The force equation of quantum mechanics.

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Abstract.

The force equation of quantum mechanics is deduced using the fact that the canonical variables $q$ and $p$ of Hamilton’s classical equations are independent. This enables the straightforward calculation of forces for the first time in quantum mechanics using the Schrödinger wavefunctions. Some examples of force eigenvalues are given for exact solutions of Schrödinger’s equation, a pure energy equation derived from the classical hamiltonian. This new method of calculating forces has essentially unlimited utility throughout quantum science.

*Keywords*: ECE theory, quantum force equation, Hamilton equations.
1. Introduction.

During the course of development of ECE unified field theory in 177 papers to date [1-10] the Schroedinger equation of quantum mechanics has been derived from Cartan geometry within the context of a unified field theory. The logical framework provided by ECE theory allowed the deduction of the quantum Hamilton equations in UFT 176 (www.aias.us).

In Section 2 a new force equation of quantum mechanics is derived using the fact that the canonical variables $q$ and $p$ of the Hamilton equations of motion are independent. This fact allows the deduction of the force equation from the Schroedinger equation, so the Schroedinger wavefunctions can be used straightforwardly to calculate force eigenvalues of quantum mechanics. The force equation of quantum mechanics has unlimited utility throughout quantum science, being as fundamentally important as the force equations of classical mechanics.

In Section 3, computer algebra is used to check the hand calculations of Section 2 and to produce tables of force eigenvalues for well known exact solutions [11, 12] of the Schroedinger equation. The existence of pure quantum force is reported for the first time in problems such as the particle on a sphere. The force equation can be applied in computational quantum chemistry to investigate intra and inter molecular forces and torques of utility in molecular dynamics simulation.

2. The force equation and some force eigenvalues.

Consider the classical hamiltonian:

$$H = T + V$$

where $T$ is kinetic energy and $V$ is potential energy. It may be written as:

$$H = E$$

where $E$ denotes total energy. The canonical variables of Hamilton are $q$ and $p$, and they are independent variables:

$$\frac{dp}{dq} = 0 \ .$$

If for the sake of argument $q$ is chosen to be $x$ in one dimension, then:

$$\frac{dp}{dx} = 0 \ .$$
The kinetic energy is:

\[ T = \frac{p^2}{m} \tag{5} \]

so it follows from the independence of \( x \) and \( p \) that:

\[ \frac{dT}{dx} = 0 \tag{6} \]

Therefore:

\[ \frac{dH}{dx} = \frac{dV}{dx} \tag{7} \]

Consider the Schroedinger axiom:

\[ \hat{p} \psi = -i \hbar \frac{d\psi}{dx} \tag{8} \]

in which \( \hat{p} \) is an operator acting on the function \( \psi \), known as the wavefunction of quantum mechanics. Here \( \hbar \) is the reduced Planck constant. It follows that the kinetic energy in quantum mechanics becomes an operator:

\[ \hat{T} \psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \tag{9} \]

and the hamiltonian becomes Schroedinger’s equation:

\[ \hat{H} \psi = (\hat{T} + V) \psi = E \psi \tag{10} \]

Now differentiate both sides of Eq. (10):

\[ \frac{d}{dx} (\hat{H} \psi) = \frac{d}{dx} (E \psi) \tag{11} \]

It follows that:

\[ \frac{d}{dx} (\hat{H} \psi) = E \frac{d\psi}{dx} \tag{12} \]

because the energy eigenvalues \( E \) are independent of \( x \). Therefore:

\[ \left( \frac{d\hat{H}}{dx} \right) \psi + \hat{H} \frac{d\psi}{dx} = E \frac{d\psi}{dx} \tag{13} \]

From the independence of \( x \) and \( p \) in Hamilton’s equations, it follows that:
\[
\frac{d\hat{H}}{dx} \psi = \left( \frac{dV}{dx} \right) \psi
\]

(14)

from Eq. (7). The force is defined as:

\[ F = - \frac{dV}{dx} . \]

(15)

Therefore the force equation of quantum mechanics follows from Hamilton´s equations:

\[
(\hat{H} - E) \frac{d\psi}{dx} = F \psi .
\]

(16)

This is a new result of unlimited utility throughout quantum science.

In Eq. (16) the hamiltonian operator:

\[
\hat{H} = - \frac{\hbar^2}{2 m} \frac{\partial^2}{\partial x^2} + V
\]

(17)

acts on the derivative of the Schroedinger wavefunction, or in general on the derivative of a quantum mechanical wavefunction obtained in any way, for example in computational quantum chemistry. The quantum Hamilton equation derived in UFT 176 is:

\[
i \hbar \frac{d}{dx} < \hat{H} > = < [\hat{H} , \hat{p} ] >
\]

(18)

where:

\[
< [\hat{H} , \hat{p} ] > = i \hbar \frac{dV}{dx}
\]

(19)

so it is found, self consistently, that:

\[
\frac{d}{dx} < \hat{H} > = \frac{dH}{dx} = \frac{dV}{dx} = - F = - \frac{dp}{dt} .
\]

(20)

The fundamental result of the independence of \( x \) and \( p \) in Hamilton´s equation means that:

\[
\frac{d}{dx} \left( \frac{p^2}{2 m} \right) = 0
\]

(21)

so it follows that:

\[
\frac{d}{dx} \left( \frac{p^2}{2 m} \right) = - \frac{\hbar^2}{2 m} \int \psi^* \frac{\partial^2 \psi}{\partial x^2} d\tau = 0 .
\]

(22)
In Eq. (18):

\[
\frac{d}{dx} < \hat{H} > = -\frac{\hbar^2}{2m} \frac{d}{dx} \int \psi^* \frac{\partial^2 \psi}{\partial x^2} \, d\tau + \int \psi^* \hat{\chi} \frac{dV}{dx} \, d\tau = < \frac{dV}{dx} > = \frac{dV}{dx} .
\]  

(23)

In general therefore:

\[
< \frac{d\hat{H}}{dx} > = \int \psi^* \frac{d\hat{H}}{dx} \psi \, d\tau
\]

(24)

and from Eq. (13) it follows that:

\[
< \frac{d\hat{H}}{dx} > = \frac{d < \hat{H} >}{dx}
\]

(25)

as used in UFT 176. This result means that:

\[
\int \psi^* \frac{d\hat{H}}{dx} \psi \, d\tau = \int \psi^* \frac{dV}{dx} \psi \, d\tau
\]

\[
= \frac{dV}{dx} = \frac{d < \hat{H} >}{dx} = -F
\]  

(26)

Eq. (16) can be used to find force eigenvalues of exact solutions of the Schroedinger equation. As far as we have been able to find by literature search, this procedure has never been carried out in quantum mechanics to date and provides fundamental information of unlimited utility. The rest of this section gives simple examples amenable to hand calculation, and in Section 3, tables of force eigenvalues are given from computer algebra.

The zero order wavefunction of the harmonic oscillator [11, 12] is:

\[
\psi_0 = \left( \frac{m\omega}{\hbar \pi} \right)^{1/4} \exp \left( -\frac{m\omega}{2\hbar} x^2 \right)
\]

(27)

where \(x\) is displacement, \(m\) is mass and \(\omega\) the angular frequency of oscillation. Therefore:

\[
\hat{H} \frac{d\psi_0}{dx} = \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \right) \frac{d\psi_0}{dx} .
\]

(28)

The energy levels of the harmonic oscillator are [11, 12]:

\[
E = ( n + \frac{1}{2} ) \hbar \omega
\]

(29)

and the zero order energy level is given by:
\( E_0 = \frac{1}{2} \hbar \omega \) . (30)

So the zero order force eigenvalue is:

\[ F_0 = -m \omega^2 x \] . (31)

This happens to be the same as the classical result. It shows that the well known zero order or “vacuum” energy (22) is accompanied by a hitherto unknown zero order force (23). It seems likely that this force is related to the Casimir force, a well known radiative correction.

The first order wavefunction of the harmonic oscillator is [11, 12]:

\[ \psi_1 = A x \exp \left( -\alpha \frac{x^2}{2} \right) \] (32)

where:

\[ A = \left( \frac{4\alpha}{\pi} \right)^{1/4} \alpha^{1/2} , \quad \alpha = \frac{m\omega}{\hbar} \] (33)

and the first order energy level is:

\[ E = \frac{3}{2} \hbar \omega , \quad n = 1 \] , (34)

so from Eq. (16), the first order force eigenvalue is:

\[ F_1 = -kx \] (35)

where the Hooke law constant is well known to be:

\[ k = m\omega^2 \] . (36)

By computer algebra it was found that all the eigenfunctions of force for the harmonic oscillator are the same as for the zero and first order eigenvalues. There is a zero order force which does not exist in classical physics, and this is the first time it has been reported. Evidently, these eigenvalues of force are all quantized, in the case of the harmonic oscillator they happen to be the same as the classical result for all wavefunctions.

The method can be extended to the 1s orbital of the H atom, whose wavefunction takes the format:

\[ \psi_{10} = e^{-r/a} \] \hspace{1cm} (37)

where \( A \) is a constant. The hamiltonian operator in this case is:
\[ \hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(r) \]  

(38)

where the potential is a Coulomb attraction between the proton and electron of the H atom together with the repulsive centrifugal force where \( l \) is the angular momentum quantum number:

\[ V(r) = -\frac{e^2}{4\pi \varepsilon_0 r} + \frac{l(l+1)\hbar^2}{2mr^2} \]  

(39)

and where \( \varepsilon_0 \) is the S.I. vacuum permittivity and where \( e \) is the proton charge [11, 12]. The energy levels of the H atom [11, 12] are:

\[ E = -\frac{\hbar^2}{2ma^2 n^2} \]  

(40)

where \( n \) is the principal quantum number and where \( a \) is the Bohr radius. For the 1s orbital:

\[ n = 1 \]  

(41)

so:

\[ E_{10} = -\frac{\hbar^2}{2ma^2} \]  

(42)

Therefore Eq. (16) gives the result:

\[ F_{10} = 0. \]  

(43)

The force eigenvalue in the 1s orbital is zero. This is an explanation of the stability of the 1s orbital. There is no way of accounting for this stability in conventional quantum mechanics [11, 12] because the 1s orbital has no angular momentum and the most probable point [11] at which the electron of the 1s orbital is found is the nucleus. The correct explanation for the stability of the 1s orbital is that the classical Coulombic force of attraction is balanced exactly by a quantum force hitherto unknown and the net force is zero.

The radial part of the 2p\(_z\) orbital of H is [11, 12]:

\[ \psi_{21} = A r e^{-r/2a} \]  

(44)

and the energy level is:

\[ E_{21} = -\frac{\hbar^2}{8ma^2} \]  

(45)

so Eq. (16) gives:
\[ F_{21} = -\frac{\hbar^2(r - 2a)}{2a mr^3}. \] (46)

In this case there is a net force on the 2p\(_x\) electron due to the radial part of its complete wavefunction. The latter is a product of the radial function (36) and a spherical harmonic as is well known. The force eigenvalues for the H atom are discussed in detail in Section 3.

For planar rotation with constant \( r \) (the particle on a ring [11]), Eq. (16) becomes:

\[ (\hat{H} - E)(\frac{d\psi}{dx} + \frac{d\psi}{dy}) = F\psi \] (47)

and the Hamiltonian operator is:

\[ \hat{H} = -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right). \] (48)

In cylindrical coordinates:

\[ \frac{df}{dx} = \cos\phi \frac{df}{dr} - \frac{\sin\phi}{r} \frac{df}{d\phi} \] (49)

\[ \frac{df}{dy} = \sin\phi \frac{df}{dr} + \frac{\cos\phi}{r} \frac{df}{d\phi} \] (50)

and if \( r \) is constant:

\[ \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = \frac{1}{r^2} \frac{\partial^2 f}{\partial \phi^2}. \] (51)

Using the results:

\[ \frac{df}{dx} + \frac{df}{dy} = \frac{1}{r} (\cos\phi - \sin\phi) \frac{df}{d\phi} \] (52)

and:

\[ \frac{\partial^3 f}{\partial x^3} + \frac{\partial^3 f}{\partial y^3} = \frac{1}{r} (\cos\phi - \sin\phi) \frac{df}{d\phi} \] (53)

it is found that:

\[ \hat{H} \left( \frac{d\psi}{dx} + \frac{d\psi}{dy} \right) = -\frac{\hbar^2}{2m r^3} (\cos\phi - \sin\phi) \frac{\partial^3\psi}{\partial \phi^3}, \] (54)
The wavefunction in general is:

\[ \psi = A \exp(\text{i} m_j \varphi) + B \exp(-\text{i} m_j \varphi) \]  

(56)

with energy levels:

\[ E = \frac{\hbar^2 m_j^2}{2mr^2} \]  

(57)

so it is found that:

\[ F = 0 \]

for all quantum numbers \( m_j \). In this case all the force eigenvalues are zero.

Finally for three dimensional rotation (the particle on a sphere), the quantum force equation becomes:

\[(\hat{A} - E) \nabla \psi = F \psi\]  

(58)

where, in spherical polar coordinates:

\[ \nabla \psi = \frac{d\psi}{dr} e_r + \frac{1}{r} \frac{d\psi}{d\theta} e_\theta + \frac{1}{r \sin \theta} \frac{d\psi}{d\varphi} e_\varphi \]  

(59)

There is no classical potential \( V \), so the hamiltonian operator is:

\[ \hat{A} = -\frac{\hbar^2}{2m} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right] \]  

(60)

The energy levels are:

\[ E = \frac{\hbar^2}{2mr^2} \ (l + 1) \]  

(61)

where \( l \) is the angular momentum quantum number \([11, 12]\) and \( mr^2 \) is the moment of inertia. There are two quantum numbers \( l \) and \( m \), and the wavefunctions are the spherical harmonics \([11, 12]\):

\[ \psi = Y_{lm} \]  

(62)

In the simplest case:
\[ \psi_{00} = \frac{1}{2\pi^{\frac{1}{2}}} \]  

so:

\[ F_{00} = 0 . \]  

In this case there is no force eigenvalue. Secondly, consider as an example:

\[ \psi_{10} = \frac{1}{2} \left( \frac{3}{\pi} \right)^{\frac{1}{2}} \cos \theta . \]  

Therefore:

\[ \nabla \psi_{10} = \frac{1}{r} \frac{d \psi_{10}}{d \theta} e_{\theta} = -\frac{A}{r} \sin \theta e_{\theta} \]  

and:

\[ \hat{H} (\nabla \psi_{10}) = -\frac{\hbar^2}{2mr^3} \left( \frac{\cos \theta}{\sin \theta} \frac{\partial^2 \psi_{10}}{\partial \theta^2} + \frac{\partial^3 \psi_{10}}{\partial \theta^3} \right) e_{\theta} \]

\[ = \frac{A\hbar^2}{2mr^3} \left( \frac{\cos^2 \theta}{\sin \theta} + \sin \theta \right) e_{\theta} \]  

with:

\[ E \nabla \psi_{10} = -\frac{A\hbar^2}{mr^3} \sin \theta e_{\theta} . \]  

So:

\[ (\hat{H} - E) \nabla \psi_{10} = F \psi_{10} = \frac{A\hbar^2}{2mr^3} \left( \frac{\cos^2 \theta}{\sin \theta} + 3 \sin \theta \right) e_{\theta} \]

\[ = A \cos \theta e_{\theta} \]  

and there is a non-zero force eigenvalue:

\[ F_{10} = \frac{\hbar^2}{2mr^3} \left( \frac{\cos \theta}{\sin \theta} + 3 \sin \theta \right) . \]  

This is a pure quantum force eigenvalue, hitherto unknown for the particle on a sphere. There is no potential and no classical force.
3. Evaluation of force eigenvalues by computer algebra.
   (Section by Dr. Horst Eckardt).

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References.