Bound States without Turning Points of Electric Dipole in Magnetic Field.

Nikita Sveshnikov* and Andrey Shirokov

Skobeltsyn Institute of Nuclear Physics, Moscow State University, Moscow 119899, Russia

and

Derek Pursey

Department of Physics and Astronomy, Iowa State University, Ames, IA 50011, U.S.A.

Abstract

We show that both rigid and non-rigid dipole can be trapped by an external uniform magnetic field in classical mechanics. The trapped states of the dipole present a non-trivial example of classical bound states embedded in continuum (BSEC) that can be treated as analogues of quantum BSECs. For example, the classical motion of the dipole is confined to a finite region in space though there are no classical turning points. We examine also the quantum motion of the dipole in magnetic field and show that for the most natural choices of the parameters (the rigid rotating dipole or the one bound by oscillator potential, uniform time-independent magnetic field, etc.) there are no quantum BSEC solutions. The possibilities of experimental investigations of BSECs are discussed.

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I. INTRODUCTION

A quantum system can have bound states with normalizable wave functions and continuum spectrum (scattering) states with non-normalizable wave functions. It is usually supposed that the energies of all of the bound states $E_i < 0$ while the continuum spectrum states have the energies $E > 0$, i. e. the continuum spectrum states are well-separated in energy from the bound ones. However, as early as 1929 von Neumann and Wigner [1] showed that a quantum system can have bound states embedded in continuum (BSEC), i. e. bound states with energies $E > 0$. Recently BSECs have been observed experimentally by F. Capasso et al [2]. The interest to BSECs was also stimulated by reported narrow e^+e^- coincidence peaks in heavy ion collisions at GSI, which were interpreted by Arbuzov et al [3] and independently by Vary and Spence [4] as due to bound states of the electron-positron system embedded in the continuum. Thus, BSECs have been studied in a number of recent papers [5]. Shirokov, Smirnov and Zaytsev [6] proposed also the so-called isolated states which are by definition the bound states that are not in correspondence with the S-matrix poles and which are a generalization of BSECs.

BSECs are conventionally regarded as exotic quantum states that do not have classical analogues. However, BSECs are very natural in classical mechanics. If the potential energy of a classical system has two barriers then any state with positive energy trapped by the barriers is a BSEC. Nevertheless, the corresponding quantum system does not have a BSEC: a double-barrier potential generates resonances instead of BSECs in quantum mechanics.

To support a BSEC in quantum mechanics, a local potential should have an infinite number of oscillations with amplitudes decreasing at large distances [1,7]. The wells of the long-range oscillating tail of the von Neumann-Wigner type potential are capable of trapping a classical particle with positive energy. Pursey and Weber [8] have analyzed this phenomenon in some detail for the three-dimensional case with zero angular momentum. Note, however, that the quantum BSEC wave function in this case decreases very slowly as the distance r tends to infinity. As a result, the probability of detecting the particle

outside the trapping potential well is much larger than the probability of detecting it within the well. Moreover the quantum BSEC in the von Neumann-Wigner type of potential can have an energy larger than the maximum of the potential energy, so that the corresponding classical motion does not have classical turning points and is not trapped. If the angular momentum $L > 0$, these potentials can also support classical BSECs with energies greater than the height of the potential barrier provided that the angular momentum is sufficiently large [9]. However this is possible only because almost all of the energy is associated with rotational motion — the energy associated with radial motion is still less than the height of the potential barrier. Therefore classical BSECs supported by the von Neumann-Wigner type of potential differ essentially from the quantum BSECs and cannot serve as analogues of quantum BSECs, in particular, such potentials do not provide a classical analogue of a quantum BSEC with no classical turning points.

BSECs are also natural in quantum mechanics when the interaction is non-local [6,10] or in the case of multichannel scattering (see, e. g., [11,12]). However, such quantum systems do not have explicit classical analogues.

In general, it seems that when a quantum system has a BSEC, the corresponding classical system does not and vice versa. The reason for this is that the mechanisms of the formation of BSEC in quantum and classical mechanics are very different: in the classical case the motion of a particle with a positive energy is confined to a finite region of space due to potential barriers that give rise to classical turning points while in the quantum case the BSEC wave function decreases at large distances due to interference of the waves reflected by an infinite number of potential barriers in the case of the von Neumann–Wigner type potential or due to the features peculiar to the quantum non-local interaction or multichannel scattering. Thus it would be interesting to find a classical system that supports BSECs with no classical turning points, i. e. where the trapping of the particle is not associated with potential barriers. Such classical BSECs can serve as analogues of quantum BSECs and may indicate the possible formation of quantum BSECs.

Classical BSECs have been discussed by Pollak and Pechukas [13] in the context of

reactive scattering theory in physical chemistry. Pollak and Pechukas have shown that a classical system can have a BSEC solution when the potential surface has a saddle point. There is a close analogy between the Pollak and Pechukas BSEC solutions and the position of unstable equilibrium of a physical pendulum. The unstable equilibrium of a classical system when the particle is stopped for an infinite time just at the maximum point of the potential barrier presents some kind of a classical BSEC. However, such BSEC is uninteresting because (i) it is unstable and any small perturbation destroys it and (ii) the corresponding quantum system does not have a BSEC solution at the same or close energy.

Recently we suggested [14] another example of a classical BSEC that seems to have some features of quantum BSECs. In particular, we demonstrated [14] that a classical rigid electric dipole can be trapped by an external magnetic field. The trapping of the dipole is not associated with any potential, thus this system presents a non-trivial example of a classical BSEC without classical turning points. However, we did not examined the quantum solutions for the dipole in the magnetic field. Thus, it is not clear whether the electric dipole in a magnetic field presents the first example of a system that has BSEC solutions both in quantum and classical cases. We discuss this problem in this paper. First, we present the classical equations for the dipole in magnetic field in the form that can be easily generalized on the quantum case, and prove the existence of the classical BSEC solutions. Unlike Ref. [14], we do not discuss the general case of the classical motion of the rigid dipole in magnetic field but restrict the discussion to a particular case that can be solved analytically. In addition we present the equations of classical motion and demonstrate the existence of classical BSEC solutions for a particular solvable case of a non-rigid dipole in magnetic field. Next, we turn to the quantum consideration of the above examples.

II. CLASSICAL TRAPPING OF ELECTRIC DIPOLE BY MAGNETIC FIELD

A. Rigid rotating dipole

Our model of the rigid dipole is a massless rod fixing the distance $2a$ between two particles each of mass m. One of the particles carries charge $+e$ while the charge of the other is $-e$. The Y axis is chosen to be in the direction of the uniform magnetic field $\boldsymbol{B}$. We restrict the center of mass motion of the dipole to the Z direction and the rotational degrees of freedom of the dipole to the XY plane. These restrictions are consistent with, and therefore provide a special case of, the general classical motion in three dimensions of the rigid dipole in magnetic field discussed in Ref. [14].

The Hamiltonian in our case is the following:

$$H = \frac{1}{4m}(P + \beta a \cos\varphi)^2 + \frac{1}{4ma^2}(\pi + \beta R a \sin\varphi)^2, \tag{1}$$

where R is the center of mass coordinate, P is the canonically conjugate momentum, φ is an angle between the X axis and $\boldsymbol{r}$ where $\boldsymbol{r}$ is the relative coordinate, $\boldsymbol{r} = \boldsymbol{r_1} - \boldsymbol{r_2}$, with $\boldsymbol{r_1}$ and $\boldsymbol{r_2}$ the coordinates of the particles, π is the momentum canonically conjugated to φ, and $\beta = eB/c$.

It is easy to check that there is an integral of motion,

$$J = P - \beta a \cos\varphi. \tag{2}$$

It is important to note that J is also an integral of motion in the quantum case, because the commutator $[\hat{H}, \hat{J}] = 0$ as seen from Eqs. (1) and (2) (hereafter we use the "hat" to denote quantum operators). Of course, the corresponding Poisson bracket $\{H, J\} = 0$ in the classical case also.

The canonical classical equations of motion are

$$\dot{R} = \frac{1}{2m}(P + \beta a \cos\varphi)\,, \tag{3}$$

$$\dot{\varphi} = \frac{1}{2ma^2}(\pi + \beta R a \sin\varphi)\,, \tag{4}$$

$$\dot{P} = -\frac{\beta}{2ma}(\pi + \beta R a \sin\varphi)\sin\varphi\,, \tag{5}$$

$$\dot{\pi} = \frac{\beta}{2m}\left[aP\sin\varphi - \frac{R}{a}\,\pi\cos\varphi - \beta(R^2 - a^2)\sin\varphi\cos\varphi\right]. \tag{6}$$

From Eqs. (3)—(6) it is easy to derive the equations of motion in the form

$$2m\ddot{R} = -2\beta a\dot{\varphi}\sin\varphi\,, \tag{7}$$

$$2ma^2\ddot{\varphi} = \beta a\dot{R}\sin\varphi\,. \tag{8}$$

The right-hand sides of Eqs. (7) and (8) are obviously the net force and the net torque, respectively, applied to the dipole.

Using (2), equation (3) can be rewritten as

$$\dot{R} = \frac{1}{2m}(J + 2\beta a\cos\varphi)\,. \tag{9}$$

The total energy of the system E is the kinetic energy. Thus, using Eq. (9) the total energy can be expressed as

$$ma^2\dot{\varphi}^2 + \frac{1}{4m}(J + 2\beta a\cos\varphi)^2 = E. \tag{10}$$

The classical bound (or trapped) state corresponds to the case when the mean value

$$\langle\dot{R}\rangle_t = 0. \tag{11}$$

Therefore classical BSECs are the solutions of Eq. (10) that fit the following equation:

$$\langle\dot{R}\rangle_t = \frac{1}{2m}\langle J + 2\beta a\cos\varphi\rangle_t = \frac{1}{2mT}\int_0^T (J + 2\beta a\cos\varphi)\,dt = 0\,, \tag{12}$$

where T is a period of motion.

If $J < -2\beta a$ or $J > 2\beta a$, then it is seen from (12) that $\langle\dot{R}\rangle_t \neq 0$, and trapping is impossible. So, let us examine the case $|J| \leq 2\beta a$.

Suppose $0 < J \leq 2\beta a$. From Eq. (10) we have:

$$\frac{d\varphi}{dt} = \sqrt{\frac{E}{ma^2} - \frac{1}{4(ma)^2}(J + 2\beta a\cos\varphi)^2}\,, \tag{13}$$

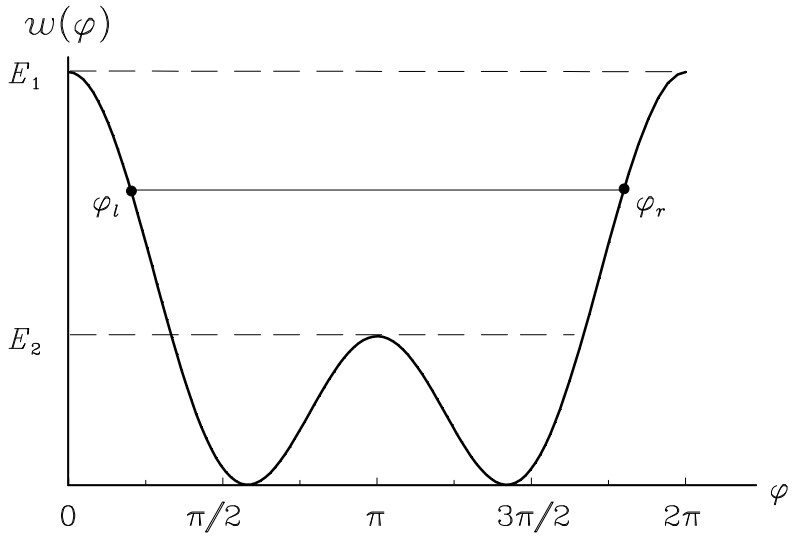

FIG. 1. Effective potential $w(\varphi)$ vs φ for $0 < J < 2\beta a$.

or

$$dt = \frac{\sqrt{m}\, a\, d\varphi}{\sqrt{E - \frac{1}{4m}(J + 2\beta a \cos\varphi)^2}} \,. \tag{14}$$

Equation (10) describes the motion of a particle in the effective potential $w(\varphi) = \frac{1}{4m}(J + 2\beta a \cos\varphi)^2$ (see Fig. 1). For $|J| < 2\beta a$, the effective potential $w(\varphi)$ has two maxima, $E_1 = \frac{1}{4m}(J + 2\beta a)^2$ at $\varphi = 0$ and $E_2 = \frac{1}{4m}(J - 2\beta a)^2$ at $\varphi = \pi$. When $E > E_1$, the dipole rotates unidirectionally. When $E < E_1$, the rotational motion is oscillatory between the left, φ_l, and the right, φ_r, classical turning points. If $E_2 < E < E_1$, then $\varphi_l + \varphi_r = 2\pi$. If $E < E_2$ then the oscillation is confined to one or other of two wells, as is clear from Fig. 1. Energy $E = E_1$ corresponds to the position of unstable equilibrium with $\varphi = 0$, while $E = E_2$ corresponds to unstable equilibrium with $\varphi = \pi$. Thus, Eq. (12) with the help of (14) is reduced to

$$\langle \dot{R} \rangle_t = \frac{a}{\sqrt{m}\, T} \int_{\varphi_l}^{\varphi_r} \frac{(J + 2\beta a \cos\varphi)\, d\varphi}{\sqrt{E - \frac{1}{4m}(J + 2\beta a \cos\varphi)^2}} \,, \tag{15}$$

where T is the period of a complete oscillation if $E < E_1$, while if $E > E_1$ then T is the period of one complete rotation while φ_l and φ_r are to be replaced by 0 and π respectively. If $E > E_1$, the numerator of the integrand in Eq. (15) is largest (and positive) and the

denominator is smallest when $\varphi = 0$. Therefore we conclude that $\langle \dot{R} \rangle_t > 0$ for $E > E_1$. Indeed, $\langle \dot{R} \rangle_t \to +\infty$ as E approaches E_1 from either above or below. By a similar argument, $\langle \dot{R} \rangle_t \to -\infty$ as $E \to E_2$ from either above or below, since the integral is then dominated by the region near $\varphi = \pi$ where $J + 2\beta a \cos\varphi < 0$. Hence $\langle \dot{R} \rangle_t$ is a continuous function of E that is negative for $E = E_2 + \varepsilon$ and positive for $E = E_1 - \varepsilon$. Thus $\langle \dot{R} \rangle_t = 0$ for some unique $E(J) \in (E_2, E_1)$, and the motion is trapped. Alternatively, for any energy $E \in (0, 2\beta a)$ there exists a unique value $J(E)$ of J for which the motion is trapped. Omitting further details, our analysis of (15) shows that the motion is untrapped for any $E > E_1$ and for any $E < E_2$, the only exception being the trivial case $E = 0$ in which the dipole is at rest. The case of $-2\beta a \leq J < 0$ can be analyzed in the same manner, leading to a trapped state when $J = -J(E)$.

The remaining case with $J = 0$ is trivial. The integrand in Eq. (15) is antisymmetric about $\varphi = \pi/2$ if $J = 0$, while $\varphi_r = \pi - \varphi_l$ in this case. Hence $\langle \dot{R} \rangle_t = 0$, and the motion is trapped for any E with the only exceptions $E = E_1$, which correspond to unstable static equilibrium.

Our conclusions are the following:

(i) If $J = 0$, then the classical motion is trapped for any energy $E > 0$ with the exception of $E = \beta^2 a^2/m$;

(ii) For any $J \neq 0$ and $E > \beta^2 a^2/m$, there are no trapped states;

(iii) For any E from the interval $0 < E < \beta^2 a^2/m$ there exists $J(E) \in (0, 2\beta a)$ such that for $J = \pm J(E)$ the classical motion is trapped. $J(E) \to 0$ when $E \to \beta^2 a^2/m$, and $J(E) \to 2\beta a$ when $E \to 0$.

A qualitative plot of the curve $J(E)$ showing the combinations of values of the energy E and of the integral of motion J corresponding to classical BSECs, is presented in Fig. 2.

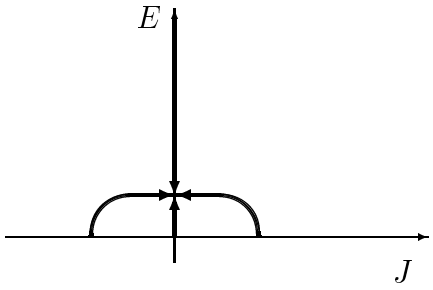

FIG. 2. A qualitative plot of $J(E)$ on the plane E vs J for the rigid dipole. Thick lines show the values of J that for a given E give rise to the trapped motion.

B. Non-rigid dipole

Our model of the non-rigid dipole is two particles of the mass m bound together by the potential $W(\boldsymbol{r})$ where $\boldsymbol{r}$ is the relative coordinate, $\boldsymbol{r} = \boldsymbol{r_1} - \boldsymbol{r_2}$. One of the particles carries the charge $+e$ while the charge of the other is $-e$. The Y axis is chosen to be parallel to the uniform magnetic field $\boldsymbol{B}$. In the same manner as for the rigid dipole, we restrict the motion of the center of mass to the Z axis and the relative motion of the particles to a plane parallel to the XY plane. Thus the relative coordinate $\boldsymbol{r}$ is always perpendicular to the center of mass velocity $\dot{\boldsymbol{R}}$, i. e. to the Z axis. These restrictions are consistent with, and therefore provide a special case of, the full classical motion of the non-rigid dipole in three dimensions.

The Hamiltonian is

$$H = \frac{1}{4m}\left(P + \frac{1}{2}\beta x\right)^2 + \frac{1}{m}\left(p_x - \frac{1}{2}\beta R\right)^2 + \frac{1}{m}p_y^2 + W(x,y), \tag{16}$$

where x and y are the projections of the relative coordinate $\boldsymbol{r}$ on X and Y axes, respectively; p_x and p_y are the momenta canonically conjugate to x and y, respectively, and $W(x,y)$ is the potential energy of the relative motion of the particles.

There is an integral of motion J given by

$$J = P - \frac{1}{2}\beta x, \tag{17}$$

which is the non-rigid equivalent of Eq. (2). As in the case of the rigid dipole, J is an integral of motion both in the classic and quantum cases.

In order to simplify the problem, we make some assumptions concerning the potential $W(x,y)$ binding the particles. In particular, we suppose that the x and y dependencies of $W(x,y)$ can be separated, i. e. $W(x,y)$ can be expressed as $W(x,y) = V(x) + \tilde{V}(y)$. This is the case, for example, of the harmonic oscillator potential $W(x,y)$. With this assumption the motion in the Y direction can be treated independently. Alternatively we may eliminate the motion in Y direction by constraining the relative motion is constrained to the X axis: this is equivalent to an approximation that ignores the rotational degrees of freedom of the dipole. So, in what follows we shall ignore the motion in the Y direction and discuss only the simplified Hamiltonian

$$H = \frac{1}{4m}\left(P + \frac{1}{2}\beta x\right)^2 + \frac{1}{m}\left(p_x - \frac{1}{2}\beta R\right)^2 + V(x). \tag{18}$$

The canonical equations of motion associated with the Hamiltonian (18) are

$$\dot{R} = \frac{1}{2m}\left(P + \frac{1}{2}\beta x\right), \tag{19}$$

$$\dot{x} = \frac{2}{m}\left(p_x - \frac{1}{2}\beta R\right), \tag{20}$$

$$\dot{P} = \frac{\beta}{m}\left(p_x - \frac{1}{2}\beta R\right), \tag{21}$$

$$\dot{p}_x = -\frac{\beta}{4m}\left(P + \frac{1}{2}\beta x\right) - \frac{dV(x)}{dx}\,. \tag{22}$$

From Eqs. (19)—(22) it is easy to derive the equations of motion in the form

$$2m\ddot{R} = \beta\dot{x}\,, \tag{23}$$

$$\frac{m}{2}\,\ddot{x} = -\beta\dot{R} - \frac{dV(x)}{dx}\,. \tag{24}$$

Eqs. (23) and (24) are just Newton's equations of motion for the center of mass and for the relative motion of the particles.

Using (17), equation (19) can be rewritten as

$$\dot{R} = \frac{1}{2m}(J + \beta x)\,. \tag{25}$$

The total energy of the system E is the kinetic energy together with $V(x)$, the potential energy of binding. Thus, using Eq. (25) the total energy can be expressed as

$$\frac{m}{4}\,\dot{x}^2 + \frac{1}{4m}(J+\beta x)^2 + V(x) = E\,. \tag{26}$$

For the trapped motion, $\langle \dot{R} \rangle_t = 0$, which from (25) is equivalent to

$$J + \beta \langle x \rangle_t = 0\,. \tag{27}$$

The average $\langle x \rangle_t$, to be derived from Eq. (26), is a function of E and J. For an arbitrary potential $V(x)$, Eq. (27) may have or have not solutions. We shall discuss a few particular choices of $V(x)$.

First, we note that if $J = 0$ then for any symmetric potential $V(x) = V(-x)$ such that the effective potential $w(x) = V(x) + \dfrac{\beta^2 x^2}{4m}$ is a monotonic increasing function for $x > 0$, a trapped state will exist at any energy E.

Next, let us discuss the case of the oscillator potential $V(x) = \dfrac{m\omega^2}{4}(x - x_0)^2$. Although this potential does not satisfy the physically necessary condition $V(x) = V(-x)$, it may be a good approximation if the motion confines x tofor a small enough interval $x \in [x_0 - \delta x_0, x_0 + \delta x_0]$. For this case from (26) we derive

$$\frac{m}{4}\,\dot{x}^2 + \left(\frac{m\omega^2}{4} + \frac{1}{4m}\,\beta^2\right)\left(x + \frac{\beta J - m^2\omega^2 x_0}{m^2\omega^2 + \beta^2}\right)^2 + \frac{m\omega^2}{4(m\omega^2 + \beta^2)}(J + \beta x_0)^2 = E\,, \tag{28}$$

and, obviously,

$$\langle x \rangle_t = \frac{m^2\omega^2 x_0 - \beta J}{\beta^2 + m^2\omega^2}\ . \tag{29}$$

From Eqs. (27) and (29), we find that for any energy E the motion is trapped if

$$J = -\beta x_0\ . \tag{30}$$

If this condition is met, then $\langle x \rangle_t = x_0$, the energy $E = \dfrac{m}{4}\,\dot{x}^2 + \dfrac{1}{4m}\left(\beta^2 + m^2\omega^2\right)(x - x_0)^2$, and the amplitude of the oscillation in x is $\sqrt{4mE \,\Big/ \left(\beta^2 + m^2\omega^2\right)}$. Hence, if the assumed form of $V(x)$ is an approximation valid

only for $|x - x_0| \leq \delta x_0$, our conclusion that Eq. (30) leads to trapped motion is valid only for energies $E \leq \frac{1}{4m}\left(\beta^2 + m^2\omega^2\right)\delta x_0^2$.

We next consider the case of a potential that has a plateau for some interval of x, that is we suppose that $V(x) = V_0 = \text{const}$ for $x \in [x_0 - L,\ x_0 + L]$, where $L > 0$. Within this range, the effective potential is $w(x) = V_0 + \frac{(J+\beta x)^2}{4m}$, which has a minimum at $x_1 = -J/\beta$. If $x_1 \equiv -J/\beta \in [x_0 - L,\ x_0 + L]$, that is if $J \in [-\beta x_0 - \beta L,\ -\beta x_0 + \beta L]$, and if the x motion is confined to the range $[x_0 - L,\ x_0 + L]$, then $\langle x \rangle_t = -J/\beta = x_1$, so that $\langle \dot{R} \rangle_t = 0$ by Eq. (25) and the classical motion is confined. The amplitude of the x oscillation is $\sqrt{4m\,(E - V_0)\,/\beta^2}$. Hence the condition that x remains in the interval $[x_0 - L, x_0 + L]$ throughout the motion is

$$\frac{\sqrt{4m\,(E - V_0)}}{\beta} \leq \inf\left(L - x_0 - \frac{J}{\beta},\ L + x_0 + \frac{J}{\beta}\right) . \tag{31}$$

(We note that $L - x_0 - J/\beta \geq 0$ by the requirement that the center of oscillation, $x_1 \equiv -J/\beta$, falls within the range $[x_0 - L, x_0 + L]$). We conclude that trapped classical motion is possible for any energy $E \in [V_0,\ V_0 + \beta^2 L^2/4m]$ provided that J takes any value from the interval

$$-\beta(L + x_0) + \sqrt{4m(E - V_0)} \leq J \leq \beta(L - x_0) - \sqrt{4m(E - V_0)} \tag{32}$$

(see Fig. 3).

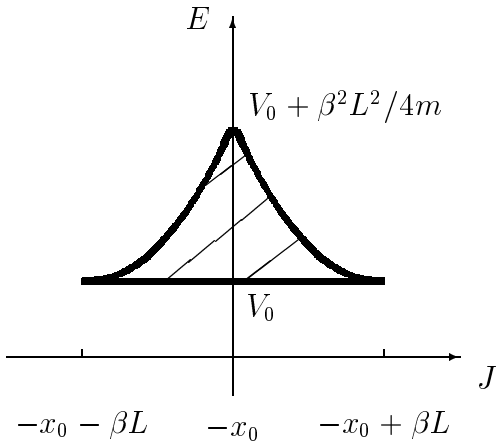

FIG. 3. The shaded area shows qualitatively the region of E and J that gives rise to the trapped motion in the case of the potential with the plateau.

This example is particularly interesting, because it shows that the dipole can be trapped for a wide and continuous range of the values of the energy E and of the integral of motion J, or, in other words, in a wide and continuous range of initial conditions.

III. QUANTIZATION

For both problems we have a Hamiltonian and an additional integral of motion commuting with the Hamiltonian. So, in the quantum case, we should search for a common solution of the Schrödinger equation

$$\hat{H}\Psi = E\Psi, \tag{33}$$

where $\hat{H}$ is given by (1) or (18), and of equation for the integral J,

$$\hat{J}\Psi = J\Psi, \tag{34}$$

where the operator $\hat{J}$ is given by (2) or (17). We shall use units in which $\hbar = 1$.

A. Rigid dipole

We use the following trick to simplify the Hamiltonian (1). We introduce a wave function ψ that is related to Ψ by

$$\Psi(R,\varphi) = e^{i\beta Ra\cos\varphi}\psi(R,\varphi). \tag{35}$$

Clearly, $\Psi(R,\varphi)$ will represent a confined state (i. e. a quantum BSEC) if and only if $\int |\psi(R,\varphi)|^2 dR < \infty$. By using Eqs. (1), (2), and (35), we reduce (33) and (34) to

$$\left[\frac{1}{4m}\left(\hat{P} + 2\beta a\cos\varphi\right)^2 + \frac{1}{4ma^2}\hat{\pi}^2\right]\psi = E\psi \tag{36}$$

and

$$\hat{P}\psi = J\psi. \tag{37}$$

Equation (37) has a continuous eigenvalue spectrum, with plane wave eigenfunctions $\exp(iJR)$. In Eq. (36), $\hat{P}$ can be replaced by its eigenvalue J, and this equation can be solved with respect to the single variable φ. Equation (36) is subjected to periodic boundary conditions, $\psi(\varphi) = \psi(\varphi+2\pi)$, thus, the spectrum of E for any given J is discrete. An infinite number of discrete energy eigenvalues $E_n(J)$ will be associated with any particular value of J. However, the lowest energy eigenvalue $E_0(J) \sim J^2$ for large J. Thus, any finite energy E can be realized only by a finite number of the plane waves with a given momentum J. It is impossible to construct a normalizable wave function as a superposition of a finite number of plane waves. Therefore, the rigid dipole in a uniform magnetic field does not have quantum BSEC solutions.

B. Non-rigid dipole

We apply to Eqs. (33) and (34) with $\hat{H}$ given by (18) and $\hat{J}$ given by (17) a trick similar to that used in the case of the rigid dipole, namely

$$\Psi = e^{i\beta Rx/2}\psi, \tag{38}$$

to obtain equations

$$\left[\frac{1}{4m}(\hat{P}+\beta x)^2 + \frac{1}{m}\hat{p}_x^2 + V(x)\right]\psi = E\psi \tag{39}$$

and

$$\hat{P}\psi = J\psi. \tag{40}$$

Due to (40), the operator $\hat{P}$ can be replaced by its eigenvalue J in Eq. (39).

The most natural choice for the potential $V(x)$ is the oscillator potential, $V(x) = \frac{1}{4}m\omega^2(x-x_0)^2$. The Schrödinger equation (39) in this case can be easily solved to yield an infinite number of discrete energy eigenvalues

$$E_n = \sqrt{\omega^2 + \frac{\beta^2}{m^2}}\left(n+\frac{1}{2}\right) + \frac{m\omega^2\left(J+\beta x_0\right)^2}{4\left(\beta^2+m^2\omega^2\right)} \tag{41}$$

for any value of the integral J. For any particular energy E, Eq. (41) and $E = E_n$ together define a functional relation between J and n. However, Eq. (41) shows that there is a maximal n consistent with any particular energy E. Hence only a finite number of eigenvalues J of $\hat{J}$ will be consistent with any fixed energy E, and this implies that there can be only a finite number of plane waves e^{iJR} associated with this energy. Thus there are also no quantum BSEC solutions for the non-rigid dipole with an oscillator binding potential.

As in the classical case, if the oscillator form for $V(x)$ is valid only for $|x - x_0| < \delta x_0$ then we should require a condition such as $\left\langle (x - x_0)^2 \right\rangle^{1/2} < \delta x_0$. This will imply a condition for the validity of Eq. (41) of the form $n < n_{\max}$, with the upper limit $n_{\max}$ deduced from $\left\langle (x - x_0)^2 \right\rangle^{1/2} < \delta x_0$.

Lastly, we consider the case when $V(x)$ has a plateau, $V(x) = V_0$ for $x_0 - L < x < x_0 + L$. In the simple but unphysical case of $L = \infty$, the Schrödinger equation (39) has the discrete energy eigenvalues

$$E_n = V_0 + \frac{\beta}{m}\left(n + \frac{1}{2}\right), \tag{42}$$

independent of J, while there are no constraints on J. However this is unphysical because the two charges are no longer bound by the potential $V(x)$. More realistically, if L is finite then a solution leading to Eq. (42) might give a good approximation provided $x_1 \equiv -J/\beta \in [x_0 - L, x_0 + L]$ and $\left\langle (x - x_1)^2 \right\rangle^{1/2} < \inf(L - x_0 - J/\beta, L + x_0 + J/\beta)$. For the state with energy E_n, the standard quantum theory of the harmonic oscillator yields $\left\langle (x - x_1)^2 \right\rangle^{1/2} = \sqrt{2m(E_n - V_0)/\beta^2}$. This leads to the constraints

$$-\beta(L + x_0) + \sqrt{4m(E_n - V_0)} < J < \beta(L - x_0) - \sqrt{4m(E_n - V_0)}, \tag{43}$$

which are very similar to those of Eq. (32). In particular, these constraints can be satisfied only if $E_n - V_0 < \dfrac{\beta^2 L^2}{4m}$, or equivalently (with Planck's constant restored) $n + \dfrac{1}{2} < \dfrac{\beta L^2}{4\hbar}$. Because a continuous range of eigenvalues J are allowed, we may construct infinitely many normalizable wave packets, all of them energy eigenfunctions with energy eigenvalue E_n. All that is required is to set

$$\Psi(R,x) = e^{\frac{1}{2}i\beta xR} \int_{J_1}^{J_2} e^{iJR} \chi_n(x + J/\beta) f(J)\, dJ, \tag{44}$$

where $\chi_n(x)$ is the oscillator eigenfunction for energy E_n and frequency β/m, the limits J_1 and J_2 are chosen well inside the range specified by Eq. (43), and $f(J)$ is chosen so that $\int_{J_1}^{J_2} |f(J)|^2\, dJ = 1$ but is otherwise arbitrary. Since there exists a countable infinity of functions $f(J)$ orthonormal in the interval (J_1, J_2), we may use this procedure to construct a countable infinity of quantum BSECs (that is, energy eigenstates with normalizable wave functions), all with energy E_n.

Note, however, that the wave functions corresponding to the energy levels (42) have small but nonzero amplitudes for $x \notin [x_0 - L, x_0 + L]$, where $V(x) \neq V_0$. It is easy to show that if the potential $V(x)$ is a rectangular well then the spectrum of J is discrete for any given energy E. Thus, due to the constraints (43), only a finite number of plane waves e^{iJR} is associated with any given energy E and the quantum BSEC is destroyed. Nevertheless, for the energies low enough the number of possible values of J can be very large. As a result, the BSEC is expected to turn into a very sharp resonant state that may appear to be indistinguishable from BSEC in applications. At the same time, we believe that it is possible to find a reasonable potential $V(x)$ binding the particles that will result in BSEC solutions for the dipole in a uniform magnetic field.

IV. DISCUSSION.

We have shown that a classical dipole can be trapped by a uniform time-independent magnetic field. The trapping is possible in all the cases which we have considered provided that the integrals of motion E and J satisfy particular constraints. The trapping of the dipole presents an interesting and non-trivial example of a classical BSEC. This classical BSEC shares some characteristics of quantum BSECs, in particular the trapping of the dipole is not associated with potential barriers and classical turning points.

We have also investigated the corresponding quantum problem. We have found out that

there are no quantum BSECs for the most natural choices of the parameters of the system, namely the rigid rotating dipole or the non-rigid dipole bound by an oscillator potential. This conclusion looks strange and intriguing. As we have already mentioned in the Introduction, all known quantum systems supporting BSECs either do not have a classical analogue (e. g., systems with non-local interaction) or the corresponding classical system does not support a classical BSEC. On the other hand, from all previously known examples of classical systems supporting BSECs we might conclude that the corresponding quantum system does not have BSEC solutions, and our study seems to confirm this conclusion even for some classical systems that support BSECs without classical turning points.

One can suspect that in the quantum case the dipole has no BSEC solutions due to the uncertainty principle. For all the cases we consider, the classical BSEC solutions for the dipole are possible only if the integrals of motion E and J satisfy certain constraints. In particular, for a rigid dipole or one bound by an oscillator potential, a classical BSEC is possible only if J has a precise value (which depends on E for the rigid case). However Eqs. (2) and (17) show that in the quantum case $\left[\hat{J},\hat{R}\right]=\left[\hat{P},\hat{R}\right]=-i$. Therefore by the uncertainty principle

$$\Delta J\Delta R\geq\frac{1}{2}. \tag{45}$$

Hence if J must have a precise value then $\Delta J=0$ so that $\Delta R=\infty$ and the quantum state cannot be confined. However the actual situation is somewhat different from this. In our analysis, the quantum mechanics for the dipole allows a quantum state with energy E to be associated with more than one eigenvalue J of $\hat{J}$, and the corresponding wave functions may be superposed to form a wave packet which is still an eigenfunction of $\hat{H}$ with the same energy eigenvalue E. However, for the rigid dipole or the dipole confined by an oscillator potential, only a finite number of eigenvalues J can be associated with any energy eigenvalue E, and this is not sufficient to produce a normalizable wave packet. Thus the reason for the absence of quantum BSECs is more subtle than is suggested by the uncertainty principle.

Note also the example of the classical potential with plateau discussed above (see Fig. 3).

As we have shown, in this case the dipole is trapped in a wide and continuous range of E and J, so that the initial conditions need not violate the uncertainty principle. Indeed, we have discussed above the possibility to construct quantum BSEC solutions in this case. The only constraint on the eigenvalue J of $\hat{J}$ seems to be an inequality very similar to an analogous inequality in the classical case. Thus it appears that a non-rigid quantum dipole bound by a potential $V(x)$ which has a flat plateau for a large enough range of x values, is remarkably similar to the corresponding classical case. We can understand this as follows. If $V(x) = V_0 =$ constant, the "dipole" consists of two non-interacting (and therefore independent) charges in an external magnetic field. In both classical and quantum physics, the motion of both charges in the plane perpendicular to the field is confined. Since the charges do not interact with each other, the relative locations of their classical orbits, or their probability distributions in the quantum case, is completely arbitrary. Hence in both the classical and quantum cases, there will be an infinity of BSEC solutions with the same energy. On the other hand, if $V(x) = V_0$ only for a finite range of x, then while there remains a continuum of classical BSEC solutions these occur only if the integrals of motion E and J satisfy a certain inequality, while the number of quantum BSEC solutions becomes countably rather than uncountably infinite or quantum BSECs can be even destroyed as in the case of the rectangular well potential $V(x)$.

Thus quantum BSEC solutions may be possible if the dipole is bound by some potential other than the harmonic oscillator potential. Our experience encourages us to search for a realistic potential $V(x)$ that will allow for an infinite number of continuous J eigenvalues associated with the same energy eigenvalue. We derive a limiting case for such a potential directly from (41), namely the limit $\beta \to 0$, or, more accurately, $\beta \ll m\omega$. This is the limit of a weak magnetic field. Note that this limit is opposite to the above limit of a potential with a plateau: the potential $V(x) = 0$ is obtained from the oscillator potential in the limit $\omega \to 0$ and corresponds to $\beta \gg m\omega$. One might expect the limit $\beta \ll m\omega$ to be just the classical limit, and that quantum BSECs in this limit equivalent to the classical ones discussed above. However, the situation is not so simple. Even in the $m \to \infty$ limit

the motion in the lowest oscillator states remains essentially quantum. The true classical limit, in which the quantum BSECs should become classical BSECs, is $n \to \infty$ and $m \to \infty$. However we saw in § III B that there might be an upper limit $n_{\max}$ to the values of n for which the harmonic oscillator approximation of the potential $V(x)$ is valid. Thus the transition from a quantum to a classical BSEC may depend on how large is the range of x for which $V(x)$ may be approximated by an oscillator potential. If n is small, only the center of mass motion is classical while the internal oscillations are quantum. If the internal oscillation is frozen in the ground state (the rms radius of the $n = 0$ oscillator state is $\sqrt{2/(m\omega)}$, so the limit $m\omega \to \infty$ guarantees that the motion is frozen in the ground state), as would be true for a typical dipole gas molecule at normal room temperatures, we get a different classical limit. In this case, if we restore the possibility of rotational motion (ignored in §§ II B and III B) we should be able to find the classical BSECs associated with a rigid dipole in § II A.

It would be interesting to find additional non-trivial and physically reasonable potentials $V(x)$ binding the particles that will provide quantum BSEC solutions for the dipole in a magnetic field. It is possible to search for such a potential $V(x)$ using the same approach that we used in the classical case, namely solving Eqs. (11) and (27). In the quantum case, $\dot{R} = i[\hat{H}, R]$. If Ψ is a normalizable BSEC wave function, then

$$\langle \Psi \mid \dot{R} \mid \Psi \rangle = i\langle \Psi \mid [\hat{H}, R] \mid \Psi \rangle = i\left(E\langle \Psi \mid R \mid \Psi \rangle - \langle \Psi \mid R \mid \Psi \rangle E\right) = 0. \tag{46}$$

If Ψ is a non-normalizable continuum spectrum wave function, then $\langle \Psi \mid R \mid \Psi \rangle$ diverges and Eq. (46) is not valid. By calculating the commutator $[\hat{H}, R]$, we immediately obtain Eq. (27) from (46). Thus, we can search for the potential $V(x)$, or (better) for the effective potential $w(x) = V(x) + \dfrac{1}{4m}(J + \beta x)^2$, that gives rise to wave functions which satisfy Eq. (27).

The quantum treatment of the non-rigid dipole shows that we should search for a potential supporting solutions with the same energy eigenvalue that satisfy Eq. (27) at least on a finite interval of the continuous variable J. We believe that it will be possible to find such physically reasonable potentials. Note that a potential $V(x)$ binding a dipole molecule (to take a specific example) can be modified to some extend by an external electric field in the

X direction. We believe that it will be valuable to find realistic potentials $V(x)$ that give rise to quantum BSEC solutions for the dipole, because (i) it will demonstrate that quantum BSECs can be present in a system that is very simple and involves only well-known local interactions; (ii) it will present an example of a system that has both classical and quantum BSECs; (iii) it may be possible to find a real system supporting BSECs that can be studied experimentally.

The rigid dipoles that we have studied in this paper may also be interesting for experimental investigation. We expect that a rigid dipole molecule should behave classically in a weak magnetic field, but in a stronger field quantum effects should become important. In a gas of dipole molecules at normal temperatures, the vibrational degrees of freedom are frozen in the ground state so that the dipole is essentially rigid. In these circumstances, some of them may be trapped by the weak magnetic field. When the field is increased, or when the temperature is lowered so that angular momentum quantization is important enough to affect the specific heat, the trapped state should be destroyed due to quantum effects. It may be possible to design experiments to investigate this effect, never discussed before in literature. A classical BSEC when destroyed by a magnetic field strong enough to give rise to quantum effects should turn into a very narrow long-lived resonance. These resonances should effect strongly the density of states in the system and give rise to some peculiarities in dispersion of some excitations.

The BSECs discussed in this paper may be also interesting for the studies of chaotic motion. The general classical Hamiltonian of the rigid dipole is non-integrable [14]. The same is true for the non-rigid dipole. Therefore, the motion of the dipole can be chaotic. The classical BSEC solutions correspond to islands of integrability in the phase space of the system. It would be interesting to study the influence of such islands of integrability on the chaotic motion in the system.

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