Small oscillations of a 3D electric dipole in the presence of a uniform magnetic field

L A del Pino¹, B Atenas¹, S Curilef⁰
1 Departamento de Física, Universidad Católica del Norte, Avenida Angamos 0610, Antofagasta, Chile
E-mail: scurilef@ucn.cl

Abstract. The classical behavior of a 3D electric dipole in the presence of a uniform magnetic field is studied in the small oscillations approximation. Using the Lagrangian formulation, the equations of motion are obtained, as well as their solutions and constants of motion. Normal modes of oscillation and their corresponding normal coordinates are obtained. Furthermore, the existence of a type of bound states without turning points, so-called trapped states conjectured by Troncoso and Curilef [Eur. J. Phys 27 (2006) 1315-1322], is investigated.

1. Introduction

Nowadays, a lot of applications are being developed in molecular-scale technologies because of the effort made to build nanobots (real intelligent nanostructures) by several specialists. Although such systems are not easy to model, we may do it through electric dipoles into external magnetic (and/or electric) fields[1, 2, 3].

In the study of this kind of systems, an atypical class of states was previously proposed[4] for a rigid electric dipole rotating around an axis into a plane perpendicular to the magnetic field, in such model the state corresponds to a bound state without turning points. In a different context[5], where the direction of axis of rotation of the electric dipole is supposed to be coincident with the magnetic field[5]. Through a prior analysis is conjectured the existence of a kind of bound states without turning points, that are so-called trapped states[5]. Recently, the motion and the relationship between the constants of motion was obtained. The trapped states [5] are shown for the model and they are completely described[6, 7]. The solutions are expressed in terms of Jacobi elliptic functions[6, 7].

In this work, the primary aim is to describe, from the perspective of the small oscillations approximation, the 3D motion of an electric dipole in the presence of an external magnetic field, without any other restriction. Particles immersed in magnetic field have been studied by several authors from different perspectives and imposing certain constraints on the motion of the center of mass and the relative coordinate[4, 5, 6, 7, 8, 9]. However, the study of small oscillations of this class of systems has not been yet addressed, and it is crucial to the creating real nanobots. The study of normal modes is a useful tool that allows classifying of molecules and studying of forces according with its symmetry.

The study of small oscillations is a relevant perspective to introduce widespread physical applications in optics, acoustics, molecular spectra, mechanical and electrical vibrations. We expect that these solutions significantly impact on the future of the applications to molecular...
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motors and their constructions, as they describe the overall behavior of a dipole from a classical perspective.

This paper is organized as follows: In Section 2, we present the model and its theoretical basis, deriving the equations and constants of motions. In Section 3, the solution of the equation of motion is obtained in the small oscillations approximation, including its normal modes and coordinates. In Section 4 we investigate the possibility of existence of trapped states as conjectured before [5]. Finally, in Section 5, we offer some concluding remarks.

2. The model

Let us consider an electric dipole composed by two identical and opposite charges \( (e_1 = -e_2) \), separated by a fixed length \( a \) and whose masses are equal, in a uniform magnetic field \( \vec{B} = B \hat{e}_{iii} \).

The Lagrangian function is given by

\[
L(r_1, \dot{r}_1, \dot{r}_2, \dot{r}_2) = \frac{1}{2} m_1 \dot{r}_1^2 + \frac{1}{2} m_2 \dot{r}_2^2 - \frac{e_1}{c} \vec{A}(r_1) \cdot \dot{r}_1 - \frac{e_2}{c} \vec{A}(r_2) \cdot \dot{r}_2 - \frac{e_1 e_2}{\kappa} \frac{r_1 - r_2}{r_1^2 - r_2^2},
\]

where \( r_{1,2} \), \( m_{1,2} \) are the position of the particles \( (1,2) \) and their corresponding masses, respectively. We additionally use the symmetric gauge for the vector potential \( \vec{A}(r_i) = \frac{1}{2} \vec{B} \times \hat{r}_i \) for \( i = 1,2 \) and by using the coordinate of the center of mass \( \vec{R} = \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m} \) and the relative coordinate \( \vec{r} = \vec{r}_2 - \vec{r}_1 \), the Lagrangian takes the following shape[5, 6, 7]:

\[
L(\vec{R}, \dot{\vec{R}}; \vec{r}, \dot{\vec{r}}) = \frac{1}{2} M \dot{\vec{r}}^2 + \frac{1}{2} \mu \vec{r}^2 + \frac{e_1}{\kappa a} \left[ \vec{B} \times \dot{\vec{R}} \cdot \dot{\vec{r}} + \vec{B} \times \vec{r} \cdot \dot{\vec{r}} \right],
\]

where \( M = m_1 + m_2 \) is the total mass, \( \mu = \frac{m_1 m_2}{m} \) is the reduce mass and the charge \( e_1 = e \).

The so-called pseudomomentum is a constant of motion[5, 9, 10] given by

\[
\vec{C} = \vec{P}_R + q \vec{A}_R + e_c \vec{A}_r,
\]

where \( q = e_1 + e_2 \) is the total charge and \( e_c = e_1 \frac{m_2}{M} - e_2 \frac{m_1}{M} \) is the coupling charge, \( \vec{A}_R = \frac{1}{2e} \vec{B} \times \vec{R} \), \( \vec{A}_r = \frac{1}{2} \vec{B} \times \vec{r} \) and \( \vec{P}_R = \frac{\partial L}{\partial \dot{\vec{R}}} = M \dot{\vec{R}} + \frac{q}{2e} \vec{B} \times \vec{r} \) is the conjugate momentum of the center of mass. Thus, the relation between the linear momentum of the center of mass and the relative coordinates, for \( q = 0 \) is given by

\[
M \dot{\vec{R}} = \vec{C} - \frac{e_c}{c} \vec{B} \times \vec{r}
\]

Additionally, we define a constant vector that we call transverse pseudomomentum \( \vec{\gamma} \).

\[
\vec{\gamma} = \vec{C} \times \hat{e}_{iii} = C_{ii} \hat{e}_i - C_i \hat{e}_{ii},
\]

where \( C_i \) and \( C_{ii} \) are the components of \( \vec{C} \) in a plane perpendicular to \( \vec{B} \). Combining the Eq.(5) with (4), we arrive at the following relation:

\[
M \dot{\vec{R}} = (-\gamma_{ii} + \frac{eB}{c} \gamma_{ii}) \hat{e}_i + (\gamma_i - \frac{eB}{c} r_i) \hat{e}_{ii} + C_{iii} \hat{e}_{iii}
\]

Certainly, other constant of motion is the energy of the system

\[
\mathcal{E}(\vec{R}, \vec{r}; \vec{\dot{R}}, \vec{\dot{r}}) = \vec{P}_R \cdot \dot{\vec{r}} + \vec{p}_{\vec{r}} \cdot \dot{\vec{r}} - L(\vec{R}, \vec{r}; \vec{\dot{R}}, \vec{\dot{r}}),
\]

where \( \vec{p}_{\vec{r}} = \frac{\partial L}{\partial \vec{r}} \) is the relative conjugate momentum. Consequently, the energy fulfills:

\[
\mathcal{E}(\vec{R}, \vec{r}; \vec{\dot{R}}, \vec{\dot{r}}) = \frac{1}{2} M \dot{\vec{R}}^2 + \frac{1}{2} \mu \vec{r}^2 - \frac{e^2}{\kappa a}.
\]
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Substituting Eq.(6) into (8), the energy may be expressed in terms of the relative variable:

\[ E = \frac{1}{2} \mu \dot{r}^2 + \frac{1}{2M} \left\{ C^2 + \frac{e^2 B^2}{c^2} (r_i^2 + r_{ii}^2) - 2 \gamma \cdot \vec{r} \right\} - \frac{e^2}{ka}. \]  

(9)

Defining a set of dimensionless variables: \( \rho = \frac{r}{a}, \xi = \frac{R}{a}, \frac{d}{dt} = \omega_c \cdot \frac{d}{d\tau} \) and \( \omega_c = \frac{eB}{Mc} \) (the cyclotron frequency). The pseudomomentum and its corresponding transverse component are also defined as dimensionless constants as follows: \( \vec{C} = \frac{\vec{C}}{M\omega_c a}, \vec{\gamma} = \frac{\vec{\gamma}}{M\omega_c a} \).

The Eqs.(9) and(6) in terms of the dimensionless variables are given by

\[ \dot{\xi} = (-\gamma_{ii} + \rho_{ii}) \hat{e}_i + (\gamma_i - \rho_i) \hat{e}_{ii} + c_{iii} \hat{e}_{iii} \]  

(10)

\[ \epsilon = \frac{1}{\alpha \hat{\rho}^2} + \{c^2 - 2 \gamma \cdot \hat{\rho} + \rho_1^2 + \rho_2^2 \} - \epsilon_c. \]  

(11)

with \( \alpha = \frac{M}{\mu}, \epsilon_c = \frac{2e^2}{\omega_c^2 Ma^2} \) and \( \epsilon = \frac{2e}{\omega_c^2 a^2 M} \). Now, using spherical coordinates:

\[ \rho_i = \cos \psi \sin \theta, \]

\[ \rho_{ii} = \sin \psi \cos \theta, \]

\[ \rho_{iii} = \cos \theta, \]  

(12)

where \( \psi \) stands for the polar angle and \( \theta \) stands for the azimuthal angle. Substituting the above equations in Eq.(11), we get:

\[ \epsilon = \frac{1}{\alpha} \left( \hat{\theta}^2 + \sin^2 \theta \hat{\phi}^2 \right) + c^2 - 2 \gamma \cos \phi \sin \theta + \sin^2 \theta - \epsilon_c. \]  

(13)

Next, we take \( \phi = \psi - \psi_0, \gamma = |\vec{\gamma}|, \epsilon = |\vec{C}^2| \). The angle subtended between the polar axis and the direction of the vector \( \vec{\gamma} \) is represented by \( \psi_0 \).

3. Small oscillations

When oscillations of systems occur about positions of equilibrium is interesting to consider the small oscillations approximation. We are interested in the motion within the immediate neighborhood of a configuration of stable equilibrium. If the deviation from equilibrium is too small, the kinetic and potential energies can be expanded in Taylor series about the equilibrium and retaining only the quadratic terms in generalized coordinates and velocities. From de Eq.(13) is easy to see that:

\[ T(\dot{\theta}, \dot{\psi}, \theta, \psi) = \frac{1}{\alpha} \left( \hat{\theta}^2 + \sin^2 \theta \hat{\phi}^2 \right), \]

\[ V(\theta, \psi) = c^2 - 2 \gamma \cos \phi \sin \theta + \sin^2 \theta - \epsilon_c, \]  

(14)

where \( T(\dot{\theta}, \dot{\psi}, \theta, \psi) \) represents the kinetic energy and \( V(\theta, \psi) \) the potential function. The potential \( V(\theta, \psi) \) has three stable configurations of equilibrium, depending on the value of the constant of motion \( \gamma \):

\[ \phi_0 = 0, \quad \theta_0 = \arcsin \gamma, \]

\[ \phi_0 = 0, \quad \theta_0 = \pi - \arcsin \gamma, \quad \gamma \leq 1 \]  

\[ \phi_0 = 0, \quad \theta_0 = \frac{\pi}{2}, \quad \gamma > 1 \]  

(15)

In Figures 1 and 2, we depict the potential as a function of the angles \( \theta \) and \( \phi \). Other parameters are defined to take the following values: \( \gamma = 0.6, \epsilon = 1 \).
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Figure 1. The potential $V$ is depicted as a function of $\theta$ for the following values of parameters:
$\gamma = 0.6$, $c = 1$ and $\phi = 0$.

Figure 2. The potential $V$ is depicted as a function of $\phi$ for $\gamma = 0.6$, $c = 1$ and $\theta = \arcsin \gamma$

For the first two configurations, we have:

\[
\begin{align*}
V & \approx c^2 - \gamma^2 + (1 - \gamma^2)(\theta - \theta_0)^2 + \gamma^2 \phi^2 \\
T & \approx \frac{1}{\alpha} \left( \dot{\theta}^2 + \gamma^2 \dot{\phi}^2 \right) \\
\epsilon & \approx \frac{1}{\alpha} \left( \dot{\theta}^2 + \gamma^2 \dot{\phi}^2 \right) + c^2 - \gamma^2 + (1 - \gamma^2)(\theta - \theta_0)^2 + \gamma^2 \phi^2 - \epsilon_c
\end{align*}
\]

and for the last one:

\[
V \approx c^2 - 2\gamma + 1 + \gamma \phi^2 + (\gamma - 1) \left( \theta - \frac{\pi}{2} \right)^2
\]
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\[ T \approx \frac{1}{\alpha} (\dot{\theta}^2 + \dot{\phi}^2) \] (17)

\[ \epsilon \approx \frac{1}{\alpha} (\dot{\theta}^2 + \dot{\phi}^2) + \epsilon^2 - 2\gamma + 1 + \gamma\phi^2 + (\gamma - 1) \left( \theta - \frac{\pi}{2} \right)^2 - \epsilon_c \] (18)

For \( \gamma < 1 \), we make the following change of variables:

\[ \theta = \theta_0 + \sqrt{\frac{\alpha}{2}} \eta_1 \]
\[ \phi = \sqrt{\frac{\alpha}{2\gamma^2}} \eta_2 \] (18)

If we substitute Eq.(18) in (16), we obtain the following energy function:

\[ \epsilon = \frac{1}{2} \eta_1^2 + \frac{1}{2} \eta_2^2 + \epsilon^2 - \gamma^2 + \frac{\alpha(1 - \gamma^2)}{2} \eta_1^2 + \frac{\alpha}{2} \eta_2^2 - \epsilon_c \] (19)

The above equation represents the energy of two uncoupled harmonic oscillators, thus \( \eta_1 \) and \( \eta_2 \) are the normal coordinates and the normal modes of oscillation are:

\[ \phi \equiv 0, \quad \omega_1 = \sqrt{\alpha(1 - \gamma^2)} \]
\[ \theta \equiv \arcsin \gamma, \quad \omega_2 = \sqrt{\alpha} \] (20)

In Figures 3 and 4, we represent graphically the oscillation modes. As seen in mode 1 (\( \phi \equiv 0 \)), the dipole oscillates about the equilibrium direction \( \vec{e}_q = \hat{\gamma} + \sqrt{1 - \gamma^2} \hat{e}_{iii} \) in a plane parallel to the magnetic field and in mode 2 (\( \theta = \arcsin \gamma \)), the swing is in a plane perpendicular to the magnetic field.

![Diagram](image)

**Figure 3.** Typical directions of mode 1 are represented.

The general solution of the Eq.(19) is:

\[ \eta_1 = A_1 \sin(\omega_1 t + \Delta_1) \]
\[ \eta_2 = A_2 \sin(\omega_2 t + \Delta_2) \] (21)
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Figure 4. Typical directions of mode 2 are represented.

$A_{1,2}$ and $\Delta_{1,2}$ are determined from the initial conditions.

For $\gamma > 1$, the normal coordinates are:

$$
\eta_1' = \sqrt{\frac{\alpha}{2}}(\theta - \frac{\pi}{2})
$$

$$
\eta_2' = \sqrt{\frac{\alpha}{2}}\phi
$$

and the normal modes of oscillation are:

$$
\phi \equiv 0, \quad \omega_1' = \sqrt{\alpha(\gamma - 1)}
$$

$$
\theta = \frac{\pi}{2}, \quad \omega_2' = \sqrt{\frac{\alpha\gamma}{2}}
$$

We have noticed that the normal modes of oscillation do not satisfy the property of isochronism, i.e. the normal frequencies of oscillation depend on the initial conditions.

It is also noteworthy that exact solutions, for the equations of motion (11), have been obtained for all values of $\gamma$ whether $\theta = \theta_0$ (mode 2). Hence, for $\theta = \theta_0$ the Eq.(13) is:

$$
\epsilon = \frac{\gamma^2}{\alpha}\dot{\phi}^2 + c^2 - 2\gamma^2 \cos \phi + \gamma^2 - \epsilon_c, \quad \gamma < 1,
$$

$$
\epsilon = \frac{1}{\alpha}\dot{\phi}^2 + c^2 - 2\gamma \cos \phi + 1 - \epsilon_c, \quad \gamma > 1,
$$

which correspond to the equations of a nonlinear pendulum, whose exact solutions are written in terms of the elliptic Jacobi function[6, 7, 11].

If $\gamma = 0$ and $\phi = 0$ (mode 1), the Eq.(11) also admits exact solution in terms of Jacobi functions. Further, $\dot{\phi} \equiv 0$ and $\theta = \varphi/2$, then Eq.(11) yields:

$$
\epsilon = \frac{1}{4\alpha}\dot{\varphi}^2 + c^2 + \frac{1}{2}(1 - \cos \varphi) - \epsilon_c
$$
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We have again obtained the equation of the nonlinear pendulum.

For \( \gamma = 1 \), the potential \( V \) is completely inharmonious in the generalized coordinate \( \theta \) and the discussion of a case as this goes beyond the scope of the present article.

4. Trapped states

Trapped states exhibit the property of having a mean velocity equal to zero[5, 4]. For the variable of the center of mass, the Eq.(11), means:

\[
\begin{align*}
\gamma_i &= \langle \rho_i \rangle \\
\gamma_{ii} &= \langle \rho_{ii} \rangle \\
\omega_{iii} &= 0,
\end{align*}
\]

where \( \langle \rho_i \rangle, \langle \rho_{ii} \rangle \), means the time average value of the \( \rho_{i,ii} \). The set of Eqs.(31) is satisfied only if the third component of the pseudomomentum is zero, then, a necessary condition for the existence of trapped states is that the center of mass moves in the plane perpendicular to the magnetic field and \( c = \gamma \).

Hereafter, we consider \( \omega_{iii} = 0 \). For \( \gamma < 1 \) and \( \phi \equiv 0 \) (mode 1), the expansions in Taylor series about the equilibrium of the spherical coordinates of Eqs.(12) are:

\[
\begin{align*}
\rho_i &\approx \gamma_i(1 - \frac{\sqrt{1 - \gamma^2}}{\gamma}(\theta - \theta_0) - \frac{1}{2}(\theta - \theta_0)^2) \\
\rho_{ii} &\approx \gamma_{ii}(1 - \frac{\sqrt{1 - \gamma^2}}{\gamma}(\theta - \theta_0) - \frac{1}{2}(\theta - \theta_0)^2)
\end{align*}
\]

Taken into account the Eqs.(18,21):

\[
\begin{align*}
\langle \rho_i \rangle &\approx \gamma_i \left(1 - \frac{A_i^2}{4} \alpha \right) \\
\langle \rho_{ii} \rangle &\approx \gamma_{ii} \left(1 - \frac{A_{ii}^2}{4} \alpha \right)
\end{align*}
\]

From the above equations, it follows that the set of Eqs.(31) only have the trivial solution \( A_i \equiv 0 \), i.e. the relative variable remains at rest. The same result is reached if \( \theta \equiv \theta_0 \) (mode 2).

If \( \gamma = 0 \), the Eqs.(31) are immediately satisfied because of the periodicity of the Jacobi functions and the center of mass is trapped by the magnetic field. For \( \gamma > 1 \), a similar analysis, leads to the conclusion of the absence of trapped states. Similarly, this result demonstrates the absence of trapped states in the neighborhood of the stable equilibrium, except for the particular case \( \gamma = 0 \).

Furthermore, it is intuitively presumed that small oscillations approximation is not valid for energies larger than the energy of the unstable equilibrium (see Figure 1,2), the challenge of finding the relationship between the constants of motion (\( \gamma \) and \( \epsilon \)), which allows the existence of trapped states, still remains[4].

5. Concluding remarks

In the present study, we obtain the normal coordinates and normal modes of oscillation of a rigid dipole in the presence of a uniform magnetic field and investigates the possibility of existence of trapped states to the coordinate of the center of mass in the small oscillations approximation.

The normal mode of oscillation depends strongly on the initial conditions via the parameter \( \gamma \) and violates the isochronous property, inherent to the potentials that depend quadratically on
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the generalized coordinates. Besides, it is shown in the energy range where the small oscillations approximation is applicable, that the coordinate of the center of mass can only be trapped by the magnetic field whether $\gamma = 0$.

We think the system has the following special properties: two degrees of freedom with several stable equilibrium points that depend on the initial conditions, the violation of the property of isochronism present in its normal modes of oscillation and the possibility of existence of trapped states of the center of mass, represents a good challenge to follow studying in the future.

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References
[1] V. V. Volchkov, M. N. Khimich, M. Ya. Melnikov, and B. M. Uzhinov, “A Fluorescence Study of the Excited State Dynamics of Boron Dipyrrin Molecular Rotors,” High Energy Chemistry 47 (2013) 224-229.
[2] Yoshida Y, Shimizu T, Yajima G, Maruta S, Takeda Y, Nakano T, Hiramatsu H, Kageyama H, Yamochi and G Saito, “Molecular Rotors of Coronene in Charge-Transfer Solids,” Chemistry-A European Journal 19 (2013) 12313-12324.
[3] Pursey D L, Sveshnikov N A, Shirokov A M “Electric dipole in a magnetic field: Bound states without classical turning points” Theoretical and Mathematical Physics 117, (1998) 1262-1273
[4] Troncoso P, Curilef S., “Bound and trapped states of an electric dipole in a magnetic field” European Journal of Physics 27 (2006) 1315-1322.
[5] Atenas B., del Pino L. A. and Curilef S. “Classical states of an electric dipole in an external magnetic field: Complete solution for the center of mass and trapped states” Annals of Physics. 350 605-614 (2014)
[6] Curilef S. and Claro F. “Dynamics of two interacting particles in a magnetic field in two dimensions” American Journal of Physics 65 (1997) 244-250.
[7] Escobar-Ruiz M. A., Turbiner A.V. “Two charges on a plane in magnetic field: special trajectories” Journal of Mathematical Physics 54 (2013) 022901.
[8] Gorkov L. P. and Dzyaloshinskii I. E. “Contribution to the theory of the Mott excition in a strong magnetic field” Zh. Eksp. Teor. Fiz. 53 717-722 (1967)
[9] Karlheinz O. “A comprehensive analytical solution of the nonlinear pendulum” European Journal of Physics 32 (2011) 479-490.
[10] P. F. Byrd and M. D. Friedmann “Handbook of Elliptical Integrals for Engineers and Scientists” (New York: Springer, 1971)
[11] M. Abramowitz and I. A. Stegun, “Handbook of Mathematical Functions with Formulas Graphs and Mathematical Tables” (New York: Dover, 1972)
[12] H. Hancock, “Elliptic Integrals” (New York: Dover, 1958)