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Exact quantum motion of a particle trapped by oscillating fields

I A Pedrosa[1], **Alexandre Rosas**[1] **and I Guedes**[2]

[1] Departamento de Física, CCEN, Universidade Federal da Paraíba, Caixa Postal 5008, 58051-970, João Pessoa, PB, Brazil
[2] Departamento de Física, Universidade Federal do Ceará, Caixa Postal 6030, 60451-970, Fortaleza, CE, Brazil

E-mail: iapedrosa@fisica.ufpb.br, arosas@fisica.ufpb.br and guedes@fisica.ufc.br

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Abstract
The exact wavefunctions for a particle trapped by oscillating fields are obtained in terms of Mathieu functions with the help of linear invariants and the dynamical invariant method. In addition, we construct Gaussian wave packet solutions and calculate the quantum fluctuations in the coordinate and momentum as well as the quantum correlations between coordinate and momentum.

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In the last few decades, the study of the quantum motion in a Paul trap has attracted a lot of attention in the literature [1–15]. The Paul trap is an important device to confine charged and neutral particles for the ultimate purpose of high resolution spectroscopy and its application to the measurement of time. Since it was reviewed by Paul in his Nobel Prize lecture [2], there has been an increasing interest in its application and mechanism. In particular, the problem of deriving the explicitly time-dependent wavefunctions for a particle in a Paul trap has been considered by some authors who have used different methods such as unitary transformations [4], Lie algebra technique [9] and trial function method [1, 10] to achieve their goals.

In this article, we take advantage of linear invariants and the dynamical invariant operator methods, devised by Lewis and Riesenfeld [16], to obtain the exact time-dependent Schrödinger wavefunctions for a particle trapped by oscillating fields. These wavefunctions are written in terms of the solution of the Mathieu–Hill equation, the Mathieu functions [17, 18]. In addition, we construct Gaussian wave packet solutions and calculate the quantum fluctuations in coordinate and momentum and the quantum correlations between coordinate and momentum.

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We model the particle in a Paul trap as a one-dimensional time-dependent harmonic oscillator described by the Hamiltonian [1–5]

$$H(t) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2(t)q^2, \tag{1}$$

where $\omega^2(t) = k\cos^2\Omega t$, Ω being the driving frequency of the external field and k a measure of its strength. To investigate the quantum motion of this system, we must solve the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(q,t)}{\partial q^2} + \frac{1}{2}m\omega^2(t)q^2\psi(q,t) = \mathrm{i}\hbar\frac{\partial\psi(q,t)}{\partial t}. \tag{2}$$

According to the invariant operator formulation [16], a solution of the Schrödinger equation (2) is found if a nontrivial Hermitian operator $I(t)$ exists and satisfies the equation

$$\frac{\mathrm{d}I}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}[I, H] + \frac{\partial I}{\partial t} = 0. \tag{3}$$

The condition above allows one to write the solutions of the time-dependent Schrödinger equation (2) as

$$\psi_\lambda(q,t) = \mathrm{e}^{\mathrm{i}\mu_\lambda(t)}\phi_\lambda(q,t), \tag{4}$$

where $\phi_\lambda(q,t)$ is an eigenfunction of $I(t)$ with time-independent eigenvalue λ and $\mu_\lambda(t)$ is a phase function that satisfies the equation

$$\hbar\frac{\mathrm{d}\mu_\lambda(t)}{\mathrm{d}t} = \langle\phi_\lambda|\left(\mathrm{i}\hbar\frac{\partial}{\partial t} - H(t)\right)|\phi_\lambda\rangle. \tag{5}$$

Hence, in order to find such an operator, we consider a Hermitian linear invariant of the form

$$I(t) = \alpha(t)q + \beta(t)p + \gamma(t), \tag{6}$$

where $\alpha(t)$, $\beta(t)$ and $\gamma(t)$ are time-dependent real functions to be determined. Thus, requiring that $I(t)$ obeys (3) we get

$$\dot{\alpha}(t) = m\omega^2(t)\beta(t), \tag{7}$$

$$\dot{\beta}(t) = -\frac{\alpha(t)}{m}, \tag{8}$$

$$\dot{\gamma}(t) = 0. \tag{9}$$

From equations (7) and (8) we find that $\beta(t)$ must obey the Mathieu–Hill equation

$$\ddot{\beta}(t) + \omega^2(t)\beta(t) = 0. \tag{10}$$

As we will discuss later, the solutions of this equation are Mathieu functions. Once $\beta(t)$ is known, $\alpha(t)$ is directly obtained from equation (8). Therefore, the linear invariant can be written as

$$I(t) = \beta(t)p - m\dot{\beta}(t)q, \tag{11}$$

where without loss of generality we set $\gamma(t) = \text{const} = 0$. Moreover, the eigenstates $|\phi_\lambda\rangle$ of $I(t)$ form a continuous complete set whose time-independent eigenvalues λ are solutions of the equation [16, 19–21]

$$I(t)\phi_\lambda(q,t) = \lambda\phi_\lambda(q,t), \tag{12}$$

with

$$\langle\phi_\lambda|\phi_{\lambda'}\rangle = \delta(\lambda - \lambda'). \tag{13}$$

It is easy to verify that the eigenstates of $I(t)$ are of the form

$$\phi_\lambda(q,t) = \left(\frac{1}{2\pi\hbar\beta(t)}\right)^{1/2} \exp\left[\frac{\mathrm{i}m\dot{\beta}(t)}{2\hbar\beta}q^2 + \frac{\mathrm{i}\lambda}{\hbar\beta(t)}q\right]. \tag{14}$$

On the other hand, after a straightforward calculation of the matrix element of equation (5), the phase functions are found to be

$$\mu_\lambda(t) = -\frac{\lambda^2}{2m\hbar}\int_0^t \frac{1}{\beta^2(t')}\,\mathrm{d}t'. \tag{15}$$

Therefore, the solutions of the Schrödinger equation (2) are given by

$$\psi_\lambda(q,t) = \left(\frac{1}{2\pi\hbar\beta(t)}\right)^{1/2} \exp\left[\mathrm{i}\mu_\lambda(t) + \frac{\mathrm{i}m\dot{\beta}(t)}{2\hbar\beta(t)}q^2 + \frac{\mathrm{i}\lambda}{\hbar\beta(t)}q\right]. \tag{16}$$

It is worth mentioning that other authors [20–29] have employed linear and quadratic invariants to study quantum time-dependent systems described by the Hamiltonian (1). Furthermore, the relationship between the linear invariant (11) and the well-known quadratic Ermakov–Lewis invariant related to the Hamiltonian (1) and the corresponding eigenstates is discussed in [30].

In order to completely determine the solutions (16), let us return to the Mathieu–Hill equation (10), whose general solution with $\omega^2(t) = k\cos^2(\Omega t)$ is [17, 18]

$$\beta(t) = AC\left(\frac{k}{2\Omega^2}, -\frac{k}{4\Omega^2}, \Omega t\right) + BS\left(\frac{k}{2\Omega^2}, -\frac{k}{4\Omega^2}, \Omega t\right), \tag{17}$$

where A and B are constants to be determined by the initial condition and C and S are, respectively, the even and odd Mathieu functions. It is worth noticing that when $\beta(t)$ vanishes the phase function $\mu_\lambda(t)$ diverges. In spite of this divergence, one can prove that the wavefunctions (16) are always finite as follows. For all times, $f_\lambda(t) \equiv \mu_\lambda(t)\beta(t)$ must be finite so that, from equation (15), we find that

$$\dot{f}_\lambda\beta - f_\lambda\dot{\beta} = -\frac{\lambda^2}{2m\hbar}. \tag{18}$$

Hence, since the leftmost term in this equation must vanish when $\mu_\lambda(t)$ diverges, the wavefunctions (16) may be rewritten in terms of $f_\lambda(t)$ (which is finite) instead of $\mu_\lambda(t)$. For a more detailed discussion, the reader may refer to [31]. Furthermore, the evolution of a general Schrödinger state can be written as

$$\psi(q,t) = \int_{-\infty}^{\infty} g(\lambda)\psi_\lambda(q,t)\,\mathrm{d}\lambda, \tag{19}$$

where $g(\lambda)$ is an arbitrary amplitude constant in time. In what follows we intend to construct Gaussian wave packet solutions of equation (2). In doing so, we write $g(\lambda)$ as

$$g(\lambda) = \frac{\sqrt{a}}{(2\pi)^{1/4}}\,\mathrm{e}^{-\frac{a^2}{4}\lambda^2}, \tag{20}$$

where a is a positive real constant. Hence, substituting equations (16) and (20) into equation (19) and performing the integral, we arrive at

$$\psi(q,t) = \left(\frac{2}{\pi}\right)^{1/4} \frac{\exp\left(-\frac{\mathrm{i}m\dot{\beta}(t)}{2\hbar\beta(t)}q^2\right)}{(\hbar a\beta(t))^{1/2}\left(1+\frac{2\mathrm{i}f(t)}{m\hbar a^2}\right)^{1/2}} \exp\left[-\frac{q^2}{\hbar^2a^2\beta^2(t)\left(1+\frac{2\mathrm{i}f(t)}{m\hbar a^2}\right)}\right], \tag{21}$$

where $f(t)$ is given by

$$f(t) = \int_0^t \frac{1}{\beta^2(t')}\,\mathrm{d}t'. \tag{22}$$

Moreover, the time-dependent probability density associated with the initial Gaussian wave packet (21) is Gaussian for all times

$$\rho(q,t) = |\psi(q,t)|^2 = \frac{1}{\sqrt{\pi}\sigma(t)}\,\mathrm{e}^{-\frac{q^2}{\sigma^2(t)}}, \tag{23}$$

with a time-dependent width

$$\sigma(t) = \sqrt{\frac{\hbar^2 a^2 \beta^2(t)}{2}\left(1 + \frac{4f^2(t)}{m^2\hbar^2 a^4}\right)}. \tag{24}$$

Therefore, the centre of the packet remains at $q = 0$ while its width changes in time, consistent with very general expectations for the oscillator case [32–34]. Furthermore, it is readily verified that the wavefunction (21) is normalized and the time-dependent probability density is conserved, i.e.,

$$\int_{-\infty}^{\infty} |\psi(q,t)|^2\,\mathrm{d}q = 1. \tag{25}$$

Next, we evaluate the quantum coordinate and momentum fluctuations in the state $\psi(q,t)$. After some algebra, these fluctuations are found to be

$$\begin{aligned}\Delta q &= \sqrt{\langle q^2\rangle - \langle q\rangle^2} = \frac{1}{2\sqrt{U(t)}},\\ \Delta p &= \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \hbar\frac{\sqrt{U^2(t)+V^2(t)}}{\sqrt{U(t)}},\end{aligned} \tag{26}$$

where we have defined

$$U(t) = \frac{1}{\hbar^2 a^2\beta^2(t)\left(1 + \frac{4f^2(t)}{m^2\hbar^2 a^4}\right)}, \tag{27}$$

$$V(t) = \frac{m\dot{\beta}(t)}{2\hbar\beta(t)} + \frac{2f(t)}{m\hbar^3 a^4\beta^2(t)\left(1 + \frac{4f^2(t)}{m^2\hbar^2 a^4}\right)}. \tag{28}$$

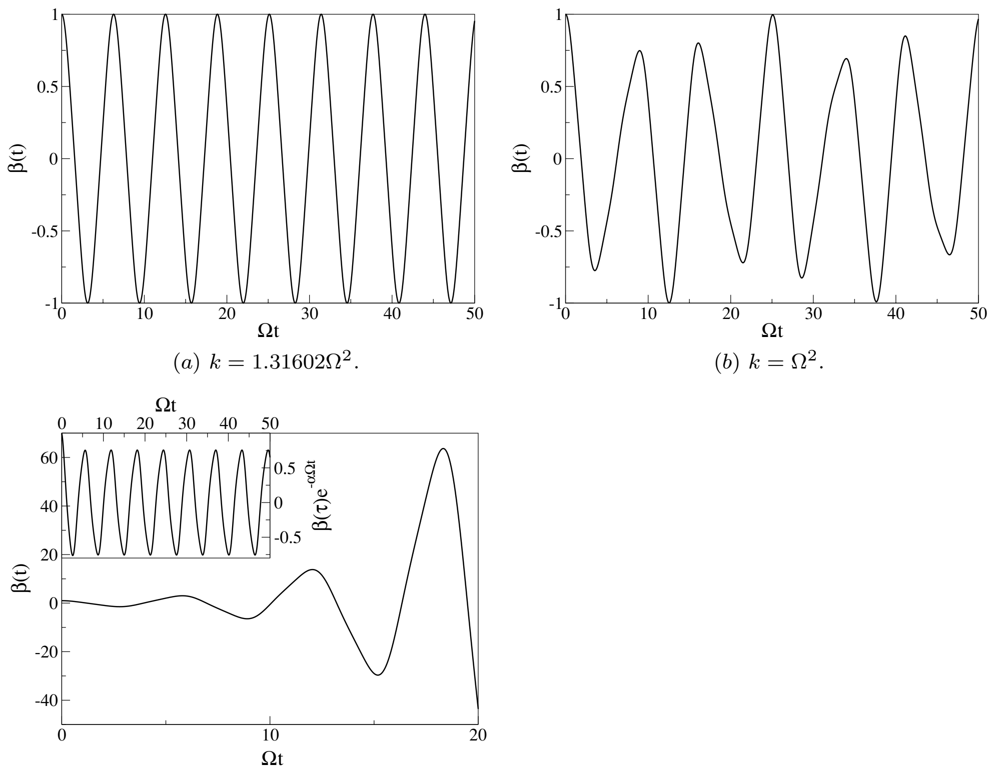
Thus, the uncertainty product takes the form

$$\begin{aligned}\Delta q\Delta p &= \frac{\hbar}{2}\sqrt{1 + \left(\frac{V}{U}\right)^2}\\ &= \frac{\hbar}{2}\sqrt{1 + \left[\frac{m\dot{\beta}(t)}{2\hbar\beta(t)} + \frac{2f(t)}{m\hbar^3a^4\beta^2(t)\left(1 + \frac{4f^2(t)}{m^2\hbar^2a^4}\right)}\right]^2\left(1 + \frac{4f^2(t)}{m^2\hbar^2a^4}\right)^2\hbar^4a^4\beta^4(t)}.\end{aligned} \tag{29}$$

If we require that the minimum uncertainty is $\hbar/2$ for a given time t, then we must have

$$\dot{\beta}(t) = -\frac{4f(t)}{\beta(t)(m^2\hbar^2a^4 + 4f^2(t))}. \tag{30}$$

For $t = 0$, this condition is obviously reduced to $\dot{\beta}(0) = 0$ (note that by definition $f(0) = 0$). On the other hand, the value of $\beta(0)$ is connected to the initial width of the Gaussian packet (see equations (21) and (23)). These are the initial conditions necessary to find the constants A and B of equation (17). As expected, $\beta(t)$ is an oscillating function as shown in figure 1. Moreover, depending on the ratio $\frac{k}{\Omega^2}$, the solution may oscillate periodically (*a*), quasiperiodically (*b*) or inside an exponential growing envelope (*c*).



(a) $k = 1.31602\Omega^2$.

(b) $k = \Omega^2$.

(c) $k = 2\Omega^2$.

Figure 1. The solution of the Mathieu–Hill equation $\beta(t)$ for an initial Gaussian packet with minimum initial uncertainty and unitary width may be periodic (*a*), quasiperiodic (*b*) or grow exponentially (*c*). The inset of (*c*) shows that when the exponential factor $\mathrm{e}^{-\alpha\Omega t}$, with $\alpha = 0.243\,15$, is scaled out, $\beta(t)$ also oscillates. In all cases, we made $\beta(0) = 1$.

Finally, we consider the quantum correlations between coordinate and momentum which are defined as [35]

$$C_{1,1} = \frac{1}{2}\int \psi^*\left[q\left(-\mathrm{i}\hbar\frac{\partial}{\partial q}\right) + \left(-\mathrm{i}\hbar\frac{\partial}{\partial q}\right)q\right]\psi\,\mathrm{d}q - \left(\int \psi^* q\psi\,\mathrm{d}q\right)\left[\int \psi^*\left(-\mathrm{i}\hbar\frac{\partial}{\partial q}\right)\psi\,\mathrm{d}q\right]. \tag{31}$$

After a minor algebra using equations (21) and (31), we obtain

$$C_{1,1} = \frac{\hbar}{2}\frac{V(t)}{U(t)} = \frac{\hbar}{2}\left[\frac{m\dot{\beta}(t)}{2\hbar\beta(t)} + \frac{2f(t)}{m\hbar^3a^4\beta^2(t)\left(1+\frac{4f^2(t)}{m^2\hbar^2a^4}\right)}\right]\left(1+\frac{4f^2(t)}{m^2\hbar^2a^4}\right)\hbar^2a^2\beta^2(t). \tag{32}$$

From this expression, we can see that although there are no correlations at time $t = 0$, the system develops correlation as time goes by. What is more, the appearance of correlation comes with an increase in the uncertainty. In fact, the condition (30) implies that the correlation is null when the uncertainty is minimum. Conversely, whenever the correlation is null the uncertainty is minimum. In figure 2 we show the behaviours of the uncertainty and the correlation. From this figure, we can see not only that the uncertainty is minimum when the correlation is zero, but also that the maximum of the uncertainty corresponds to the

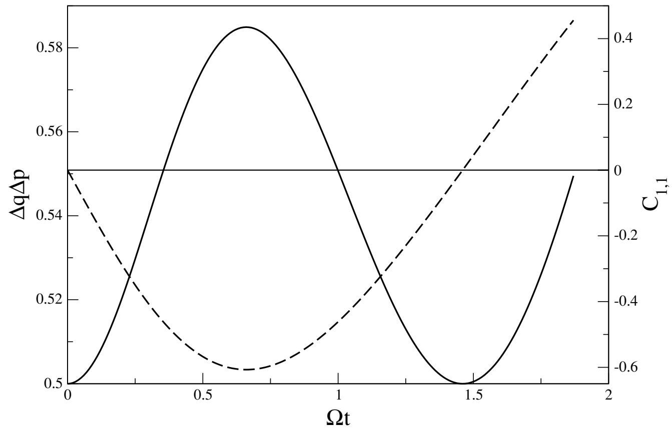


Figure 2. Uncertainty (solid line, left axis) and correlation (broken line, right axis) as a function of time. Once again we have set $k = \Omega^2$, $a = 1$, $\hbar = 1$ and $m = 1$, so that the minimum uncertainty is $1/2$ and occurs whenever the packet is uncorrelated.

minimum correlation. This striking relationship can be understood once the uncertainty can be written as a function of the correlation

$$\Delta q \Delta p = \frac{\hbar}{2}\sqrt{1 + \left(\frac{2}{\hbar}C_{1,1}\right)^2}. \tag{33}$$

In summary, in this short article we have combined linear invariants and the dynamical invariant method of Lewis and Riesenfeld [16] to derive the exact wavefunctions for a particle trapped by oscillating fields. These wavefunctions were completely determined and written in terms of Mathieu functions. In addition, we have constructed Gaussian wave packet solutions whose probability density, quantum fluctuations, correlation and uncertainty were calculated. Finally, we would like to point out that the results of this paper may be useful for the analysis of ion-cooling processes and quantum statistical effects in atomic ensembles at low temperatures, such as the Bose–Einstein condensation, since the quantum aspect of the Paul trap is essential for the analysis of these systems [1, 36].

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