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Quantum dynamics of a charged particle in a Penning trap

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Abstract. With the help of the exact classical path representation of the time dependent propagator the dynamics of a charged particle in a Penning trap in the presence of an additional classical, time-dependent electric field is investigated. In this way the connection between quantum and classical dynamics is exhibited in a clear way. The possibility of localizing a particle in the ground state of a Penning trap with unit probability by a suitably chosen electric field is discussed.

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The quantum dynamics of charged particles which are confined by external electromagnetic fields is a physical problem of current interest. Taking advantage of the fact that for Lagrangians which are at most quadratic in space and velocity variables the quantum dynamics can be constructed exactly from the knowledge of the corresponding classical dynamics [1, 2, 3, 4, 5] the time evolution of wave packets in an ideal Paul trap has been discussed recently in a series of papers [6, 7]. These one-dimensional studies show that this exact relation between classical and quantum dynamics offers the possibility of using the Paul trap in a simple way as a device for the preparation of various interesting experiments, for example for the well defined preparation of wave packets or the preparation of squeezed states of a charged particle [7]. Though this exact relation between quantum dynamics and classical dynamics also applies to the Penning trap [8] much less is known about the dynamics of wave packets in this case.

In this letter the quantum dynamics of a structureless charged particle in a Penning trap in the presence of an additional time dependent, classical electric field is discussed. Within the dipole approximation this problem is equivalent to the dynamics of a three-dimensional anisotropic harmonic oscillator whose equilibrium position varies with time. This implies that the exact path integral representation of the time dependent propagator of this problem can be constructed completely by a knowledge of the corresponding classical dynamics. With the help of this propagator the time evolution of an initially prepared Gaussian wave packet is studied. It is shown that in certain cases, by the application of a suitably chosen electric field in combination with a sudden change of the trap parameters, it is possible to localize a charged particle in the ground state of a Penning trap with unit probability. Furthermore, the use of the classical path integral representation of the propagator exhibits in a natural way the connection between the quantum dynamics of the charged particle in the Penning trap and its corresponding classical dynamics.

In the dipole approximation the Lagrangian which describes the classical dynamics of a structureless charged particle (mass M and charge q) in an ideal Penning trap (with magnetic field $\mathbf{B}=B\mathbf{e}_z$ and electric quadrupole field $V(x,y,z)=\Phi\times(2z^2-x^2-y^2)$ with $\Phi>0$) in the presence of an additional, time dependent classical electric field $\mathbf{E}(t)$ is given by

$$L(\dot{\mathbf{x}},\mathbf{x},t)=\frac{M}{2}\dot{\mathbf{x}}^2+\frac{1}{4}M\omega_z^2(x^2+y^2) -\tfrac{1}{2}M\omega_z^2z^2+\tfrac{1}{2}\omega_c L_z+q\mathbf{x}\cdot\mathbf{E}(t). \tag{1}$$

The z-component of the angular momentum is $L_z=xp_y-yp_x$ and the cyclotron and quadrupole-frequencies are $\omega_c=qB/(Mc)$ and $\omega_z=\sqrt{4\Phi/M}$. The corresponding modified cyclotron and magnetron frequencies are given by $\omega_+=\omega_c/2+\Omega$ and $\omega_-=\omega_c/2-\Omega$ with $\Omega=\sqrt{\omega_c^2/4-\omega_z^2/2}$. In terms of this Lagrangian the exact path integral representation of the propagator which describes the quantum mechanical time evolution of the charged particle is given by

$$G(\mathbf{x},t;\mathbf{x}_0,t_0)=\left[Det\left(\frac{i}{2\pi\hbar}\frac{\partial^2S}{\partial x^m\partial x_0^n}\right)\right]^{1/2}e^{iS(\mathbf{x},t;\mathbf{x}_0,t_0)/\hbar}. \tag{2}$$

It is completely determined by properties of the unique classical trajectory $\mathbf{x}_{cl}(t)$ which fulfills the classical equations of motion of the Lagrangian of (1) and which starts at position $\mathbf{x}_0$ at time t_0 and reaches position $\mathbf{x}$ at time t. Its classical action

$$S(\mathbf{x}, t; \mathbf{x}_0, t_o) = \int_{t_0}^{t} d\tau\, L(\dot{\mathbf{x}}_{cl}(\tau), \mathbf{x}_{cl}(\tau), \tau). \tag{3}$$

is a quadratic function of the variables $(\mathbf{x}-\mathbf{x}_0)$. An explicit expression for this classical action has been given by Papadopoulos and Jones [5]. From a knowledge of this propagator the time evolution of any initially prepared state $\psi(\mathbf{x}_0, t_0)$ of a charged particle in a Penning trap is determined by

$$\psi(\mathbf{x}, t) = \int d^3\mathbf{x}_0\, G(\mathbf{x}, t; \mathbf{x}_0, t_0)\, \psi(\mathbf{x}_0, t_0). \tag{4}$$

This expression shows that it is the quantum mechanical interference between the contributions of all classical trajectories which start from any initial point $\mathbf{x}_0$ at time t_0 and reach point $\mathbf{x}$ at time t which determines the wave function at point $\mathbf{x}$. In general, $\psi(\mathbf{x}, t)$ has to be determined from (4) by numerical integration. In the following we concentrate on the time evolution of initially prepared Gaussian wave packets of the form

$$\psi(\mathbf{x}_0, t_0) = (2\pi)^{-3/4}[Det(\sigma_0)]^{-1/2} e^{i\mathbf{p}_0\cdot\mathbf{x}/\hbar} \cdot e^{-(\mathbf{x}-\mathbf{x}_0)^T \sigma_0^{-2} (\mathbf{x}-\mathbf{x}_0)/4} \tag{5}$$

with the spatial variance matrix

$$\sigma_0^2 = \begin{pmatrix} \langle \Delta x^2 \rangle & \langle \Delta x \Delta y \rangle & 0 \\ \langle \Delta x \Delta y \rangle & \langle \Delta y^2 \rangle & 0 \\ 0 & 0 & \langle \Delta z^2 \rangle \end{pmatrix}.$$

For simplicity we restrict our following discussion to initial conditions without any correlations between the z and the x, y directions, i.e. $\langle \Delta x \Delta z \rangle = \langle \Delta y \Delta z \rangle = 0$. In this case the quadratic dependence of the classical action of (3) on the variables $(\mathbf{x}-\mathbf{x}_0)$ implies that (4) reduces to a Gaussian integral and can be evaluated easily. Thus we find for the time evolution of the probability density of the charged particle in the Penning trap

$$|\psi(\mathbf{x}, t)|^2 = (2\pi)^{-3/2}[Det(\sigma(t))]^{-1} \cdot e^{-(\mathbf{x}-\mathbf{x}_{cl}(t))^T \sigma(t)^{-2} (\mathbf{x}-\mathbf{x}_{cl}(t))/2} \tag{6}$$

with the time dependent spatial variance matrix

$$\sigma^2(t) = U(\sigma_0^2 \cos^2[\omega(t-t_0)] + r_0^4 \sigma_0^{-2} \sin^2[\omega(t-t_0)])\, U^T.$$

The orthogonal matrix U describes a rotation around the magnetic field z-axis with angle $\omega_c t/2$. The diagonal 3×3 matrices ω and r_0^2 are given by

$$\omega = \begin{pmatrix} \Omega & 0 & 0 \\ 0 & \Omega & 0 \\ 0 & 0 & \omega_z \end{pmatrix}$$

and

$$r_0^2 = \begin{pmatrix} \frac{\hbar}{2M\Omega} & 0 & 0 \\ 0 & \frac{\hbar}{2M\Omega} & 0 \\ 0 & 0 & \frac{\hbar}{2M\omega_z} \end{pmatrix}$$

and determine the characteristic frequencies and the spatial variances of the ground state of the Penning trap. Besides the rotation matrix U, the time dependent spatial variance matrix $\sigma^2(t)$ has the same form as for a driven forced three dimensional harmonic oscillator with frequency Ω in the x−y plane and with frequency ω_z in the z-direction. This can be understood easily, because the Lagrangian of (1) can be transformed into this problem by a rotation around the magnetic field axis with frequency $\omega_c/2$. The initial canonical momentum $\mathbf{p}_0$ is related to the initial velocity $\dot{\mathbf{x}}_0$ of a particle in the trap by $\mathbf{p}_0 = M\dot{\mathbf{x}}_0 + M\omega_c(-y_0\mathbf{e}_x + x_0\mathbf{e}_y)/2$.

Within the framework of the dipole approximation (6) implies that

(1) an initially prepared Gaussian state remains always Gaussian,
(2) the mean values $\mathbf{x}_{cl}(t)$ and $\mathbf{p}_{cl}(t)$ fulfill the classical equations of motion of the Lagrangian of (1) and
(3) the width of the Gaussian wave packet oscillates with time. These oscillations of the width are *independent* of the applied external electric field. They are a typical quantum phenomenon and arise from quantum mechanical interferences between probability amplitudes of the classical trajectories which contribute to $\psi(\mathbf{x}, t)$ according to (4) [7].

This special form of the time evolution of a Gaussian wave packet suggests a mechanism for localizing a charged particle in the ground state of a Penning trap with the help of a suitably chosen external (classical) electric field. The basic idea of this "coherent cooling mechanism" rests on the fact that according to the classical equations of motion which are derived from the Lagrangian of (1) for given initial values of position and velocity, $\mathbf{x}_0$ and $\dot{\mathbf{x}}_0$, we can always find an electric field which brings the particle to rest.

In Fig. 1a the time evolution of the mean position of a charged particle in the plane perpendicular to the magnetic field direction is shown. Its initial mean position and velocity are indicated by the cross and the arrow in Fig. 1a. The time evolution in the absence of the applied electric field is shown by the dashed curve. The applied electric field is circularly polarized and in resonance with the magnetron frequency, i.e.

$$\mathbf{E}(t) = (\mathcal{E}/\sqrt{2\pi}) \exp(-(t-t_p)^2/(2\tau^2)) \cdot [\mathbf{e}_x \cos(\omega_-(t-t_p)) - \mathbf{e}_y \sin(\omega_-(t-t_p))].$$

As apparent from Fig. 1a after application of this electric field in the mean the particle comes to rest in the center of the Penning trap. In Fig. 1b the corresponding time

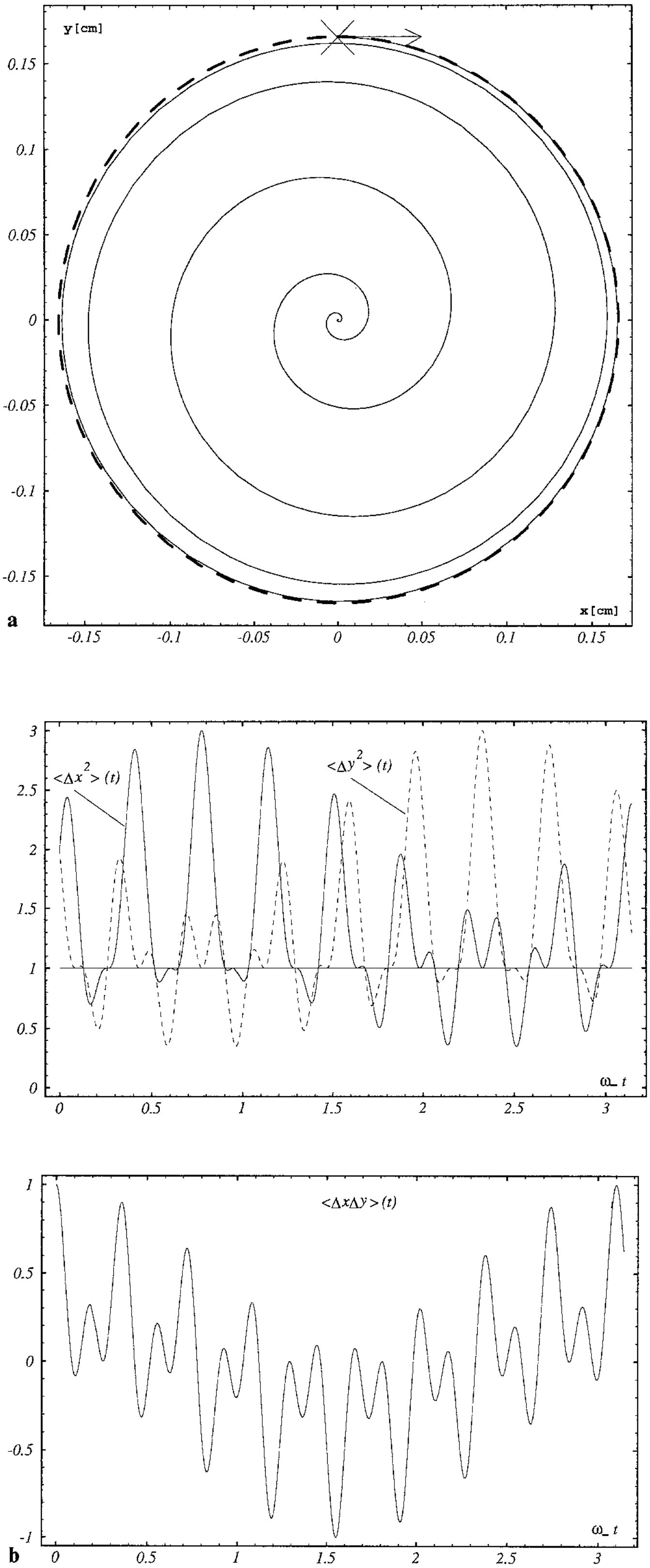

Fig. 1. **a** Time evolution of $\langle \mathbf{x}_{\perp cl}\rangle(t)(\langle \mathbf{x}_{\perp cl}\rangle(t)\cdot\mathbf{B}=0)$ for $0<t<T$ with (*full curve*) and without (*dashed curve*) applied, time dependent electric field; $t_p=12\pi/\omega_-$, $\tau=2\pi/\omega_-$, $T=24\pi/\omega_-$, $\omega_+/2\pi=580.6\,kHz$, $\omega_-/2\pi=33.7\,kHz$; **b** Time evolution of the spatial variances with $\langle \Delta x^2\rangle(0)=\langle \Delta y^2\rangle(0)=2\times\langle \Delta x \Delta y\rangle(0)=2$ (in units of the width of the ground state $\sqrt{\hbar/(2M\Omega)}$). Characteristic frequencies as in *a*

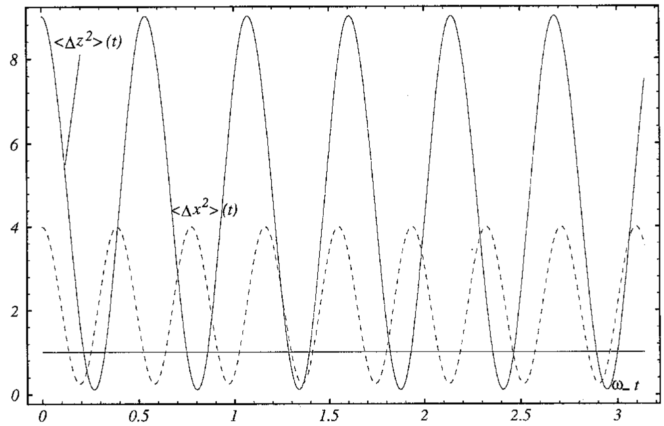

Fig. 2. Time evolution of the spatial variances with $\langle \Delta x^2\rangle(0)=\langle \Delta y^2\rangle(0)=4$, $\langle \Delta x \Delta y\rangle(0)=0$ and $\langle \Delta z^2\rangle(0)=9$ (in units of the corresponding widths of the ground state)

evolution of the variances $\langle \Delta x^2\rangle(t)$, $\langle \Delta y^2\rangle(t)$ and $\langle \Delta x \Delta y\rangle(t)$ is shown.

Although after the interaction with the circularly polarized electric field in the mean the charged particle is positioned in the center of the Penning trap with zero mean velocity, the corresponding spatial variances are still oscillating. However, under certain circumstances an instantaneous change of the parameters of the Penning trap may be used to "freeze" these oscillations of the spatial variances and localize the charged particle with unit probability in the ground state of a newly configured Penning trap. For this purpose it is necessary that a time t_1 can be found at which the variances fulfill the relations

$$\begin{aligned}\langle \Delta x^2\rangle(t_1) &= \langle \Delta y^2\rangle(t_1)\\ \langle \Delta x \Delta y\rangle(t_1) &= 0.\end{aligned} \tag{7}$$

If at this instant of time the trap parameters are changed instantaneously from (B,Φ) to (B',Φ') in such a way that

$$\langle \Delta x^2\rangle(t_1)=\langle \Delta y^2\rangle(t_1)=\frac{\hbar}{2M\Omega'}$$

and

$$\langle \Delta z^2\rangle(t_1)=\frac{\hbar}{2M\omega'_z}$$

(the primes indicate the new characteristic frequencies corresponding to (B',Φ')), the state $\psi(\mathbf{x},t_1)$ is the ground state of the new trap with parameters (B',Φ'). It should be mentioned that the spatial variances of this new ground state can be much smaller than the corresponding variances of the ground state of the original Penning trap with parameters (B,Φ). The conditions of (7) can be fulfilled most easily if $\langle \Delta x^2\rangle(t_0)=\langle \Delta y^2\rangle(t_0)$ and $\langle \Delta x \Delta y\rangle(t_0)=0$, initially, which implies $\langle \Delta x^2\rangle(t)=\langle \Delta y^2\rangle(t)$ and $\langle \Delta x \Delta y\rangle(t)=0$ for all subsequent times. Figure 2 shows the time evolution of the non-zero spatial variances $\langle \Delta x^2\rangle(t)=\langle \Delta y^2\rangle(t)$ and $\langle \Delta z^2\rangle(t)$ in such a case.

The strongest localization of a charged particle by this "coherent cooling mechanism" would be achieved, if the trap parameters were changed at a time t_1 where $\langle \Delta x^2 \rangle (t_1) = \langle \Delta y^2 \rangle (t_1)$ and $\langle \Delta z^2 \rangle (t_1)$ assume their minimum values.

For the experimental realization of the "coherent cooling mechanism" discussed above besides the initial preparation of a sufficiently symmetric Gaussian wave packet two points seem to be of major importance. First of all, the application of the classical electric field at time t_p has to be synchronized with the initial preparation time t_0 of the charged particle in the trap. Furthermore, the trap parameters have to be changed instantaneously on the time scales determined by $2\pi/\Omega$ and $2\pi/\omega_z$. This may be achieved by a suitable change of the static electric quadrupole field, for example. Considering typical trap parameters both conditions might be fulfilled by using ions, because in this case the fundamental frequencies of the trap are sufficiently small (typically of the order of Mhz or less).

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