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QUALITATIVE THEORY OF STOCHASTIC DIFFERENTIAL EQUATIONS AND QUANTUM MECHANICS OF DISORDERED SYSTEMS

G. Jona-Lasinio
Istituto di Fisica "G.Marconi" Università di Roma, Italy.

Abstract

In this talk we shall review some recent applications of ideas and methods from the qualitative theory of stochastic differential equations to problems in Quantum Mechanics. An interesting phenomenon revealed by this approach is the instability of tunneling states under small deformations of the potential. This result may be relevant for a deeper understanding of localization in random potentials. As a second application we will show that the theory of small random perturbations allows a direct estimate of the asymptotic behaviour for large negative energies of the density of states in a white noise potential. In addition it provides a description of the local shape of the wave function in such a situation.

In this talk I shall review some ideas from the qualitative theory of stochastic differential equations which appear of interest in the study of a number of quantum mechanical problems.

Here we shall emphasize quantum mechanical applications that may lead to a better understanding of those disordered systems that can be described in terms of a Schrödinger equation with random potential.

The first problem we have in mind is a fundamental one: the localization of the wave function due to disorder. This is a very striking phenomenon: in one dimension, where a germ of a general theory begins to exist, it is a theorem that any amount of disorder will produce a point spectrum and a complete localization of the states /1/. This theorem applies for instance to such a simple situation like that of Fig. 1 where the potential is a random sequence of two types of barriers differing only in their height.

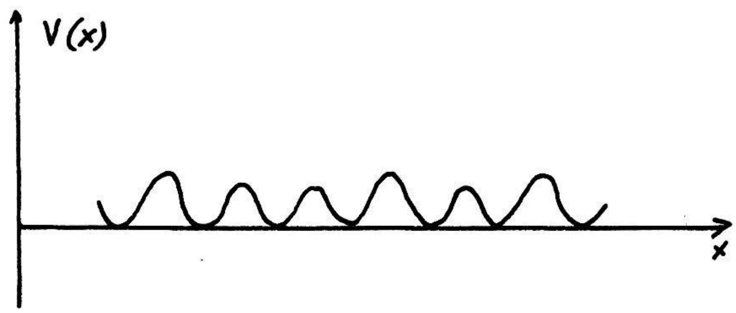

Fig. - 1 -

A less satisfactory aspect of such a theorem is that its proof does not provide much insight into the mechanism which produces localization. It is one of the purposes of this talk to point out that tunneling instability may be a relevant physical concept on which to build a more detailed picture of the behaviour of a particle in certain types of random potentials. This idea is partly suggested by the experience gained in some recent study of the low-lying states in unsymmetric potential barriers or imperfect periodic structures in one dimension /2/. It is also in agreement, although formulated in a different language, with the very interesting proof of localization for the Schrödinger equation on a lattice recently produced by Frölich and Spencer /3/.

In the following we shall give a more precise description of what we mean by tunneling in stationary states and briefly discuss its stability properties in one dimension. We shall work in a semiclassical limit $\hbar \to 0$. However we believe that our considerations have a more general validity and we shall briefly comment on this later.

The starting point of our method is the following canonical transformation which is certainly well defined if we enclose initially our system in a large box whose volume will become eventually infinite. Let $\psi_o(x)$ be the ground state wave function which can be chosen to be real and positive (no nodes) and define the transformation

$$H \longrightarrow \psi_o^{-1} H \psi_o = -\hbar L + E_o \tag{1}$$

where

$$\begin{aligned} L &= \frac{\hbar}{2} \Delta + \underline{b} \cdot \underline{\nabla} \\ \underline{b} &= \frac{\hbar}{2} \underline{\nabla} \ln \psi_o^2 \end{aligned} \tag{2}$$

There is a simple relation between the eigenvalues λ_k and eigenfunctions f_k of L and those of H

$$\begin{aligned} E_k - E_o &= \hbar \lambda_k \\ \psi_k &= \psi_o f_k \end{aligned} \tag{3}$$

The reader will recognize in L the generator of a diffusion process with diffusion constant $\hbar$ and drift $\underline{b}$. We can forget about ψ_o and consider directly the equation for $\underline{b}$

(4) $$\hbar \operatorname{div} \underline{b} + \underline{b}^2 = 2(V - E_o)$$

An equivalent way of describing a diffusion is by means of a stochastic differential equation of the form

(5) $$d\underline{x} = \underline{b}\, dt + \epsilon\, d\underline{w}$$

where $\underline{w}$ is the Wiener process and $\epsilon = \sqrt{\hbar}$ in our case. This is how stochastic differential equations come into play. To understand how (5) can provide useful information on the original Schrödinger equation, it is necessary to obtain some qualitative picture of the stochastic process generated by (5). For small ϵ, i.e. in a semiclassical limit the picture which emerges from a rigorous analysis is the following. The process will spend very long times performing small fluctuations near the stable equilibrium positions $\underline{x}_i$ of the vector field $\underline{b}$ (actually it is sufficient to consider $\underline{b}_o = \lim_{\epsilon \to 0} \underline{b}(\underline{x}, \epsilon)$. From time to time a large fluctuation will drive the process from one equilibrium position to another (tunneling) where it will spend again a long time. From this it follows that the behaviour of the process over long times can be approximated by that of a Markov chain whose state space is discrete and given by the stable positions of $\underline{b}_o$.

Let us call $P = |P_{ij}|$ the transition matrix associated with the chain. If we define the eigenvalues and eigenvectors of P

(6) $$P f_k = e^{-\eta_k} f_k$$

then the η_k can be identified with very good approximation with the λ_k (and therefore with the splittings $E_k - E_o$) and the $(f_k)_i$

with the values of the ratios ψ_k/ψ_o at the equilibrium points $\underline{x}_i$. Therefore P provides direct information on the low-lying states produced by tunneling. The next important fact is that one can write an explicit expression for the P_{ij}

$$P_{ij} \approx e^{-\frac{V_{ij}}{2\epsilon^2}} \tag{7}$$

where

$$V_{ij} = \inf_{\substack{T, \underline{\varphi} \\ \underline{\varphi}(0)=\underline{x}_i \quad \underline{\varphi}(T)=\underline{x}_j}} \int_0^T |\dot{\underline{\varphi}} - \underline{b}_o(\underline{\varphi})|^2 dt \tag{8}$$

From the previous discussion it is clear that if we are able to calculate the vector field $\underline{b}_o$ we have a complete scheme of calculation.

We now describe the situation for d = 1. First of all in order that we may speak of tunneling we need two or more stable equilibrium positions of b_o.

For d = 1 from (4) we have that $b_o(x) = \pm\sqrt{2V(x)}$

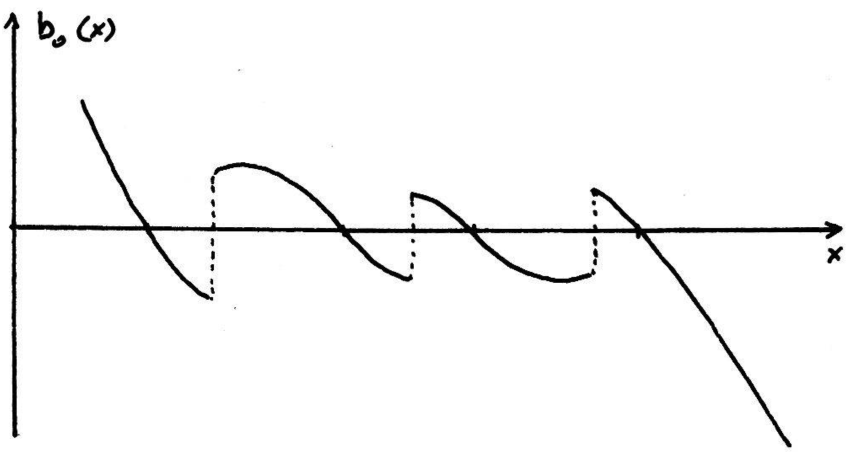

Fig. - 2 -

b_0 could be for example something like in Fig. 2 for a potential exhibiting four degenerate minima. The points where b_0 changes sign are stable. The difficult part consists in locating the jumps of b_0 from $-\sqrt{2V}$ to $\sqrt{2V}$, and for this one has to study in detail the one-dimensional version of (4) which is a Riccati equation. The result of the analysis is that the position of these jumps is in fact extremely sensitive to the whole shape of the potential, and it can be seen that given a potential V(x) with many degenerate minima, rather special conditions have to be satisfied in order that they give rise to stable equilibrium points for b_0. For most potentials instead of the situation of Fig. 2 we can expect for b_0 a form

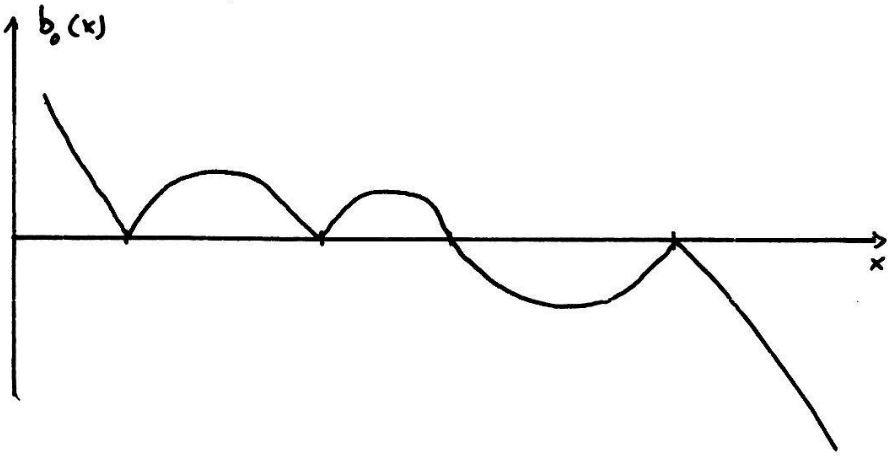

Fig. - 3 -

where only one minimum survives. But this means (remember that b is the log-derivative of ψ_0) localization of the wave function in this minimum. To give an idea of the mechanism for this peculiar behaviour we mention an identity, which follows easily from the Riccati equation and the boundary conditions. Take any point x_0 and consider the symmetric and antisymmetric parts of b(x) and of the potential with respect to this point

$$b_s(x) = b(x) + b(2x_0 - x)$$
$$b_a(x) = b(x) - b(2x_0 - x)$$
$$V_a(x) = V(x) - V(2x_0 - x)$$

The following equation holds

$$(9) \qquad b_s(x) = -\frac{2}{\hbar} \int_x^{\infty} V_a(x')\, e^{\frac{1}{\hbar}\int_x^{x'} b_a(x'')dx''} dx'$$

Consider then as an example a case in which V is obtained by slightly deforming a function symmetric with respect to x_o. Eq. (9) shows that the effect of the deformation can be felt everywhere and be quite large for $\hbar \to 0$. This is why stable minima of the potential do not necessarily correspond to stable minima of b_o. For examples where the consequences of (9) are worked out in detail we refer the reader to /2/. If we do not take the limit $\hbar \to 0$ what we expect is that even if the stable minima of the potential survive in $\underline{b}$, the stability region for most of them will be very small and the corresponding wave function will have very few large peaks.

In conclusion on the basis of the above discussion we propose the following qualitative description of the behaviour in a random potential: most realizations of the potential will give rise to very few stable positions of the vector field $\underline{b}_o$. This in turn implies localization and very few tunneling levels in the vicinity of the ground state.

We hope to come back elsewhere to a more quantitative formulation of this point of view. In the above formulation our problem has also some connections with the random walk and the diffusion in a random environment.

We now consider a <u>different way</u> in which the ideas of the qualitative behaviour of stochastic differential equations are helpful to obtain an insight into the behaviour of a disordered system. The following application is due to Høegh-Krohn and Jona-Lasinio /4/. We consider the Schrödinger equation in a white-noise stochastic potential

(10) $$(-\Delta + V(\underline{x}))\psi = E\psi$$

with $E(V(\underline{x})\ V(\underline{y})) = \delta(\underline{x} - \underline{y})$. We have set $\hbar = 2m = 1$. We first perform a scale transformation $\underline{y} = |E|^{\frac{1}{2}}\underline{x}$

$$(-\Delta + \frac{1}{|E|} V(\frac{\underline{y}}{|E|^{1/2}}))\psi =$$

(11)

$$(-\Delta + \frac{1}{|E|^{1-d/4}} V(\underline{y}))\psi = \text{sign}\, E\,\psi$$

where we have used the homogeneity property of the white noise. We then see that for large $|E|$ the potential is a small perturbation for $d < 4$, We now specialize (11) in one dimension. It is well known that in such a case the problem of calculating the density of states can be reduced to the problem of calculating the average density of nodes of a solution of the Schrödinger equation satisfying an arbitrary initial condition for example at x = 0. Between one node and the next we are allowed to make the transformation of variables

(12) $$b(x) = \frac{1}{2}\frac{d}{dx} \ln \psi^2$$

which leads again to a Riccati equation.

(13) $$\frac{db}{dx} = -b^2 - \text{sign}\, E + \frac{1}{|E|^{3/4}} V(x)$$

Due to our choice of V this is now a stochastic differential equation which for large $|E|$ can be interpreted as a small random perturbation of a deterministic system. In other words we are in a situation similar to that described earlier in connection with Eq. (5), if we now identify $\epsilon = |E|^{-3/4}$.

The average distance between two nodes corresponds to the average distance necessary for the stochastic process b(x) to go from $+\infty$ to $-\infty$. When $E < 0$ the deterministic part of (13) has two equilibrium positions at $b = \pm 1$

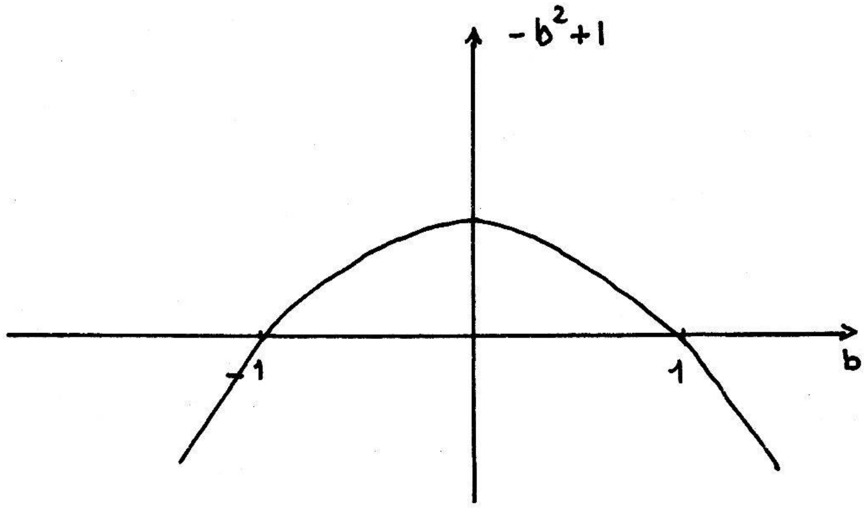

Fig. - 4 -

and the one at b = 1 is stable. According to our previous discussion the process will reach the value b = 1 and spend there a long "time" until a large fluctuation will bring it to -1 ("tunneling") from where it escapes to $-\infty$. Since the "time" to go from $+\infty$ to + 1 and from -1 to $-\infty$ are finite, for large enough $|E|$ the average distance between two nodes will coincide to a good approximation with the time spent by b near + 1, that is with the tunneling time. This is proportional to the inverse transition probability $P_{+1,-1}$ from + 1 to - 1. Using (7) and (8) whose application in one dimension is straightforward we find

$$N(E) \underset{E\to -\infty}{\longrightarrow} e^{-8/3\,|E|^{3/2}} \tag{14}$$

This is a well known result/5/. The interest of our calculation however resides besides its simplicity, in the fact that it gives also information on the local shape of the wave function. This can be seen as follows. Let us consider the segment between two nodes of a given eigenfunction corresponding to the energy $-|E|$. The shape of the wave function will be determined by the matching of two solutions, one starting at the left of the segment and propagating forward, the other starting at the right end and then propagating backward. The first can be described by a typical trajectory of Eq. (13), the second one by a typical trajectory of the equation which is obtained from (13) by changing the sign of the left hand side. This trajectory will now spend a long time near -1. The conclusion is that the wave function locally will increase or decrease exponentially with high probability and with a rate $\pm\ |E|^{3/2}$, i.e. ψ has the form $e^{\pm |E|^{3/2} y}$. We now expect something like this

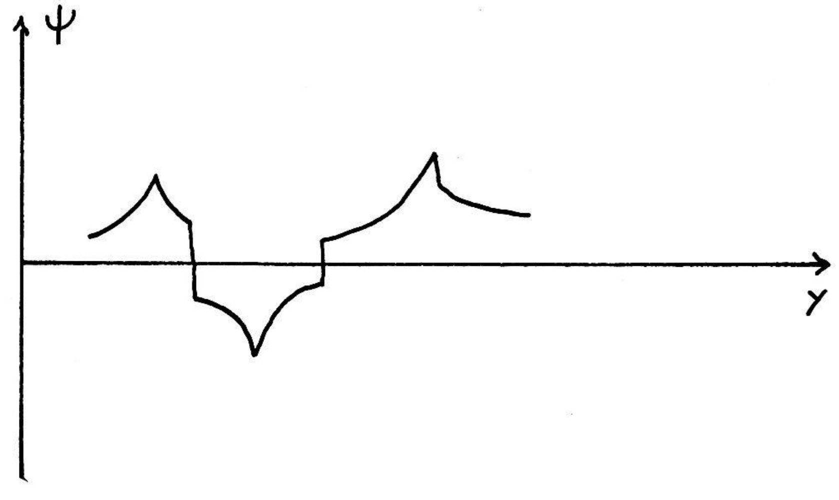

Fig. - 5 -

This local exponential behaviour must not be confused with the global exponential decay connected with localization and which is an ergodic property.

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/5/ For a rigorous proof see M.Fukushima, S.Nakao , Z.für Warscheinlichkeits theorie 37, 267 (1977).