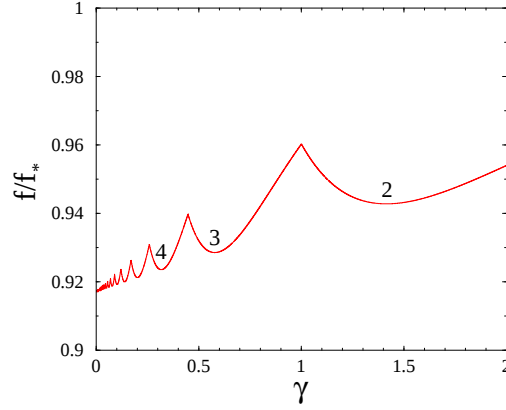


Fig. 6.4 Plot of the ratio f/f_* against γ . Numbers: values of the integer $k(\gamma)$ labeling the first few regions where this integer is constant (Color online).

This exact result involves the non-trivial factor f , defined in (6.24) and plotted in Figure 6.3, which only depends on the trapping strength γ .

7 Higher-dimensional disordered systems

This section is devoted to an extension of the results of Section 6 to higher-dimensional disordered systems.

7.1 A classical particle

We start with a reminder on a classical particle diffusing on a d -dimensional lattice, chosen to be hypercubic for simplicity, in the presence of a random distribution of traps with density c . We again assume that all traps have the same strength γ . We are thus led to consider the stationary equation

$$-E p_{\mathbf{n}} = \sum_{\mathbf{m}(\mathbf{n})} (p_{\mathbf{m}} - p_{\mathbf{n}}) - \gamma \eta_{\mathbf{n}} p_{\mathbf{n}}, \quad (7.1)$$

where $\mathbf{m}(\mathbf{n})$ are the $2d$ neighbors of site $\mathbf{n}$.

In analogy with the one-dimensional situation, investigated in Section 6.1, the smallest eigenvalues of (7.1) correspond to the lowest modes living in *Lifshitz spheres*,² i.e., large and almost spherical regions of the lattice which are free of traps. Consider such a sphere of radius $R \gg 1$, and translate the

² We keep with the long tradition in mathematical physics [15, 16] of using the word *sphere*, even though the word *ball* would be more appropriate to describe the volume delimited by a sphere.

co-ordinate system so that the sphere is centered at the origin. The probability of occurrence of such a large trap-free sphere per unit volume scales as

$$P(R) \sim (1 - c)^{\omega_d R^d}, \quad (7.2)$$

where

$$\omega_d = \frac{\pi^{d/2}}{\Gamma\left(\frac{d+2}{2}\right)} \quad (7.3)$$

is the volume of the unit d -dimensional sphere.

As we are only interested in the lowest mode of the discrete difference equation (7.1), it is legitimate to replace it by its continuum approximation,

$$-Ep = \Delta p, \quad (7.4)$$

where Δ is the Laplace operator inside the sphere, with Dirichlet boundary conditions. The lowest mode of the above equation is spherically symmetric and reads

$$p(r) = L_d(qr), \quad (7.5)$$

where $q = \sqrt{E}$ is the wavevector, while the scaling function L_d , normalized to be unity at the center, reads

$$L_d(x) = \Gamma\left(\frac{d+2}{2}\right) \left(\frac{2}{x}\right)^{(d-2)/2} J_{(d-2)/2}(x), \quad (7.6)$$

where $J_{(d-2)/2}$ is a Bessel function. The boundary condition $p(R) = 0$ yields

$$q = \frac{j_d}{R}, \quad (7.7)$$

where j_d is the first zero of $J_{(d-2)/2}$. Table 7.1 gives the value of ω_d , L_d and j_d in one, two, and three dimensions.

d	ω_d	$L_d(x)$	j_d
1	2	$\cos x$	$\pi/2$
2	π	$J_0(x)$	2.404825
3	$4\pi/3$	$(\sin x)/x$	π

Table 7.1 Values of various characteristics of Lifshitz spheres in one, two, and three dimensions: ω_d is the volume of the unit sphere, $L_d(x)$ is the scaling function of the lowest mode of the Laplace-Dirichlet equation in the sphere, j_d is the first zero of the latter function.

The asymptotic decay of the survival probability $P(t)$ can again be estimated by superposing the contributions of Lifshitz spheres of all sizes. Working with exponential accuracy and going to a continuum approximation, we get

$$P(t) \sim \int_0^\infty \exp\left(-\frac{j_d^2 t}{R^2} - \omega_d |\ln(1 - c)| R^d\right) R^{d-1} dR. \quad (7.8)$$

Evaluating the integral by the saddle-point method, we obtain

$$P(t) \sim \exp \left(-C_d |\ln(1-c)|^{2/(d+2)} t^{d/(d+2)} \right). \quad (7.9)$$

This is the stretched exponential law of the survival probability announced in (1.1), with

$$A_d = C_d |\ln(1-c)|^{2/(d+2)}, \quad (7.10)$$

where the exact prefactor reads

$$C_d = \frac{d+2}{d} \left(\frac{d\omega_d j_d^d}{2} \right)^{2/(d+2)}. \quad (7.11)$$

7.2 A quantum particle

Let us now consider a quantum particle on a d -dimensional lattice, in the presence of a random distribution of traps with strength γ and density c . We are thus led to study the stationary tight-binding equation

$$\varepsilon p_{\mathbf{n}} = \sum_{\mathbf{m}(\mathbf{n})} p_{\mathbf{m}} - i\gamma \eta_{\mathbf{n}} p_{\mathbf{n}}. \quad (7.12)$$

On a very large but finite sample, the survival probability decays exponentially fast, as

$$\Pi(t) \sim e^{-\lambda t}, \quad (7.13)$$

where the decay rate λ is dictated by the eigenvalue of (7.12) whose imaginary part is the smallest, i.e.,

$$\lambda = -2 \operatorname{Im} \varepsilon_1. \quad (7.14)$$

It is to be expected that ε_1 is close to the band edge (i.e., $\varepsilon_{\max} = 2d$ on the hypercubic lattice). This legitimates the use of a continuum description, and therefore the analysis in terms of Lifshitz spheres, recalled in Section 7.1 within the classical framework. More precisely, setting

$$\varepsilon = 2d - q^2, \quad (7.15)$$

the lowest mode in a sphere of large radius ($R \gg 1$) is still given by (7.5), and so the real part of the wavevector q is still given by (7.7). We thus obtain

$$\operatorname{Re} \varepsilon \approx 2d - \frac{j_d^2}{R^2}. \quad (7.16)$$

The decay rate λ is given by the imaginary part of ε (see (7.14)), which is typically much smaller than $1/R^2$, and whose determination is accordingly more delicate. In the one-dimensional situation, the Riccati formalism allowed us to derive the quantitative result (6.23), including the exact expression (6.24) for the factor f . In the present higher-dimensional situation, no such quantitative approach is available.

An approximation which can be dealt with by analytical means consists in considering a trap-free spherical cavity of radius R embedded in an infinite space with a uniform optical potential iW , with $W = c\gamma$ [28]. For a large enough cavity, and with the present notations, this model yields the prediction

$$\lambda_{\text{cavity}} \approx \frac{2j_d^2 \Lambda}{R^3} \approx \frac{4j_d^2}{R^3 \sqrt{2c\gamma}}, \quad (7.17)$$

where $\Lambda = \sqrt{2/W}$ is the penetration depth of a particle with very long wavelength ($q \rightarrow 0$) into the medium endowed with the optical potential. The proportionality of the penetration depth (and hence of the decay rate) to $1/\sqrt{\gamma}$ is an artifact of the continuum description of the trapping medium. A $1/\gamma$ behavior is indeed expected to universally hold in the presence of discrete traps, in accord with all the results obtained so far. We are thus led to make the following Ansatz for the lowest decay rate λ_{min} associated with a large Lifshitz sphere of fixed radius R :

$$\lambda_{\text{min}} \approx \frac{\phi}{R^3 \gamma}. \quad (7.18)$$

The above Ansatz is meant to capture the leading dependence of the decay rate on R and γ in the regime where these parameters are large. The numerator ϕ is a higher-dimensional analogue of the factor f which enters the exact one-dimensional result (6.23). It is assumed to be of order unity, and possibly depends on the trap density c .

The asymptotic decay of the survival probability can now be estimated as

$$\Pi(t) \sim \int_0^\infty \exp\left(-\frac{\phi t}{R^3 \gamma} - \omega_d |\ln(1-c)| R^d\right) R^{d-1} dR. \quad (7.19)$$

Evaluating the integral by the saddle-point method, we obtain

$$\Pi(t) \sim \exp\left(-Q_d |\ln(1-c)|^{3/(d+3)} \left(\frac{\phi t}{\gamma}\right)^{d/(d+3)}\right). \quad (7.20)$$

This is the stretched exponential law announced in (1.2), with

$$B_d = Q_d \left(\frac{\phi}{\gamma}\right)^{d/(d+3)} |\ln(1-c)|^{3/(d+3)}, \quad (7.21)$$

where the prefactor reads

$$Q_d = \frac{d+3}{d} \left(\frac{d\omega_d}{3}\right)^{3/(d+3)}. \quad (7.22)$$

The only part of the result (7.21) which is not known analytically is the factor ϕ , which has been introduced in the Ansatz (7.18).

8 Concluding remarks

In this work we have investigated the survival probabilities of a classical and of a quantum particle in the presence of traps in a whole range of finite or infinite geometries. Our main goal was to present a thorough comparison of the temporal behavior of the classical and quantum survival probabilities, in order to better grasp the qualitative differences between both situations. This systematic kind of approach had not been adopted so far, in spite of the appreciable number of published works on the trapping of continuous-time quantum walks [26–29, 31–33, 52–60].

It is worth recalling the leitmotiv of the present study: static traps are far less efficient to absorb quantum particles than classical ones. Free quantum particles indeed benefit from interference effects in order to efficiently avoid any particular site, much more easily than diffusing classical particles. This qualitative difference manifests itself in all the geometries that we have considered in this work. On the chain with a single trap, a classical walker is eventually absorbed with certainty, while a quantum one may escape forever with a rather high probability Π_∞ . This asymptotic probability bears a non-monotonic dependence on the trapping strength, and goes paradoxically to unity in the nominal strong-trapping regime. On a finite ring of N sites with a single trap, we have the extra feature that characteristic times scale differently. In the classical case the relevant time scale is the diffusive one, scaling as N^2 , whereas the much longer quantum absorption time grows as $N^3\gamma$. Furthermore, for some configurations of several traps on a ring, the quantum particle may have a non-zero asymptotic survival probability, owing to the existence of avoiding modes. In higher dimensions, virtually all questions concerning these avoiding modes are entirely open: What is the number of these modes, their nature, their relevance to quantum percolation? We plan to return to these matters in future work.

In the presence of a random distribution of traps with fixed density, both the classical and the quantum survival probabilities were known to obey a stretched exponential asymptotic decay, albeit with different exponents, i.e., respectively $d/(d+2)$ and $d/(d+3)$ (see (1.1), (1.2)). One of our main goals was to determine the amplitude B_d of the quantum survival probability, and chiefly its dependence on the trap density c and on the trapping strength γ . This task is far more involved than the evaluation of the classical amplitude A_d . Indeed, at variance with the classical case, the decay rate of the quantum particle depends to leading order on the whole environment.

In the one-dimensional situation, the strong contrast between the classical and the quantum situations can be illustrated explicitly. In the classical case, in order to evaluate the amplitude A_1 (see (6.15)), one has to perform a single averaging over the size N of the Lifshitz region. In the quantum case, however, in order to evaluate the amplitude B_1 (see (6.49)), one is naturally led to perform a double averaging, first on the environment at fixed N , obtaining thus the non-trivial factor f exactly, and then over the size N . In higher dimension, however, the first averaging cannot be performed exactly. We have replaced

it by a motivated but heuristic Ansatz. It seems plausible that evaluating the amplitude B_d by analytical means is just as difficult as evaluating the survival probability of the classical situation throughout the Lifshitz regime, beyond its leading term [19–25].

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