APPLICATION OF CLASSICAL MECHANICS FOR THE DETERMINATION OF ENERGY LEVELS IN HELIUM ATOMS

THESIS

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By

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To

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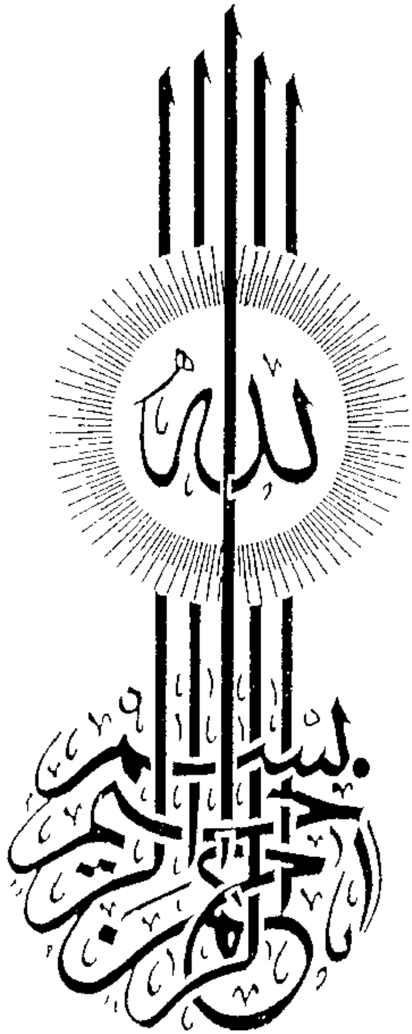
TO MY FATHER

TO MY HUSBAND

AND TO MY DAUGHTERS


بسم الله الرحمن الرحيم

ABSTRACT

Using Einstein-Brillouin-Keller quantisation, the semi-classical treatment based on the first-order perturbation of the energy levels of the Helium atom has been applied for different values of quantum numbers. Results show an agreement with the quantal approach (first order perturbation). Different classical models for the atom have been considered corresponding to different atomic levels. The pattern of these models is discussed. For the non overlapping case an analytical formula is obtained, while the partial and total overlapping cases are calculated numerically. The effect of Maslov's number in the calculation of the energy levels is also discussed.

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CONTENTS

INTRODUCTION

INTRODUCTION

The study of atomic structure and atomic collision problems require a precise estimation of the ground-state and excited-states energies. Various methods have been used quantum mechanically such as the perturbation theory and Ritz variational method, for the calculation of binding energy for the two electron system.

On the other hand, classically, Leopold, Percival and Tworkowski (1980) developed a semiclassical method which depends on the first order perturbation theory (FOP), based on a theory developed by Percival (1971, 1977). Also they obtained and applied a semiclassical equivalent of the Hylleraas (1928, 1929) variational method for helium atom. The accuracy is comparable to the early quantal results of Hylleraas (1929) and Eckart (1930).

In the historical development for the classical model of the He atom, many trials have been done to construct quantum mechanical models for the ground-state helium atom. The first picture was the Bohr model (1913) in which the two electrons are assumed to revolve about the nucleus at the extremities of a diameter as shown in figure 1.

Secondly, in 1921 Langmiur changed the Bohr idea of circular orbit into semicircular orbits. The two electrons here are symmetrically situated with respect to an axis passing through the nucleus as shown in figure 2.

In the work of Lande', Frank and Reiche (Van Velck, 1922) the electrons have more complicated orbits of unequal size, which are coplanar only in Lande's model as described in figure 3.

Again Langmiur changed his semicircular model to a double circle model. In this model, each electron revolve in a separate circle such that the two circles lie in two parallel planes (figure 4). Some reformation are also introduced taking the symmetrical and the other previous shapes into consideration but all of them are incorrect if Sommerfeld action integrals for the principal and azimuthal quantum numbers are accepted.

Finally, Kramers (1923) obtained the energies of a non-planar model first proposed by Bohr as shown in figure 5 (Born 1927) with circular orbits. This is closest to our model (figure 8). Unfortunately, all the previous models fail to produce acceptable results for ground-state energy for helium because of the choice of integer value for orbital angular momentum. Einstein-Brilleuin-Keller (1958) or (EBK) quantisation imposes the unique value for orbital and total angular momenta for unperturbed system. It is given by a half-odd-integer multiple of $\hbar$. So the eccentricity of each electron orbit in the EBK unperturbed model is given by

$$\varepsilon = (1 - I_{\ell}^{2}/I_{n}^{2})^{\frac{1}{2}} = (1 - \tfrac{1}{4})^{\frac{1}{2}} = \sqrt{3}/2$$

and the angle between the orbits is 120°, as in Kramers model.

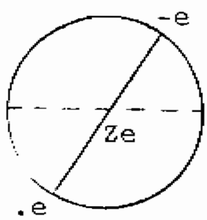

Fig. (1)
Bohr (1913)

E_1 = (3.063) a.u.

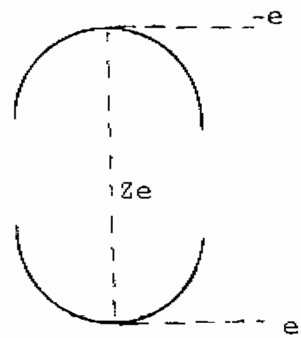

Fig. (2)
Langmuir (1921)a

E_1 = (-2.17) a.u.

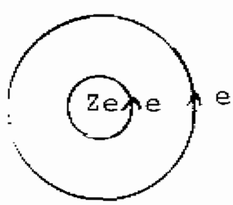

Fig. (3)
Lande (1922)

E_1 = (-2.7) a.u.

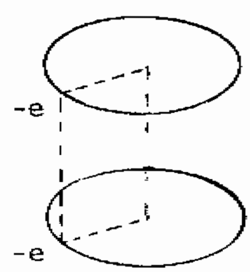

Fig. (4)
Langmuir (1921)b

E_1 = (2.3) a.u.

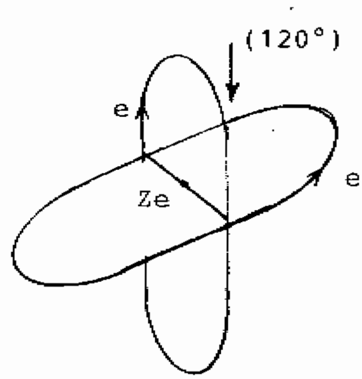

Fig. (5)
Bohr-Kramers (1923)

E_1 = (-2.76) a.u.

In table I, we show the different values of the ground-state energy obtained by these different models. Also in this table, we mentain the year of each work to clarify the historical background for this atomic calculation of energy.

Table 1

Ground-state energy values for different models for helium.

Year	Method	Model	Ground state energy in a.u
1913	Classical	Bohr, Fig. 1	-3.063
1921_a	Classical	Langmuir, Fig. 2	-2.17
1921_b	Classical	Langmuir, Fig. 4	-2.31
1922	Classical (Van Vleck)	-----	-2.765
1022	Experimental (Franck)	-----	-2.909
1923	Classical	Bohr-Kramers, Fig.5	-2.762
1928	Variational (quantal), (Hylleraas)	1 parameter	-2.8476
1929	Variational (quantal), (Hylleraas, Kinoshita)	38 parameters	-2.9037
1977	Experimental (Herzberg)	-----	-2.9037
1979_a	Semiclassical (FOP), (Leopold et al 1980)	EBK, quantisation	-2.7410
1979_b	Semiclassical(variation), (Leopold and Percival)	EBK, quantisation	-2.8407

In this thesis we will use Leopold and Percival (1980) semiclassical perturbation method which can be summarized and described as follows :

(1) This method is developed by using semiclassical quantisation which leads to analyticals first order perturbation formula.

(2) It is also developed by using concepts suggested by the analogous quantal theory.

(3) It is successfuly applied for both ground-state and doubly excited states of helium atom and helium like-ions. These doubly excited states are frequently known as Reasonance states.

In particular, this method has proved to be effective for high Rydberg states (HRS) i.e.states with high quantum numbers (Percival and Richards 1975, Banks and Leopold 1973).

On the other hand, pure quantum mechanical methods are lengthy and tedius to apply for those HRS (Percival 1977a). The difficulties of semiclassical quantisation of non-separable systems have been removed through (EBK) approximation and Maslov work in 1972.

Therefore, it is easy to carry out the precise calculation using the semiclassical method and facilitate the comparison between semiclassical and quantal results (FOP) for the energy of the atom.

In this thesis, we emphasize on the calculation of binding energy of the He atom, in its ground and different excited states using the Leopold et al (1980) semiclassical model. In addition, we calculate some of those binding energies quantum mechanically, for the purpose of comparison with the semi-classical theory.

In order to test the validity of this semi-classical method, for ground and excited states of He atom, we compare the radial and angular integrals separately.

Although, Leopold et al semi-classical model depends mainly on the treatment of the angular part semi-classically or more specifically the formalism of $1/r_{12}$ semi-classically, the energies do not different drastically.

The agreement of the energies is a clear manifestation that Leopold et al semi-classical model can be considered as a powerfull simple method for the calculation of binding energy especially for HRS of He atom compared with the Hylleraas variational method, in which tens of parameters were used.

In chapter I : we will give a brief review on the theoretical method of energy calculation using the semi-classical perturbation theory. Our formulation of the ground state and many excited states energies using this semi-classical method are presented.

In chapter 2 : we present the quantum mechanical perturbation theory together with our formulation of the He atom energies.

In chapter 3 : A comparison between semi-classical and quantum mechanical results is presented. Also discussion and comments on the obtained results are investigated, the tables of comparison are included.

The Gaussian quadrature formula (Francis, S. 1982), Demiovich and Maron (1973) is explained in appendix A, the Clebsch Gorden coefficients (Rose (1968), Richard and Liboff (1980)) are explained in appendix B, and some important integrals used in our calculation are presented in appendix C (Tables of integrals, Herbert Bristol Dwight).

CHAPTER 1

SEMI-CLASSICAL PERTURBATION THEORY OF THE HELIUM ATOM