Ground states and dynamics of a trapped charged particle in the magnetic field

Maciej Janowicz and Jan Mostowski

1Institute of Physics of the Polish Academy of Sciences, Aleja Lotników 32/46, 02-668 Warsaw, Poland

(Dated: October 16, 2013)

Abstract

A system of two charged particles in a harmonic trap with additional magnetic field is considered. The problem is reduced to a single-particle one in relative coordinates. The ground- and lowest excited-state energies and wave functions are found. The ground state exhibits non-zero expectation value of the velocity (kinetic momentum) and the probability current density does not vanish as well. When the ground state becomes degenerate the expectation value of velocity becomes discontinuous. The effects associated with turning on of the magnetic field are studied by solving the appropriate time-dependent Schrödinger equation. No substantial differences between abrupt (discontinuous in time) and continuous switching on have been observed. Evolution of a wave packet which is initially Gaussian is also investigated. The wave packet loses its Gaussian nature and, after sufficiently large time, a system of diffractive maxima and minima is built.

I. INTRODUCTION

Time crystals and their dynamics became an interesting problem after recent publications of [1], etc. In short time crystals are systems where natural symmetry is not compatible with gauge field. A good example is a system of two or more ions in a cylindrically symmetric harmonic trap and in an additional constant homogeneous magnetic field directed along the symmetry axis. Because of cylindrical symmetry in the ground state the system wave function should be an eigenstate of the angular momentum component along the symmetry axis. On the other hand in is a property of the magnetic field that the total flux of the field should be a multiple of the flux quantum. These two conditions are not compatible with each other. It has been argued [1]that the ground state as well as excited state of the system show a nontrivial dynamics. In particular the ground state of a time crystal is not stationary, but instead exhibits time dependence characteristic for motion. We will explore this idea in detail in this paper.

A system of ions on a trap with additional magnetic field was recently investigated by [2] from the point of view of time crystal dynamics. It was shown there that two or more ions indeed provide a good example of a time crystal and the dynamics was discussed.

In this paper we will further investigate similar systems. In particular we will discuss the dynamics, i.e. time dependence of the wave function. We will restrict ourselves to the simplest case of two ions, this simple system exhibits all the characteristic features of a time crystal. More ions add complications not giving any new aspects to the problem. There is no need to discuss more ions.

The problem of interaction of two charged non-relativistic particles in a trap with additional homogeneous magnetic field is interesting also from another point of view. This is one of the simplest systems in which non-trivial effects associated with the difference between the canonical and kinetic momentum can be studied. The particular form of the coupling of the electromagnetic field to the matter fields appears as a consequence of the gauge invariance of quantum electrodynamics. Even in the realm of non-relativistic quantum mechanics that coupling leads quite profound effects, in particular, to the necessity to distinguish between the canonical and kinetic momentum. In the presence of (non-static) electromagnetic field the canonical momentum while retaining its role in the Hamiltonian formalism loses its status of a physical observable and is to be replaced with the velocity. This happens even in the simplest situation when the electromagnetic field reduces itself to the constant homogeneous magnetic field when the corresponding vector potential is linear in the coordinate.

One may suspect that a system with non-zero expectation value of the radial coordinate (hence non-zero expectation value of the vector potential) can be of particular interest. Indeed, in such a system the expectation value of velocity does not vanish in the ground state because the minimum of the effective potential is displaced from zero. One way to achieve that is to introduce a repulsive Coulomb potential with the center at the same point as the center of the trap potential. This can be realized by placing to ions with identical charges in a trap. Then the problem reduces to a one-body problem in the relative coordinates. Similar ring-shaped traps have been considered, e.g., in [3-7]. A remarkable comparison of the energy spectra as produced by the propagation of a semiclassical wave packet and those computed from the WKB approximation has been performed in [8]. A real and very interesting related systems are composed of aromatic molecules in the magnetic field [9, 10].

The main part of this work is organized as follows. In Section 2, the construct the mathematical model and describe the basis states. Section 3 contains the results of the calculation of lowest energy levels as well as the ground-state expectation value of the velocity. In Section 4 we investigate the effects associated with abrupt turning on of the magnetic field. Section 5 is devoted to the evolution of the wave packet, and Section 6 contains some concluding remarks.
II. THE MODEL

Let us consider a system of two identically charged particles which are trapped in a harmonic external potential with additional homogeneous magnetic field. The Hamiltonian of one of the particles in the relative coordinates (in two spatial dimensions) can be written as:

\[ H = \frac{1}{2\mu} (p - eA)^2 + \frac{1}{2}\mu\omega^2 r^2 + \frac{ke^2}{|r|}, \quad (1) \]

where \( \mu \) is the reduced mass, \( e \) is the charge of each particle, \( p \) is the relative canonical momentum, \( A \) is the vector potential, \( \omega \) is the frequency of the trap, \( k = 1/(4\pi\epsilon_0) \), and \( r = (x, y) \) are the relative coordinates. We choose the so-called symmetric gauge for the vector potential, \( \omega \) the vector potential, \( \mu \) where

\[ A = \frac{1}{2} B \times r, \]

where \( B = (0, 0, B_z) \) is the magnetic induction.

Before we proceed let us briefly discuss the motion of particles within the framework of classical mechanics. It is clear that the lowest energy solution of the classical equations of motion are obtained when the velocities \( \frac{1}{\mu} (p - eA) \) equal to zero. Thus there is no motion if the system is in the lowest energy configuration. The canonical momentum \( p \) is different from zero, but this does not relate to movement.

We will now proceed with description of the system within the framework of quantum mechanics. Let us introduce the dimensionless coordinates \( \xi, \eta \) such that

\[ x = \frac{\sqrt{\hbar}}{\sqrt{\mu\omega_1}} \xi, \quad y = \frac{\sqrt{\hbar}}{\sqrt{\mu\omega_1}} \eta. \]

Then the Hamiltonian takes the form:

\[ H = \hbar\omega_1 \left( -\frac{1}{2} \frac{\nabla^2}{2} + \frac{1}{2} + \frac{\nu^2}{8} \right) \rho^2 + \frac{i}{2} (\nu (\xi \partial_\eta - \eta \partial_\xi) + b/\rho), \quad (2) \]

where \( \rho = \sqrt{\xi^2 + \eta^2}, \partial_\xi = \partial/\partial_\xi, \partial_\eta = \partial/\partial_\eta, \nabla^2 = \partial^2_\xi + \partial^2_\eta, \nu = \omega_c/\omega_1, \) \( b = (ke^2/\hbar)\sqrt{(m/\hbar\omega_1)}, \) and \( \omega_c = eB_z/m \) is the cyclotron frequency. Thus, the parameter \( \nu \) is a measure of strength of the magnetic field. The dynamics of the system are determined by the two parameters \( \nu \) and \( b \).

In polar coordinates \( \rho, \phi \) such that \( \xi = \rho \cos \phi, \eta = \rho \sin \phi \) the Hamiltonian takes the form:

\[ H = \hbar\omega_1 \left[ -\frac{1}{2} \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{2} \frac{\nu^2}{4} \rho^2 + \frac{i}{2} \left( \nu (\xi \partial_\eta - \eta \partial_\xi) + b/\rho \right) \right]. \quad (3) \]

Clearly, the \( z \)-component of the angular momentum commutes with the Hamiltonian, and the latter admits separation of variables in the radial coordinates \( \rho \) and \( \phi \).

Let us consider the time-independent Schrödinger equation

\[ H\psi = E\psi, \quad (4) \]

and let us write the wave function \( \psi = \psi(\rho, \phi) \) in terms of separated variables \( (\rho, \phi) \) as:

\[ \psi(\rho, \phi) = \frac{1}{\sqrt{\rho}} \chi(\rho) e^{im\phi}. \quad (5) \]

Then the time-independent Schrödinger equation takes the form:

\[ H'\chi(\rho) = E\chi(\rho), \quad (6) \]

where

\[ H' = \frac{1}{2} \hbar\omega_1 \left[ -\frac{\partial^2}{\partial \rho^2} - m\nu + \left( 1 + \frac{\nu^2}{4} \right) \rho^2 + \left( m^2 - \frac{1}{4} \right) \rho^{-2} + \frac{b'}{\rho} \right], \quad (7) \]

where \( b' = 2b. \) \( H' \) can also be written as a sum of the kinetic term and dimensionless effective potential term:

\[ H' = \frac{1}{2} \hbar\omega_1 \left( -\frac{\partial^2}{\partial \rho^2} + V(\rho) \right). \]

With the above forms of the Hamiltonian we are well-prepared to study the spectral and dynamical features of the system.

In Fig. 1 we have displayed the effective potential \( V(\rho) \) as a function of \( \rho \).

III. THE GROUND-STATE ENERGY AND PROBABILITY CURRENT

In the presence of the Coulomb interactions the system is not exactly solvable and the numerical calculations are necessary (although analytical approximations like WKB or dominant balance are readily available). To solve Eq. \( \psi \) we have used the standard Rayleigh-Ritz variational method [11] with radial Gaussian functions \( \rho^{(1/2)+m+k} \exp(-(1/2)\rho^2), \) \( k = 0, 1, 2, \ldots, \) as the basis set.
FIG. 1: Shape of the dimensionless effective potential $V(\rho)$ as a function of the radial coordinate $\rho$. (a) $\nu = 0.5$, $b = 0.1$; (b) $\nu = 0.5$, $b = 10.0$; (c) $\nu = 5.0$, $b = 1.0$. In all figures the solid line corresponds to $m = 0$, and the dashed line to $m = 1$.

The spectrum of the system is determined by two parameters $\nu$, $b$ and labelled by the angular momentum quantum number $m$. For sufficiently small magnetic field (i.e. sufficiently small parameter $\nu$), the ground state of the system is contained in the manifold of states labelled by $m = 0$. With growing $\nu$, however, the ground state can be associated with larger $m$.

In Fig. 2 we have shown the dependence of the ground-state energy on the dimensionless strength of the magnetic field for two values of $b$ and several values of the quantum number $m$. It is clear that there exist values of the magnetic induction for which the ground states becomes degenerate. More importantly, if the magnetic field is sufficiently strong, the ground state corresponds to the non-zero value of $m$. Clearly, this is a result of the interplay between the terms in the Hamiltonian which are linear and quadratic in the magnetic potential. As the latter approaches zero, the energy spectra for positive and negative $m$ cease to differ, of course.

Let us notice that no anticrossing appears at the points where various branches of the spectrum are about to meet. The energy of the ground state is a non-differentiable function of the magnetic induction.

As one might expect, a good approximation of the spectrum can be obtained just by taking the expectation values of the Hamiltonian with the crude approximate
wave functions with correct behavior at zero and infinity, i.e.

\[ \chi_m = \rho^{m+1/2} \exp(- (1/2) a \rho^2), \]

where \( a = \sqrt{1 + \nu^2 / 4}. \)

In the context of the present paper, the probability current density in the stationary states is of considerable interest. It is the current that gives adequate meaning to possible motion of the system, in the ground state in particular. In radial coordinates, the only nonvanishing component of the probability current density is the angular component, \( j(\rho, \phi) = (0, j(\rho)) \) which does not depend on \( \phi. \) The natural unit of the probability current is obtained from the natural unit of length \( \sqrt{\mu \omega_s / \hbar} \) and frequency \( \omega_s. \) Hence we define the dimensionless current density \( J(\rho) = (0, J(\rho)) \) by \( j(\rho) = \sqrt{\mu \omega_s / \hbar \omega_s} J(\rho). \) In Fig. 3 we have shown the behavior of \( J \) as a function of its argument \( \rho \) for \( b = 5, \nu = 1, m = 1. \) For those values of \( b \) and \( \nu \) it is \( m = 1 \) for which the ground state is achieved. Fig. 3(a) displays the dependence of \( J \) on \( \rho \) while Fig. 3(b) shows the vector plot of \( J(\rho) \) in the \( xy \)-plane as computed in the ground state.

Interestingly, the probability current density changes its sign with growing \( \rho \) for positive angular momentum. The probability current itself (the density integrated over the whole plane) does not vanish, however, in spite of the sign changes. Thus, the expectation value of velocity (kinetic momentum) is non-zero in the ground state of the system. This must be the case since the expectation value of the radial coordinate does not vanish, hence the expectation value of the vector potential is also non-zero. The fact that the expectation value of velocity cannot vanish is especially obvious for the zero angular momentum \( m: \) indeed, the azimuthal coordinate of the gradient of the wave function is equal to zero, but the expectation value of the vector potential is not.

What we found very interesting is the behavior of the expectation value of the velocity as dependent on the magnetic field. If Fig. 4(a) and 4(b) we have displayed that dependence for several values of the angular momentum. Again, for positive values of the angular momentum the expectation value of velocity changes its sign. The magnetic field attempts to move the particle in the positive direction of \( \phi. \) Thus, in order to “work out” the positive angular momentum the particle must acquire negative (azimuthal) velocity. Fig. 4(c) illustrates the dependence of the ground-state expectation value of the velocity as a function of the magnetic field \( \nu. \) It contains discontinuities because different value of the angular momentum \( m \) correspond to the ground-state energy as the magnetic field grows as shown in Fig. 2.

### IV. DYNAMICS OF THE WAVE PACKET

In the next step in our considerations we have studied the dynamics of the wave function which has initially been prepared as a Gaussian wave packet of the form:

\[ \psi(\xi, \eta; 0) = N \exp(- a ((\xi - \xi_0)^2 + \eta^2)). \]

One can identify the following physical mechanisms which influence the dynamics of the wave packet. The first is the harmonic force which, if present alone, would simply yield the oscillations of the packet. The second one is the magnetic field with twofold effect: the quadratic part introduces a new frequency to the system which results in the “breathing” of the wavepacket; the linear part generates its overall rotation. Finally, there is the “scattering” by the repulsive Coulomb potential which leads to deformation of the packet as shown below.

The dynamics has been studied with the help of the standard split-operator technique working in Cartesian coordinates. It has been convenient to work in the dimensionless time \( \tau = (1/2 \hbar \omega_s t). \) The time-evolution operator \( U \) can be written in the form:
The action of $U_2$ on $\psi$ has been computed according to:

$$
\psi(\xi, \eta, \tau + \Delta\tau) \approx \exp(-i(V_2/2)\Delta\tau) \cdot 
\cdot \exp\left(i/2\left(\partial_{\xi}^2 + \partial_{\eta}^2\right)\Delta\tau\right) 
\cdot \exp\left(-i(V_2/2)\Delta\tau\psi(\xi, \eta, \tau)\right),
$$

(10)

where $V_2 = (1/2)(1+1/4\nu^2)(\xi^2 + \eta^2) + b/\rho$. The action of the exponential of the kinetic term has been computed using two-dimensional fast Fourier transformation and its inversion.

The snapshots of shape of the resulting wave functions have been displayed in Fig. 5.

As can be seen from the above figure, the (initially Gaussian) wave packet does not return to its initial shape and becomes spread out in the azimuthal coordinate due to the Coulomb “scattering”.

V. CONCLUDING REMARKS

We have also investigated whether the values of the magnetic induction leads to any unusual characteristic in the ground state. Instead of the expansion in terms of the basis sets, we have rather employed the dynamics in the imaginary time as an alternative way to find the ground state. However, we have not observed any spectacular changes in the imaginary time dynamics, which might be associated with such a value of magnetic field which makes the ground state degenerate.

Let us also notice that we have tested the system for adiabatic versus abrupt turning on of the magnetic field, looking for any unusual behavior like phase discontinuities. However, no such effects have been found.

To summarize, we have investigated a system of two identically charged particles trapped in the harmonic potential with additional constant and homogeneous magnetic field. The problem becomes effectively one-particle upon introduction of the relative coordinates. The
FIG. 5: Shaded contour plots of the time-dependent wave packets in the rotating frame for $b = 1, \nu = 1$. (a) Initial Gaussian wave packet localized at the point $\xi' = 4, \eta' = 0$. (b)-(e) Shapes of the wave packet at the time $\tau = j\pi/12$, $j = 1, 2, ..., 5$. The darker regions corresponds to larger values of the modulus of wave function.

The ground state of such a system can be degenerate for specific values of the magnetic induction. Also, the ground state of the system can be that of non-vanishing eigenvalue of the third component of the angular momentum. The ground-state expectation value of velocity turns out to be non-zero. As a function of the magnetic field, it is discontinuous at the points where the ground state becomes degenerate. An interesting feature of the system is the sign change of the azimuthal component of the probability current density in the ground state as a function of the radial coordinate. We have also investigated the dynamics of the wave packet. Due to the presence of the Coulomb potential, the wavepacket partially loses its Gaussian shape and symmetry while retaining its coherence. It becomes spread out in the ring trap. No unusual behavior of the wavepacket have been observed while varying the magnetic field.

[1] F. Wilczek, Phys. Rev. Lett. 109, 160401 (2012)
[2] T. Li, Z.-X. Gong, Z-Q Yin, H.T. Quan, Z. Yin, P. Zhan, L.-M. Duan, and X. Zhang, Phys. Rev. Lett. 109, 163001 (2012)
[3] T. Schätz, U. Schramm, and D. Habs, Nature (London) 412, 7171 (2001)
[4] M.J. Madsen and C.H. Gorman, Phys. Rev. A 82, 043423 (2010)
[5] K. Okada, K. Yasuda, T. Takayanagi, M. Wada, H.A. Schuessler, and S. Ohtani, Phys. Rev. A 75, 033409 (2007)
[6] C. Champenois, M. Marciane, J. Pedregosa-Gutierrez, M. Houssin, M. Knoop, and M. Kajita, Phys. Rev. A 81, 043410 (2010)
[7] R.J. Clark, App. Phys. B, DOI: 10.1007/s00340-013-5451-0 (2013)
[8] F. Grossmann and T. Kramer, J. Phys. A 44, 445309 (2011)
[9] J.A.N.F. Gomes and R.B. Mallion, Chem. Rev. 101, 1349 (2001)
[10] G. Merino, T. Heine, G. Seifert, Chem. Eur. J. 10, 4367 (2004)
[11] A. Messiah, *Quantum Mechanics* (Dover, Mineola 1999)
FIG. 5: (Continued) Shaded contour plots of the time-dependent wave packets in the rotating frame for $b = 1, \nu = 1$.

(g)-(k) Shapes of the wave packet at the time $\tau = j \pi/12$, $j = 6, 7, \ldots, 10$. The darker regions corresponds to larger values of the modulus of wave function.