Physics Letters A 378 (2014) 691–698

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Validity of the time-dependent variational approximation to the Gaussian wavepacket method applied to double-well systems

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ARTICLE INFO

Article history:
Received 23 October 2013
Received in revised form 15 December 2013
Accepted 18 December 2013
Available online 2 January 2014
Communicated by P.R. Holland

Keywords:
Gaussian wavepacket
Time-dependent variational approximation
Spectral method
Double-well potential

ABSTRACT

We have examined the validity of the time-dependent variational approximation (TDVA) to the Gaussian wavepacket method (GWM) for quantum double-well (DW) systems, by using the quasi-exact spectral method (SM). Comparisons between results of wavefunctions, averages of position and momentum, the auto-correlation function, and an uncertainty product calculated by SM and TDVA have been made. It has been shown that a given initial Gaussian wavepacket in SM is quickly deformed at $t > 0$ where a wavepacket cannot be expressed by a *single* Gaussian, and that assumptions on averages of higher-order fluctuations in TDVA are not justified. These results cast some doubt on an application of TDVA to DW systems. Gaussian wavepacket dynamics in anharmonic potential systems is studied also.

1. Introduction

Dynamical properties of nonrelativistic quantum systems may be described by the Schrödinger equation [1], in which the time-dependent wavefunction $\Psi(x,t)$ for the one-dimensional system with the potential $U(x)$ is described by

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = H\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)\right]\Psi(x,t). \tag{1}$$

It is generally difficult to obtain exact solutions of the Schrödinger equation which are available only for limited cases like a harmonic oscillator (HO) system. For general quantum systems, various approaches such as perturbation and spectral methods have been developed to obtain approximate solutions [1]. From Eq. (1), we may derive equations of motion for $\langle x\rangle$ and $\langle p\rangle$ expressed by

$$\frac{d\langle x\rangle}{dt} = \frac{\langle p\rangle}{m}, \qquad \frac{d\langle p\rangle}{dt} = -\left\langle\frac{\partial U(x)}{\partial x}\right\rangle, \tag{2}$$

where the bracket $\langle\cdot\rangle$ denotes the expectation value. Although equations of motion given by Eq. (2) are closed within $\langle x\rangle$ and $\langle p\rangle$ for a HO system, they generally yield equations of motion including higher-order fluctuations such as $\langle\delta x^2\rangle$, $\langle\delta p^2\rangle$ and $\langle\delta x\delta p + \delta p\delta x\rangle$ where $\delta x = x - \langle x\rangle$ and $\delta p = p - \langle p\rangle$. It is necessary to develop an approximate method to close or truncate a hierarchical chain of equations of motion.

The Gaussian wavepacket method (GWM) is one of such methods whose main aim is a semi-classical description of quantum systems (for a recent review on GWM, see Ref. [2]). If the wavefunction is Gaussian at $t = 0$ in a HO system, it remains at all $t > 0$. Heller [3] proposed that even for more realistic potentials, we may adopt a (thawed) Gaussian wavepacket given by

$$\Psi_H(x,t) = \exp\left[\frac{i}{\hbar}\left[A\big(x-\langle x\rangle\big)^2 + \langle p\rangle\big(x-\langle x\rangle\big) + \gamma\right]\right], \tag{3}$$

where A and γ are time-dependent complex parameters. Heller [3] derived equations of motion for $\langle x\rangle$, $\langle p\rangle$, A and γ, employing an assumption that the potential expanded in the Taylor series at $x = \langle x\rangle$ may be truncated by

$$U(x) \cong U^{(0)}\big(\langle x\rangle\big) + U^{(1)}\big(\langle x\rangle\big)\big(x-\langle x\rangle\big) + \frac{1}{2}U^{(2)}\big(\langle x\rangle\big)\big(x-\langle x\rangle\big)^2, \tag{4}$$

where $U^{(k)}(x)$ signifies the kth derivative of $U(x)$. The concept of the Gaussian wavepacket has been adopted in many fields [2]. Dynamics is well described by GWM for a HO system where motions of fluctuations are separated from those of $\langle x\rangle$ and $\langle p\rangle$, leading to the uncertainty relation: $\langle\delta x^2\rangle\langle\delta p^2\rangle \geqslant \hbar^2/4$. Various types of variants of GWM such as the frozen [4] and generalized Gaussian wavepacket methods [5] have been proposed [2]. Among them, we pay our attention into the time-dependent variational approximation (TDVA) which employs the normalized squeezed coherent-state Gaussian wavepacket given by [6–10]

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0375-9601/$ – see front matter
http://dx.doi.org/10.1016/j.physleta.2013.12.035

$$\Psi_G(x,t) = \frac{1}{(2\pi\mu)^{1/4}} \times \exp\left[-\frac{(1-i\alpha)}{4\mu}\big(x-\langle x\rangle\big)^2 + i\frac{\langle p\rangle(x-\langle x\rangle)}{\hbar}\right], \quad (5)$$

μ and α being time-dependent parameters. For the introduced squeezed coherent state, equations of motion given by Eq. (2) are closed within $\langle x\rangle$, $\langle p\rangle$, $\langle \delta x^2\rangle$ and $\langle \delta x\delta p + \delta p\delta x\rangle$ (see Eqs. (33)–(36)). A comparison between Heller's GWM and TDVA is made in Refs. [9,10].

There have been many studies on GWM which is applied to HO, anharmonic oscillator (AO) and Morse potentials [2]. However, GWM has some difficulty when applied to a potential $U(x)$ including terms of x^n with $n > 2$. Although it has been claimed that GWM yields a fairly good result for AO systems [6], we wonder whether it actually works for double-well (DW) systems. DW potential models have been employed in a wide range of fields including physics, chemistry and biology (for a recent review on DW systems, see Ref. [11]). Lin and Ballentine [12], and Utermann, Dittrich and Hänggi [13] studied semi-classical properties of DW systems subjected to periodic external forces, calculating the Husimi function [14]. Their calculations showed a chaotic behavior in accordance with classical driven DW systems. Igarashi and Yamada [15] studied a coherent oscillation and decoherence induced by applied polychromatic forces in quantum DW system. By using TDVA, Pattanayak and Schieve [8] pointed out that a chaos is induced by quantum noise in DW systems without external forces although classical counterparts are regular. This is in contrast to the usual expectation that quantum effects suppress classical chaos. Chaotic-like behavior was reported in a square DW system obtained by the exact calculation [16]. Quantum chaos pointed out in Ref. [8] is still controversial [17–22].

Quite recently, Hasegawa has studied effects of the asymmetry on the specific heat [23] and tunneling [24] in the asymmetric DW systems, by using the spectral method (SM) in which expansion coefficients are evaluated for energy matrix elements with a finite size of $N_m = 30$ (Eqs. (16) and (17)). Model calculations in Refs. [23,24] have pointed out intrigue phenomena which are in contrast with earlier relevant studies. It is worthwhile to examine the validity of TDVA applied to DW systems with the use of quasi-exact SM [23,24], which is the purpose of the present paper. Such a study has not been reported as far as we are aware of. It is important to clarify the significance of TDVA for DW systems.

The paper is organized as follows. In Section 2, we mention the calculation method employed in our study. We consider quantum systems described by the symmetric DW (SDW) model. In solving dynamics of a Gaussian wavepacket in the SDW, we have adopted the two methods: SM and TDVA. In Section 3, we report calculated results of the magnitude of wavefunction ($|\Psi(x,t)|^2$), an expectation value of x ($\langle x\rangle$), the auto-correlation function ($C(t)$) and the uncertainty product ($\langle \delta x^2\rangle\langle \delta p^2\rangle$). In Section 4 we apply our method also to an AO model. Section 5 is devoted to our conclusion.

2. The adopted method

2.1. Symmetrical double-well potential

We consider a DW system whose Hamiltonian is given by [23,24]

$$H = \frac{p^2}{2m} + U(x) = H_0 + V(x), \quad (6)$$

where

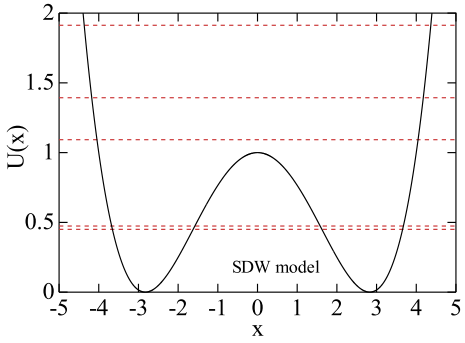

Fig. 1. (Color online.) The symmetric DW potential (solid curve) with $x_s = 2\sqrt{2}$ and $\Delta = 1.0$ in Eq. (7), dashed curves expressing eigenvalues of E_ν ($\nu = 0$–4).

$$U(x) = C\left(x^2 - x_s^2\right)^2 \quad \left(C = \frac{m\omega^2}{8x_s^2}\right), \quad (7)$$

$$H_0 = \frac{p^2}{2m} + U_0(x), \quad (8)$$

$$U_0(x) = \frac{m\omega^2 x^2}{2}, \quad (9)$$

$$V(x) = U(x) - U_0(x). \quad (10)$$

Here m, x and p express mass, position and momentum, respectively, of a particle, $U(x)$ stands for the DW potential, and H_0 is the HO Hamiltonian with the oscillator frequency ω. The SDW potential $U(x)$ has stable minima at $x = \pm x_s$ and an unstable maximum at $x_u = 0$ with the potential barrier of $\Delta = U(0) - U(\pm x_s) = m\omega^2 x_s^2/8$. A prefactor of C in Eq. (7) is chosen such that the DW potential $U(x)$ has the same curvature at the minima as the HO potential $U_0(x)$: $U''(\pm x_s) = U_0''(0) = 1.0$. Fig. 1 expresses the adopted quartic DW potential $U(x)$ with $x_s = 2\sqrt{2}$ and $\Delta = 1.0$ in Eq. (7). Eigenfunction and eigenvalue for H_0 are given by

$$\phi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega x^2}{2\hbar}\right)\mathcal{H}_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right), \quad (11)$$

$$E_{0n} = \left(n + \frac{1}{2}\right)\hbar\omega \quad (n = 0, 1, 2, \ldots), \quad (12)$$

where $\mathcal{H}_n(x)$ stands for the nth Hermite polynomial.

2.2. Spectral method

Various approximate analytical and numerical methods have been proposed to solve the Schrödinger equation given by Eq. (1) [1]. Assuming $\Psi(x,t) = \Psi(x)e^{-iEt/\hbar}$, we first solve the steady-state Schrödinger equation, $H\Psi(x) = E\Psi(x)$, with the eigenvalue E. The stationary wavefunction $\Psi(x)$ is expanded in terms of $\phi_n(x)$

$$\Psi(x) = \sum_{n=0}^{N_m} c_n\phi_n(x), \quad (13)$$

leading to the secular equation

$$Ec_n = \sum_{k=0}^{N_m} H_{nk}c_k, \quad (14)$$

with

$$H_{nk} = E_{0n}\,\delta_{n,k} + \int_{-\infty}^{\infty}\phi_n(x)^* V(x)\,\phi_k(x)\,dx, \quad (15)$$

where N_m is the maximum quantum number.