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CLASSICAL DIFFUSION IN SOFT POTENTIALS AND SUPERSYMMETRIC QUANTUM MECHANICS

F. MARCHESONI[*,**], P. SODANO[*,**], P. BICCHERI[**], C. PRESILLA[**] and M. ZANNETTI[***]

[*] *MIDIT, The Technical University of Denmark, DK-2800 Lyngby, Denmark*
[**] *Dipartimento di Fisica, Universitá di Perugia, I-06100 Perugia, Italy*
[***] *Dipartimento di Fisica, Universitá di Napoli, I-80100 Napoli, Italy*

Résumé : Nous analysons l'emploi de la supersymétrie de la mécanique quantique pour la diffusion classique d'un particule brownienne dans des potentiels faiblement liés. En particulier, nos calculs numériques ont permis la détermination analytique précise de la forme du mode de fréquence d'un "kink" statique de l'équations de sine-Gordon double.

Abstract - We review the use of supersymmetric quantum mechanics in the analysis of the classical diffusion of a brownian particle in weakly binding (soft) potentials. In particular, our computations are shown to provide an accurate analytical determination of the shape–mode frequency of the static double sine–Gordon kink.

1. Introduction

The usage of the Langevin equation formalism to describe the dynamics of localized solutions (solitons) of non-linear field theories perturbed by random fields of force is now common practice [1]. In the present Communication we wish to show how the very same formalism also provides a useful tool for the stability analysis of soliton–like solutions through the connection between Schrödinger and Fokker–Planck equation [2–5]. We shall specialize our approach to the discussion of the stability of the static double sine–Gordon soliton and to the related problem of the brownian diffusion in weakly binding (soft) potentials.

2. Classical diffusion and quantum mechanics

Consider the classical diffusion problem described by the Langevin equation

$$\frac{dx}{dt} = -\frac{dW}{dx} + \eta(t) \tag{2.1}$$

where $W(x)$ is a binding potential function and $\eta(t)$ is a gaussian white noise with zero mean and auto–correlation function

$$< \eta(t)\eta(t') > = 2D\delta(t-t') \tag{2.2}$$

The associated Fokker-Planck equation for the probability density $P(x,t)$

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[\frac{dW}{dx} + D\frac{\partial}{\partial x}\right]P(x,t) \tag{2.3}$$

is trasformed [5] into an imaginary-time Schrödinger equation

$$-\frac{\partial \Psi(x,t)}{\partial t} = H_{-}\Psi(x,t) \tag{2.4}$$

through the substitution

$$P(x,t) = e^{\frac{-W(x)}{2D}}\Psi(x,t) \tag{2.5}$$

where the hamiltonian in (2.4) is given by

$$H_- = -D\frac{\partial^2}{\partial x^2} + V_-(x) \tag{2.6}$$

and the quantum potential $V_-(x)$ is related to the "classical" potential by the Riccati equation

$$V_-(x) = \frac{1}{4D}\left(\frac{dW}{dx}\right)^2 - \frac{1}{2}\frac{d^2W}{dx^2} \tag{2.7}$$

The connection with quantum mechanics is obtained by setting $D = \frac{\hbar}{2m}$ for the diffusion coefficient [5].

The hamiltonian (2.6) is a positive operator

$$H_- = A^+A \tag{2.8}$$

with

$$A = \sqrt{D}\frac{\partial}{\partial x} + \frac{1}{\sqrt{4D}}\frac{dW}{dx} \qquad A^+ = -\sqrt{D}\frac{\partial}{\partial x} + \frac{1}{\sqrt{4D}}\frac{dW}{dx} \tag{2.9}$$

which implies a non–negative spectrum $E_n^- \geq 0$. Introducing the set of eigenfunctions $\varphi_n^-(x)$, $H_-\varphi_n^- = E_n^-\varphi_n^-$, the transition probability of the classical diffusion process can be expanded as

$$R(x,t|x',0) = e^{\frac{W(x')-W(x)}{2D}} \sum_{n=0}^{\infty} \varphi_n^-(x')\varphi_n^-(x)e^{-E_n^- t} \tag{2.10}$$

thus implying that the lowest non–vanishing eigenvalue $\lambda \equiv E_1^-$ provides an estimate of the rate of approach to equilibrium of the brownian particle. Furthermore, if the classical problem admits of a stationary state there must exist

$$\lim_{t\to\infty} R(x,t|x',0) = P_{eq}(x) \tag{2.11}$$

independent of x'. From (2.10) and (2.11) it follows that in this case $E_0^- = 0$ and

$$\varphi_0^-(x) \sim e^{-\frac{W(x)}{2D}} \tag{2.12}$$

with

$$P_{eq}(x) = [\varphi_0^-(x)]^2 \tag{2.13}$$

3. Supersymmetric quantum mechanics

It is well known [6] that the quantum mechanics generated through the transformation (2.5) is supersymmetric. Introducing the two–component wave–functions

$$\Psi = \begin{pmatrix} \varphi^- \\ \varphi^+ \end{pmatrix} \tag{3.1}$$

and the supercharges

$$Q = \begin{pmatrix} 0 & 0 \\ A & 0 \end{pmatrix} \qquad Q^+ = \begin{pmatrix} 0 & A^+ \\ 0 & 0 \end{pmatrix} \tag{3.2}$$

the supersymmetric hamiltonian is given by

$$H = Q^+Q + QQ^+ = \begin{pmatrix} H_- & 0 \\ 0 & H_+ \end{pmatrix} \tag{3.3}$$

with $H_- = A^+A$ and $H_+ = AA^+$, i.e.

$$H_\mp = -D\frac{\partial^2}{\partial x^2} + V_\mp \tag{3.4}$$

$$V_\mp = \frac{1}{4D}\left(\frac{dW}{dx}\right)^2 \mp \frac{1}{2}\frac{d^2W}{dx^2} \tag{3.5}$$

It is well known that if the classical diffusion problem (2.1) admits an equilibrium state with a normalizable probability distribution (2.11), the supersymmetry is not broken, the ground state has zero energy ($E_0^- = 0$) with wave–function given by (2.12). Furthermore the partner hamiltonians $H_\mp$ have the same spectra, $H_\mp \varphi^\mp = E^\mp \varphi^\mp$, with

$$E_{n+1}^- = E_n^+ \tag{3.6}$$

and the eigenfunctions corresponding to the same eigenvalues are related by

$$A\varphi_{n+1}^- = \sqrt{E_n^+}\varphi_n^+ \tag{3.7}$$

$$A^+\varphi_n^+ = \sqrt{E_n^+}\varphi_{n+1}^- \tag{3.8}$$

The supersymmetric partner of the ground state of H_- is not normalizable.

The use of supersymmetric quantum mechanics for solving a bistable Fokker-Planck equation has, indeed, several major advantages over other computational methods. First of all, in the Schrödinger equation corresponding to H_+ the bistable potential is replaced with an essentially monostable (single-well) supersymmetric partner. The zero-eigenvalue appearing in the spectrum of the Fokker-Planck equation is deleted and the determination of λ does not require then any difficult tunneling calculation (we recall that in the low temperature limit λ is exceedingly small) [2]. Secondly, supersymmetry provides a way to construct a family of Schrödinger equations, the eigenvalue spectrum of which differs only for a finite number of states [6]; as a consequence diffusion problems with a different number of time scales might be related to each other.

Furthermore supersymmetric quantum mechanics provides a sistematic and simple method for determining λ also when the brownian particle experiences a constant binding force at infinity [4]: we agree to term these potentials soft. Soft potentials are relevant not only for physical applications, but also because they allow to verify the assumptions underlying Kramers' method [7,8] to evaluate the time of approach to equilibrium of a brownian particle in a bistable potential. In these cases supersymmetry may provide an exact solution even when Kramers' theory is inadequate. This we shall investigate in the next section.

4. A soft potential

We consider a one–dimensional system defined by the stochastic differential equation (2.1) with potential

$$W(x,R) = -2\beta ln[\frac{ch\gamma x}{ch^2\gamma x + sh^2 R}] \tag{4.1}$$

For $\gamma \to 0$ (4.1) produces the free particle potential while for $\gamma \to \infty$ with $\gamma\beta = const$ (4.1) gives the exactly solvable wedge potential [5]. From now on, we set $\gamma = \beta = 1$. On varying the tunable parameter R the potential shape changes from a single–well structure for $R < R^* = 0.88$ to a double–well structure (Fig. 1). Note that the potential is linear as $x \to \pm\infty$ and $W(x;0) = -W(x;\infty)$.

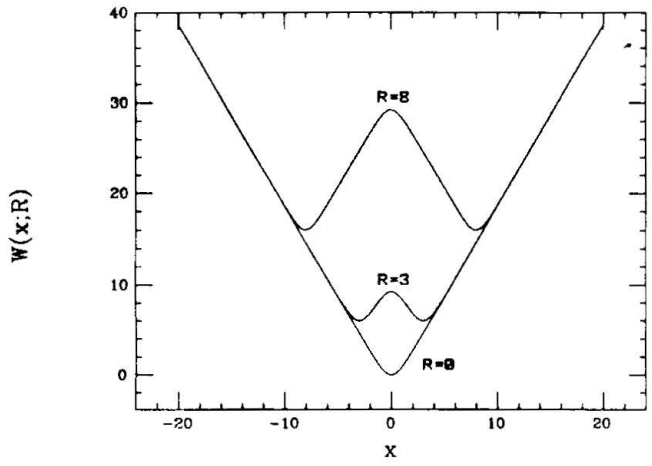

Fig.1 – Plot of the potential $W(x;R)$.

We shall now estimate the smallest eigenvalue λ for all values of R and D. The transformation (2.5) for $D = 1$

leads to the eigenvalue problem

$$H_-\varphi^- = E^-\varphi^- \tag{4.2}$$

with H_- given by

$$H_- = -\frac{d^2}{dx^2} + 1 - \frac{2}{ch^2(x-R)} - \frac{2}{ch^2(x+R)} + \frac{2}{ch^2R + sh^2x} \tag{4.2a}$$

With (4.2a) is associated [9] the supersymmetric partner H_+

$$H_+ = -\frac{d^2}{dx^2} + 1 - \frac{2}{ch^2x} + \frac{2}{sh^2R + ch^2x} \tag{4.2b}$$

which, in turn, may be approximated to a symmetric Pöschl–Teller hamiltonian of the form

$$H_{PT} = -\frac{d^2}{dx^2} + 1 - \frac{U_0}{ch^2\alpha x} \tag{4.3}$$

with

$$U_0 = 2th^2R \tag{4.4a}$$

$$\alpha = th^2R\frac{sh2R}{sh2R - 2R} \tag{4.4b}$$

The eigenvalue spectrum of (4.3) is known analytically [9]. The smallest non–vanishing eigenvalue is then computed as [4]

$$\lambda = \frac{<\varphi_b^+(x)|H_+|\varphi_b^+>}{<\varphi_b^+\varphi_b^+>} \tag{4.5}$$

where $H_{PT}\varphi_b^+ = 0$ and

$$\varphi_b^+ = (\frac{1}{ch\alpha x})^s \tag{4.6a}$$

with

$$s = \frac{1}{2}(-1 + \sqrt{1 + \frac{8th^2R}{\alpha^2}}) \tag{4.6b}$$

The behavior of λ as a function of R is displayed in Fig. 2 and is compared with λ obtained from the numerical integration of the Schrödinger equation [9]. We see that the agreement is excellent for all values of R, including the range $R < 2$ where the usual semiclassical approximations are no longer tenable.

We notice that (4.5) provides also an analytical expression – valid for all values of R – of the frequency of the shape mode [9] of the 4π double sine–Gordon kink.

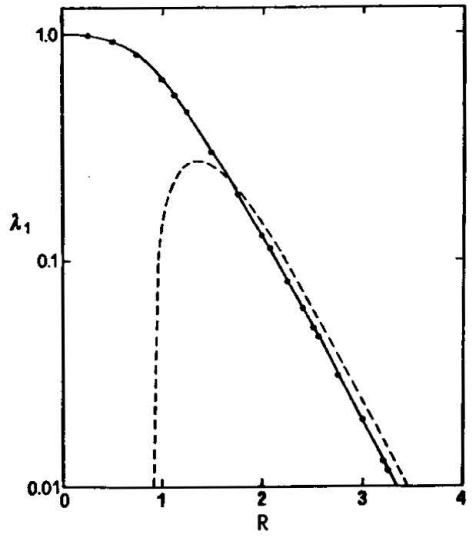

Fig.2 – The supersymmetric result (4.5) (solid line) is compared with the numerical integration of (4.2) (dots) and Kramers' approximation (4.7) (dotted-dashed line)

To obtain the correct result for λ using standard FP techniques is less straightforward. In fact, the computation

of λ through Kramers' formula turns out to hold only for $D << 1$. The assumptions implicit in Kramers' method are often summarized by the requirement that $D << \Delta W \equiv W(0,R) - W(\pm x_m; R) = 2ln\frac{ch^2R}{2sh\bar{R}}$, where x_m denotes the position of the potential minima for $R > R^*$. Such a condition is meant to guarantee by one token that the potential barrier ΔW is much larger than the average energy fluctuation D and that the bistable potential can be approximated by parabolic curves in the vicinity of the extremal points $x = 0$ and $\pm x_m$. This is not the case of soft potential where the second condition corresponds [4] to the further inequality $D << [W^{ii}(0;R)]^2/W^{iv}(0;R) \simeq O(1)$.

This explains why Kramers' formula for λ

$$\lambda^K = \frac{8}{\pi}\frac{sh^2R - 1}{ch^4R}thR \tag{4.7}$$

is inadequate at $D = 1$ even for $R \to \infty$, where $\Delta W \simeq 2R$ becomes infinitely large.

For $D \neq 1$ the Schrödinger problem is not amenable to an easy analytical solution. We may use in this case the variational method proposed by Bernstein and Lowell–Brown [2] to investigate the behavior of λ as a function of both D and R. To obtain a good variational estimate for the ground state level, λ, of the hamiltonian H_+, one first notices that $H_+ exp\frac{W(x;R)}{2D} = 0$. As the operator H_+ is positive definite a natural choice for the trial function is

$$\varphi_+(x) = exp\frac{\psi(x)}{2D} \tag{4.8a}$$

with

$$\psi(x) = \psi(-x) = \begin{cases} W(x;R) & 0 \leq x \leq c \\ W(c) + W'(c)(x-c) & x \geq c \end{cases} \tag{4.8b}$$

where c is the only variational parameter in this scheme. To guarantee that $\varphi_+(x)$ is normalizable, one requires that $0 < c < x_m$, so that $W'(c)$ is negative definite.

The variational method provides then an upper bound for λ

$$\lambda \leq \lambda^V = \min_{\{c\}} \frac{< \varphi_+(x)|H_+|\varphi_+ >}{< \varphi_+\varphi_+ >} \tag{4.9}$$

The variational computation of $\lambda(D;R)$ for the potential (4.1) has been reported elsewhere [10]. Here we recall only that

i) λ^V is well defined only for $R > R^*$ as understood in the variational approach where the bistable structure of $W(x;R)$ is always assumed. For $R > 2$ λ^V approximates λ within up to 40 % for the whole range of values of D considered; an excellent agreement (within 1 %) is obtainable for both $D << \Delta W$ and $D >> \Delta W$.

ii) in the limit $\Delta W >> D$ and $D << 1$ λ^V and λ^K (the eigenvalue computed via Kramers' formula) come close to each other.

iii) there is a critical value D_c such that for $\Delta W >> D \geq D_c$ the activation rate is no longer reproduced by Kramers' formula; a good approximation for λ has been obtained from (4.9) [10].

In summary, we have shown how supersymmetric quantum mechanics could provide – in an easy and systematic fashion – an estimate of the time of approach to equilibrium of a brownian particle even in cases (soft potentials) in which FP techniques are hard to use. For $D = 1$, supersymmetric quantum mechanics is able to reproduce the exact activation rate.

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