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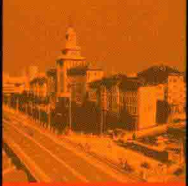
Applications of Quantum and Classical Connections in Modeling Atomic, Molecular and Electrodynamic Systems



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［罗］Popa, A.（波帕） 著

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INTRODUCTION

In the first volume, we presented a review and synthesis of our theoretical work, available until now only in journal articles, in which we establish an exact connection between the quantum and classical equations describing the same system. This connection was proved starting from the basic equations, without using any approximation. For stationary multidimensional atomic and molecular systems, the connection between the quantum and classical equations is based on the fact that the geometric elements of the wave described by the Schrödinger equation, namely the wave surface and their normals, are given by the Hamilton–Jacobi equation. For electrodynamic systems composed of a particle in an electromagnetic field, we established a similar connection using the fact that the Klein–Gordon equation is verified exactly by a wave function that corresponds to the classical solution of the relativistic Hamilton–Jacobi equation.

In this volume, we present applications of the above theory, for the modeling of the properties of atomic, molecular, and electrodynamic systems. In the case of the atomic and molecular systems, whose behavior is described by the Schrödinger equation, the principle of our calculation method is based on the fact that the wave function and geometric elements of the wave described by the Schrödinger equation are mathematical objects which describe the same physical system and depend on its constants of motion. It follows that we can use the geometric elements of the wave, to calculate the energetic values and the symmetry properties of the system. Accuracy of our method is comparable to the accuracy of the Hartree–Fock method, for numerous atoms and molecules.

For electrodynamic systems composed of a particle in an electromagnetic field, the connection between the Klein–Gordon and relativistic Hamilton–Jacobi equation is related to a periodicity property, which leads to an accurate method for studying systems composed of very intense laser fields and electrons or atoms. We present a series of applications of this method, such as the calculation of angular and spectral distributions of the radiations generated at interactions between very intense laser beams and electron plasmas or relativistic electron beams. Our results are in good agreement with experimental data from literature. The study of these systems is particularly important, due to the recent emergence of a new generation of ultraintense lasers, whose applications can be predicted using the model described here.

This volume is structured into three chapters, numbered by 1, 2, and 3. Chapters 1 and 2 present wave models for the calculation of the energies and symmetry properties for atomic and molecular systems, while Chapter 3 presents models for the properties of radiations generated at the interaction between very intense laser beams and electron plasmas, electron beams, or atomic gases. For completeness, in Appendices we include the programs which are used for the numerical calculations. The equations are written in the International System.

This book presents applications of the theoretical models, which are described in the first volume, entitled "Theory of Quantum and Classical Connections in Modeling Atomic, Molecular and Electrodynamic Systems." This volume will be referred as "Volume I" throughout the present book.

CONTENTS

CHAPTER 1

Wave Model for Atomic Systems

Abstract

In the first chapter from Volume I, we have shown that the normal curves C of the wave surface of a system described by the Schrödinger equation, can be used to calculate the constants of motion of the system. We show that the motions of the electrons can be separated, and the projection of the C curve from the R^{3N} space of coordinates on the space x_a, y_a, z_a of the electron e_a, denoted by C_a, can be calculated with the aid of the central field approximation. Our method is similar to the central field method, applied in the frame of the atomic and molecular orbitals model. The energy of the system is calculated with the aid of the Bohr quantization relation, which is valid for the C_a curves. The accuracy of our calculations is comparable to the accuracy of the Hartree–Fock method.

Key Words: wave surface; wave surface normals; Hamilton–Jacobi equation; constants of motion; energetic values; Bohr quantization relation; central field approximation; central field method; geometrical symmetries; periodic solutions

1.1 GENERAL CONSIDERATIONS

In this chapter, we review the applications of the wave model presented in the first chapter of Volume I to the case of atomic systems, which were treated in the papers (Popa, 1998b, 1999b, 2008a, 2009a).

The central idea of our approach is that the wave surface and its normals can be used to study the properties of the system, just as well as the wave function. This is because the wave surface and its normals are mathematical elements of the wave described by Schrödinger equation, and depend on the constants of motion of the system. More specifically, we calculate the curves C_a with the aid of the central field method, in a similar manner as the atomic orbital wave functions

Table 1.1 Values of L and $p_{\theta T}$ for the Atoms Analyzed in This Chapter

Atom	State	Spectral Term	L	$p_{\theta T}$
Helium	$1s^2$	$^1S_0$	0	0
Lithium	$1s^22s$	$^2S_{1/2}$	0	0
Lithium	$1s^22p$	$^2P_{1/2}$	1	$\hbar\sqrt{2}$
Beryllium	$1s^22s^2$	$^1S_0$	0	0
Boron	$1s^22s^22p$	$^2P_{1/2}$	1	$\hbar\sqrt{2}$
Carbon	$1s^22s^22p^2$	$^3P_0$	1	$\hbar\sqrt{2}$
Nitrogen	$1s^22s^22p^3$	$^4S_{3/2}$	0	0
Oxygen	$1s^22s^22p^4$	$^3P_2$	1	$\hbar\sqrt{2}$

Ψ_a are calculated in the frame of the atomic orbital method. This similitude explains the fact that the accuracy of our method is comparable to the accuracy of the Hartree–Fock method. In addition, our calculations lead to symmetry properties of the C_a curves, which are similar to the symmetry properties of the wave function.

In virtue of Eq. (1.52) from Volume I, the curve C corresponds to the same constants of motion as those resulting from the Schrödinger equation. For example, the total angular momentum of the curve C is $p_{\theta T} = \hbar\sqrt{L(L+1)}$, where L is the corresponding quantum number. The value of L can be found from the expression of the spectral term corresponding to a given element, as it results from Table 1.1. Using the data from Landau (1991), in this table we give the spectral terms and the values of L and $p_{\theta T}$ for all the atoms, which will be analyzed in this chapter.

1.2 SOLUTION FOR HELIUM-LIKE SYSTEMS

The helium-like systems (He, Li^+, Be^{2+}, B^{3+}, and so on) are composed of a nucleus and two 1s electrons, which are denoted by e_1 and e_2. The corresponding C_a curves, for $a = 1, 2$, are the periodic solutions of the equations of motion of the electrons. In a Cartesian system of coordinates with origin at nucleus, these equations are:

$$-\frac{K_1 Z\bar{r}_a}{r_a^3} + \frac{K_1(\bar{r}_a - \bar{r}_b)}{|\bar{r}_a - \bar{r}_b|^3} = m\frac{d^2\bar{r}_a}{dt^2} \quad \text{with} \quad a, b = 1, 2 \text{ and } a \neq b \qquad (1.1)$$

where $\bar{r}_a$ is the position vector of the electron e_a and K_1 is given by Eq. (B.3) from Volume I. The system (Eq. (1.1)) has the following solution:

$$\bar{r}_1 = -\bar{r}_2 = \bar{r}, \quad \bar{r}_1 \cdot \bar{k} = \bar{r}_2 \cdot \bar{k} = 0, \quad \bar{v}_1 = -\bar{v}_2 = \bar{v} \tag{1.2}$$

It follows that the motions of the electrons are separated, and the solution of the system (Eq. (1.1)) reduces to the solution of the following equation:

$$-\frac{K_1 Z_a \bar{r}_a}{r_a^3} = m\frac{\mathrm{d}^2\bar{r}_a}{\mathrm{d}t^2}, \quad \text{where} \quad Z_a = Z - s_{12e} \tag{1.3}$$

and $s_{12e} = s_{21e} = 1/4$. Here, Z_a has the significance of an effective order number while s_{12e} and s_{21e} have the significance of reciprocal screening coefficients of the electrons e_1 and e_2.

In virtue of Eq. (1.3), written for $a = 1$ and $a = 2$, we have

$$E_1 = \frac{m}{2}\left(\frac{\mathrm{d}r_1}{\mathrm{d}t}\right)^2 - \frac{K_1 Z_1}{r_1}, \quad E_2 = \frac{m}{2}\left(\frac{\mathrm{d}r_2}{\mathrm{d}t}\right)^2 - \frac{K_1 Z_1}{r_2} \tag{1.4}$$

where E_1 and E_2 are the total energies of the electrons e_1 and e_2. It follows that the total energy is $E = E_1 + E_2$, where, due to the symmetry, $E_1 = E_2$. We note that one half of the electrostatic interaction energy between the two electrons enters in the expression of E_1 through the quantity s_{12e} from the expression of Z_1. The other half of the interaction energy enters in the expression of E_2.

The relation (1.3) is the equation of a motion in central field. It follows that the C_1 curve is an ellipse in the xy plane and, in virtue of Eq. (1.2), the curve C_2 is an ellipse symmetrical to C_1 with respect to the nucleus, as shown in Figure 1.1A.

Since the motions of the electrons are separated, we apply the quantization condition (1.43) from Volume I for the electron e_1 and find its energy, which is E_1. Since its expression is given by Eq. (B.10) from Volume I, we have:

$$E = E_1 + E_2 = 2E_1 = -2R_\infty \frac{Z_1^2}{n_1^2} \tag{1.5}$$

The total angular momentum is:

$$\bar{p}_{\theta\mathrm{T}} = \bar{p}_{\theta 1} + \bar{p}_{\theta 2} = 2\bar{p}_{\theta 1} = p_{\theta\mathrm{T}}\bar{k} \tag{1.6}$$

where $\bar{p}_{\theta 1}$ and $\bar{p}_{\theta 2}$ are the angular moments corresponding to the curves C_1 and C_2, which are equal.

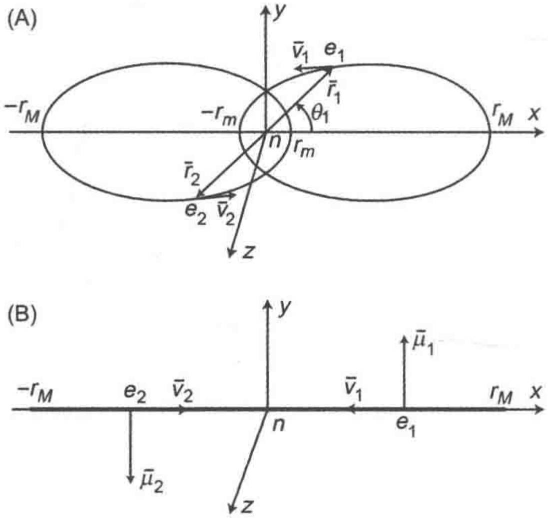

Figure 1.1 (A) C_1 and C_2 curves for helium-like systems. (B) Quasilinear trajectories for the $1s^2$ *states.*

In agreement with the data from Table 1.1, it follows that the angular moments of the C_1 and C_2 curves have negligible values, and we have:

$$p_{\theta 1} = p_{\theta 2} = \varepsilon \quad \text{with} \quad \varepsilon \ll \hbar \tag{1.7}$$

where ε is a very small positive number. It follows that the C_1 and C_2 curves are ellipses with eccentricity e very close to unity, for which the following inequality is strongly fulfilled: $r_m \ll r_M$. These curves are quasilinear along the ox axis, as shown in Figure 1.1B. For these curves, the value of the energy given by Eq. (1.5) must be corrected, taking into account the average spin magnetic interaction energy of the electrons (Gryzinski, 1973):

$$E_{m1s} = -\frac{1}{\tau_1}\int_{\tau_1} \overline{\mu}_1 \overline{B}_2 \, \mathrm{d}t = -\frac{1}{\tau_1}\int_{\tau_1} \overline{\mu}_2 \overline{B}_1 \, \mathrm{d}t \tag{1.8}$$

where τ_1, given by Eq. (B.11) from Appendix B of Volume I, is the period of the electrons motion, while $\overline{\mu}_1$, $\overline{\mu}_2$ and $\overline{B}_1$, $\overline{B}_2$ are, respectively, the magnetic moments and magnetic induction vectors of the two electrons:

$$\mu_1 = \mu_2 = \frac{e\hbar}{2m} \quad \text{and} \quad \overline{B}_2 = \frac{\mu_0}{4\pi}\left[\frac{3\overline{d}(\overline{\mu}_2 \cdot \overline{d})}{d^5} - \frac{\overline{\mu}_2}{d^3}\right] \tag{1.9}$$

a similar relation being valid for $\overline{B}_1$. In the above relations, μ_0 is the magnetic permeability of vacuum and $\overline{d}$ is the vector having its origin on the electron e_2 and the tip on the electron e_1.

In Section 1.3, we prove that E_{m1s} is given by the following relation:

$$E_{m1s} = R_\infty \frac{Z_1^{3/2}}{8n_1^3} \tag{1.10}$$

We use normalized quantities: the energies are normalized to R_∞ and distances to $2a_0$. The normalized quantities are underlined. For example, $\underline{E}_{m1s} = E_{m1s}/R_\infty$. Introducing the correction term $\underline{E}_{m1s}$ in Eq. (1.5), the normalized expression of the total energy becomes:

$$\underline{E} = 2\underline{E}_1 + \underline{E}_{m1s} = -\frac{2Z_1^2}{n_1^2} + \frac{Z_1^{3/2}}{8n_1^3} \tag{1.11}$$

where $Z_1 = Z - 1/4$ and $n_1 = 1$.

The experimental value of the total energy, denoted by E_{exp}, is obtained by summing the two ionization energies of helium. The experimental ionization energies are taken from Lide (2003). In Table 1.2, we give a comparison between the experimental value of the total energy of helium and the theoretical values, calculated with the aid of Eq. (1.11), and in papers from literature, with the aid of the Hartree–Fock method (Slater, 1960; Hartree, 1957; Coulson, 1961).

For ions with the same structure as helium, E_{exp} is the sum of the last two ionization energies. The comparison between the theoretical and experimental values of the total energy for helium and for ions with the same structure is presented in Table 1.3.

1.3 EVALUATION OF THE CORRECTION TERM E_{M1S}

The calculation of E_{m1s} is based on the following assumptions:

(a1.1) The vectors $\overline{\mu}_1$ and $\overline{\mu}_2$ are normal to the *ox* axis, as shown in Figure 1.1B.

(a1.2) The total magnetic moment is equal to zero, corresponding to the $1s^2$ states of helium-like systems.

(a1.3) We suppose that the magnetic forces act only as a perturbation, and it does not change the elliptic character of the C_1 and C_2 curves. When calculating the integral from Eq. (1.8), we approximate these curves by their projections on the *xoy* plane.

Table 1.2 Normalized Values of the Total Energy Calculated by Popa (2008a, 2009a) and in Literature, with the Aid of the Hartree–Fock Method, as Compared to Experimental Values

Atom	$\underline{E}$ (Our Model)	$\underline{E}$ (Literature)	$\underline{E}_{\mathrm{exp}}$
Helium	−5.83562	−5.723359[a]	−5.80692[b]
		−5.7233598[c]	
		−5.7233600[d]	
Lithium ($1s^22s$ state)	−14.9563	−14.8654514[c]	−14.95634[b]
		−14.8654516[d]	
		−14.8654475[e]	
Lithium ($1s^22p$ state)	−14.8174	−14.760174[f] −14.760382[h]	−14.82147[g]
Beryllium	−29.2533	−29.146044[a]	−29.33766[b]
		−29.146042[c]	
		−29.146042[d]	
Boron	−49.1475	−49.058114[c]	−49.3177[b]
		−49.058116[d]	
		−49.058114[e]	
Carbon	−75.5248	−75.377224[c]	−75.7133[b]
		−75.377232[d]	
		−75.377224[e]	
Nitrogen	− 109.018	−108.80185[c]	−109.2266[b]
		−108.80187[d]	
		108.80184[e]	
Oxygen	−149.428	−149.61874[c]	−150.2206[b]
		−149.61879[d]	
		−149.61876[e]	

The values are given in Rydbergs.
[a] *Huzinaga and Aranu (1970).*
[b] *Lide (2003).*
[c] *Clementi and Roetti (1974).*
[d] *Koga et al. (1993).*
[e] *de Castro and Jorge (2001).*
[f] *Ladner and Goddard (1969).*
[g] *Slater (1960).*
[h] *Beebe and Lunell (1975).*

Assumption (a1.3) is sustained by the fact that the attraction force of the nucleus is overwhelmingly dominant over the most part of the trajectory. We have to check that this force is dominant even in the configuration where the Lorentz force has the maximum value in the vicinity of the nucleus.

Table 1.3 Theoretical and Experimental Normalized Values of the Total Energy for Some Atoms and Ions with the Same Structure

Z	2	3	4	5
System	He	Li^+	Be^{2+}	B^{3+}
State	$1s^2$	$1s^2$	$1s^2$	$1s^2$
$\underline{E}$	−5.83562	−14.555	−27.2173	−43.831
$\underline{E}_{\mathrm{exp}}$[a]	−5.806921	−14.56004	−27.31391	−44.07097
System	–	Li	Be^+	B^{2+}
State	–	$1s^22s$	$1s^22s$	$1s^22s$
s_{31e}	–	0.854942	0.824677	0.80852
s_{13e}	–	0.0013792	0.0031737	0.0045637
$\underline{E}$	–	−14.9563	−28.5522	−46.6073
$\underline{E}_{\mathrm{exp}}$[a]	–	−14.956336	−28.65244	−46.85889
System	–	Li	Be^+	B^{2+}
State	–	$1s^22p$	$1s^22p$	$1s^22p$
s_{31e}	–	0.979092	0.956543	0.941069
s_{13e}	–	0.000831799	0.00257599	0.00415845
$\underline{E}$	–	−14.8174	−28.2684	−46.1839
$\underline{E}_{\mathrm{exp}}$[b]	–	−14.82147	−28.36230	−46.41877

The values are given in Rydbergs.
[a] *Lide (2003).*
[b] *Slater (1960).*

In virtue of Eq. (1.6), we obtain the total orbital magnetic moment:

$$\overline{\mu}_{\theta \mathrm{T}} = -\frac{e}{2m}\overline{p}_{\theta \mathrm{T}} = -\frac{e}{m}p_{\theta 1}\overline{k} \tag{1.12}$$

The total magnetic moment is:

$$\overline{\mu}_{\mathrm{T}} = \overline{\mu}_{\theta \mathrm{T}} + \overline{\mu}_1 + \overline{\mu}_2 \tag{1.13}$$

With the aid of assumption (a1.2), we have $\overline{\mu}_{\mathrm{T}} = 0$. We write this relation by components, taking into account Eqs. (1.12), (1.13) and assumption (a1.1), and have $-(e/m)p_{\theta 1}\overline{k} + \mu_{1y}\overline{j} + \mu_{1z}\overline{k} + \mu_{2y}\overline{j} + \mu_{2z}\overline{k} = 0$, from where obtain:

$$\mu_{1z} + \mu_{2z} = \frac{e}{m}p_{\theta 1} \quad \text{and} \quad \mu_{1y} = -\mu_{2y} \tag{1.14}$$

From relation $\mu_1^2 = \mu_{1y}^2 + \mu_{1z}^2 = \mu_2^2 = \mu_{2y}^2 + \mu_{2z}^2$ and Eq. (1.14), we have $\mu_{1z} = \pm \mu_{2z}$. From Eq. (1.14), we have also $\mu_{1z} + \mu_{2z} > 0$, resulting that $\mu_{1z} = \mu_{2z}$. From this relation, together with Eqs. (1.7) and (1.14), we obtain:

$$\mu_{1z} = \mu_{2z} = \frac{e}{2m} p_{\theta 1} \ll \frac{e}{2m} \hbar \tag{1.15}$$

From the first relation of Eqs. (1.9) and (1.15), we have:

$$\mu_{1z} = \mu_{2z} \ll \mu_1 \tag{1.16}$$

Using Eqs. (1.14) and (1.16), we obtain:

$$\bar{\mu}_1 \cong \mu_1 \bar{j} \quad \text{and} \quad \bar{\mu}_2 \cong -\mu_2 \bar{j} \tag{1.17}$$

as shown in Figure 1.1B.

Figure 1.2A shows the forces which act on the electrons, when the electrons approach the nucleus: the forces in the radial direction, $\overline{F}_{r1}$ and $\overline{F}_{r2}$, the Lorentz forces, $\overline{F}_{m1}$ and $\overline{F}_{m2}$, and the repelling forces between the two electrons, $\overline{F}_{e1}$ and $\overline{F}_{e2}$. It results that the C_1 and C_2 curves are slightly different from the elliptic trajectories described by Eqs. (B.1) and (B.2) from Volume I. In Figure 1.2B, we show the projection of these curves on the plane xy, where γ is the angle between the velocity vector $\bar{v}_1$ and the oy axis, corresponding to $\theta_1 = \pi/2$.

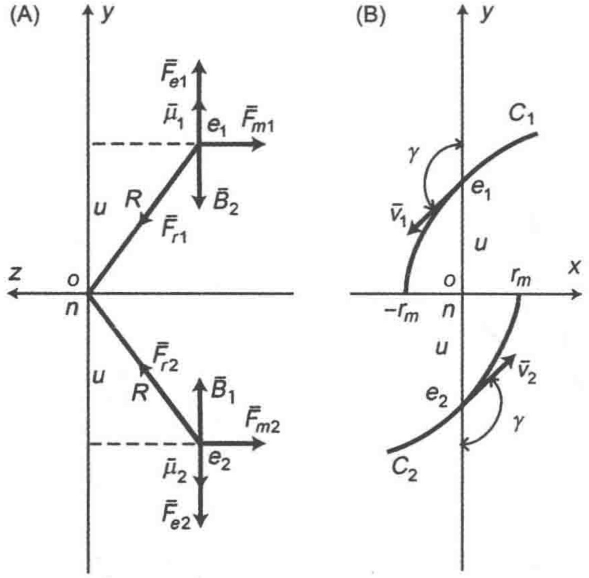

Figure 1.2 (A) Configuration of the electrons in the vicinity of nucleus for $1s^2$ *states. (B) Projection of the* C_1 *and* C_2 *curves on the* xy *plane.*

The C_1 and C_2 curves have a spatial configuration in the vicinity of the nucleus, where the Lorentz forces cannot be neglected. When the electrons e_1 and e_2 move toward the nucleus, the forces $\overline{F}_{m1}$ and $\overline{F}_{m2}$ act in the direction $-\overline{k}$, as illustrated in Figure 1.2A. It follows that the electrons are situated in the domain corresponding to $z<0$. When the electrons move away from the nucleus, the forces $\overline{F}_{m1}$ and $\overline{F}_{m2}$ act in the direction $\overline{k}$, and the electrons are situated in the domain for which $z>0$.

In virtue of assumption (a1.3), we approximate the C_1 and C_2 curves by their projections on the xy plane. From Eq. (1.2), we have $\overline{r}_1 = -\overline{r}_2$. For simplicity, we write $\overline{r}_1 = \overline{r}$ and $\theta_1 = \theta$. From these relations, together with Eqs. (1.8) and (B.1) from Volume I, we have:

$$E_{m1s} = -\frac{1}{\tau_1}\int_{\tau_1} \overline{\mu}_1 \overline{B}_2 \, \mathrm{d}t = -\frac{2}{\tau_1}\sqrt{\frac{m}{2|E_1|}}\int_{r_m}^{r_M} \overline{\mu}_1 \overline{B}_2 \frac{r\,\mathrm{d}r}{\sqrt{(r_M - r)(r - r_m)}} \tag{1.18}$$

From assumption (a1.3), we can write $\overline{d} \cong 2\overline{r}_1 = 2\overline{r}$. From this relation, together with Eqs. (1.9) and (1.18), we have:

$$E_{m1s} = -\frac{2}{\tau_1}\cdot\frac{\mu_0}{4\pi}\sqrt{\frac{m}{2|E_1|}}\int_{r_m}^{r_M}\left[\frac{12(\overline{r}\cdot\overline{\mu}_1)(\overline{r}\cdot\overline{\mu}_2)}{(2r)^5} - \frac{\overline{\mu}_1\cdot\overline{\mu}_2}{(2r)^3}\right]\frac{r\,\mathrm{d}r}{\sqrt{(r_M - r)(r - r_m)}} \tag{1.19}$$

We have $\overline{r} = r\cos\theta\overline{i} + r\sin\theta\overline{j}$, and from Eq. (1.17), we obtain $\overline{r}\cdot\overline{\mu}_1 = r\mu_1\sin\theta$, $\overline{r}\cdot\overline{\mu}_2 = -r\mu_2\sin\theta$, and $\overline{\mu}_1\cdot\overline{\mu}_2 = -\mu_1^2$. On the other hand, from Eq. (B.8) of Volume I, we have $|E_1| = (K_1 Z_1)/r_M$. Introducing these relations in Eq. (1.19), we have:

$$E_{m1s} = \frac{\mu_1^2}{4\tau_1}\frac{\mu_0}{4\pi}\sqrt{\frac{m r_M}{2K_1 Z_1}}I \quad \text{where} \quad I = \int_{r_m}^{r_M}\frac{(2 - 3\cos^2\theta)\mathrm{d}r}{r^2\sqrt{(r_M - r)(r - r_m)}} \tag{1.20}$$

In Appendix A, we prove that the processing of Eq. (1.20) leads to the expression of the correction term E_{m1s}, which is given by Eq. (1.10).

1.4 SOLUTION FOR LITHIUM-LIKE SYSTEMS

1.4.1 The States $1s^2 2s$

The lithium-like systems (Li, Be^+, B^{2+}, C^{3+}, and so on) are composed of a nucleus and three electrons. The 1s electrons are denoted by e_1 and e_2 while the 2s electron is denoted by e_3.

We consider the following assumptions (Gryzinski, 1973; Popa, 2008a):

(a1.4) The motion of the 1s electrons is like in the helium atom, and it is not influenced significantly by the motion of the 2s electron. This assumption is strongly sustained by the fact that the mean distance between a 1s electron and nucleus is much smaller than the mean distance between the 2s electron and nucleus. The C_1 and C_2 curves corresponding to the 1s electrons are quasilinear. In a Cartesian system of coordinates with origin at nucleus (Figure 1.3), we have $r_1 = r_2$, $r_{m1} \cong 0$, and $r_{m2} \cong 0$. They are situated in the plane *xoy*, very close to the *ox* axis, as illustrated in Figure 1.3A.

(a1.5) The 2s electron has a quasilinear motion, and the C_3 curve is situated in the plane *yoz*, very close to the *oy* axis. The following relation is valid: $r_{m3} \cong 0$. The assumption is sustained by the fact that for this configuration the energy of the system is minimum.

Our solution of the equations of the electron motion is based on a central field method, which has the following stages.

1.4.1.1 Definition of the Screening Coefficients

Since the motions of the e_1 and e_2 electrons are symmetrical, the equation of the energy can be written as:

$$E = -\frac{ZK_1}{r_3} + \frac{m}{2}\left(\frac{\mathrm{d}r_3}{\mathrm{d}t}\right)^2 + \frac{2K_1}{\sqrt{r_1^2 + r_3^2}} + 2\left[-\frac{(Z - s_{12e})K_1}{r_1} + \frac{m}{2}\left(\frac{\mathrm{d}r_1}{\mathrm{d}t}\right)^2\right] \tag{1.21}$$

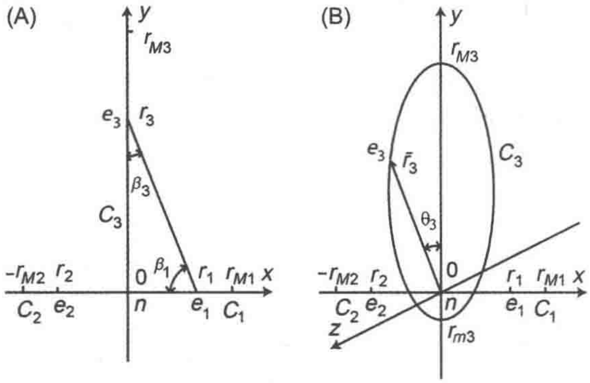

Figure 1.3 Configuration of the curves C_1, C_2, and C_3 for the $1s^22s$ *(A) and* $1s^22p$ *(B) states of lithium.*