WKB Wave Function of the General Time-Dependent Quadratic Hamiltonian System

Jeong Ryeol Choi¹

We derived the WKB wave function for the general time-dependent quadratic Hamiltonian system using a unitary transformation method. We applied our research to sinusodially drived Caldirola–Kanai oscillator and confirmed that the time evolution of our approximated WKB wave function is similar to that of the exact one. This wave function can be used to analyze the interference between the probability amplitudes contributed by the area of overlap in phase space of quantum states.

KEY WORDS: WKB wave function; time dependent Hamiltonian; unitary operator; invariant operator; Caldirola-Kanai oscillator.

1. INTRODUCTION

In recent years, many researches have been contributed to the transition from classical physics to the semiclassical and quantum physics. Especially, much of the work in quantum mechanics of the time-dependent harmonic oscillator, we may recall, accomplished with the intermediate aid of the adiabatic invariants (Hu, 1998; Neishtadt, 1981). It is known that the problem of the harmonic oscillator with time-variable frequency was first solved in 1880 by Ermakov (Hass, 2002; Qian, Huang, and Gu, 2001) in view of the classical mechanics. Therefore, such systems are named Ermakov systems owned a related constant of motion that often called as an Ermakov invariant quantity. A generalization of the Ermakov systems are found in Hass (2002) and a detailed discussion about them in view of quantum point are found in Hartley and Ray (1981).

After the publication of the work of Kramers (see Robicheaux *et al.* (1987) and references there in) in 1926 for WKB approximation in order to solve onedimensional wave equations, vivid research for the WKB calculation has been performed in the literature (Guérin, 1996; Robicheaux *et al.*, 1987; Robnik and Salasnich, 1997). WKB method is a nice technique especially for computing approximate eigenvalues of the one-dimensional Schrödinger equation of the slowly

¹Department of New Material Science, Division of Natural Sciences, Sun Moon University, Asan 336-708, Korea; e-mail: choiardor@hanmail.net.

varying potentials (Fröman and Fröman, 1965; Geldart and Kiang, 1986). Hence, it is a good tool to bridge the interval between classical and quantum theory (Kromer, 1994; Merzbacher, 1970). In this paper, we derive WKB wave function of the general time-dependent harmonic oscillator using an invariant operator that was introduced by Lewis (1967). The invariant operator is very useful in order to derive exact solutions of the time-dependent quantum-mechanical Hamiltonian systems. Recently, the exact invariant quantities for the three-dimensional Hamiltonian systems which can be applicable to the time-dependent nonlinear harmonic oscillator are derived (Struckmeier and Riedel, 2000). The exact wave function of the general time-dependent harmonic oscillator has been reported in the literature (Choi, 2003; Yeon *et al.*, 1997). However, the derivation of the semiclassical WKB wave function is worth because it can be applied to analyze the interference between the probability amplitudes contributed by the areas of overlap in phase space of quantum states (Schleich, Walls, and Wheeler, 1988).

This paper is organized as follows. In Section II, we survey how to transform complicated time-dependent Hamiltonian to the simple one that can be easily treated. We derived the WKB wave function in Section III. We discussed the approximated wave function at the classical turning point in Section IV. Finally, in the last section, we apply our research to sinusoidally driven Caldirola–Kanai oscillator.

2. SURVEY OF THE UNITARY TRANSFORMATION FOR THE TIME-DEPENDENT HAMILTONIAN SYSTEM

In this section, we review the unitary transformation method (Li *et al.*, 1994) for the general time-dependent quadratic Hamiltonian system of the form (Choi, 2003; Yeon *et al.*, 1997)

$$H(x, p, t) = A(t)p^{2} + B(t)(xp + px) + C(t)x^{2} + D(t)x + E(t)p + F(t), \quad (1)$$

where A(t) - F(t) are time-variable functions that differentiable with respect to time. Note that A(t) is not zero. The system evolves according to the following Schrödinger equation as time goes by

$$i\hbar\frac{\partial}{\partial t}\psi = H(x, p, t)\psi.$$
 (2)

The original Hamiltonian can be transformed to another form by a unitary operator U (Li *et al.*, 1994):

$$H' = U^{-1}HU - i\hbar U^{-1}\frac{\partial U}{\partial t}.$$
(3)

If we choose U as

$$U = U_1 U_2 U_3, \tag{4}$$

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with

$$U_1 = \exp\left(\frac{i}{\hbar}p_p x\right) \exp\left(-\frac{i}{\hbar}x_p p\right),\tag{5}$$

$$U_2 = \exp\left(-\frac{i(2B\rho - \dot{\rho})}{4A\hbar\rho}x^2\right),\tag{6}$$

$$U_3 = \exp\left[-\frac{i}{4\hbar}(xp+px)\ln(2\rho^2)\right],\tag{7}$$

where $\rho(t)$ is the solution of the following differential equation

$$\ddot{\rho}(t) - \frac{\dot{A}}{A}\dot{\rho}(t) + \left(2\frac{\dot{A}B}{A} - 4B^2 + 4AC - 2\dot{B}\right)\rho(t) - kA^2\frac{1}{\rho^3(t)} = 0, \quad (8)$$

and $x_p(t)$ and $p_p(t)$ stand for the particular solutions (Choi, 2002a, Yeon *et al.*, 1997) of the classical equation of motion of the system, i.e., they satisfies

$$\begin{split} \ddot{x}_{p}(t) &- \frac{\dot{A}}{A} \dot{x}_{p}(t) + \left(2\frac{\dot{A}B}{A} - 4B^{2} + 4AC - 2\dot{B} \right) x_{p}(t) \\ &= -\frac{\dot{A}E}{A} + 2BE - 2AD + \dot{E}, \end{split}$$
(9)
$$\ddot{p}_{p}(t) &- \frac{\dot{C}}{C} \dot{p}_{p}(t) + \left(4AC - 2\frac{\dot{C}B}{C} - 4B^{2} + 2\dot{B} \right) p_{p}(t) \\ &= \frac{\dot{C}D}{C} + 2BD - 2CE - \dot{D}. \end{split}$$
(10)

Then, Eq. (3) can be simplified to

$$H' = g(t)I'(x) + \mathcal{L}_p(x_p(t), \dot{x}_p(t), t) - \frac{E^2(t)}{4A(t)} + F(t),$$
(11)

where

$$g(t) = \frac{A(t)}{\rho^2(t)},\tag{12}$$

$$I'(x) = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2,$$
(13)

$$\mathcal{L}_p(x_p(t), \dot{x}_p(t), t) = \frac{1}{4A(t)} \dot{x}_p^2(t) - \frac{B(t)}{A(t)} x_p(t) \dot{x}_p(t) - \left(C(t) - \frac{B^2(t)}{A(t)}\right) x_p^2(t).$$
(14)

Note that I'(x) is the invariant operator of the transormed system and the form of $\mathcal{L}_p(x_p(t), \dot{x}_p(t), t)$ is same as the Langrangian of the system with D = E = 0

except that x and \dot{x} replaced with x_p and \dot{x}_p . The relation between invariant operator, I(x, t), of the untransformed system and invariant operator, I'(x), of the transformed system is (Li *et al.*, 1994).

$$I(x,t) = UI'(x)U^{-1}.$$
(15)

The system of the transformed Hamiltonian evolves acording to the following Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi' = H'\psi'.$$
 (16)

We can proceed by writing that

$$\psi'(x, \{p\}, t) = T(t)\phi'(x, \{p\}).$$
(17)

When we substitute Eqs. (11) and (17) into Eq. (16), we find that

$$I'\phi' = \lambda\phi',\tag{18}$$

$$\frac{\partial T(t)}{\partial t} = \frac{1}{i\hbar} \bigg[\lambda g(t) + \mathcal{L}_p(x_p(t), \dot{x}_p(t), t) - \frac{E^2(t)}{4A(t)} + F(t) \bigg] T(t), \quad (19)$$

where λ is a separation constant (or an eigenvalue of the transformed invariant operator). If we consider Eqs. (13) and (18), the separation constant is discrete:

$$\lambda_n = \hbar \sqrt{k} \left(n + \frac{1}{2} \right). \tag{20}$$

We see that Eq. (19) can be readily solved as

$$T(t) = \exp\left[-i\sqrt{k}\left(n+\frac{1}{2}\right)\int_{0}^{t}\frac{A(t')}{\rho^{2}(t')}dt' - \frac{i}{\hbar}\int_{0}^{t}\left[\mathcal{L}_{p}(x_{p}(t'),\dot{x}_{p}(t'),t') - \frac{E^{2}(t')}{4A(t')} + F(t')\right]dt'\right].$$
 (21)

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Using Eq. (20), Eq. (18) can be written in the form

$$\frac{d^2\phi'}{dx^2} + \frac{p^2}{\hbar^2}\phi' = 0,$$
(22)

where

$$p = \sqrt{2\lambda_n - kx^2}.$$
 (23)

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In the discussion of the WKB wave function, it can be shown that wave function can be approximated by

$$\phi' = \phi'_0 \exp\left[\pm \frac{i}{\hbar} \int^x p(x) \, dx\right],\tag{24}$$

where $\phi'_0(x)$ and p(x) are slowly varying functions. By substitution of this approximate solution into Eq. (22) under the assumption that \hbar/p is small than the other dimensions in problem, we can show that (Powell and Crasemann, 1961)

$$\frac{d^2\phi'_0}{dx^2} \pm \frac{i}{\hbar} \left(2p \frac{d\phi'_0}{dx} + \phi'_0 \frac{dp}{dx} \right) = 0.$$
⁽²⁵⁾

If we neglect the first term of the above equation, we can derive ϕ'_0 as

$$\phi_0' = \frac{C}{\sqrt{p}},\tag{26}$$

so that Eq. (24) becomes

$$\phi' = \frac{C}{\sqrt{p}} \exp\left[\pm \frac{i}{\hbar} \int^x p(x) \, dx\right]. \tag{27}$$

We may determine how good an approximation the WKB wave function is. To do this, using Eqs. (25)–(27) we derive the differential equation

$$\frac{d^2\phi'}{dx^2} + \left[\frac{p^2}{\hbar^2} - \frac{3}{4}\left(\frac{p'}{p}\right)^2 + \frac{p''}{2p}\right]\phi' = 0,$$
(28)

where

$$p' = \frac{dp}{dx}, \quad p'' = \frac{d^2p}{dx^2}.$$
 (29)

If we compare Eq. (28) with Eq. (22) we can confirm that the last two terms in the left-hand side of Eq. (28) are extra terms. In order to Eq. (28) be a good approximation, these extra terms must become negligible quantity compared to the other terms in the left-hand side, i.e., (Kroemer, 1994; Powell and Crasemann, 1961),

$$\frac{\hbar^2}{4} \left| 2\frac{p''}{p} - 3\left(\frac{p'}{p}\right)^2 \right| \ll |p|^2.$$
(30)

The unnormalized eigenstate approximated using WKB method to the bound system is (Powell and Crasemann, 1961)

$$\phi' = (-1)^n \frac{1}{\sqrt{p}} \exp\left(-\frac{1}{\hbar} \int_x^{x_{n-}} p \, dx\right) \quad \text{for } x < x_{n-}, \tag{31}$$

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$$= (-1)^n \frac{2}{\sqrt{p}} \cos\left(\frac{1}{\hbar} \int_{x_{n-}}^x p \, dx - \frac{\pi}{4}\right) \quad \text{for } x_{n-} < x < x_{n+}, \qquad (32)$$

$$= \frac{1}{\sqrt{\mathsf{p}}} \exp\left(-\frac{1}{\hbar} \int_{x_{n+}}^{x} \mathsf{p} \, dx\right) \quad \text{for } x_{n+} < x, \tag{33}$$

where x_{n-} is lower turning point and x_{n+} is upper turning point of the transormed oscillator:

$$x_{n\pm} = \pm \sqrt{\frac{2\lambda_n}{k}},\tag{34}$$

and p is defined only when p is imaginary as

$$\mathbf{p} = |p| = \sqrt{kx^2 - 2\lambda_n}.$$
(35)

Integrating after substitution of Eqs. (23) and (35), we obtain from Eqs. (31)–(33)

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$$\phi' = (-1)^n \frac{1}{\sqrt[4]{kx^2 - 2\lambda_n}} \exp\left\{-\frac{1}{\hbar} \left\lfloor \frac{|x|}{2} \sqrt{kx^2 - 2\lambda_n} - \frac{\lambda_n}{\sqrt{k}} \cosh^{-1}\left(\sqrt{\frac{k}{2\lambda_n}}|x|\right)\right]\right\} \quad \text{for } x < x_{n-},$$
(36)
$$= (-1)^n \frac{2}{\sqrt[4]{2\lambda_n - kx^2}} \cos\left\{\frac{1}{\hbar} \left\lfloor \frac{x}{2} \sqrt{2\lambda_n - kx^2} + \frac{\lambda_n}{\sqrt{k}} \sin^{-1}\left(\sqrt{\frac{k}{2\lambda_n}}x\right) - \frac{\lambda_n \pi}{\sqrt{k}} \left(2m + \frac{3}{2}\right)\right] - \frac{\pi}{4}\right\} \quad \text{for } x_{n-} < x < x_{n+},$$
(37)
$$= \frac{1}{\sqrt[4]{kx^2 - 2\lambda_n}} \exp\left\{-\frac{1}{\hbar} \left\lfloor \frac{x}{2} \sqrt{kx^2 - 2\lambda_n} - \frac{\lambda_n}{\sqrt{k}} + \frac{\lambda_n}{\sqrt{k}} \right\rfloor\right\} \quad \text{for } x_{n+} < x,$$
(38)

where m = 0, 1, 2, ... Hereafter, we will choose m = 0. In the derivation Eq. (36), we altered the interval of the integration from (x, x_{n-}) into $(x_{n+}, |x|)$ for the sake of the symmetry of the simple harmonic potential. The eigenstate of the untransformed invariant operator can be derived from (Choi and Zhang, 2002b)

$$\phi = U\phi'. \tag{39}$$

Applying Eq. (4) to the above equation, we can obtain that

$$\phi = (-1)^{n} \frac{1}{\sqrt[4]{k(x-x_{p})^{2}-4\rho^{2}\lambda_{n}}} e^{ip_{p}x/\hbar} \exp\left(-\frac{i(2B\rho-\rho)}{4A\hbar\rho}(x-x_{p})^{2}\right)$$

$$\times \exp\left\{-\frac{1}{\hbar}\left[\frac{1}{2\sqrt{2}}\left|\frac{x-x_{p}}{\rho}\right|\sqrt{\frac{k}{2\rho^{2}}(x-x_{p})^{2}-2\lambda_{n}}\right]$$

$$-\frac{\lambda_{n}}{\sqrt{k}}\cosh^{-1}\left(\sqrt{\frac{k}{4\lambda_{n}}}\left|\frac{x-x_{p}}{\rho}\right|\right)\right]\right\} \quad \text{for } x < x_{n-}, \qquad (40)$$

$$= (-1)^{n} \frac{2}{\sqrt[4]{4\rho^{2}\lambda_{n}}-k(x-x_{p})^{2}} e^{ip_{p}x/\hbar} \exp\left(-\frac{i(2B\rho-\rho)}{4A\hbar\rho}(x-x_{p})^{2}\right)$$

$$\times \cos\left\{\frac{1}{\hbar}\left[\frac{1}{2\sqrt{2}}\frac{x-x_{p}}{\rho}\sqrt{2\lambda_{n}}-\frac{k}{2\rho^{2}}(x-x_{p})^{2}\right] + \frac{\lambda_{n}}{\sqrt{k}}\sin^{-1}\left(\sqrt{\frac{k}{4\lambda_{n}}}\frac{x-x_{p}}{\rho}\right) - \frac{3\lambda_{n}\pi}{2\sqrt{k}}\right] - \frac{\pi}{4}\right\} \quad \text{for } x_{n-} < x < x_{n+}, \qquad (41)$$

$$= \frac{1}{\sqrt[4]{k(x-x_{p})^{2}-4\rho^{2}\lambda_{n}}} e^{ip_{p}x/\hbar} \exp\left(-\frac{i(2B\rho-\rho)}{4A\hbar\rho}(x-x_{p})^{2}\right)$$

$$\times \exp\left\{-\frac{1}{\hbar}\left[\frac{1}{2\sqrt{2}}\frac{x-x_{p}}{\rho}\sqrt{\frac{k}{2\rho^{2}}(x-x_{p})^{2}-2\lambda_{n}}\right] - \frac{\lambda_{n}}{\sqrt{k}}\cosh^{-1}\left(\sqrt{\frac{k}{4\lambda_{n}}}\frac{x-x_{p}}{\rho}\right)\right]\right\} \quad \text{for } x_{n+} < x. \qquad (42)$$

The WKB wave function of the original system related to Hamiltonian Eq. (1) is given by

$$\psi = T(t)\phi. \tag{43}$$

4. EIGENSTATE NEAR THE TURNING POINTS

In the previous section, we derived wave function of the system using the WKB approximation method. However, it is known that near the classical turning points, $x_{n\pm}$, of the transformed oscillator, these approximations fail. The eigenstate ϕ' near the turning points are the Airy functions (Powell and Crasemann, 1961):

$$\phi' \simeq Ai(z) = \frac{1}{\pi} \int_0^\infty \cos\left(\frac{s^3}{3} + sz\right) ds,\tag{44}$$

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where

$$z = -\left(\frac{2}{\hbar^2}k|x_{n-1}|\right)^{1/3}(x - x_{n-1}) \quad \text{at the neighborhood of } x_{n-1}, \qquad (45)$$

$$= \left(\frac{2}{\hbar^2}kx_{n+1}\right)^{1/3}(x - x_{n+1}) \quad \text{at the neighborhood of } x_{n+1}.$$
(46)

For large z, Eq. (44) asymptotically becomes (Powell and Crasemann, 1961)

$$\phi' \simeq \frac{1}{2\sqrt{\pi}z^{1/4}} \exp\left(-\frac{2}{3}z^{3/2}\right) \quad \text{for } z > 0,$$
 (47)

$$\simeq \frac{1}{\sqrt{\pi}(-z)^{1/4}} \sin\left[\frac{2}{3}(-z)^{3/2} + \frac{\pi}{4}\right] \quad \text{for } z < 0.$$
 (48)

Applying the same relation in Eq. (39), we have

$$\phi \simeq \frac{1}{2\sqrt{2^{1/2}\pi\rho}Z^{1/4}} e^{ip_{\rho}x/\hbar} \exp\left(-\frac{i(2B\rho - \dot{\rho})}{4A\hbar\rho}(x - x_{p})^{2}\right)$$

$$\times \exp\left(-\frac{2}{3}Z^{3/2}\right) \quad \text{for } z > 0, \qquad (49)$$

$$\simeq \frac{1}{\sqrt{2^{1/2}\pi\rho}(-Z)^{1/4}} e^{ip_{\rho}x/\hbar} \exp\left(-\frac{i(2B\rho - \dot{\rho})}{4A\hbar\rho}(x - x_{p})^{2}\right)$$

$$\times \sin\left[\frac{2}{3}(-Z)^{3/2} + \frac{\pi}{4}\right] \quad \text{for } z < 0, \qquad (50)$$

where

$$Z = -\left(\frac{2}{\hbar^2}k|x_{n-1}|\right)^{1/3}\left(\frac{1}{\sqrt{2\rho}}(x-x_p) - x_{n-1}\right) \quad \text{at the neighborhood of } x_{n-1},$$
(51)

$$= \left(\frac{2}{\hbar^2}kx_{n+}\right)^{1/3} \left(\frac{1}{\sqrt{2\rho}}(x-x_p) - x_{n+}\right) \quad \text{at the neighborhood of } x_{n+}.$$
 (52)

The form of the wave function for the original system is given by Eq. (43) with Eqs. (21), (49), and (50).

5. APPLICATION TO CALDIROLA-KANAI OSCILLATOR

As an example, let us apply our theory to the Caldirola–Kanai oscillator (Kanai, 1948) driven by a periodical force $F_0 \cos(\omega_1 t + \theta)$, where F_0 , ω_1 , and θ

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Fig. 1. Absolute square of WKB wave function for the Caldirola–Kanai oscillator with a sinusoidal driving force as functions of position *x* and time *t*. This drawing is based on Eq. (43) with Eqs. (21) and (41). We used quantum number n = 4 and used parameters of $\omega_0 = 1$, $\omega_1 = 0.5$, $\gamma = 0.1$, m = 1, $\hbar = 1$, $F_0 = 1$, k = 1 and $\theta = 0$.



Fig. 2. Absolute square of the exact wave function for the Caldirola–Kanai oscillator with a sinusoidal driving force as functions of position x and time t. We depicted this figure on the basis of the results in Choi (2003) and used the same quantum, number and parameters as in Fig. 1.



Fig. 3. Comparisons between the absolute square of the WKB wave function (thick line) and exact wave function (dotted line) at (a) t = 0 and (b) t = 2. The exact wave function is based on the results in Choi (2003). We used the same quantum number and parameters as in Fig. 1.

are real constants. In this case, A(t) - F(t) in Eq. (1) is given by

$$A(t) = \frac{1}{2m} e^{-\gamma t},\tag{53}$$

$$C(t) = \frac{1}{2}m\omega_0^2 e^{\gamma t},$$
(54)

$$D(t) = -F_0 e^{\gamma t} \cos(\omega_1 t + \theta), \qquad (55)$$

$$B(t) = E(t) = F(t) = 0.$$
(56)

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Then, the solutions of Eqs. (8)–(10) can be evaluated as

$$\rho(t) = \sqrt{\frac{k^{1/2}}{2m\omega}} e^{-\gamma t/2},\tag{57}$$

$$x_{p}(t) = \frac{F_{0}/m}{\sqrt{\left(\omega_{0}^{2} - \omega_{1}^{2}\right)^{2} + \gamma^{2}\omega_{1}^{2}}}\cos(\omega_{1}t + \theta - \delta),$$
(58)

$$p_p(t) = -\frac{F_0\omega_1}{\sqrt{(\omega_0^2 - \omega_1^2)^2 + \gamma^2 \omega_1^2}} e^{\gamma t} \sin(\omega_1 t + \theta - \delta),$$
(59)

where ω and phase δ are given by

$$\omega = \sqrt{\omega_0^2 - \frac{\gamma^2}{4}},\tag{60}$$

$$\delta = \tan^{-1} \frac{\gamma \omega_1}{\omega_0^2 - \omega_1^2}.$$
(61)

In Fig. 1, we depicted the absolute square of the WKB wave function as functions of x and t on the base of Eq. (43) with Eqs. (21) and (41). If we compare this figure with the exact one in Fig. 2 depicted using the result of Choi (2003), we can confirm that the time evolution of our approximated WKB wave function is similar to that of the exact one. For a more detailed comparision between them, see Fig. 3. Near the classical turning point of the oscillator, e.g., $x = \pm 3$ at t = 0, the WKB approximation deviates remarkably from the exact one like the standard harmonic oscillator. In conclusion, we plan to investigate interference and overlap in phase space Wigner pseudoprobabilities (Schleich, Walls, and Wheeler, 1998) for the time-dependent harmonic oscillator in the near future by using the result of this paper.

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