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Quantization of Friction for Nano Isolated Systems

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ABSTRACT

A wide variety of materials have mechanical friction. This friction plays an important role in determine the mechanical properties and the electrical properties of the matter. The most popular physical theory that is used to describe the physical properties of matter is quantum mechanics. Recently quantum laws found to be incapable of describing the behavior of some new materials like super conductors and Nano materials. This may be attributed to the fact that quantum laws have no terms sensitive to friction. This work aims to derive Schrodinger quantum equation having frictional term. This equation is used to solve the problem of particle in a box. The solution shows quantized frictional energy.

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Introduction

Quantum theory has been extremely successful at describing the features of microscopic particles, for example the energy levels in atoms. However, in order to calculate any specific property of such a microscopic particle, one usually considers it in isolation - as if there was nothing else around in the whole world. In many cases this is justified in the sense that the impact of the rest of the world has only a very marginal effect on this microscopic particle and its properties, but there are also quite a few cases where this is not true and where the immediate vicinity of a microscopic particle radically alters the particle's properties and behavior [1]. The effect of surrounding atoms, on specific atomic electrons, was observed in bulk matter. In bulk matter the electrons distribution, and the energy levels of atoms changes radically as compared to one isolated atom. For example, the energy levels are converted to energy gaps in between [2,3] but still the macroscopic properties of the bulk matter obeys classical laws.

However the situation is different for Nano particles which are isolated aggregates of atoms, having nano scale dimension. Nano particles cannot behave as a single atom as far as they consist of a large amount of atoms having fields that affect the electronic configuration of each single atom. They cannot obey classical laws since the nano scale particles obeys quantum laws [4,5]. The behavior of aggregates of atoms which form a bulk matter or nano particles in relation to their physical properties was take led by different models. In the models like free electrons model, Krong-Benny model and tight binding approximation, the periodicity, and crystal field and electrons wave functions interference are used to account for the effect of the surrounding atoms [6]. In the so called mean field theory the effect of surrounding atoms manifests itself through the super position of atomic wave functions [7].

Despite the successes of these models, they unfortunately suffer from noticeable setbacks and some deceases which need to be cured. One of the main setbacks comes from the fact that the wave function and energy of two systems having the same crystal and atomic potentials, but having different friction coefficient, is the same. I.e. the presence of friction or its absence does not affect the wave function and energy distribution. This becomes in direct conflict with the fact their electrical properties is macroscopically different [8].

For example the atomic potential on elements is the same, in gaseous state, liquid state and solid state. Despite the quantity of this potential, in all these states, they have different microscopic and macroscopic properties. This reflects the importance of inter atomic interactions of the neighboring atoms including collision and frictional force. Where these interactions become important, due to the fact that the change from gaseous state to liquid state to solid state, decreases atomic spacing and increases their mutual interaction [9].

Unfortunately ordinary Schrödinger Equation has no terms to account for mutual a atomic interaction which includes collision that is related to thermal energy and force of friction. Thus there is an urgent need to construct a new Schrödinger Equation which accounts for these effects, strictly speaking, thermal and friction effects. Different attempts were made to incorporated friction and thermal terms in Schrodinger Equation [10]. Some of them in Maxwell wave equation [11]. Attempts are also based on correspondence principle, where the expectation value is equal to the classical macroscopic value [12] Some authors also uses classical harmonic oscillator model to derive statistical distribution laws [13]. Despite the remarkable successes of these models, they suffer from some draw backs. First of all some of them are not take into account the wave nature of microscopic world, which requires that Schrödinger energy equation should be based on energy expression for oscillating system. The models do nothing about the quantization of frictional energy.

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Thus a new Schrodinger model incorporating the effect of thermal energy and friction is needed. This is done in section three. Before this section, one have introduction in section one, while section two is devoted for plasma equation, where as section four and five are concerned with the solutions of Schrödinger equation for a particle in a box and a harmonic oscillators respectively.

Plasma equations

In plasma state atoms and molecules are highly ionized. Thus it can be described by the laws of fluid mechanics beside Maxwell's equations. The use of fluid mechanics comes from the fact that plasma resembles gaseous state . Maxwell's equations can describe ionized moving particles generating electric and magnetic fields inside the plasma . Thus the equation of plasma particles having density ρ ,velocity \mathbf{v} , pressure \mathbf{P} ,and force \mathbf{F} is given by [14]

$$\rho \left[\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right] + \nabla P = \mathbf{F} \quad (1)$$

$$\text{Where } \rho \text{ is given by } \rho = nm \quad (2)$$

And n being the number density , m is the particle mass . In presence of a field of potential V beside a frictional force F_r , the force is given by

$$\mathbf{F} = -\nabla V - F_r \quad (3)$$

The electric force F_{elec} on a charge q , is given by

$$F_{elec} = qnE \quad (4)$$

E is the electric field intensity.

The electric field satisfies Maxwell's equations

$$\nabla \cdot \mathbf{D} = qn \quad (5)$$

$$\mathbf{D} = \epsilon \mathbf{E} \quad (6)$$

\mathbf{D} is the electric flux density.

The thermal pressure is given by

$$P = nkT \quad (7)$$

k is the Boltzmann constant , and T is the temperature .The frictional force can be assumed to be[15]

$$F_r = \frac{mv}{\tau} \quad (8)$$

Where τ the relaxation time and m is is the moving particle.

Schrodinger Equation in Presence of Thermal and Resistive Energy:

The energy of ordinary Schrödinger equation includes kinetic and potential energy .However, there are other energy types which should be considered , for example the energy lost E_r by friction for oscillating system which is given by[16]

$$\int F_r dx \quad (9)$$

The thermal energy is given in terms of temperature T and Boltzman constant k as

$$E_r = kT \quad (10)$$

Where there is no room in ordinary conventional Schrödinger equation for feeling the effect of friction and heating does not recognize these energy types.

To incorporate energy consider the plasma equation [1]

$$mn \left(\frac{\partial v}{\partial t} + v \cdot \nabla v \right) = F - \nabla P - F_r \quad (11)$$

Where P stands for the force, thermal pressure.

The resistive force is given by

$$F_r = \frac{nmv}{\tau} \quad (12)$$

Suggesting the displacement to be

$$x = x_0 e^{-i\omega t}$$

$$\frac{\partial x}{\partial t} = x_0 e^{-i\omega t} = -i\omega x$$

$$v = -i\omega x \quad (13)$$

It follows that

$$F_r = -i \frac{nm\omega x}{\tau} \quad (14)$$

Since v is function of t and x , it follows that

$$dv = \frac{\partial v}{\partial t} dt + \frac{\partial v}{\partial x} dx$$

$$\frac{dv}{dt} = \frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x}$$

$$\frac{dv}{dt} = \frac{\partial v}{\partial t} + v \cdot \nabla v \quad (15)$$

Thus by using equation (15)and equation (11)reduces to

$$mn \frac{dv}{dt} = F - \nabla P - F_r \quad (16)$$

If the field potential per particle is given by v , then the field force F takes the form

$$F = - \frac{\partial(nv)}{\partial x} \quad (17)$$

The left hand side of equation (16) is given by:

$$mn \frac{dv}{dt} = mn \frac{dv}{dx} \frac{dx}{dt} = mnv \frac{dv}{dx}$$

The pressure is given in turn to be:

$$\nabla P = \frac{\partial p}{\partial x} = \frac{dp}{dx} = \frac{d(nkT)}{dx} \quad (18)$$

Where the thermal pressure takes the form

$$P = nkT \quad (19)$$

Then equation (16) can be re expressed with the aid of equations (17), and (18) to be:

$$\frac{dmnv^2}{dx} = -\frac{d(nv)}{dx} - \frac{d(nKT)}{dx} + i \frac{m\omega xn}{\tau}$$

Thus

$$\frac{d}{dx} \left(\frac{1}{2} mnv^2 + nv + nKT \right) = i \frac{m\omega xn}{\tau} \quad (20)$$

Integrating both sides of equation (20) one gets

$$-C_0 + \int d \left(\frac{1}{2} mnv^2 + nv + nKT \right) = i \frac{m\omega n}{\tau} \int x dx$$

$$\left(\frac{1}{2} mnv^2 + nV + nKT \right) - i \frac{m\omega nx^2}{2\tau} = C_0$$

$$(nE_{kin} + nv + nKT) - i \frac{m\omega nx^2}{2\tau} = C_0 \quad (21)$$

The left hand side is a constant of motion and has a dimension of energy. Thus one can define the total energy E_T to be

$$E_T = nE = n \left(\left(\frac{1}{2} mV^2 + V + KT \right) - i \frac{m\omega A^2}{2\tau} \right) \quad (22)$$

But

$$\frac{1}{2} mv^2 = \frac{m^2 v^2}{2m} = \frac{p^2}{2m} \quad (23)$$

Thus the total energy of one particle can be rewritten in the form:

$$E = \frac{p^2}{2m} + v + kT - i \frac{m\omega x^2}{2\tau} \quad (24)$$

This expression stands for the total energy of a single particle, which consists beside kinetic energy, additional terms. The third term represents the thermal energy, while the fourth term stands for the frictional energy.

To derive Schrödinger equation, for this new energy expression, equation (24) must be multiplied by the wave function ψ to get

$$E\psi = \frac{p^2}{2m} \psi + V\psi + kT\psi - i \frac{m\omega x^2}{2\tau} \psi \quad (25)$$

The wave function for a free particle is given by

$$\psi = Ae^{-\frac{i}{\hbar}(Px - Et)} \quad (26)$$

Differentiating ψ with respect to t and x yields

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} E\psi$$

$$i\hbar \frac{\partial \psi}{\partial t} = E\psi$$

$$\frac{\partial \psi}{\partial x} = \frac{i}{\hbar} p\psi$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{p^2}{\hbar^2} \psi \quad (27)$$

Substitute equation (27) in equation (25) yields

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2 v^2}{2m} \psi + v\psi + kT\psi - i \frac{m\omega x^2}{2\tau} \psi \quad (28)$$

If one rewrites the frictional term in the form

$$E_r = i \frac{m\omega A^2}{2\tau} = i \frac{m\omega^2 A^2}{2\tau\omega} = i \frac{mV^2}{2\tau\omega} = i \frac{m^2 V^2}{2\tau m\omega} = i \frac{m^2 V^2 \hbar}{2\tau m \hbar \omega}$$

$$= i \frac{\hbar m^2 v^2}{2\tau m \hbar \omega} = i \frac{\hbar p^2}{2\tau m^2 c^2} = i \frac{\hbar}{2\tau m^2 c^2} p^2 \quad (29)$$

$$\text{Where: } \omega \hbar = mc^2$$

And equation (13) gives:

$$v^2 = |v^2| = v \cdot v^* = (-i\omega x)(i\omega x) = \omega^2 x^2$$

Substitute equation (14) in equation (25) to get

$$E\psi = \frac{p^2}{2m} \psi + V\psi + kT\psi - i \frac{\hbar}{2\tau m^2 c^2} p^2 \psi \quad (30)$$

Substitute equation (14) in equation (25) yields

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + kT\psi - i \frac{\hbar^3}{2\tau m^2 c^2} \frac{\partial^2 \psi}{\partial x^2} + v\psi$$

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + kT\psi - i \frac{\hbar^3}{2\tau m^2 c^2} \nabla^2 \psi + v\psi \quad (31)$$

Which is the Schrödinger equation for thermal resistive medium.

Particle in box

The motion of the particle in box can be described by Schrodinger Equation. The potential per particle is given by

$$V = 0 \quad (32)$$

Substituting equation (32) in equation (31) yields

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + kT\psi - i \frac{\hbar^3}{2\tau m^2 c^2} \nabla^2 \psi \quad (33)$$

Consider a solution of the form

$$\psi = e^{-i\omega t} u \quad (34)$$

Inserting equation (34) in (33) yields:

$$\hbar\omega e^{-i\omega t}u = -\frac{\hbar^2}{2m}\nabla^2 e^{-i\omega t}u + kTe^{-i\omega t}u - i\frac{\hbar^3}{2\tau m^2 c^2}\nabla^2 e^{-i\omega t}u \quad (35)$$

By considering

$$E = \hbar\omega$$

And eliminating common terms one gets:

$$Eu = -\frac{\hbar^2}{2m}\nabla^2 u + kTu - i\frac{\hbar^3}{2\tau m^2 c^2}\nabla^2 u \quad (36)$$

To solve this equation consider the solution

$$u = A \sin \alpha x \quad (37)$$

Differentiating u with respect to x yields

$$\frac{\partial u}{\partial x} = \alpha \cos \alpha x$$

Thus

$$\frac{\partial^2 u}{\partial x^2} = -\alpha^2 \sin \alpha x = -\alpha^2 u \quad (38)$$

Substituting equation (38) in equation (36) to get

$$Eu = \frac{\hbar^2}{2m}\alpha^2 u + kTu + i\frac{\hbar^3}{2\tau m^2 c^2}\alpha^2 u$$

$$E = \frac{\hbar^2}{2m}\alpha^2 + kT + i\frac{\hbar^3}{2\tau m^2 c^2}\alpha^2 \quad (39)$$

Rearranging for getting α , yields

$$\left[\frac{\hbar^2}{2m} + i\frac{\hbar^3}{2\tau m^2 c^2}\right]\alpha^2 = E - kT \quad (40)$$

$$\alpha^2 = \frac{E - kT}{\left[\frac{\hbar^2}{2m} + i\frac{\hbar^3}{2\tau m^2 c^2}\right]} \quad (41)$$

$$\alpha = \sqrt{\frac{E - kT}{\left[\frac{\hbar^2}{2m} + i\frac{\hbar^3}{2\tau m^2 c^2}\right]}} \quad (42)$$

$$\alpha = \sqrt{\frac{E - kT}{\frac{\hbar^2}{2m}\left(1 + \frac{i\hbar}{\tau mc^2}\right)}} \quad (43)$$

For particle in a box

$$u(x = L) = 0$$

Thus from (37)

$$u = A \sin \alpha L = 0$$

$$\alpha L = 0, \pm\pi, \pm 2\pi, \dots$$

$$= n\pi$$

$$\alpha = \frac{n\pi}{L} \quad n = 0, \pm 1, \pm 2, \dots \quad (44)$$

Thus from (21)

$$E - kT = \frac{n^2\pi^2}{L^2} \frac{\hbar^2}{2m} \left(1 + \frac{i\hbar}{\tau mc^2}\right)$$

$$E = kT + \frac{n^2\hbar^2}{8L^2m} \left(1 + \frac{i\hbar}{\tau mc^2}\right) \quad (45)$$

Where

$$\hbar = \frac{h}{2\pi}$$

The energy in equation (45) can be written in the form :

$$E = E_1 + iE_2$$

Where

$$E_1 = kT + \frac{n^2\hbar^2}{8L^2m} \quad (46)$$

$$E_2 = \frac{n^2\hbar^2\hbar}{8L^2\tau m^2 c^2} \quad (47)$$

E_1 Stands for the energy gained by the particle , while E_2 is the energy lost by the particle .

Harmonic Oscillator

The Harmonic Oscillator is characterized by the potential:

$$V = +\frac{1}{2}kx^2 \quad (48)$$

Inserting equation (48) in equation (36) yields:

$$-\frac{\hbar^2}{2m}\nabla^2 u + kTu - \frac{i\hbar^3}{2\tau m^2 c^2}\nabla^2 u - \frac{1}{2}kx^2 u = Eu \quad (49)$$

Consider the solution:

$$u = Ae^{-\alpha x^2} \quad \nabla u = -2\alpha x u$$

$$\nabla^2 u = -2\alpha u - 2\alpha x \nabla u = -2\alpha u + 4\alpha^2 x^2 u \quad (50)$$

A direct substitution of equation (50) in equation (49) yields:

$$+\frac{\hbar^2}{2m}[2\alpha - 4\alpha^2 x^2]u + kTu + i\frac{\hbar^3}{2m}\left[\frac{2\alpha - 4\alpha^2 x^2}{\tau mc^2}\right]\hbar u + \frac{1}{2}kx^2 u = Eu$$

Equating the coefficients of u and $x^2 u$ on both sides yields:

$$-\frac{4\hbar^2}{2m} \left[1 + \frac{i\hbar}{\tau mc^2} \right] \alpha^2 - \frac{1}{2} k = 0 \quad 2 \frac{\hbar^2}{2m} \left[1 + \frac{i\hbar}{\tau mc^2} \right] \alpha + kT = E$$

By ignoring temperature term, one gets:

$$E = \alpha \left[1 + \frac{i\hbar}{\tau mc^2} \right] \frac{\hbar^2}{m} \quad (51)$$

The energy quantization can be obtained from equation (31) by separating variables, and assuming ψ to be:

$$\psi = \omega(\mathbf{t})v(\mathbf{x}) \quad (52)$$

To get:

$$\frac{i\hbar}{\omega} \frac{d\omega}{dt} = \frac{1}{u} \left[-\frac{\hbar^2}{2m} \left[1 + \frac{i\hbar}{\tau mc^2} \right] \right] \nabla^2 u + V = E$$

Thus:

$$\frac{i\hbar}{\omega} \frac{d\omega}{dt} = E$$

$$L_n \omega = c_1 - i \frac{E}{\hbar} t$$

$$\int \frac{d\omega}{\omega} = \frac{E}{i\hbar} \int dt + c_1$$

$$\omega = e^{c_1} e^{-\frac{iEt}{\hbar}} = c_2 e^{-\frac{iEt}{\hbar}} \quad (53)$$

The periodicity condition requires:

$$\omega(t+T) = \omega(t)$$

$$e^{-\frac{iET}{\hbar}} = 1$$

$$\cos \frac{ET}{\hbar} = 1$$

$$\frac{E}{\hbar} T = 2n\pi$$

$$e^{-\frac{iE}{\hbar}(t+T)} = e^{-\frac{iE}{\hbar}(t)}$$

$$\cos \frac{E}{\hbar} T - i \sin \frac{E}{\hbar} T = 1$$

$$\sin \frac{E}{\hbar} T = 0$$

$$E = \frac{n\hbar}{T} = n\hbar f \quad (53)$$

Therefore energy is quantized according to equation (51) and equation (52) beside equation (53), one gets:

$$nhf = \frac{(mk)^{1/2}}{2\hbar \left[1 + \frac{i\hbar}{\tau mc^2} \right]^{1/2}}$$

$$E = nhf = \frac{\hbar}{2} \left(\frac{k}{m} \right)^{1/2} \left[\frac{i\hbar}{\tau mc^2} \right]^{1/2} = \frac{1}{2} \hbar \omega c \left[1 + \frac{i\hbar}{\tau mc^2} \right]^{1/2} \quad (54)$$

Discussion

Plasma equation in the presence of friction and thermal energy equations (1, 3, and 7) is utilized to derive new Schrödinger Equation which is sensitive to temperature and friction as shown by equation (31). The friction term and manifests itself through (τ), where

$$\gamma = \frac{m}{\tau}$$

For particle in a box equation (45) shows the energy is quantized, including the energy loss due to friction which appear as an imaginary part. This imaginary energy resembles the optical potential which describes inelastic collision in a sea herring process. It also resembles the role of imaginary wave number in electromagnetic theory which is related to the damping term in the expression of light intensity that describes the energy loss by light when it enters a certain medium. Equations (45) and (46) show that the energy for a particle in a box reduces to the ordinary one in the absence of friction and thermal energy.

For a harmonic oscillator the solution equation (50) and the value of (α) is complex. This solution reduces to the ordinary one in the ordinary one in the absence of friction. Equation (53), shows that the energy is quantized. Equation (54) indicates the existence of friction term as an imaginary part.

Conclusion

The new Schrodinger Equation derived in this work is capable of describing a physical system in which temperature and friction plays an important role. It shows that friction energy appear as an imaginary part and is quantized.

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