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Time evolution of an atomic system in the presence of a time dependent electric field

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Abstract

In this work we analyze the time evolution of an atomic system in the presence of an electromagnetic field. The interaction between the field and the system is modeled within the dipole approximation. As a zero approximation we first model the system with a harmonic oscillator and consider the field as classical. As is well known, in this case the quantal result is identical with the classical one. Then we model the system with a Morse oscillator which we expand keeping up to fourth order terms in the displacement coordinate. We compare the response of the system for different depths of the potential and different intensities of the field.

Key words: Harmonic oscillator; Lie algebra; Morse oscillator.

Evolución temporal de un sistema atómico en la presencia de un campo eléctrico dependiente del tiempo

Resumen

En este trabajo analizamos la evolución temporal de un sistema atómico en la presencia de un campo electromagnético. La interacción entre el campo y el sistema es modelada de acuerdo a la aproximación dipolar. Como aproximación cero, modelamos primero el sistema como un oscilador armónico y consideramos el campo como clásico. Tal como es conocido, en este caso el resultado cuántico es idéntico con el resultado clásico. Luego, modelamos el sistema como un oscilador de Morse el cual desarrollamos hasta el término de cuarto orden en la coordenada de desplazamiento. Comparamos la respuesta del sistema para diferentes tipos de potencial y distintas intensidades del campo.

Palabras clave: Algebras de Lie; oscilador armónico; oscilador de Morse.

Introduction

Laser cooling has been the subject of much theoretical and experimental work because it provides a method to reduce first and second order Doppler shifts in ultra high resolution spectroscopy and also because it allows for the possibility of controlling the positions and velocities of a collection of atomic particles to within the limits imposed by quantum fluctuations (1). The method of laser cooling can be applied to reduce the temperature of a gas of neutral at-

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oms as well as to ions bound in an electromagnetic trap with near resonant laser radiation (2). Using this technique, it was possible to cool a single trapped ion into its quantum ground state of motion for approximately 95% of the time (3). Not long ago, the experimental generation of a Schrödinger cat-like state of matter at the single atom level was reported (4).

In order to create this non classical state of the harmonic oscillator they first laser-cool the ion to the quantum ground state of motion and then coherently manipulate its internal (electronic) and external (motional) state by applying pairs of off resonant laser beams which drive two-photon stimulated Raman transitions. As pointed out by Zurek (5) a macroscopic superposition of the form of a Schrödinger cat state decays to a statistical mixture on a short time scale (decoherence time) which is related to the size of the cat and is much faster than the energy dissipation time, this provides an explanation for the absence of superpositions in the macroscopic world. A numerical study of the experiment studying the importance of nonlinearities of the electromagnetic field, and its effects in the temporal evolution of this non classical state is under way and will be presented elsewhere (6). Here we analyze the temporal evolution of an atomic system modeled via harmonic and anharmonic oscillators interacting with an electromagnetic field using algebraic techniques.

Harmonic Oscillator

Let us start by considering the Hamiltonian

$$H = H_0 + V(t) = H_0 - exE(t) \quad [1]$$

with H_0 the unperturbed Hamiltonian $H_0 = p^2/2m + m\omega_0^2 x^2/2$, where x is the displacement from the equilibrium position, e is the electric charge and $E(t)$ is the external, classical electric field, given by $E(t) = E_0 \cos(\omega t)$. Expressing the displacement coordinate and the momentum in terms of the creation and annihilation operators $a^\dagger$, a, we obtain:

$$H = \hbar\omega_0\left(a^\dagger a + 1/2\right) - e\sqrt{\frac{\hbar}{2m\omega_0}}\,E_0 \cos(\omega t)(a + a^\dagger) \quad [2]$$

In order to study the temporal evolution of the system, it is convenient to transform into the interaction picture where the free evolution has been frozen. Schrödinger's equation in the interaction picture takes the form

$$i\hbar\partial_t U_I = H_I U_I, \text{ with } U_I(t_0, t_0) = 1 \quad [3]$$

where the Hamiltonian H_I is given by $H_I(t) = U_0^+ V U_0$ with U_0 being the time evolution operator corresponding to the unperturbed Hamiltonian. In this simple case, it is given by:

$$U_0(t, t_0) = e^{-i\omega_0(t-t_0)(a^\dagger a + 1/2)} \quad [4]$$

In the interaction picture, the creation and annihilation operators are

$a_I(t) = U_0^\dagger a U_0 = a e^{-i\omega_0 t}$, and $a_I^\dagger(t) = U_0^\dagger a^\dagger U_0 = a^\dagger e^{i\omega_0 t}$

so that, the interaction picture Hamiltonian takes the form (7)

$$\begin{aligned} H_I(t) &= -e\sqrt{\frac{\hbar}{2m\omega_0}}\,E_0 \cos(\omega t)\left(a e^{-i\omega_0 t} + a^\dagger e^{i\omega_0 t}\right) \\ &= f_1(t) a^\dagger + f_1^*(t) a \end{aligned} \quad [5]$$

Since this a linear combination of operators which form a finite Lie algebra, the time evolution operator can be written as a product of exponentials (8,9)

$$U_I(t, t_0) = e^{-\alpha_2 a^\dagger} e^{-\alpha_2 a} e^{-\alpha_3} \quad [6]$$

with unknown, complex, time dependent functions α_i. Substitution of Equation [6] into Equation [3] yields the following set of first order differential equations:

$$\alpha_1 = \frac{i}{\hbar} f_1 \quad [7]$$

$$\alpha_2 = \frac{i}{\hbar} f_1^* \quad [8]$$

$$\alpha_3 = -\frac{i}{\hbar} \alpha_1 f_1^* \quad [9]$$

Due to the simple form of the function $f_1(t)$, these can be integrated obtaining:

$$\alpha_1(t) = - \frac{\hbar}{2m\omega_0} \frac{e^{i\omega_0 t} eE_0}{2\hbar} \left(\frac{e^{i\omega t}}{\omega + \omega_0} - \frac{e^{-i\omega t}}{\omega - \omega_0} \right) \quad [10]$$

$$\alpha_2(t) = - \frac{\hbar}{2m\omega_0} \frac{e^{-i\omega_0 t} eE_0}{2\hbar} \left(\frac{e^{i\omega t}}{\omega - \omega_0} - \frac{e^{-i\omega t}}{\omega + \omega_0} \right) \quad [11]$$

Once we have the explicit form of the time evolution operator, we can evaluate the temporal evolution of a given observable through its matrix elements, that is:

$$O(t) = U_I^\dagger U_0^\dagger O U_0 U_I \quad [12]$$

Using Equations [4] and [6], the operators a and $a^\dagger$ transform according to:

$$\tilde{a}(t) = U_I^\dagger U_0^\dagger a U_0 U_I = e^{-i\omega_0 t}(a - \alpha_1) \quad [13]$$

$$\tilde{a}^\dagger(t) = U_I^\dagger U_0^\dagger a^\dagger U_0 U_I = e^{i\omega_0 t}(a^\dagger + \alpha_2) \quad [14]$$

so that, the temporal evolution of the dipolar moment of the system is:

$$\begin{aligned} n \mid ex(t) \mid n &= -e \frac{\hbar}{2m\omega_0} \left(\alpha_1 e^{-i\omega_0 t} - \alpha_2 e^{i\omega_0 t}\right) \\ &= \frac{e^2/m}{\omega_0^2 - \omega^2} E(t) \end{aligned} \quad [15]$$

where we have used Equations [10] and [11] and we see that the linear polarizability of the system (harmonic oscillator) coincides with the classical result

$$\alpha(\omega) = \frac{e^2/m}{\omega_0^2 - \omega^2} \quad [16]$$

We can also evaluate the temporal evolution of the momentum:

$$\begin{aligned} n \mid p \mid n &= -i \frac{\hbar m\omega_0}{2} \left(\alpha_1 e^{-i\omega_0 t} + \alpha_2 e^{i\omega_0 t}\right) \\ &= eE_0 \left(\frac{\omega}{\omega_0^2 - \omega^2} \right) \sin(\omega t) \end{aligned} \quad [17]$$

and of the dispersions in the displacement and the momentum operators:

$$\Delta x = x^2 - x^2 \text{ and } \Delta p = p^2 - p^2$$

For example, the squared of the displacement operator is given by:

$$\begin{aligned} n \mid x^2 \mid n = \frac{\hbar}{2m_0} &\left(e^{-2i\omega_0 t}\alpha_1^2 + 2n + 1 \right. \\ &\left. - 2\alpha_1\alpha_2 + e^{2i\omega_0 t}\alpha_2^2\right) \end{aligned} \quad [18]$$

In a similar form we can construct the expression for the square of the momentum operator, the result obtained for the ground state of the oscillator

$$\Delta x = \frac{\hbar}{2m\omega_0} \quad [19]$$

$$\text{and } \Delta p = \frac{\hbar m\omega_0}{2} \quad [20]$$

so that the ground state is a minimum uncertainty state at all times.

Anharmonic Oscillator

Consider now a quartic oscillator given by the following expression:

$$H_0 = \frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 x^2 + \lambda x^4 \quad [21]$$

where λ is an annharmonicity parameter with units of energy/distance^4. First we introduce creation-annihilation operators defined in the usual form and the unperturbed Hamiltonian takes the form:

$$H_0(a, a^+) = \tilde{H}_0(a, a^+) + H_0^{ho}(a, a^+) \quad [22]$$

where

$$\tilde{H}_0(a,a^\dagger) = \hbar\omega_0\left(a^\dagger a + 1/2\right) + 6\lambda\left(\frac{\hbar}{2m\omega_0}\right)^2 \left(a^{\dagger^2} + a^2 + 2a^\dagger a + 1/2\right)$$

$$H_0^{ho}(a,a^\dagger) = \lambda\left(\frac{\hbar}{2m\omega_0}\right)^2 \left(a^4 + 4a^\dagger a^3 + 6a^{\dagger^2}a^2 + 4a^{\dagger^3}a + a^{\dagger^3}\right)$$

notice that we have separated the contribution which arises from the quartic (q) term and we have written it as a sum of two terms, the first one being a bilinear form and the second one containing higher order terms. If we approximate the unperturbed Hamiltonian and neglect the part containing terms higher than quadratic we get

$$H_0(a,a^\dagger) \approx \tilde{H}_0(a,a^\dagger) \quad [23]$$

We now introduce a Bogoliubov transformation (10), which defines operators b and $b^\dagger$ through:

$$b = t_1 a + t_2 a^\dagger \quad [24]$$

$$b^\dagger = t_1 a^\dagger + t_2 a \quad [25]$$

with real transformation coefficients t_i. For the transformation to be unitary the commutation relation must be preserved:

$$\left[a^\dagger, a\right] = \left[b^\dagger, b\right] = 1$$

and we thus obtain the condition

$$t_1^2 - t_2^2 = 1 \quad [26]$$

To single out the transformation coefficients we impose the condition that the Hamiltonian in the new variables must have the form of a displaced harmonic oscillator

$$H_0(b,b^\dagger) = \hbar\Omega b^\dagger b + \Delta E \quad [27]$$

where Ω is an effective frequency and ΔE gives an estimate of the ground state energy. Using the inverse of the transformation equations [24], [25] and substituting into Equation [23], we obtain a set of algebraic equations whose solutions yield:

$$\Omega = \omega_0(t_1 + t_2)^2,$$

$$\Delta E = \frac{\hbar\omega_0}{2}\left(1 + \frac{1}{N}\left(1 - 4t_2(t_1 - t_2)\right) + 2t_2^2\right) \quad [28]$$

$$\text{with } t_2^2 = \frac{\left[-1 + \left(1 + 2/N\right)^{1/2}\right]}{2}$$

$$\text{and } N = 6\lambda\left(\frac{\hbar}{2m\omega_0}\right)^{-2} \hbar\omega_0 \quad [29]$$

Notice that when $\lambda \to 0$, $t_1 \to 1$ and $t_2 \to 0$. Writing the interaction in terms of operators $b^\dagger$ and b, we obtain the following effective Hamiltonian:

$$H(b,b^\dagger) = \hbar\Omega b^\dagger b + \Delta E + \left(f_1 t_1 - f_1^* t_2\right)b^\dagger + \left(f_1^* t_1 - f_1 t_2\right)b$$

$$= \hbar\Omega b^\dagger b + \Delta E + g(t)b^\dagger + g^*(t)b \quad [30]$$

with the function $f_1(t)$ defined in Equation [5]. In analogy with the previous case, we go into the interaction picture where the Hamiltonian takes the form:

$$H_I(t) = g(t)b^\dagger e^{i\Omega t} + g^*(t)be^{-i\Omega t} \quad [31]$$

Since the set of operators appearing in Equation [31] forms a finite Lie algebra, the time evolution operator can be written as a product of exponentials with unknown complex functions β_i (see Equation [6] which fulfill equations similar to Equations [7-9] with $g(t)$ instead of $f_1(t)$.

In order to study the temporal evolution of the displacement and the momentum operators, we first transform the operators b and $b^\dagger$

$$b = U_I^\dagger U_0^\dagger b U_0 U_I = e^{-i\Omega t}(b - \beta_1) \quad [32]$$

$$b^\dagger = U_I^\dagger U_0^\dagger b^\dagger U_0 U_I = e^{i\Omega t}(b^\dagger + \beta_2) \quad [33]$$

Expressing the displacement operator in terms of these, we obtain:

$$n \mid x \mid n = \frac{\hbar}{2m\omega_0} (t_1 - t_2)\left(e^{i\Omega t}\beta_2 - e^{-i\Omega t}\beta_1\right) \quad [34]$$

$$n \mid p \mid n = i \frac{\hbar m\omega_0}{2} (t_1 + t_2)\left(e^{i\Omega t}\beta_2 + e^{-i\Omega t}\beta_1\right) \quad [35]$$

and

$$n \mid x^2 \mid n = \frac{\hbar}{2m\omega_0} \left[(t_1 - t_2)^2\left(2n + \left(e^{-i\Omega t}\beta_1 - e^{i\Omega t}\beta_2\right)^2\right) - 2t_2(t_1 - t_2) + 1\right] \quad [36]$$

$$n \mid p^2 \mid n = -\frac{\hbar m\omega_0}{2} \left[(t_1 + t_2)^2\left(-2n + \left(e^{-i\Omega t}\beta_1 + e^{i\Omega t}\beta_2\right)^2\right) - 2t_2(t_1 + t_2) - 1\right] \quad [37]$$

from the above equations we find the dispersions in the two quadratures to be:

$$(\Delta x)^2 = \frac{\hbar}{2m\omega_0} \left[2n(t_1 - t_2)^2 - 2t_2(t_1 - t_2) + 1\right] \quad [38]$$

$$(\Delta p)^2 = \frac{\hbar m\omega_0}{2} \left[2n(t_1 + t_2)^2 + 2t_2(t_1 + t_2) - 1\right] \quad [39]$$

finally:

$$\Delta x \Delta p = \left(\frac{\hbar}{2}\right)\left(1 + 8t_2^2\right)^{1/2} \quad [40]$$

and we see that the ground state of the anharmonic oscillator is no longer a minimum uncertainty state. If the anharmonicity parameter λ is time dependent, the transformation coefficients t_1 and t_2, and the effective frequency Ω also become time dependent and the effective Hamiltonian becomes that of a linearly driven parametric harmonic oscillator with the possibility of squeezing (11).

In order to evaluate the evolution of the transition and permanency probabilities we have to calculate the matrix elements of the time evolution operator in the interaction picture. This can be accomplished in the harmonic and the anharmonic cases using the fact that the operator U_I has the form of a product of exponentials. Consider first the matrix element

$$A_{n,n'} = n' \mid U_I \mid n = n' \mid e^{-\delta_1 c^\dagger} e^{-\delta_2 c} e^{-\delta_3 I} \mid n \quad [41]$$

where I is the identity operator and where the functions δ are used instead of either α or β and the operators and c, $c^\dagger$ are used to designate a, $a^\dagger$ or b, $b^\dagger$. The matrix element can be calculated as follows:

$$A_{n',n} = e^{-\delta_3} \sum_m < n' \mid e^{-\delta_1 c^\dagger} \mid m > < m \mid e^{-\delta_2 c} \mid n > [42]$$

each one of the matrix elements in the summation give:

$$< n' \mid e^{-\delta_1 c^\dagger} \mid m > = \sum_p \frac{(-\delta_1)^p}{p!} \sqrt{\frac{(m+p)!}{m!}} < n' \mid m + p > [43]$$

$$< m \mid e^{-\delta_2 c} \mid n > = \sum_{q=0} \frac{(-\delta_2)^q}{q!} \sqrt{\frac{n!}{(n-q)!}} < m \mid n - q > [44]$$

so that when the summations over m and p are done one is left with a finite summation over q where the maximum number of terms is n. Taking the absolute value squared we obtain the transition probabilities $P_{n,n'}$ +:

$$P_{n,n'} = \mid A_{n,n'} \mid^2 = \left| \sqrt{n!n'!} e^{-\delta_3} \sum_{q=0}^{n} \frac{(-\delta_1)^{n'-n+q}(-\delta_2)^q}{(n'-n+q)!q!(n-q)!} \right|^2 \quad [45]$$

Numerical Results

In order to set the parameters defining the oscillator we used those given by Clark and Dickinson (12) in their calculation of transition probabilities in collinear collisions between an atom and a diatom which was modeled through harmonic and Morse oscillators.

In Figure 1 we show the time evolution of the displacement operator for a harmonic oscillator and an anharmonic one. The frequency of the harmonic oscillator is $\omega_0 = 8.05 \times 10^{14}$ / *sec*, the effective frequency $\Omega = 22.57 \times 10^{14}$ / *sec*, the external electric field frequency is $\omega = 9.585 \times 10^{14}$ / *sec* and the anharmonicity parameter $\lambda = 8.44$. The units of time are 10^{-14} sec., and those of the displacement are Å. Notice that the effect of the anharmonicity is manifested by a shortening of the amplitude of the oscillation and the appearance of a secondary frequency giving rise to a beating phenomena. In Figure 2 we also show the average value of the displacement operator (for the anharmonic case) with the same set of parameters describing the atomic system but with a field intensity twice and three times that of Figure 1. The amplitude of the oscillation is increased and the beating behavior is maintained.

In Figure 3 we show the transition probabilities $P_{1,0}$ and $P_{1,2}$ for de-excitation from the first excited state to the ground

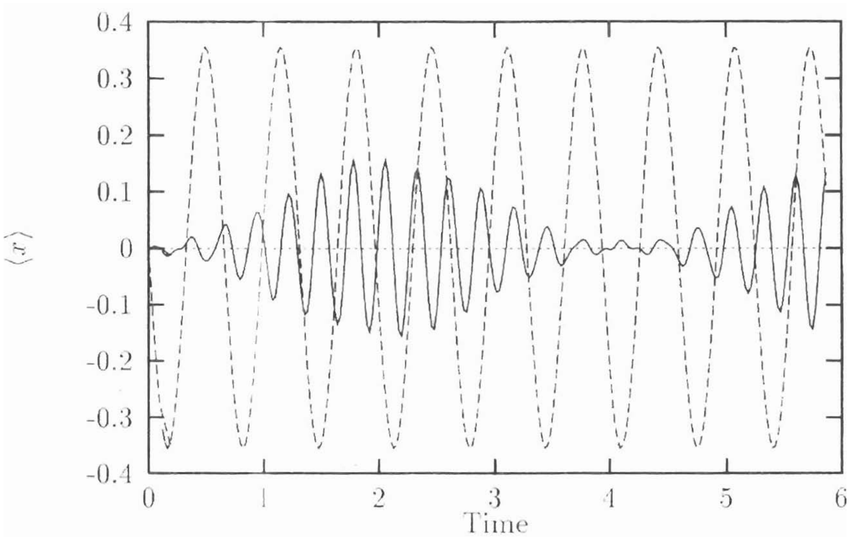

Figure 1. Average value of the displacement operator as a function of time. The dotted line corresponds to the harmonic case; the continuous line to the anharmonic case.

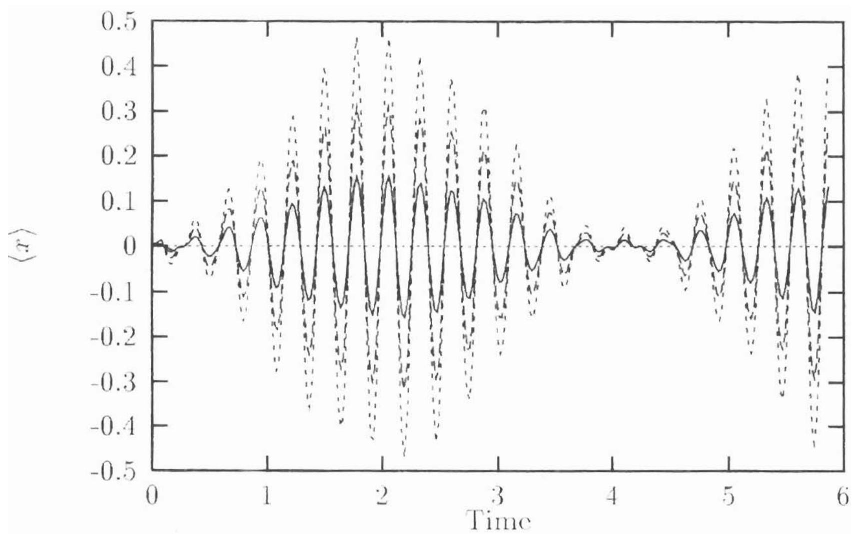

Figure 2. Average value of the displacement operator as a function of time for a anharmonic oscillator and several values of the field intensity. The largest amplitude corresponds to $E_3 = 3E_0$, the next to $E_2 = 2E_0$, and the smallest to $E_0 = 1$.

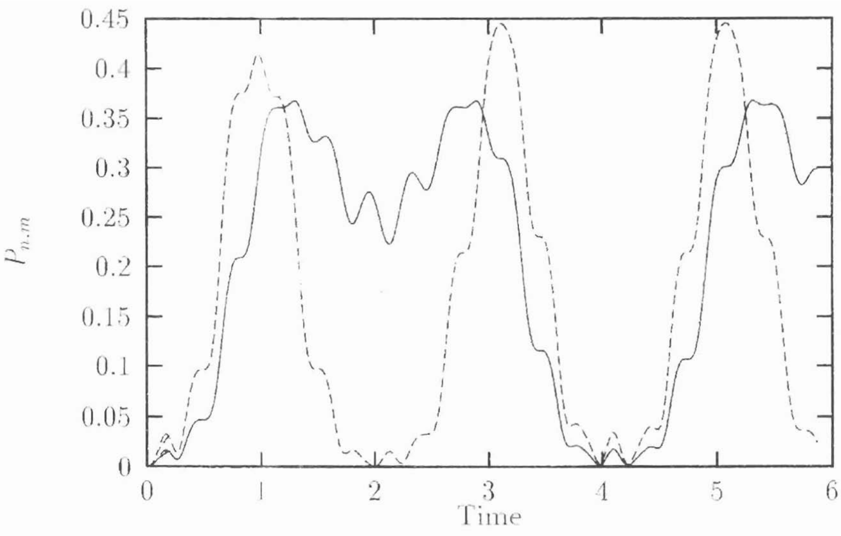

Figure 3. Transition probabilities $P_{1,0}$ (full line) and $P_{1,2}$ (dotted line) for the anharmonic oscillator as a function of time. The effective frequency of the oscillator is $\Omega = 22.96$ and the field frequency is $\omega = 9.58$.

state and excitation from the first excited state to the second excited state as a function of time for a system characterized by the same set of parameters as the one used in the previous figure. We can see a semi periodic behavior for both with marked differences. The (1-0) transitions, first increases as the system interacts with the field until it gets to a maximum value, then it starts to decrease and after a short time (when $t \approx 2$) it starts to increase again reaching a value near the previous maximum and then it decreases again but this time it attains a value a practically zero (at $t \approx 4$), after that the cycle starts again. On the other hand, the (1-2) transition follows a similar conduct as the previous one with the difference that when the (1-0) transition gets to a local minima (when $t \approx 2$) the (1-2) transition becomes almost zero, then the (1-2) transition increases to a maximum value and decreases again to a zero when $t \approx 4$.

Conclusions

In this work we have presented an algebraic method which allows us to construct an approximation for the time evolution operator of a anharmonic oscillator forced by an external classical field. The method relies in the fact that when the Hamiltonian can be written as a linear combination of operators which form a finite Lie algebra, the corresponding time evolution operator can be expressed as a product of exponentials. Using this fact, the temporal evolution of physical observables like the position and momentum can be evaluated. It is also possible to obtain an explicit expression for the permanency and transition probabilities. The method can be applied to the case of a parametric oscillator since its validity depends only upon the algebraic properties of the Hamiltonian.

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