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Differential Geometry of Atomic Structure and the Binding Energy of Atoms

R. RAMANNA AND S. JYOTHI

Bhabha Atomic Research Centre, Bombay, India

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Abstract

The geometric theory of partial differential equations due to E. Cartan is applied to atomic systems in order to solve the many-body problems and to obtain the binding energies of electrons in an atom. The procedure consists in defining a Schrödinger equation over an Euclidean patch which overlaps with other Euclidean patches in a specified way to form a manifold. If the energy of the system has to be a minimum, it is shown using the Dirichlet principle that the coordinate systems are related by the Cauchy-Riemann relations. The invariance of the Schrödinger equations in the overlapping region leads to a nonlinear second-order equation which is invariant to automorphic transformations and whose solutions are doubly periodic functions. There are only two possible single-valued solutions to this nonlinear partial differential equation and these correspond to lattices of points in the complex space, which are (a) corners of an array of equilateral triangles, and (b) corners of an array of isosceles right-angled triangles. The first solution was used in an earlier work to derive many static properties of nuclei. In this paper it is shown that the second solution gives binding energies of atoms in agreement of about 3% for the few experimental points that are available and also in good agreement with the binding energies of atoms obtained by the perturbation theory. It is also shown that this lattice under certain approximations is equivalent to a pure Coulomb law and the Bohr orbits of the hydrogen atom are correctly predicted. In obtaining the binding energies of atoms, no free parameters are required in the theory, except for the value of the binding energy of the ^{4}He atom, as the theory is developed only for spinless systems. All other constants turn out to be fundamental constants.

It was shown in earlier papers (Ramanna, 1968; Ramanna & Jyothi, 1969) that many of the static properties of nuclei could be accounted for by studying the differential geometry of nuclear space using the geometric theory of partial differential equations due to E. Cartan. This was done by considering a system of Schrödinger equations, each representing a nucleon having its own Euclidean coordinate system. Two such equations are related to one another by the overlap of their respective coordinate systems, i.e. by an appropriately defined manifold. If in the region of overlap, the coordinates of the two systems are related to one another by the Cauchy-Riemann relations, the energy of the system in ground state can be obtained through the Dirichlet principle. The invariance of the equations in any two overlapping systems leads to a non-linear partial differential equation whose solutions are doubly periodic functions, giving rise to a specific geometry in complex space which determines the nature of interaction responsible for the binding of the system.

The method is an extremely general one and can be applied to any system obeying a set of Schrödinger equations and the description of a specific system depends on the choice of doubly-periodic functions satisfying the non-linear differential equation. In the case of nuclei in the ground state, for stable systems, these functions turned out to be equianharmonic Weierstrass functions, giving a geometry which leads to a lattice of points forming the corners of equilateral triangles in complex space and the static properties of nuclei were obtained by linear mapping of those complex points onto the real line (Ramanna & Jyothi, 1969). In this paper the same procedure is applied to a system of electrons held together in the Coulomb field of a nucleus. We show that in this case, the mapping functions turn out to be simple Jacobian elliptic functions which lead to a lattice of points which are the corner of squares corresponding to the lemniscate Weierstrass functions. There are in fact only two distinct types of mappings possible where the solutions are single-valued functions, and it seems that these lead respectively to the only known stable quantum systems, with two different laws of interaction, one electromagnetic and the other nuclear (strong interaction).

It is shown in this paper that it is possible to predict the periodic table of elements and obtain the total binding energy of atoms directly without recourse to perturbation theory, and with only one constant, that being the binding energy of the electrons of the He atom. This fixed constant is required as the present theory is developed only for spinless systems. The agreement with the few experimental points is remarkable, the difference being of the order of 3%. The predictions are also in good agreement with those based on the Thomas-Fermi model and the more recent calculation of Foldy (1951).

The principle of the new approach to the solution of many-body problems described here consists of looking at the many-body system simultaneously from several coordinate systems each of which can be mapped into one another by some appropriate functions. Any of the several coordinate systems can be chosen to be the basis of the description of the system. The fact that in each of the coordinate systems the same phenomena are observed, i.e. the description are invariant, leads to a correct description of the system, if the appropriate mapping functions between the coordinate systems are known.

Consider two Schrödinger equations, one describing a proton and another an electron, each moving in a potential V_1 and V_2 respectively. Let the coordinate system of the proton be described by (x_1, t_1) and that of the electron by (x_2, t_2) where x_1 and t_1 are the space and time coordinates of the proton system and x_2 and t_2 similarly for the electron. The potentials V_1 and V_2 are in general functions of (x_1, t_1) and (x_2, t_2) respectively. We restrict the discussion to one-dimensional systems which in special cases correspond to spherically symmetrical systems. If m_1 and m_2 are the masses of the proton and electron respectively, we have

$$\frac{\hbar^2}{2m_1}\frac{\partial^2\psi_1(x_1,t_1)}{\partial x_1^2} + V_1(x_1,t_1)\psi_1(x_1,t_1) = \frac{i\hbar\,\partial\psi_1}{\partial t_1}(x_1,t_1) \tag{1}$$

$$\frac{\hbar^2}{2m_2}\frac{\partial^2\psi_2(x_2,t_2)}{\partial x_2^2} + V_2(x_2,t_2)\psi_2(x_2,t_2) = \frac{i\hbar\,\partial\psi_2}{\partial t_2}(x_2,t_2) \tag{2}$$

The coordinates x_1, x_2, t_1 and t_2 are related to one another thus.

Let

$$p = \frac{\partial x_1}{\partial x_2} = \frac{\partial t_1}{\partial t_2} \quad \text{and} \quad q = \frac{\partial x_1}{c\,\partial t_2} = -c\frac{\partial t_1}{\partial x_2}$$

which implies

$$\frac{\partial p}{\partial x_1} = \frac{1}{c}\frac{\partial q}{\partial t_1} \quad \text{and} \quad \frac{\partial q}{\partial x_1} = -\frac{1}{c}\frac{\partial p}{\partial t_1} \tag{3}$$

We multiply all quantities involving time by c the velocity of light to make p and q dimensionless quantities. These relations as shown by Ramanna & Jyothi (1969) and in Appendix II ensure that the total interaction energy of the system is minimised.

Let

$$\psi_2(x_2,t_2) = \omega(x_1,t_1)\,\psi_1(x_1,t_1) \tag{4}$$

where $\omega(x_1, t_1)$ is some complex valued function of x_1 and t_1. In the following discussion we consider cases where ω is purely a function of space only.

Eliminating ψ_2 and ψ_1 by putting (3) and (4) in (1) and (2) and by separating the purely space-dependent part and the time-dependent part and setting them each equal to zero, we get (Appendix I)

$$p\frac{\partial^2 p}{\partial x_1^2} - \frac{1}{2}\left(\frac{\partial p}{\partial x_1}\right)^2 - \frac{2c^2}{\hbar^2 q^2}(m_2 - m_1 p)\left[m_1 p^3 - m_2(p^2 + 2q^2)\right]$$
$$- \frac{2i}{\hbar p q}\frac{\partial p}{\partial x_1}\left[m_1 p^3 - m_2(2p^2 + q^2)\right] = \frac{4}{\hbar^2}(m_2 V_2 - m_1 V_1 p^2) \tag{5}$$

If the potentials V_2 and V_1 are real, we can set the imaginary part of equation (5) equal to 0, giving

$$m_1 p^3 - m_2(2p^2 + q^2) = 0 \tag{6}$$

and

$$p\frac{\partial^2 p}{\partial x_1^2} - \frac{1}{2}\left(\frac{\partial p}{\partial x_1}\right)^2 - 2c^2\frac{(m_2 - m_1 p)}{\hbar^2 q^2}\left[m_1 p^3 - m_2(p^2 + 2q^2)\right]$$
$$= \frac{4}{\hbar^2}(m_2 V_2 - m_1 V_1 p^2) \tag{7}$$

Eliminating q from (7) using (6) we get

$$p\frac{\partial^2 p}{\partial x_1^2}-\frac{1}{2}\left(\frac{\partial p}{\partial x_1}\right)^2-\frac{2m_2c^2}{\hbar^2}\frac{(m_2-m_1p)(3m_2-m_1p)}{(2m_2-m_1p)} = \frac{4}{\hbar^2}(m_2V_2-m_1p^2V_1) \quad (8)$$

Equation (8) is a non-linear differential equation which is invariant to automorphic transformations and whose solutions are usually doubly periodic functions (Davis, 1961).

Let

$$m_2=\mu m_1, \qquad \text{where } \mu=\frac{1}{1836}$$

We write

$$S=\frac{m_2V_2}{m_1V_1}, \qquad L=\frac{2m_1m_2c^2}{\hbar^2} \qquad \text{and} \qquad M=\frac{4m_1e^2}{\hbar^2} \quad (9)$$

where c is the velocity of light and its value is taken to be 1. In the region of invariance, we consider V_2/V_1 to be a constant since both V_1 and V_2 measure the same potential except that they are measured in two different coordinate systems. Equation (8) becomes

$$-\left[p\frac{\partial^2 p}{\partial x_1^2}-\frac{1}{2}\left(\frac{\partial p}{\partial x_1}\right)^2\right]\frac{1}{p^2-S}-\frac{L(p-\mu)(p-3\mu)}{(p-2\mu)(p^2-S)}=\frac{M}{e^2}V_1 \quad (10)$$

We now show that under certain circumstances V_1 approximates to an e^2/x_1 law.

We note that

$$\frac{2L}{M}=\frac{1}{r_0} \qquad \text{and} \qquad \frac{L}{M^2}=\frac{\mu}{8}\frac{\alpha_H}{r_0}$$

where

$$\alpha_H \text{ (the radius of the first Bohr orbit)} = \hbar^2/m_2e^2$$

and

$$r_0 \text{ (the classical electron radius)} = e^2/m_2c^2$$

Let us assume that

$$p=A\exp\left(-\mu\,\mathrm{sn}\frac{4Kx_1}{n\alpha_H}\,\mathrm{dn}\frac{4Kx_1}{n\alpha_H}\right)+B \quad (11)$$

is a solution of equation (10), where A and B are two constants chosen suitably, K is the complete elliptical integral of the first type with modulus $1/\sqrt{2}$ and n is an integer which as we see later corresponds to the various excited states with $n=1$ corresponding to the ground state. The elliptic functions

$$\mathrm{sn}\left[\frac{4Kx_1}{n\alpha_H},\frac{1}{\sqrt{2}}\right]\mathrm{dn}\left[\frac{4Kx_1}{n\alpha_H},\frac{1}{\sqrt{2}}\right]$$

with modulus $= k = k' = \sin 45° = 1/\sqrt{2}$ have been chosen as they generate a lattice on the complex plane with its points forming the corners of squares; any selection of these points forming an isosceles right-angled triangle can be mapped on to a real line by means of a single-valued analytical function. In fact triangles (Kober, 1957) with angles (a) $\pi/2$, $\pi/4$, $\pi/4$, (b) $2\pi/3$, $\pi/6$, $\pi/6$, (c) $\pi/2$, $\pi/3$, $\pi/6$ and (d) $\pi/3$, $\pi/3$, $\pi/3$ are the only cases where a triangle can be mapped into a half-plane by an analytic function which is single-valued. The triangles of the type (b), (c) and (d) can be arranged to form a lattice of points which are the corners of a Rhombus and the triangles of the type (a) form a lattice of points which are the corners of a square. The mapping corresponding to an equilateral triangle was used in the nuclear case and that of a right-angled isosceles triangle is used in the present study of atomic structure.

As shown below, the choice of the right-angled isosceles triangle in the present case leads to the Bohr periodic table and predicts correctly the many-body binding energy of atoms. Besides, under certain approximations, it can be shown to lead to the usual Coulomb law of interaction. In view of these successes and that of the nuclear case where two states, one for a neutral particle and the other for a particle with a charge, are predicted, it seems reasonable to conjecture that the equilateral triangle lattice corresponds to strong interactions and the isosceles right-angled triangles to electromagnetic interactions. It is to be noted that these are the only two stable systems with two different kinds of interaction.

In equation (11) since $\mu \ll 1$ we can approximate

$$\exp\left(-\mu \operatorname{sn}\frac{4Kx_1}{n\alpha_H}\operatorname{dn}\frac{4Kx_1}{n\alpha_H} \text{ to } 1-\mu \operatorname{sn}\frac{4Kx_1}{n\alpha_H}\operatorname{dn}\frac{4Kx_1}{n\alpha_H}\right)$$

Considering only those values of x_1 for which the expansion

$$\operatorname{sn} U \operatorname{dn} U = U - \frac{U^3}{3} + \cdots$$

is valid and retaining terms of first order only we can write

$$p = \frac{-4KA\mu x_1}{n\alpha_H} + A + B$$

The values of A, B determine the nature of the interaction and it is shown that for

$$\frac{-4KA\mu}{n\alpha_H} = -\frac{L}{M} \quad \text{and} \quad A + B = \frac{-L}{2M^2}$$

i.e. for

$$A = \frac{n\alpha_H}{4K\mu}\frac{L}{M} = \frac{n}{8K\mu}\frac{\alpha_H}{r_0} \quad \text{and} \quad A + B = \sqrt{S} = \frac{-\mu}{16}\frac{\alpha_H}{r_0} \qquad (12)$$

where $S=\mu(V_2/V_1)$, V_1 approximates to a e^2/x_1 law. It is easily verified that $2KA\mu/n\alpha_H=-M(A+B)$ and $\mu \ll A+B$. Also that

$$B=\frac{-\alpha_H}{r_0}\left(\frac{K\mu^2+2n}{16K\mu}\right) \tag{13}$$

Substituting for p in equation (10), we get

$$\frac{8K^2A^2\mu^2}{n^2\alpha_H^2}-\frac{L\left\{\dfrac{-4KA\mu x_1}{n\alpha_H}+A+B-\mu\right\}\left\{\dfrac{-4KA\mu x_1}{n\alpha_H}+A+B-3\mu\right\}}{\left\{\dfrac{-4KA\mu x_1}{n\alpha_H}+A+B-2\mu\right\}}$$
$$=\frac{MV_1}{e^2}\left\{\frac{16K^2A^2\mu^2x_1^2}{n^2\alpha_H^2}-\frac{8KA\mu(A+B)}{n\alpha_H}+(A+B)^2-S\right\}$$

As $\mu \ll (A+B)$ terms like $A+B-2\mu$, $A+B-3\mu$, $A+B-\mu$ can be replaced by $A+B$ in each case and we get

$$\frac{8K^2A^2\mu^2}{n^2\alpha_H^2}-L\left(\frac{-4KA\mu x_1}{n\alpha_H}+A+B\right)$$
$$=\frac{MV_1}{e^2}\frac{4KA\mu x_1}{n\alpha_H}\left(\frac{4KA\mu x_1}{n\alpha_H}-2(A+B)\right)$$

This simplifies to

$$M\left(\frac{4KA\mu x_1}{n\alpha_H}-2(A+B)\right)=\frac{MV_1x_1}{e^2}\left(\frac{4KA\mu x_1}{n\alpha_H}-2(A+B)\right)$$

Since this is true for all x_1, $V_1=e^2/x_1$. From equation (3) we have

$$x_2=\int\frac{dx_1}{p}$$

Substituting for p from equation (11) we get

$$x_2=\int\frac{dx_1}{p}=\int\frac{dx_1}{\{A\exp[-\mu\,\mathrm{sn}(4Kx_1/n\alpha_H)\,\mathrm{dn}(4Kx_1/n\alpha_H)]+B\}} \tag{14}$$

from equations (12) and (13), it follows that $B\simeq A$ so that

$$\sqrt{S}=A+B\simeq 2B \qquad \text{and} \qquad \left|\frac{A\mu}{2B}\right|=\left|\frac{-2n\mu}{2(K\mu^2+2n)}\right|<1$$

Since $\mu \ll 1$, we can approximate

$$\exp\left(-\mu\,\mathrm{sn}\frac{4Kx_1}{n\alpha_H}\,\mathrm{dn}\frac{4Kx_1}{n\alpha_H}\right) \text{ to } \left(1-\mu\,\mathrm{sn}\frac{4Kx_1}{n\alpha_H}\,\mathrm{dn}\frac{4Kx_1}{n\alpha_H}\right)$$

From equation (13) we get

$$x_2 = \int \frac{dx_1}{(A+B) - A\mu \operatorname{sn}(4Kx_1/n\alpha_H)\operatorname{dn}(4Kx_1/n\alpha_H)}$$

viz.

$$x_2 = \frac{1}{A+B}\int \frac{dx_1}{[1-(A\mu/A+B)\operatorname{sn}(4Kx_1/n\alpha_H)\operatorname{dn}(4Kx_1/n\alpha_H)]}$$

Since

$$\frac{A\mu}{A+B} \simeq \frac{A\mu}{2B} \ll 1$$

we get

$$x_2 = \frac{1}{\sqrt{S}}\int\left(1+\frac{A\mu}{\sqrt{S}}\operatorname{sn}\frac{4Kx_1}{n\alpha_H}\operatorname{dn}\frac{4Kx_1}{n\alpha_H}\right)dx_1$$

i.e.

$$x_2 = \frac{x_1}{\sqrt{S}} - \frac{n\alpha_H}{4K}\frac{A\mu}{S}\operatorname{cn}\frac{4Kx_1}{n\alpha_H} + Q \tag{15}$$

where Q is a constant of integration.

We define the radius of the Bohr orbit as the distance between the origins of the two overlapping coordinate systems measured in one of the systems:

If $(x_2)_{x_1=0}$ is the distance measured in the x_2 system for the point corresponding to $x_1=0$ in the x_1 system and $(x_1)_{x_2=0}$ is the distance measured in the x_1 system for the point corresponding to $x_2=0$ in the x_2 system, then from equation (15) we have

$$(x_2)_{x_1=0} = \frac{-A\mu}{S}\frac{n\alpha_H}{4K} + Q$$

and

$$\frac{(x_1)_{x_2=0}}{\sqrt{S}} = \frac{A\mu}{S}\frac{n\alpha_H}{4K}\operatorname{cn}\left[\frac{4K}{n\alpha_H}(x_1)_{x_2=0}\right] - Q$$

Therefore

$$(x_2)_{x_1=0} + \frac{(x_1)_{x_2=0}}{\sqrt{S}} = -\frac{n\alpha_H}{4K}\frac{A\mu}{S}\left[1-\operatorname{cn}\left\{\frac{4K}{n\alpha_H}(x_1)_{x_2=0}\right\}\right] \tag{16}$$

The left-hand side of this equation is 0, since the two distances measured in the two coordinate systems are equal and opposite except, for a normalisation constant $1/\sqrt{S}$. That this constant is $1/\sqrt{S}$ is seen from equation (11) where if $x_1 = \alpha_H$, then

$$p_{(x_1=\alpha_H)} = \left(\frac{\partial x_1}{\partial x_2}\right)_{x_1=\alpha_H} = A + B = \sqrt{S}$$

Since

$$\mathrm{cn}\left[\frac{4K}{n\alpha_H}(x_1)_{x_2=0}\right]=1$$

i.e. $4K/n\alpha_H(x_1)_{x_2=0}=4nK$, we get

$$(x_1)_{x_2=0}=n^2\alpha_H \tag{17}$$

which is the usual expression for the Bohr orbits.

In the above discussion we have considered only two Schrödinger equations, one representing a proton and the other an electron. We now extend it to a system which has many electrons around a central Coulomb field arising from the protons in the nucleus. We, therefore, have for the nucleus of the system with a charge Ze and mass M_{nuc}.

$$\frac{\hbar^2}{2M_{\mathrm{nuc}}}\frac{\partial^2\psi_1(x_1,t_1)}{\partial x_1{}^2}+V_1(x_1,t_1)\psi_1(x_1,t_1)=i\hbar\frac{\partial\psi_1}{\partial t_1}(x_1,t_1)$$

and similar such equations for the other pairs between the nucleus and each of the other electrons. For each pair of electrons we have

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi_2(x_2,t_2)}{\partial x_2{}^2}+V_2(x_2,t_2)\psi_2(x_2,t_2)=i\hbar\frac{\partial\psi_2}{\partial t_2}(x_2,t_2)$$

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi_3(x_3,t_3)}{\partial x_3{}^2}+V_3(x_3,t_3)\psi_3(x_3,t_3)=i\hbar\frac{\partial\psi_3}{\partial t_3}(x_3,t_3)$$

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi_N(x_N,t_N)}{\partial x_N{}^2}+V_N(x_N,t_N)\psi_N(x_N,t_N)=\frac{i\hbar\,\partial\psi_N(x_N,t_N)}{\partial t_N} \tag{18a}$$

where m is the mass of the electron.

In this many-particle system, the physical meaning of x_1, x_2 etc. can be given the following interpretation. Equation (18a) represents the motion of the nucleus with the origin of the coordinate systems at some average point determined by all the other electrons in whose field the nucleus moves. Similarly (18b) describes the motion of the first electron with the origin of coordinates at some average point determined by the nucleus and the several other electrons and so forth. Since the system is the same in whatever frame of reference it is described in, all the equations are invariant to the coordinate transformations. Considering only time-independent situations and following the same procedure described above, we get for the overlapping region between the first particle (nucleus) and the second particle (electron) the non-linear partial differential equation

$$-\left[p_{12}\frac{\partial^2 p_{12}}{\partial x_1{}^2}-\frac{1}{2}\left(\frac{\partial p_{12}}{\partial x_1}\right)^2\right]-\frac{L(p_{12}-\mu)(p_{12}-3\mu)}{(p_{12}-2\mu)}=MV_1(p_{12}^2-S) \tag{18b}$$

where

$$p_{12}=\frac{\partial x_1}{\partial x_2},\qquad \mu_1=\frac{m}{M_{\mathrm{nuc}}}$$

For the overlap region between two electrons we note that $\mu = 1$. As before we assume

$$p_{12} = \frac{\partial x_1}{\partial x_2} = A_{12} \exp\left(-\mu_1 \operatorname{sn} \frac{4Kx_1}{n\alpha_H} \operatorname{dn} \frac{4Kx_1}{n\alpha_H}\right) + B_{12}$$

as a solution for the overlap region between the nucleus and the first electron. In general for the overlap region between the first particle (nucleus) and the nth particle (electron), we assume

$$p_{1N} = \frac{\partial x_1}{\partial x_N} = A_{1N} \exp\left(-\mu_1 \operatorname{sn} \frac{4Kx_1}{n\alpha_H} \operatorname{dn} \frac{4Kx_1}{n\alpha_H}\right) + B_{1N}$$

and for the overlap region between the second particle (electron) and the nth particle (electron) we have

$$p_{2N} = \frac{\partial x_2}{\partial x_N} = A_{2N} \exp\left(-\mu_1 \operatorname{sn} \frac{4Kx_2}{n\alpha_H} \operatorname{dn} \frac{4Kx_2}{n\alpha_H}\right) + B_{2N}$$

p_{2N} has to satisfy the equation

$$-\left[p_{2N} \frac{\partial^2 p_{2N}}{\partial x_2^2} - \frac{1}{2}\left(\frac{\partial p_{2N}}{\partial x_2}\right)^2\right] - \frac{L(p_{2N} - 1)(p_{2N} - 3)}{(p_{2N} - 2)} = MV_{2N}(p_{2N}^2 - S) \quad (19)$$

Since $\mu_1 = 1$ as both particles are electrons and $V_{2N} \to -e^2/x_2$ by putting these in equation (19) and equating coefficients of like powers in x_2, we get $A_{2N} \to 0$, $B_{2N} \to 1$ and $x_N = x_2 + C$ where C is a constant, giving a translation of the coordinate systems for each of the electrons.

From the following equations, since $p_{13} = p_{12}p_{23}$,

$$\frac{\partial x_1}{\partial x_2} = p_{12} = A_{12} \exp\left(-\mu_1 \operatorname{sn} \frac{4Kx_1}{n\alpha_H} \operatorname{dn} \frac{4Kx_1}{n\alpha_H}\right) + B_{12}$$

$$\frac{\partial x_2}{\partial x_3} = p_{23} = A_{23} \exp\left(-\mu_1 \operatorname{sn} \frac{4Kx_2}{n\alpha_H} \operatorname{dn} \frac{4Kx_2}{n\alpha_H}\right) + B_{23}$$

$$\frac{\partial x_1}{\partial x_3} = p_{13} = A_{13} \exp\left(-\mu_1 \operatorname{sn} \frac{4Kx_1}{n\alpha_H} \operatorname{dn} \frac{4Kx_1}{n\alpha_H}\right) + B_{13}$$

it follows that

$$\begin{aligned}
&A_{13} \exp\left(-\mu_1 \operatorname{sn} \frac{4Kx_1}{n\alpha_H} \operatorname{dn} \frac{4Kx_1}{n\alpha_H}\right) + B_{13} \\
&\quad = A_{12} A_{23} \exp\left(-\mu_1 \operatorname{sn} \frac{4Kx_1}{n\alpha_H} \operatorname{dn} \frac{4Kx_1}{n\alpha_H}\right) \exp\left(-\mu_1 \operatorname{sn} \frac{4Kx_2}{n\alpha_H} \operatorname{dn} \frac{4Kx_2}{n\alpha_H}\right) \\
&\qquad + B_{23} A_{12} \exp\left(-\mu_1 \operatorname{sn} \frac{4Kx_1}{n\alpha_H} \operatorname{dn} \frac{4Kx_1}{n\alpha_H}\right) \\
&\qquad + A_{23} B_{12} \exp\left(-\mu_1 \operatorname{sn} \frac{4Kx_2}{n\alpha_H} \operatorname{dn} \frac{4Kx_2}{n\alpha_H}\right) + B_{12} B_{23}
\end{aligned}$$

Since $A_{23} = 0$.

$$A_{13}\exp\left(-\mu\,\mathrm{sn}\,\frac{4Kx_1}{n\alpha_H}\,\mathrm{dn}\,\frac{4Kx_1}{n\alpha_H}\right) + B_{13}$$

$$= B_{23}A_{12}\exp\left(-\mu\,\mathrm{sn}\,\frac{4Kx_1}{n\alpha_H}\,\mathrm{dn}\,\frac{4Kx_1}{n\alpha_H}\right) + B_{12}B_{23}$$

$$\frac{A_{13}}{A_{12}} = B_{23} = \frac{B_{13}}{B_{12}}$$

As B_{2N} and hence $B_{23} \rightarrow 1$, $A_{12} = A_{13} = \ldots A_{1N}$ and $B_{12} = B_{13} \ldots = B_{1N}$; therefore, the solutions for the different regions of overlap between the proton and the various electrons are identical.

We now show that purely on the basis of the minimisation of energy, only certain points of the lattice can be considered for the purpose of their representation as possible stable states of the atom. In Fig. 1 we have empirically drawn on a complex plane, a set of isosceles right-angled triangles through the lattice points, each one enclosing the other in the form of shells. An even atomic number is associated with each point along the hypotenuse of the right-angled triangle and the vertex opposite it. Only even atomic number systems are considered, as in the present theory the spin of the system has not been specifically put in. In this way starting with ^{4}He at the vertex of shell No. 1, it is seen that it is possible to reproduce the entire Bohr periodic table of elements. We note the following:

(a) All the rare gases fall along the vertices of the triangles and the chemical similarities can be traced in exactly the same way as in the Bohr table of elements.

(b) It is necessary to have two entries along the hypotenuse of each shell, or each shell can have a mirror reflection through the vertex.

(c) Along the real axis, the length of the sides of the triangle in some arbitrary units are $\Delta = \pm 2, \pm 7, \pm 14$, which can be represented as

$$\Delta = \sum_{j=1} (2j+1) - 1$$

where j is an integer.

As shown earlier (Ramanna & Jyothi, 1969), and in Appendix II, the total interaction energy of a system is given by the Dirichlet integral

$$E^2 = \iint_D |a|^2 + |b|^2\,dx\,dt \tag{20}$$

where D is the domain of the integral.

For E or E^2 to be minimum $|a| + i|b|$ and $|a| - i|b|$ have to be harmonic functions. Guided by the preceding discussion, we assume

$$\begin{aligned} |a| + i|b| &= \mathrm{sn}\left(\frac{4Kx}{n\alpha_H} + \frac{i4Kt}{nT_0}\right)\mathrm{dn}\left(\frac{4Kx}{n\alpha_H} + \frac{i4Kt}{nT_0}\right) \\ |a| - i|b| &= \mathrm{sn}\left(\frac{4Kx}{n\alpha_H} - \frac{i4Kt}{T_0}\right)\mathrm{dn}\left(\frac{4Kx}{n\alpha_H} - \frac{i4Kt}{nT_0}\right) \end{aligned} \tag{21}$$

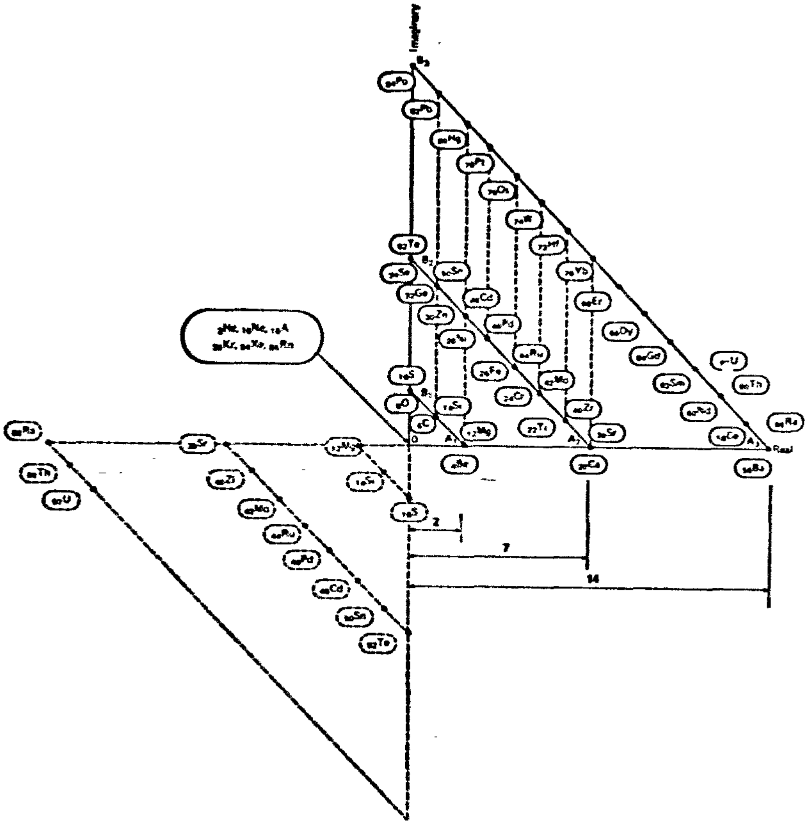

Figure 1.—The periodic table of elements obtained by arranging the even number atoms on the sides of right angled isosceles triangles on the complex plane. The Pauli principle appears as the exclusion of more than one atom with real or imaginary position having the same domain width. The dotted-lines drawn vertically link up atoms with similar chemical properties.

So that

$$E^2 = \iint_D \operatorname{sn}\left(\frac{4Kx}{\alpha_H} + \frac{i4Kt}{T_0}\right) \operatorname{sn}\left(\frac{4Kx}{\alpha_H} - \frac{i4Kt}{T_0}\right) \operatorname{dn}\left(\frac{4Kx}{\alpha_H} + \frac{i4Kt}{T_0}\right) \times \operatorname{dn}\left(\frac{4Kx}{\alpha_H} - \frac{i4Kt}{T_0}\right) d\left(\frac{4Kx}{\alpha_H}\right) d\left(\frac{4Kt}{T_0}\right) \tag{22}$$

As we are concerned with systems in the ground state only, we have set $n = 1$ in (21) just as in equation (11). Due to the double periodicity of the integrand, we can choose a characteristic time $t = T_0$ such that

$$E^2 = Q \int_{D_t} \frac{\partial 4Kt}{T_0} \int_{D_x} \operatorname{sn}^2 \frac{4Kx}{\alpha_H} \operatorname{dn}^2 \frac{4Kx}{\alpha_H} \partial \frac{(4Kx)}{\alpha_H} \tag{23}$$

Here Q is a constant with dimensions of square of energy and D_s, D_t are the space and time domains respectively.

As already observed in the discussion following equation (11), the very choice of the integrand in equation (22) as a function of the type

$$\operatorname{sn}(x+it)\operatorname{dn}(x+it)$$

implies that the integration is over an isosceles right-angled triangle.

If the upper and lower limits of D_s are X_U and X_L respectively

$$E^2 = \frac{Q}{3} D_t[(X_U - X_L) - (\operatorname{sn} X_U \operatorname{cn} X_U \operatorname{dn} X_U - \operatorname{sn} X_L \operatorname{cn} X_L \operatorname{dn} X_L)] \quad (24)$$

The integration of $\operatorname{sn}^2 x \operatorname{dn}^2 x$ depends on the path along which x varies and this gives rise to three cases:

(i) The path of integration is along the real axis; i.e. the domain-limits X_U, X_L are real.
(ii) The path of integration is along the imaginary axis; i.e. the domain-limits X_U, X_L are pure imaginary.
(iii) The path of integration is along the hypotenuse of the isosceles right-angled triangle.

In case (i) the integrand $\operatorname{sn}^2 x \operatorname{dn}^2 x$ has turning points whenever the domain-limit X_U or X_L is an odd multiple of K. At these points the integrand is a maximum and the system will be in a stable state whenever the domain-width D_s is an odd multiple of K. The sum Δ, of real domain-widths is given by

$$\sum D_s \quad \text{and} \quad \Delta = \sum_{j=0}^{l} (2j+1)K$$

where j, l are integers.

The present theory deals with spin-less systems and as the first atom without spin is Helium, the domain-width corresponding to this atom has to be subtracted from Δ, making the domain-width of Helium to be K. We therefore write

$$\Delta = \left[\sum_{j=1}^{l} (2j+1)K - K\right] \quad (25)$$

where $l = 1, 2$ or 3 and $j = 1, 2, 3$.

It is easily verified from equation (25) that for $l = 1$, $\Delta = 2$; for $l = 2$, $\Delta = 7$; and for $l = 3$, $\Delta = 14$. It is seen thus, that the numbers 2, 7 and 14 assumed empirically in Fig. 1 to correspond to the different shells come out to be the total domain-measures on the real line.

In case (ii), by symmetry considerations, we expect the system to be in a stable state whenever the domain-width is an odd multiple of K. The analysis is exactly the same as in case (i).

In case (iii) the integrand $\operatorname{sn}^2 x \operatorname{dn}^2 x$ has turning points whenever the domain-limit X_L or X_U is an odd multiple of $\frac{1}{2}(K+iK)$. At these points the integrand is a minimum and the system will be in a stable state if the domain-width is an integral multiple of $-K+iK$.

An atom in its stable state is characterised by its average position and the domain width Δ. The average position of the atom is given by two parameters, the real part and the imaginary part. It is assumed that no two atoms can be fitted into domains of the same width unless the real and imaginary parts of their average positions are different and the shell structure arises because of the restriction that no two atoms can have the same three parameters, the real and imaginary parts of the average positions and the domain width. The above restriction can be considered as the geometrical equivalent of the Pauli principle which gives rise to a shell-behaviour in the usual quantum theory of atomic structure.

Considering the cases (i), (ii), (iii) together; we expect the system to be in a stable state for domain-widths which are either odd multiples of K or odd multiples of $(-K+iK)$ corresponding to the following points of the complex plane:

$$\begin{array}{lll} \text{(a)} & (2-j)K+ijK, & 0\leqslant j\leqslant 2 \\ \text{(b)} & (7-j)K+ijK, & 0\leqslant j\leqslant 7 \\ \text{(c)} & (14-j)K+ijK, & 0\leqslant j\leqslant 14 \end{array} \qquad (26)$$

The discussion following equation (24) remains valid when one replaces D_s by $-D_s$ and D_t by $-D_t$. This means that in Fig. 1 we could have put the double entries like (4,12), (20,38) etc. on two triangular shells, one corresponding to D_s, the other to $-D_s$ as shown by the dotted lines in Fig. 1. The points of the complex space enumerated in equation (26) lie in the form of shells along the sides of an isosceles right-angled triangle in the complex plane. The domain-lengths D_s corresponding to these points are measured continuously along the sides of the triangle and are terminated by one of the points enumerated above. Since the values of D_s are integral multiples of K, the second term of equation (24) vanishes and we can write

$$E^2=(Q/3)\,|D_t\,D_s| \qquad (27)$$

This implies that

$$E=\sqrt{(Q/3)}\,\sqrt{(|D_s\,D_t|)}=\sqrt{(Q/3)}\,K|\Phi| \qquad (28)$$

Here we have written $|D_s D_t|^{1/2}=K|\Phi|$ where Φ is a complex number associated with each permitted domain length corresponding to the selected point along the sides of the isosceles right-angled triangle. In order to get the energies of interaction in a linear order of the atomic weights, these points are mapped on to a real line by means of the Schwarz-Christoffel transformation of the triangle onto a real half-plane. This is done by first mapping the vertices to the points 0, 1 and ∞ respectively on the real line and then proceeding to the θ plane. This mapping is given by the following integrals:

$$\text{(a)} \int_x^{\infty} \frac{dt}{(t^2-1)^{3/4}} \qquad \text{(b)} \int_x^{1} \frac{dt}{(1-t^2)^{3/4}} \qquad \text{and (c)} \int_{-\infty}^{x} \frac{dt}{(1+t^2)^{3/4}}$$

The corresponding linear map to the θ plane is given by

$$\text{(a)} \quad \cos\theta = \frac{1-\sqrt{(x^2-1)}}{1+\sqrt{(x^2-1)}}, \qquad 1 < x < \infty$$

$$\text{(b)} \quad \cos\theta = \frac{1}{(1-x^2)^{1/4}}, \qquad 0 < x < 1$$

$$\text{(c)} \quad \cos\theta = \frac{1}{(1+x^2)^{1/4}}, \qquad -\infty < x < 0$$

depending on the side of the triangle under consideration. We note that (a) corresponds to points on the hypotenuse. In Fig. 1 as one moves along OA from O to A, θ changes through an angle $\pi/2$. From A to B, the variation in θ is π and it is again $\pi/2$ from B to O. Thus the entire triangle is mapped as θ moves through an angle of 2π.

The corresponding regions of the mappings in the different space can be schematically expressed as follows:

Complex space	From O to A	A to B	B to O
x-space	0 to 1	1 to ∞	∞ to 0
θ-space	$\langle\pi/2\rangle$	$\langle\pi\rangle$	$\langle\pi/2\rangle$

The Schwarz-mapping gives

$$\Phi = \frac{\sqrt{(2)}\Delta}{4K} F(\theta, K) \tag{29}$$

where Δ is the length of the hypotenuse of the triangle that is mapped. The constant Q in equation (23) as stated earlier has the dimensions of the square of energy.

We set $Q = [Zm_0 C^2 \alpha^2]^2$, where $Zm_0 C^2$ is the rest energy of all the electrons in the system and α is the fine structure constant. This implies that the number $E/Zm_0 C^2$ which is also the average binding energy of each electron in the system in terms of the rest energies, is a constant in each domain, the mean position of which is given by one of the allowed complex points and the distances in the complex plane are measured in terms of α^2, the square of the fine structure constant. The above conformal transformation maps the complex points Φ to θ on a real line to give a linear ordering which in turn gives the energy in real space.

From equation (29) we have

$$E = \sqrt{(Q/3)}\,|D_t D_s|^{1/2} = \sqrt{(Q/3)}\,4K|\Phi| = \sqrt{(Q/3)}\,\Delta\sqrt{(2)}\,F(\theta, K) \tag{30}$$

Introducing the value of Q

$$E = \sqrt{(\tfrac{2}{3})}\, m_0 C^2 \alpha^2 \Delta Z F(\theta, K)$$

$$E_{(ev)} = 22{\cdot}20775\, \Delta Z F(\theta, K)$$

Since $m_0 C^2 \alpha^2 = 27{\cdot}2$ ev.

As the theory is applicable only to spinless systems, the binding energy of the ^{4}He atom has to be removed from E. This is because the first triangle representing atoms lighter than ^{4}He is a point and therefore is of arbitrary measure.

The total binding-energy of atoms is therefore given by

$$E_B - E_B(^4\mathrm{He}) = 22{\cdot}20775\, \Delta Z F(\theta, K) \tag{31}$$

We note that the length of the hypotenuse Δ for the range of $2 < Z \leqslant 18$ is 2; for $18 < Z \leqslant 54$ is 7 and for $54 < Z \leqslant 86$ is 14 and the values of E_B are obtained from the following equations:

For

$$\begin{aligned} 2 < Z \leqslant 10, &\quad E_B = E_2 + 22{\cdot}20775 \times 2 \times ZF(\theta, k) \\ 10 < Z \leqslant 18. &\quad E_B = E_{10} + 22{\cdot}20775 \times 2 \times ZF(\theta, k) \\ 18 < Z \leqslant 36, &\quad E_B = E_{18} + 22{\cdot}20775 \times 7 \times ZF(\theta, k) \\ 36 < Z \leqslant 54, &\quad E_B = E_{36} + 22{\cdot}20775 \times 7 \times ZF(\theta, k) \end{aligned} \tag{32}$$

and

$$54 < Z \leqslant 86, \quad E_B = E_{54} + 22{\cdot}20775 \times 14 \times ZF(\theta, k)$$

The values of E_{10}, E_{18}, E_{36} and E_{54} are obtained from the respective previous equations and $E_2 = E_B(^4\mathrm{He}) = 78{\cdot}884$.

In Table 1 the values of θ, $F(\theta, k)$ and E for all even values of Z are given. It is seen that the agreement with the few available experimental points† is within 3% and the agreement with the perturbation theories (Foldy, 1951) is quite impressive, especially considering the fact that no arbitrary parameters are used in the present theory. At the present moment, no experimental values are available for the total binding energies beyond $Z = 8$. A value of this energy for some $Z > 62$ would provide a very good test for the theory.

The theory deals with stable spinless systems. To extend the theory to systems with spin the Dirac equation will have to be used instead of the Schrödinger equation. It may, however, be possible to introduce spin by using the third type elliptic integrals as solutions to the non-linear differential equation rather than the first type as suggested in an earlier paper (Ramanna, 1968).

Acknowledgement

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† *C.R.C. Handbook of Chemistry and Physics*, 50th Edition (1969–70).

TABLE 1. Electron-binding energy values in electron-volts of present theory compared with experimental values† and the existing calculated values based on the Fermi-Thomas model and that due to Foldy (1951).

	Z	θ	$F(\theta,k)$	E_B exptl.	E_B Foldy	E_B Fermi-Thomas	E_B cal. (present theory)
2	2	0	0	78·884	78·63	79·274	78·884
	4	$\pi/2$	1·8541	399·033	400·30	399·520	408·300
	6	π	3·7082	1029·805	1041·00	1029·000	1067·100
	8	$3\pi/2$	5·5623	2043·189	2068·00	2013·400	2055·400
	10	2π	7·4164	—	3535·00	3388·900	3373·100
	12	$5\pi/2$	9·2705	—	—	5·186 × 10^3	8·314 × 10^3
	14	3π	11·1246	—	—	7·431 × 10^3	1·029 × 10^4
	16	$7\pi/2$	12·9787	—	—	1·015 × 10^4	1·260 × 10^4
	18	4π	14·8328	—	—	1·336 × 10^4	1·523 × 10^4
7	20	$\pi/2$	1·8541	—	1·833 × 10^4	1·708 × 10^4	2·100 × 10^4
	22	$9\pi/14$	2·3157	—	—	2·133 × 10^4	2·315 × 10^4
	24	$11\pi/14$	2·8032	—	—	2·614 × 10^4	2·569 × 10^4
	26	$13\pi/14$	3·3900	—	—	3·150 × 10^4	2·893 × 10^4
	28	$15\pi/14$	3·9361	—	—	3·745 × 10^4	3·237 × 10^4
	30	$17\pi/14$	4·3959	—	4·811 × 10^4	4·399 × 10^4	3·573 × 10^4
	32	$19\pi/14$	4·9400	—	—	5·114 × 10^4	3·981 × 10^4
	34	$3\pi/2$	5·5623	—	—	5·891 × 10^4	4·463 × 10^4
	36	2π	7·4164	—	—	6·731 × 10^4	5·674 × 10^4
	38	$5\pi/2$	9·2705	—	—	7·636 × 10^4	1·115 × 10^5
	40	$37\pi/14$	9·7321	—	9·590 × 10^4	8·607 × 10^4	1·173 × 10^5
	42	$39\pi/14$	10·2196	—	—	9·645 × 10^4	1·235 × 10^5
	44	$41\pi/14$	10·8064	—	—	1·075 × 10^5	1·307 × 10^5
	46	$43\pi/14$	11·3525	—	—	1·193 × 10^5	1·379 × 10^5
	48	$45\pi/14$	11·8123	—	—	1·317 × 10^5	1·449 × 10^5
	50	$47\pi/14$	12·3564	—	1·637 × 10^5	1·449 × 10^5	1·528 × 10^5
	52	$7\pi/2$	12·9787	—	—	1·588 × 10^5	1·617 × 10^5
	54	4π	14·8328	—	—	1·734 × 10^5	1·818 × 10^5
14	56	$\pi/2$	1·8541	—	—	1·887 × 10^5	2·135 × 10^5
	58	$8\pi/14$	2·0820	—	—	2·048 × 10^5	2·188 × 10^5
	60	$9\pi/14$	2·3157	—	2·532 × 10^5	2·217 × 10^5	2·245 × 10^5
	62	$10\pi/14$	2·5612	—	—	2·393 × 10^5	2·306 × 10^5
	64	$11\pi/14$	2·8032	—	—	2·577 × 10^5	2·370 × 10^5
	66	$12\pi/14$	3·0859	—	—	2·769 × 10^5	2·446 × 10^5
	68	$13\pi/14$	3·3900	—	—	2·969 × 10^5	2·529 × 10^5
	70	π	3·7082	—	3·663 × 10^5	3·177 × 10^5	2·620 × 10^5
	72	$15\pi/14$	3·9361	—	—	3·392 × 10^5	2·694 × 10^5
	74	$16\pi/14$	4·1698	—	—	3·616 × 10^5	2·772 × 10^5
	76	$17\pi/14$	4·3959	—	—	3·849 × 10^5	2·851 × 10^5
	78	$18\pi/14$	4·6573	—	—	4·089 × 10^5	2·942 × 10^5
	80	$19\pi/14$	4·9400	—	5·049 × 10^5	4·338 × 10^5	3·041 × 10^5
	82	$20\pi/14$	5·2441	—	—	4·595 × 10^5	3·150 × 10^5
	84	$3\pi/2$	5·5623	—	—	4·861 × 10^5	3·265 × 10^5
	86	2π	7·4164	—	—	5·135 × 10^5	3·796 × 10^4

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† *C.R.C. Handbook of Chemistry and Physics*, 50th Edition (1969–70).

Appendix 1

Using the coordinate transformation of the (x_2, t_2) into (x_1, t_1) as prescribed in (3) and transforming equation (2) to the (x_1, t_1) system, we get

$$\begin{aligned}
&\frac{\partial^2 \psi_1}{\partial x_1{}^2} + \frac{\partial \psi_1}{\partial x_1}\left[\frac{2}{\omega}\frac{\partial \omega}{\partial x_1} + \frac{2q}{pc}\frac{1}{\omega}\frac{\partial \omega}{\partial t_1} + \frac{1}{p}\frac{\partial p}{\partial x_1} + \frac{q}{pc^2}\frac{\partial p}{\partial t_1} + \frac{2m_2 iqc}{\hbar p^2}\right] + \frac{2q}{pc}\frac{\partial^2 \psi_1}{\partial x_1 \partial t_1} \\
&+ \frac{q^2}{p^2 c^2}\frac{\partial^2 \psi_1}{\partial t_1{}^2} + \frac{\partial \psi_1}{\partial t_1}\left[\frac{2q}{pc}\frac{1}{\omega}\frac{\partial \omega}{\partial x_1} + \frac{2q^2}{p^2 c^2}\frac{1}{\omega}\frac{\partial \omega}{\partial t_1} + \frac{q}{p^2 c}\frac{\partial p}{\partial x_1} - \frac{1}{pc^2}\frac{\partial p}{\partial t_1} - \frac{2m_2 i}{\hbar p}\right] \\
&+ \psi_1\left[\frac{1}{\omega}\frac{\partial^2 \omega}{\partial x_1{}^2} + \frac{2q}{pc}\frac{1}{\omega}\frac{\partial^2 \omega}{\partial x_1 \partial t_1} + \frac{q^2}{p^2 c^2}\frac{1}{\omega}\frac{\partial^2 \omega}{\partial t_1{}^2} + \frac{1}{\omega}\frac{\partial \omega}{\partial x_1}\left(\frac{1}{p}\frac{\partial p}{\partial x_1} + \frac{q}{p^2 c}\frac{\partial p}{\partial t_1}\right.\right. \\
&\left.\left.+ \frac{2m_2 qci}{\hbar p^2}\right) + \frac{1}{\omega}\frac{\partial \omega}{\partial t_1}\left\{\frac{q}{p^2 c}\frac{\partial p}{\partial x_1} - \frac{1}{pc^2}\frac{\partial p}{\partial t_1} - \frac{2m_2 i}{\hbar p}\right\} + \frac{2m_2 V_2}{\hbar^2 p^2}\right] = 0 \qquad \text{(A1.1)}
\end{aligned}$$

Comparing this with the Schrödinger equation:

$$\frac{\partial^2 \psi_1}{\partial x_1{}^2} + \frac{2m_1}{\hbar^2} V_1 \psi_1 = \frac{2m_1 i}{\hbar}\frac{\partial \psi_1}{\partial t_1}$$

we find that in the overlap region, the following relations hold:

$$\begin{aligned}
&\frac{\partial \psi_1}{\partial x_1}\left[\frac{2}{\omega}\frac{\partial \omega}{\partial x_1} + \frac{2q}{pc}\frac{1}{\omega}\frac{\partial \omega}{\partial t_1} + \frac{1}{p}\frac{\partial p}{\partial x_1} + \frac{q}{p^2 c}\frac{\partial p}{\partial t_1} + \frac{2m_2 qic}{\hbar p^2}\right] \\
&\qquad\qquad + \frac{2q}{pc}\frac{\partial^2 \psi_1}{\partial x_1 \partial t_1} + \frac{q^2}{p^2 c^2}\frac{\partial^2 \psi_1}{\partial t_1{}^2} = 0 \qquad \text{(A1.2)}
\end{aligned}$$

$$\begin{aligned}
&\frac{1}{\omega}\frac{\partial^2 \omega}{\partial x_1{}^2} + \frac{2q}{pc}\frac{1}{\omega}\frac{\partial^2 \omega}{\partial x_1 \partial t_1} + \frac{q^2}{p^2 c^2}\frac{1}{\omega}\frac{\partial^2 \omega}{\partial t_1{}^2} + \frac{1}{\omega}\frac{\partial \omega}{\partial x_1}\left\{\frac{1}{p}\frac{\partial p}{\partial x_1} + \frac{q}{p^2 c}\frac{\partial p}{\partial t_1} + \frac{2m_2 qci}{\hbar p^2}\right\} \\
&+ \frac{1}{\omega}\frac{\partial \omega}{\partial t_1}\left\{\frac{q}{p^2 c}\frac{\partial p}{\partial x_1} - \frac{1}{pc^2}\frac{\partial p}{\partial t_1} - \frac{2m_2 i}{\hbar p}\right\} + \frac{2}{\hbar^2 p^2}(m_2 V_2 - m_1 p^2 V_1) = 0 \quad \text{(A1.3)}
\end{aligned}$$

$$\frac{2q}{pc}\frac{1}{\omega}\frac{\partial \omega}{\partial x_1} + \frac{2q^2}{p^2 c^2}\frac{1}{\omega}\frac{\partial \omega}{\partial t_1} + \frac{q}{p^2 c}\frac{\partial p}{\partial x_1} - \frac{1}{pc^2}\frac{\partial p}{\partial t_1} - \frac{2m_2 i}{\hbar p} = \frac{-2m_1 i}{\hbar} \quad \text{(A1.4a)}$$

In a time-independent case $\partial\omega/\partial t_1 = 0$. From (A1.4a) it follows that

$$\frac{1}{\omega}\frac{\partial \omega}{\partial x_1} + \frac{1}{2p}\frac{\partial p}{\partial x_1} - \frac{1}{2qc}\frac{\partial p}{\partial t_1} = \frac{ic}{\hbar q}(m_2 - m_1 p) \qquad \text{(A1.4b)}$$

$$\frac{2q}{pc}\frac{1}{\omega}\frac{\partial \omega}{\partial x_1} + \frac{q}{p^2 c}\frac{\partial p}{\partial x_1} - \frac{1}{pc^2}\frac{\partial p}{\partial t_1} = \frac{2i}{\hbar p}(m_2 - m_1 p) \qquad \text{(A1.4c)}$$

Differentiating (A1.4b) with respect to x_1, and (A1.4c) with reference to t_1 and adding we get

$$\begin{aligned}\frac{1}{\omega^2}\frac{\partial^2\omega}{\partial x_1{}^2}+\frac{2q}{pc}\frac{1}{\omega}\frac{\partial^2\omega}{\partial x_1\,\partial t_1}=\frac{1}{\omega^2}\left(\frac{\partial\omega}{\partial x_1}\right)^2-\frac{2}{\omega}\frac{\partial\omega}{\partial x_1}\left(\frac{1}{p}\frac{\partial p}{\partial x_1}-\frac{q}{p^2c}\frac{\partial p}{\partial t_1}\right)\\ -\frac{1}{2p}\frac{\partial^2 p}{\partial x_1{}^2}-\frac{1}{2p^2}\left(\frac{\partial p}{\partial x_1}\right)^2-\frac{m_1 ic}{\hbar q}\frac{\partial p}{\partial x_1}\\ +\left(\frac{1}{2q^2c^2}-\frac{1}{p^2c^2}\right)\left(\frac{\partial p}{\partial t_1}\right)^2+\frac{1}{pc^2}\frac{\partial^2 p}{\partial t_1{}^2}\\ +\left(\frac{1}{2qc}-\frac{q}{p^2c}\right)\frac{\partial^2 p}{\partial x_1\,\partial t_1}+\frac{2q}{p^3c}\frac{\partial p}{\partial x_1}\frac{\partial p}{\partial t_1}\\ +\frac{i}{\hbar q^2}\frac{\partial p}{\partial t_1}(m_2-m_1p)-\frac{2im_2}{\hbar p^2}\frac{\partial p}{\partial t_1}\end{aligned}$$

Introducing in (A1.3) we get

$$\begin{aligned}&\frac{1}{\omega^2}\left(\frac{\partial\omega}{\partial x_1}\right)^2+\frac{1}{\omega}\frac{\partial\omega}{\partial x_1}\left\{\frac{1}{p}\frac{\partial p}{\partial x_1}+\frac{q}{p^2c}\frac{\partial p}{\partial t_1}+\frac{2m_2qci}{\hbar p^2}-\frac{2}{p}\frac{\partial p}{\partial x_1}+\frac{2q}{cp^2}\frac{\partial p}{\partial t_1}\right\}\\ &\quad-\frac{1}{2p^2}\left(\frac{\partial p}{\partial x_1}\right)^2-\frac{1}{2p}\frac{\partial^2 p}{\partial x_1{}^2}+\frac{p^2-2q^2}{2q^2p^2c^2}\left(\frac{\partial p}{\partial t_1}\right)^2+\frac{1}{pc^2}\frac{\partial^2 p}{\partial t_1{}^2}+\frac{2q}{p^3c}\frac{\partial p}{\partial x_1}\frac{\partial p}{\partial t_1}\\ &\quad+\frac{i}{\hbar q^2}\frac{\partial p}{\partial t_1}(m_2-m_1p)-\frac{m_1ic}{\hbar q}\frac{\partial p}{\partial x_1}-\frac{2im_2}{\hbar p^2}\frac{\partial p}{\partial t_1}+\left(\frac{1}{2qc}-\frac{q}{cp^2}\right)\frac{\partial^2 p}{\partial x_1\,\partial t_1}\\ &\quad+\frac{2}{\hbar^2p^2}(m_2V_2-m_1p^2V_1)=0 \qquad \text{(A1.5a)}\end{aligned}$$

Eliminating $\partial\omega/\partial x_1$ using (A1.4b), we get, after some simplification,

$$\begin{aligned}&\frac{1}{4p^2}\left(\frac{\partial p}{\partial x_1}\right)^2-\frac{1}{2p}\frac{\partial^2 p}{\partial x_1{}^2}+\frac{c^2(m_2-m_1p)}{\hbar^2p^2q^2}\{m_1p^3-m_2(p^2+2q^2)\}\\ &\quad+\frac{2}{\hbar^2p^2}(m_2V_2-m_1p^2V_1)+\frac{ic}{\hbar p^3q}\frac{\partial p}{\partial x_1}\{m_1p^3-m_2(2p^2+q^2)\}+\frac{1}{pc^2}\frac{\partial^2 p}{\partial t_1{}^2}\\ &\quad-\frac{2p^2-q^2}{2qp^3c}\frac{\partial p}{\partial x_1}\frac{\partial p}{\partial t_1}+\frac{3p^2+2q^2}{4p^2q^2c^2}\left(\frac{\partial p}{\partial t_1}\right)^2+\frac{p^2-2q^2}{2qp^2c}\frac{\partial^2 p}{\partial x_1\,\partial t_1}\\ &\quad-\frac{i}{\hbar p^2q^2}\frac{\partial p}{\partial t_1}\{m_1p(2p^2+3q^2)-2m_2(p^2+q^2)\}=0 \qquad \text{(A1.5b)}\end{aligned}$$

We assume that in a time-independent case

$$\begin{aligned}\frac{1}{pc^2}\frac{\partial^2 p}{\partial t_1{}^2}+\frac{3p^2+2q^2}{4p^2q^2c^2}\left(\frac{\partial p}{\partial t_1}\right)^2-\frac{2p^2-q^2}{2qp^3c}\frac{\partial p}{\partial x_1}\frac{\partial p}{\partial t_1}+\frac{p^2-2q^2}{2qp^2c}\frac{\partial^2 p}{\partial x_1\,\partial t_1}\\ -\frac{i}{\hbar p^2q^2}\frac{\partial p}{\partial t_1}\{m_1p(2p^2+3q^2)-2m_2(p^2+q^2)\}=0\end{aligned}$$

so that (A1.5b) is equivalent to

$$\frac{1}{4p^2}\left(\frac{\partial p}{\partial x_1}\right)^2-\frac{1}{2p}\frac{\partial^2 p}{\partial x_1{}^2}+\frac{c^2(m_2-m_1p)}{\hbar^2p^2q^2}\{m_1p^3-m_2(p^2+2q^2)\}$$

$$+\frac{2}{\hbar^2p^2}(m_2V_2-m_1p^2V_1)+\frac{ic}{\hbar p^3q}\frac{\partial p}{\partial x_1}\{m_1p^3-m_2(2p^2+q^2)\}=0 \quad \text{(A1.5c)}$$

If further the potentials are real, viz., $m_1p^3=m_2(2p^2+q^2)$ then from (A1.5c) we get

$$p\frac{\partial^2 p}{\partial x_1{}^2}-\frac{1}{2}\left(\frac{\partial p}{\partial x_1}\right)^2-\frac{2c^2(m_2-m_1p)}{\hbar^2q^2}\{m_1p^3-m_2(p^2+2q^2)\}$$

$$=\frac{4}{\hbar^2}(m_2V_2-m_1p^2V_1)$$

which is equation (7) of the paper.

Appendix 2

We now show that the choice of harmonic functions for the coordinate transformation automatically minimises the total energy of the systems described by Schrödinger equations. This is done in an elegant manner by resorting to the calculus of differential forms and to the Dirichlet principle. The energy of the systems are found directly without a knowledge of ψ, the state-function.

If $\omega_1=a_1dx_1+b_1dt_1$, $\omega_2=a_2dx_2+b_2dt_2$ are two differential forms of order one defined in two overlapping domains h_1, h_2 over a Riemann surface then from the calculus of differential forms (Ahlfors & Sario, 1960), it follows that the complex functions a_1, b_1, a_2, b_2 of the coordinates (x_1, t_1) and (x_2, t_2) respectively are connected by the following relations.

$$\begin{aligned} a_1&=a_2\frac{\partial x_2}{\partial x_1}+b_2\frac{\partial t_2}{\partial x_1}\\ b_1&=a_2\frac{\partial x_2}{\partial t_1}+b_2\frac{\partial t_2}{\partial t_1}\end{aligned} \quad \text{(A2.1)}$$

and

$$\begin{aligned} a_1&=-b_2\frac{\partial x_2}{\partial t_1}+a_2\frac{\partial t_2}{\partial t_1}\\ -b_1&=-b_2\frac{\partial x_2}{\partial x_1}+a_2\frac{\partial t_2}{\partial x_1}\end{aligned} \quad \text{(A2.2)}$$

A one-form in general is of the form $\omega = a\,dx + b\,dt$ and its exterior derivative is given by

$$d\omega = \left(\frac{\partial b}{\partial x} - \frac{\partial a}{\partial t}\right) dx\,dt$$

The differential form ω is said to be closed if $d\omega = 0$. The invariance of a differential form ω under coordinate transformations implies the invariance of the conjugate differential ω^* defined by $\omega^* = -b\,dx + a\,dt$; the complex conjugate of the conjugate differential is $\bar{\omega}^* = -\bar{b}\,dx + \bar{a}\,dt$ where $\bar{a}$ and $\bar{b}$ are complex conjugates of a and b respectively. The integral I defined by the equation

$$I = \int_D \omega\bar{\omega}^* = \int_D (|a|^2 + |b|^2)\,dx\,dt \qquad \text{(A2.3)}$$

is finite and positive. This can be seen to be a Dirichlet integral and by Dirichlet principle it takes a minimum value when the integrand $|a|^2 + |b|^2$ is a harmonic function. The type of functions the integrand can take depends on the Riemann manifold chosen, i.e. one gets spherical harmonics if the Riemann surface is that of the sphere, doubly-periodic functions (elliptic integrals) if the surface is that of a torus and other meromorphic functions for higher punctured surfaces. The Dirichlet principle also ensures that this integral is invariant under conformal transformations.

We now write a set of Schrödinger equations and their complex conjugates into their respective differential forms and compare with the differential forms $d\omega$, $d\bar{\omega}^*$ defined above.

The Schrödinger equation can be written as

$$H_{\text{op}}\,\psi(x,t) - i\hbar\frac{\partial\psi(x,t)}{\partial t} = 0 \qquad \text{(A2.4)}$$

where $\psi(x,t)$ is a complex-valued function of space x and time t and H_{op} is the energy operator.

Comparing (A2.4) with the closed differential form $d\omega$, we find that

$$\frac{\partial b}{\partial t} = H_{\text{op}}\,\psi(x,t) = \frac{\partial a}{\partial x} \qquad \text{(A2.5)}$$

If similarly one compares the conjugate equation of the Schrödinger equation with the closed differential form $d\bar{\omega}^*$, we find that

$$-\frac{\partial \bar{b}}{\partial x} = [H_{\text{op}}\,\psi(x,t)]^* = \frac{\partial \bar{a}}{\partial t} \qquad \text{(A2.6)}$$

where $[H_{\text{op}}\,\psi(x,t)]^*$ is the complex conjugate of $[H_{\text{op}}\,\psi(x,t)]$.

From (A2.5) and (A2.6) we find after integration that

$$\begin{aligned} a &= \int H_{op}\,\psi(x,t)\,dx + f_a(t) \\ \bar{a} &= \int [H_{op}\,\psi(x,t)]^*\,dt + f_{\bar{a}}(x) \\ b &= \int H_{op}\,\psi(x,t)\,dt + f_b(x) \\ \bar{b} &= \int [H_{op}\,\psi(x,t)]^*\,dx + f_b(t) \end{aligned} \qquad \text{(A2.7)}$$

Since $a\bar{a}$ and $b\bar{b}$ have to be real, one writes

$$\begin{aligned} &f_a(t) = \int H_{op}\,\psi(x,t)\,dt, \qquad f_{\bar{a}}(x) = \text{complex conjugate of} \int H_{op}\,\psi(x,t)\,dx \\ &\hfill \text{(A2.8)} \\ &f_b(x) = \int H_{op}\,\psi(x,t)\,dx, \qquad f_b(x) = \text{complex conjugate of} \int H_{op}\,\psi(x,t)\,dt \end{aligned}$$

From (A2.7) and (A2.8) it follows that

$$\begin{aligned} a\bar{a} + b\bar{b} = 2\Big[&\Big(\int H_{op}\,\psi(x,t)\,dx\Big)\Big(\int \{H_{op}\,\psi(x,t)\}^*\,dx\Big) \\ &+ \Big(\int H_{op}\,\psi(x,t)\,dt\Big)\Big(\int \{H_{op}\,\psi(x,t)\}^*\,dt\Big)\Big] \end{aligned} \qquad \text{(A2.9)}$$

The positive square root of the integral

$$I = \int |a|^2 + |b|^2\,dx\,dt$$

i.e. the norm $\|\omega\|$ gives the interaction energy E within a domain.

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