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Effective quantum dynamics in a weakly anharmonic interaction in the vicinity of a focusing point

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ABSTRACT

We describe here the dynamic behaviors of a quantum ensemble of particles in a one-dimensional anharmonic potential well and of the corresponding classical ensemble in the vicinity of a focusing point. The anharmonicity of the interaction is chosen to be very small and small. Accordingly, the perturbation theory is used, and the accurate analytical solutions of the problem in both the quantum and classical cases are obtained. The dynamics of the quantum ensemble is considered through a detailed morphological analysis of the families of amplitudes squared and phases of the particle wave functions. We explore the dependence of the quantum solution of the problem on the anharmonicity and its relation to the classical solution. In addition, a solution of the problem based on catastrophe theory is given and compared with the quantum solution. It has been proven that an effective quantum dynamics of the ensemble can be clearly observed. In addition, we have concluded that, when the anharmonicity increases, the difference between the effective quantum behavior and classical behavior becomes larger.

1. Introduction

It is well-known that the anharmonic component of the potential energy of a crystal plays a crucial role in describing and explaining its properties [1]. In the harmonic approximation, in which only the quadratic terms in the perturbation expansion of the potential energy in the displacements of crystal's nuclei from their equilibrium positions are taken into account, the crystal, for example, would show no thermal expansion or its specific heat would become constant at high temperatures, which is certainly wrong.

Bender and Wu [2] studied in detail the eigenvalue problem of a simple one-dimensional (1D) anharmonic oscillator using the We ntzel–Kramers–Brillouin (WKB) method. The potential energy of the system contained the quadratic and quartic terms in its perturbation expansion in the space coordinate. The quadratic term coefficient was positive and the quartic term coefficient was varied in the complex plane. It was established that the ground-state energy of the system, which was a power series in the quartic term coefficient, was divergent. It should be mentioned that a similar anharmonic oscillator, with the potential energy containing the quadratic and quartic terms with the quadratic term coefficient being positive or negative and the quartic term positive, has been explored and used in development of 1D quantum field theory [3]. A 1D system having the linear, quadratic and quartic terms in the perturbation expansion of its potential energy was investigated by Delabaere and Pham [4]. They varied the coefficients of these terms in the complex plane and used the WKB method. We would also like to mention the work of Martin-Delgado *et al.* [5]. They accurately determined two lowest energy levels of a 1D anharmonic oscillator using the continuum limit of the density matrix renormalization group method. The potential energy of the system included the quadratic and quartic terms with the coefficients of both terms being positive, and the calculations were performed for various values of the quartic term coefficient. The anharmonic interactions are also employed in investigations of the non-perturbative effects in quantum field theory [6]. These effects are connected, for example, to non-trivial solutions of the Newton's equations of a system, or to the situations in which a property of a system appears in a term of its power series expansion but not in the resummed expansion.

Demkov and Meyer [7] showed that the potential in a crystal channel can be used for reducing the radius of an impinging proton beam to several picometers. They used the harmonic approximation of the potential. This effect is known as the superfocusing effect in charged particle channeling. A study of the effect with the anharmonicity of the interaction taken into account revealed that its origin was the reduction of a spatial rainbow (or caustic) line to a point [8,9]. It has been demonstrated that the

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superfocusing effect might be employed for developing a measurement technique with the picometer resolution—rainbow subatomic microscopy [7–9]. The results presented in Refs. [7–9] can be treated as part of a long-term study of ion channeling in thin crystals involving three dedicated groups [10–17].

Schulman [18] analyzed a 1D system with the (anharmonic) potential energy containing the quadratic and inverse quadratic terms with the coefficients of both terms being positive. He used the time-dependent propagator of the system to explore its semiclassical behavior in the vicinity of a spatial caustic (or rainbow) point, where the line representing the corresponding classical principal Hamilton's function had a singular point. Petrović *et al.* [19] and Ćosić *et al.* [20] studied the quantum rainbow effect in positron channeling in very short carbon nanotubes. The incident positrons were represented as the Gaussian wave packets. The observed spatial and angular rainbows were successfully explained using the semiclassical approach. However, in continuation of that study, it was demonstrated that the behavior of an ensemble of positrons, represented initially as the Gaussian wave packets, transmitted through a very short carbon nanotube could be fully understood through a detailed morphological analysis of the families of amplitudes squared and phases of the positron wave functions, without any help of the semiclassical approach [21]. In the analysis, special attention was paid to the shapes of the lines representing the classical and quantum principal Hamilton's functions of the ensemble in the vicinities of the spatial and angular rainbow points.

In this paper, we shall present the results of a detailed exploration of the dynamics of an ensemble of particles in a simple 1D anharmonic potential well. The anharmonicity of the interaction will be very small and small. The potential energy of the system will contain the quadratic and quartic terms in its perturbation expansion with the coefficients of both terms being positive. The incident particles will be represented as the Gaussian wave packets. Our attention will be focused on the morphological characteristics of the quantum and classical solutions of the problem in the vicinity of a spatial double rainbow point and on the relation between them. As a result, we shall be able to directly compare the effective dynamics of the quantum ensemble and the dynamics of the classical ensemble. The solution of the problem based on catastrophe theory will be presented as well. We shall demonstrate that the behavior of the chosen ensemble is exceptionally rich.

This work was undertaken with the intention to pave the way for formulation of a quantum theory of the superfocusing effect in positron channeling in chiral carbon nanotubes, which can be treated as 1D targets [7–9]. Namely, the system we shall consider was chosen because it could be viewed as a simple model of a positron propagating along such a nanotube. The above mentioned spatial double rainbow point is a simple analogue of the first superfocusing point for positrons channeled in the nanotube, being the limiting point at which the nanotube is very short. In this sense, the paper appears as a natural continuation of our works on positron channeling in nanotubes [19–21], in which nanotubes were very short.

2. Theory

We study the quantum and classical motions of a particle in a simple 1D anharmonic potential well. The potential energy of the system contains the quadratic and quartic terms in its perturbation expansion in the space coordinate, *i.e.*, the harmonic and anharmonic terms, respectively. It reads

$$V(x) = \frac{k}{2}x^2 + \frac{g}{4}x^4, \tag{1}$$

where x is the spatial coordinate, and k and g are positive constants.

2.1. Quantum dynamics

The 1D time-dependent Schrödinger equation that determines the motion of the particle under consideration reads

$$i\hbar\partial_t\Psi = -\frac{\hbar^2}{2m}\partial_x^2\Psi + V(x)\Psi, \tag{2}$$

where $\Psi = \Psi(x,t)$ is the particle wave function, t is the time coordinate, $\partial_t = \partial/\partial t$, $\partial_x^2 = \partial^2/\partial x^2$, m is the particle mass, $\hbar$ is the reduced Planck constant, and $V(x)$ is given by Eq. (1). Let us introduce the units of time and space T_0 and L_0, respectively, such that $T_0^2 = m/k$ and $L_0^2 = \hbar T_0/m = \hbar/(mk)^{1/2}$. The time and space coordinates in these units, which will be referred to as the natural units, are $\tau = t/T_0$ and $\xi = x/L_o$. Now, Eq. (2) can be rewritten in the form

$$i\partial_\tau\psi = -\frac{1}{2}\partial_\xi^2\psi + \frac{1}{2}\xi^2\psi + \frac{\lambda}{4}\xi^4\psi, \tag{3}$$

where $\psi = \psi(\xi,\tau) = \Psi(x,\tau)L_0^{1/2}$, $\partial_\tau = \partial/\partial\tau$, $\partial_\xi^2 = \partial^2/\partial\xi^2$, and $\lambda = \hbar g/(mk^3)^{1/2}$. It is clear that the dynamics of the particle is governed solely by parameter λ, which is determined by k and g. We shall call this parameter the anharmonicity of the interaction.

It is assumed that initially, at $\tau = 0$, the particle is a Gaussian wave packet at rest defined by the expression,

$$\psi(\xi,0;\eta) = \varphi(\xi;\eta) = \frac{1}{(2\pi\sigma^2)^{1/4}}\exp\left[-\frac{(\xi-\eta)^2}{4\sigma^2}\right], \tag{4}$$

where η and σ are the wave packet initial position and spatial standard deviation, respectively, in the natural units. This means that $\eta = x_0/L_0$, where x_0 is the particle impact parameter.

Eq. (3) with Eq. (4) as the initial condition cannot be solved analytically. However, if λ is small, *i.e.*, if the anharmonic term in $V(x)$ can be treated as a perturbation, the equation can be solved analytically using the perturbation theory. We assume that λ is small enough to approximate ψ with its first order perturbation expansion. Hence,

$$\psi(\xi,\tau;\eta) = \psi_0(\xi,\tau;\eta) + \lambda\psi_1(\xi,\tau;\eta); \tag{5}$$

the unperturbed wave function of the particle, ψ_0, and its perturbation wave function, ψ_1, are given by expressions

$$\begin{aligned}\psi_0(\xi,\tau;\eta) &= \int_{\xi\prime} K(\xi,\tau;\xi\prime,\tau\prime)\varphi(\xi\prime;\eta)d\xi\prime,\\ \psi_1(\xi,\tau;\eta) &= -\frac{i}{4}\int_{\xi\prime}\int_{\tau\prime} K(\xi,\tau;\xi\prime,\tau\prime)\xi\prime^4\psi_0(\xi\prime,\tau\prime;\eta)d\xi\prime d\tau\prime,\end{aligned} \tag{6}$$

respectively, where K denotes the kernel of the evolution operator corresponding to the harmonic term in $V(x)$ [7]. This function reads

$$\begin{aligned}K(\xi,\tau;\xi\prime,\tau\prime) = &\frac{1}{[4i\pi\mu^2\sin(\tau-\tau\prime)]^{1/2}}\\ &\times\exp\left\{\frac{i}{4\mu^2\sin(\tau-\tau\prime)}\left[(\xi^2+\xi\prime^2)\cos(\tau-\tau\prime)-2\xi\xi\prime\right]\right\},\end{aligned} \tag{7}$$

where $\mu = 2^{-1/2}$ is the spatial standard deviation of the wave packet in its ground state corresponding to the harmonic term in $V(x)$ in the natural units.

The amplitude squared of the unperturbed wave function of the particle reads

$$|\psi_0(\xi,\tau;\eta)|^2 = \frac{1}{[2\pi\sigma_\tau^2(\tau)]^{1/2}}\exp\left[-\frac{(\xi-\eta\cos\tau)^2}{2\sigma_\tau^2(\tau)}\right], \tag{8}$$

with

$$\sigma_\tau(\tau) = \sigma\left(\frac{\mu^4}{\sigma^4}\sin^2\tau + \cos^2\tau\right)^{1/2}, \tag{9}$$