QUANTIZATION RULES APPLIED TO ANALYTICAL SOLUTIONS OF THE SCHROEDINGER EQUATION.

by

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ABSTRACT

The quantization rules of m theory developed in immediately preceding papers are applied to the analytical solutions of the Schroedinger equation. In each case the solution becomes one of generally covariant quantum mechanics, i.e. quantum mechanics unified with general relativity.

Keywords: ECE2 theory, quantization rules of m theory, generally covariant quantum mechanics.

UFT 436

1. INTRODUCTION

In the immediately preceding papers of this series {1 - 41}, quantization rules were developed for generally covariant quantum mechanics (quantum mechanics unified with general relativity). In Section 2 of this paper they are applied to some well known analytical solutions of the Schroedinger equation such as the harmonic oscillator. It is shown that the use of the most general spherically symmetric space results in shifts of the well known solutions in the non relativistic limit of the Schroedinger equation. In Section 3 the method is applied in computational quantum mechanics with an ab initio technique. The use of an m space produces small but significant effects. The m space can be thought of as "the vacuum", and the most well known vacuum effect is the Lamb shift. So the m theory can be used to eliminate the non Baconian ideas of quantum electrodynamics.

This paper is a brief synopsis of notes accompanying UFT436 on www.aias.us . Note 436(1) deals with the harmonic oscillator, Note 436(2) with the anharmonic oscillator, Note 436(3) gives a general law of spectral effects of m space, or the vacuum, and Note 436(4) gives a separation of variables solution of the Schroedinger equation. Note 436(5) discusses the expectation values of the complete Schroedinger equation.

2. EFFECT OF m THEORY ON ANALYTICAL SOLUTIONS.

Consider the non relativistic limit of quantum mechanics, governed by the Schroedinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial r^2}+U(r)\psi=i\hbar\frac{\partial\psi}{\partial t}\qquad-(1)$$

where ψ is the complete wavefunction, U (r) is the potential energy, $\hbar$ is the reduced Planck constant and m the mass of the particle under consideration. As shown in detail in Note 436(4), Eq. (1) can be solved by writing:

$$\psi = \psi_1(r)\psi_2(t) \quad -(2)$$

thus producing two equations:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi_1}{\partial r^2} + U(r)\psi_1 = E\psi_1 \quad -(3)$$

and

$$i\hbar \frac{\partial \psi_2}{\partial t} = E\psi_2 \quad -(4)$$

giving the complete solution:

$$\psi(r,t) = \psi_1(r)\psi_2(t) = \exp\left(-\frac{iEt}{\hbar}\right)\psi_1(r) \quad -(5)$$

where E are the energy levels.

The quantization rules of the immediately preceding papers modify the wavefunction as follows:

$$t \rightarrow m^{1/2}(r)\, t \quad -(6)$$

$$r \rightarrow \frac{r}{m^{1/2}(r)} \quad -(7)$$

to produce the generally covariant wavefunction, the wavefunction in the presence of the vacuum. So the general solution (5) becomes

$$\psi\left(\frac{r}{m(r)^{1/2}},\, m^{1/2}(r)\, t\right) = \exp\left(-\frac{iEm^{1/2}(r)\, t}{\hbar}\right)\psi_1\left(\frac{r}{m(r)^{1/2}}\right) \quad -(8)$$

Some examples of well known analytical wavefunctions in the absence of the vacuum are given as follows.

1) The free particle energy levels are:

$$E = \hbar\omega \qquad -(9)$$

and the time dependent wavefunction is:

$$\psi_2(t) = \exp(-i\omega t). \qquad -(10)$$

2) The harmonic oscillator energy levels are:

$$E = \left(n + \frac{1}{2}\right)\hbar\omega \qquad -(11)$$

where n is the vibrational quantum number, and the time dependent wavefunction is:

$$\psi_2(t) = \exp\left(-i\left(n + \frac{1}{2}\right)\omega t\right). \qquad -(12)$$

3) The anharmonic oscillator energy levels are:

$$E = \hbar\omega\left(n + \frac{1}{2}\right)\left(1 - x\left(n + \frac{1}{2}\right)\right) \qquad -(13)$$

where x is a measure of anharmonicity, and

$$\psi_2(t) = \exp\left(-i\omega t\left(n + \frac{1}{2}\right)\left(1 - \left(n + \frac{1}{2}\right)x\right)\right). \qquad -(14)$$

4) The energy levels of the particle in a box in well known notation are:

$$E = \frac{n^2\hbar^2\pi^2}{2mL^2} \qquad -(15)$$

and:

$$\psi_2(t) = \exp\left(-i\frac{n^2\hbar\pi^2}{2mL^2}t\right). \qquad -(16)$$

5) The well known energy levels of the H atom are:

$$E = -\frac{\mu e^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} \quad -(17)$$

so its time dependent wavefunction is:

$$\psi_2(t) = \exp\left(-\frac{i\mu e^4 t}{32\pi^2 \epsilon_0^2 \hbar^3 n^2}\right) \quad -(18)$$

The expectation value of energy from Eq. (4) is:

$$\langle E \rangle = i\hbar \int \psi_2^* \frac{\partial \psi_2}{\partial t} d\tau \quad -(19)$$

Using:

$$\psi_2(t) = \exp\left(-i\frac{Et}{\hbar}\right) \quad -(20)$$

it follows that:

$$\frac{\partial \psi_2}{\partial t} = -i\frac{E}{\hbar}\psi_2 \quad -(21)$$

so:

$$\langle E \rangle = E \int \psi_2^* \psi_2 \, d\tau \quad -(22)$$

If the wavefunction is correctly normalized then:

$$\int \psi_2^* \psi_2 \, d\tau = 1 \quad -(23)$$

so:

$$\langle E \rangle = E \quad -(24)$$

However, in m space:

$$\psi_2(t) = \exp\left(-i\frac{E}{\hbar} m(r)^{1/2} t\right) \quad -(25)$$

so:
$$\frac{\partial \phi_2(t)}{\partial t} = -\frac{iE}{\hbar} m(r)^{1/2} \phi_2(t) \quad -(26)$$

and the energy expectation value is:
$$\langle E \rangle = E \int \phi_2^* m(r)^{1/2} \phi_2 \, d\tau. \quad -(27)$$

Therefore in the generally covariant quantum mechanics of m space, the energy levels are shifted. The extent of the shift is determined by the m function and the time dependent wavefunction.

The energy levels of the Schroedinger equation (1) are given in general by the expectation value calculated over the complete wavefunction (ϕ). So:

$$\langle E \rangle = \int \phi^* E \phi \, d\tau = \int \phi_1^*(r) \phi_2^*(t) E \phi_1(r) \phi_2(t) \, d\tau. \quad -(28)$$

However:
$$\phi_2^*(t) = \exp\left(\frac{iEt}{\hbar}\right) \quad -(29)$$

so Eq. (28) reduces to:
$$\langle E \rangle = \int \phi_1^*(r) \exp\left(\frac{iE}{\hbar} t\right) E \phi_1(r) \exp\left(-\frac{iE}{\hbar} t\right) d\tau \quad -(30)$$

In m space this becomes:
$$r \to \frac{r}{m(r)^{1/2}}, \quad t \to m(r)^{1/2} t. \quad -(31)$$

and in m space there are shifts and splittings produced by the m (r) function, Q. E. D.

Generally covariant quantum mechanics can be thought of as quantum mechanics in the presence of the vacuum. The most well known vacuum induced shift is the Lamb shift, which requires consideration of the spin quantum number, but in the non relativistic approximation the Schroedinger equation can be used. Finally, as shown in Note 436(5), the same energy levels E appear in both Eqs. (3) and (4), so it follows that:

$$\langle E\rangle = \int \psi_1^* E \psi_1 \, d\tau = -\frac{\hbar^2}{2m}\int \psi_1^* \frac{\partial^2 \psi_1}{\partial r^2} \, d\tau + \int \psi_1^* U(r) \psi_1 \, d\tau = \int \psi_2^* E \psi_2 \, d\tau \quad -(32)$$

In m space:

$$\psi_2(t) = \exp\left(-i\frac{E}{\hbar} m^{1/2}(r)\, t\right) \quad -(33)$$

so:

$$\langle E\rangle = E\int \psi_2^* m^{1/2}(r) \psi_2 \, d\tau. \quad -(34)$$

In the same m space Eq. (32) becomes:

$$r \rightarrow \frac{r}{m(r)^{1/2}}, \quad -(35)$$

$$t \rightarrow m(r)^{1/2} t \quad -(36)$$

so the energy levels of the complete Schroedinger equation in m space are:

$$E = \frac{1}{\int \psi_2^* m^{1/2}(r) \psi_2 \, d\tau}\left[-\frac{\hbar^2}{2m}\int \psi_1^*\left(\frac{r}{m(r)^{1/2}}\right)\frac{\partial^2}{\partial r^2}\left(\psi_1\left(\frac{r}{m(r)^{1/2}}\right)\right) d\tau + \int \psi_1^*\left(\frac{r}{m(r)^{1/2}}\right) U\left(\frac{r}{m(r)^{1/2}}\right)\psi_1\left(\frac{r}{m(r)^{1/2}}\right) d\tau\right] \quad -(37)$$

Quantization rules applied to analytical solutions of the Schrödinger equation

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3 Graphical examples and application to quantum chemistry

3.1 Examples of wave functions in m theory

First we present some graphics of analytical solutions of the Schrödinger equation. One basic system often used for describing quantum effects is the harmonic oscillator. It exhibits energy levels and time eigenfunctions as given by Eqs. (11) and (12). The radial eigenfunctions are complicated functions of Hermite polynomials and given in note 436(1). A remarkable property is the existence of a zero point energy $E = \frac{1}{2}\hbar\omega$ for the lowest quantum state $n = 0$. The eigen functions of the harmonic oscillator are graphed in Fig. 1 for the lowest states. They are even and odd functions around the centre $r = 0$. In case of m theory the radial coordinate is replaced by

$$r \rightarrow \frac{r}{\mathrm{m}(r)^{1/2}}. \tag{38}$$

This leads to sharp edges and stretching in the eigenstates at $r = 0$ as can be seen from Fig.2. The symmetry or antisymmetry remains intact.

The anharmonic oscillator is much more complicated to handle but an analytical solution for the Schrödinger equation is known, see note 436(2). There is an asymmetry factor $x \propto 1/\omega$ in energies and eigenfunctions. The asymmetric potential of this oscillator type leads to asymmetric eigenstates as graphed in Fig. 3. The eigenstates depend on generalized Laguerre polynomials. Using the transformation (38) to m space, a similar effect as for the harmonic oscillator appears: The functions have wide jumps or get sharp edges at the origin (Fig. 4). This is a consequence of the m function which is effective near to the origin.

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3.2 m theory in Quantum Chemistry

We have developed an example of m space effects impacting Quantum Chemistry. The computer code used is based on an ab initio method, the Local Density Approximation (LDA), and solves either the Schrödinger equation (non-relativistic case) or the Dirac equation (relativistic case) or the squared Dirac equation (so-called scalar-relativistic calculation)[1]. Spin-polarized calculations can be performed with the first two cases.

In the LDA method the equations for the N-electron system are reduced to effective 1-electron equations for each electron (i.e. orbital occupation). The effective potential to be used is (in atomic units)

$$U_{\text{eff}}(\mathbf{r}) = U_{\text{core}}(\mathbf{r}) + U_{\text{el}}(\mathbf{r}) + U_{\text{xc}}(\mathbf{r}) \tag{39}$$

with core potential

$$U_{\text{core}}(\mathbf{r}) = -Z/r, \tag{40}$$

electron potential

$$U_{\text{el}}(\mathbf{r}) = \int \frac{\rho(\mathbf{r}')}{\mathbf{r} - \mathbf{r}'} d\tau', \tag{41}$$

and so-called exchange-correlation potential

$$U_{\text{xc}}(\mathbf{r}) = U_{\text{xc}}[\rho(\mathbf{r})]. \tag{42}$$

The main problem is the handling of exchange and correlation of the N-electron system (interaction of electrons according to Pauli's exclusion principle) so that an effective 1-electron equation remains to be solved. There are several approaches to this problem but the differences cannot be seen in charge density plots we provided as examples below.

The wave functions ψ_i follow as solutions of e.g. the Schrödinger equation and the charge density is

$$\rho(\mathbf{r}) = \sum_i |\psi_i(\mathbf{r})|^2 . \tag{43}$$

Because the charge density enters the potential which in turn determines the solutions of the Schrödinger equation, both computations have to be iteratively repeated until self-consistency is reached. A similar problem was already discussed for Hydrogen bonding[2] where the full ECE potential including the spin connection was considered. In order to obtain resonant states, a similar self-consistency cycle was proposed.

We computed the atomic charge density of a Nickel atom as an example. Ni has 18 core electrons and 10 valence electrons in configuration $3d^8 4s^2$. The configuration can be changed e.g. to compute ionization energies for the ion $3d^8 4s^1$ or spin-ordered states which play a role in the Ni solid. The relevant quantity in such calculations is the total energy.

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[1] H. Gollisch and L. Fritsche; "Relativistic One-Particle Equation for Electron States of Heavy Metals", phys. stat. sol. (b)86, 145 (1978)

[2] Myron Evans, Douglas Lindstrom, Horst Eckardt; "ECE Theory of Hydrogen Bonding", International Conference on Water, Hydrogen Bonding Nanomaterials and Nanomedicine; Banja Luka, September 4, 2010

In our example we have first graphed the total charge density concentrated in spherical shells, $4\pi r^2 \rho$, see Fig. 5. This is what can be sampled by XPS experiments for example. The three shells of the principal quantum numbers can be seen. For a more detailed view the valence charge density ρ_{val} alone is shown in Fig. 6. The $3d$ shell, which is separated from the s electrons, is well visible. When performing the radial coordinate transformation (38), the charge density near to the origin is shifted to larger radii. This effect can be observed in Fig. 6 where we have used the exponential m function with parameter $R = 5 \cdot 10^{-4} a_0$. Due to the logarithmic scale, differences near to the origin are clearly visible. As a second modification we have graphed the modified density $\frac{\rho(r)}{\mathrm{m}(r)^{1/2}}$. Near to the lowest radial grid points, the density is enlarged by a factor of 2. The question is if this has a remarkable effect on the total charge which is the integral over the charge density. The integral

$$\int \frac{\rho(r)}{\mathrm{m}(r)^{1/2}} d\tau \tag{44}$$

which gives the number of electrons in the case m(r)=1, deviates from N=28 (for atomic nickel) only in the fifth decimal place. The differences are not visible if the charge density of spherical shells of Fig. 5 is considered. This shows that for quantum-chemical calculations it could be sufficient to apply m theory a posteriori as a perturbation effect, although the density is altered significantly near to the origin. The situation is different for nuclear physics where the structure of the nucleus is impacted – and possibly completely determined – by m theory.

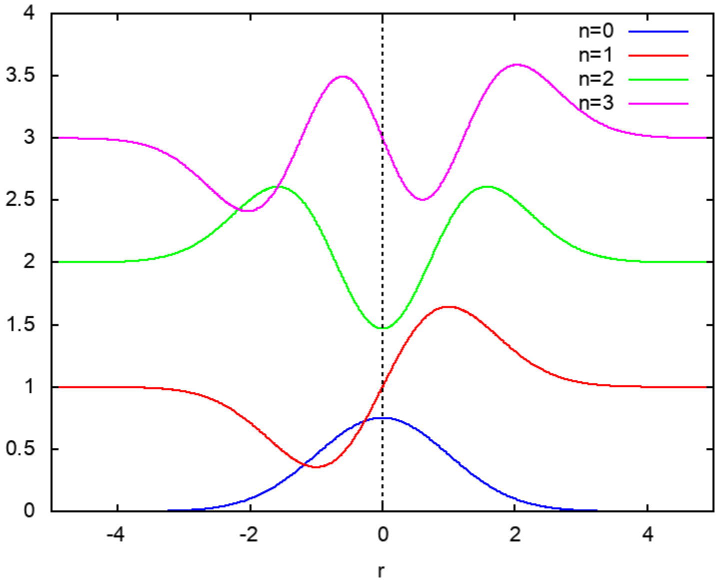

Figure 1: Eigenstates of the harmonic oscillator.

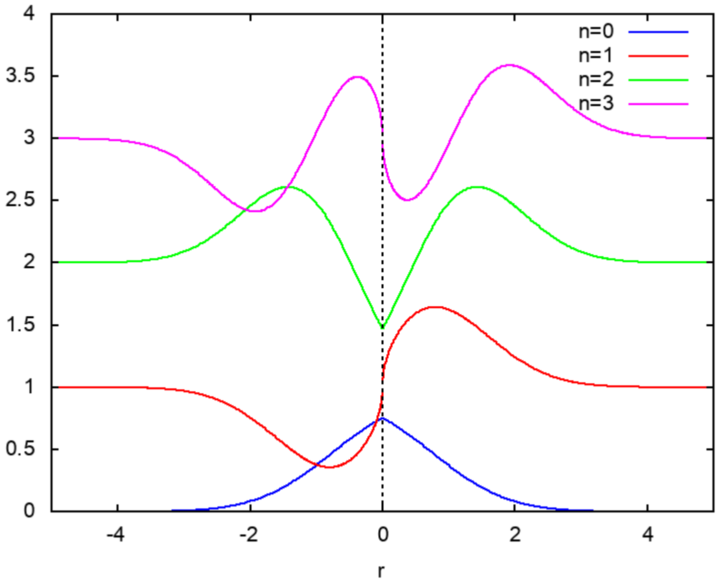

Figure 2: Eigenstates of the harmonic oscillator, m theory.

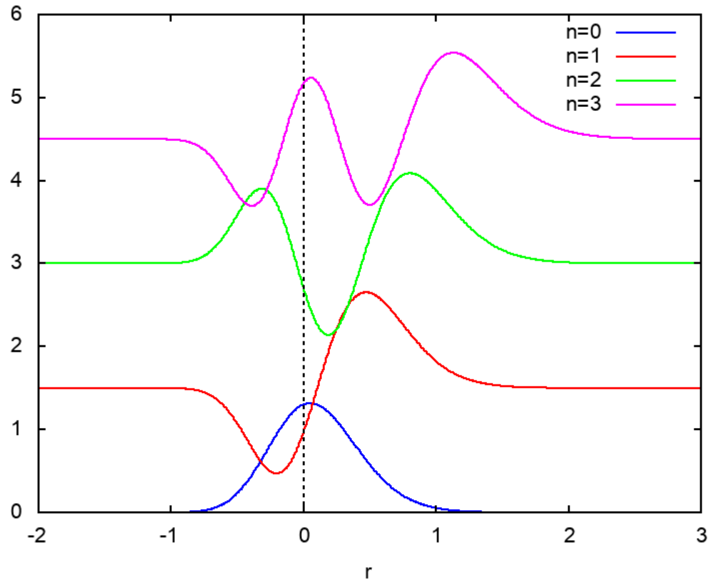

Figure 3: Eigenstates of the anharmonic oscillator.

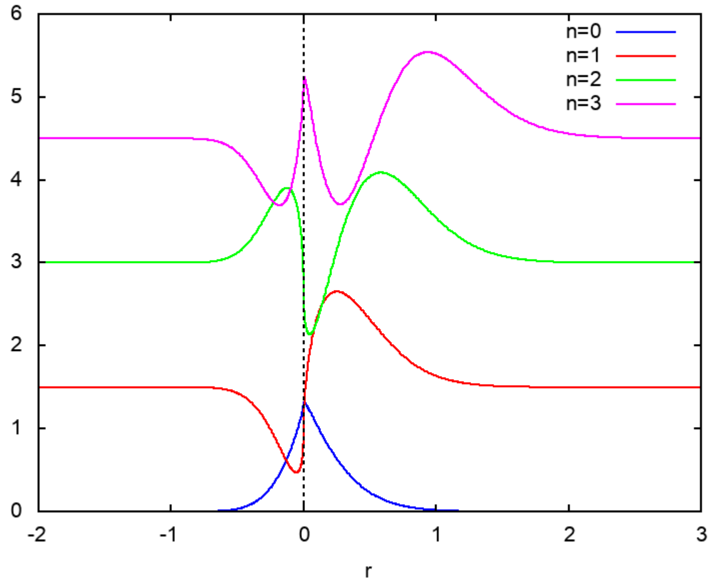

Figure 4: Eigenstates of the anharmonic oscillator, m theory.

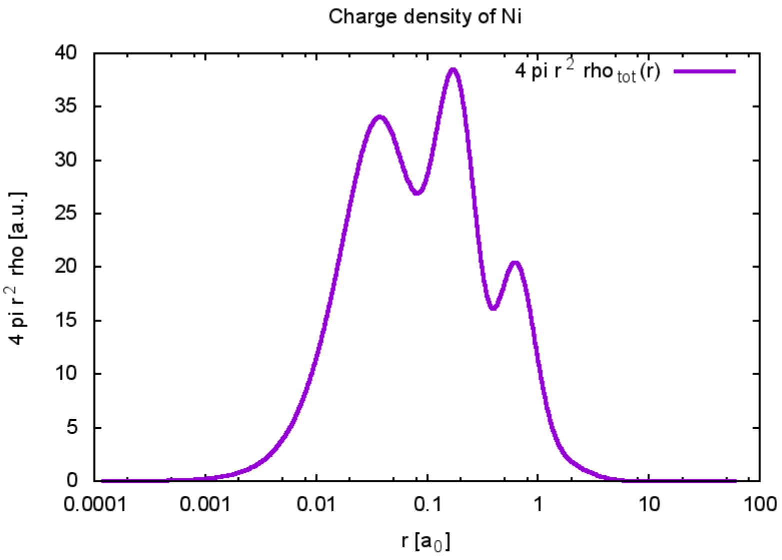

Figure 5: Total charge density of a Ni atom, spherical $4\pi r^2\rho$.

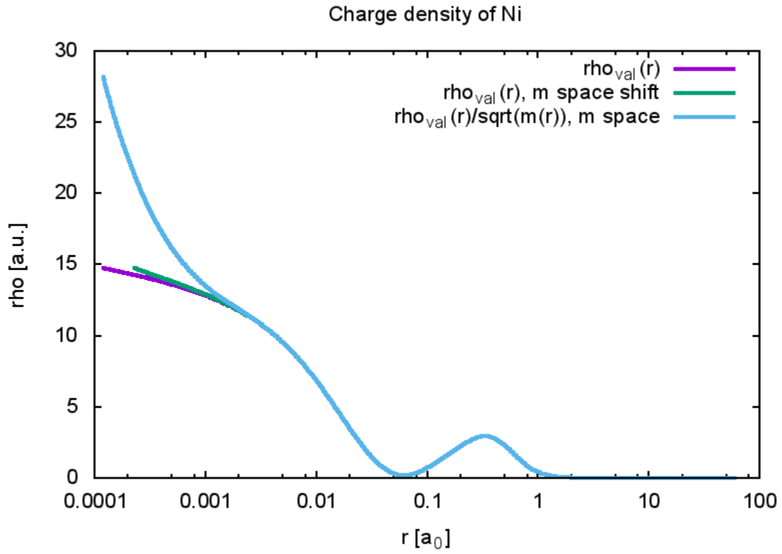

Figure 6: Valence charge density ρ_{val} of a Ni atom, effects of m space.

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