Minimal length implications on the Hartree-Fock theory

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Hartree-Fock approximation suffers from two shortcomings including i) the divergence of the electron Fermi velocity, and ii) the existence of bandwidth which is not confirmed experimentally. Here, we study the effects of the minimal length on the ground state energy of the electron gas in the Hartree-Fock approximation. Our results indicate that, mathematically, the correction of minimal length to the phase space, which plays a vital, and predominant role below the Fermi surface, eliminates the weaknesses of the Hartree-Fock approximation. On the other hand, the effect of the Hamiltonian correction, which has the same form as the relativistic correction of electrons in solids, becomes dominant at energy levels above the Fermi surface. Physically, it is concluded that electrons in metals may be employed to test the quantum gravity scenario, if the value of its parameter ($\beta$) lies within the range of 2 to 10, depending on the used metal. Indeed, the latter addresses an upper bound on $\beta$ parameter which is comparable with previous works meaning that these types of systems may be employed as a benchmark to examine quantum gravity scenarios. To overcome the Fermi velocity divergence in the Hartree-Fock method, the screening potential is used based on the Lindhard theory. In the context of this theory, we also find that considering the generalized Heisenberg uncertainty leads to some additional oscillating terms in the Friedel oscillations.

Keywords: Hartree-Fock model, Exchange energy, Electron gas, Planck Scale, Minimal Length, Generalized Uncertainty Principle

I. INTRODUCTION

The quantum features of gravity, and indeed quantum gravity, are amongst the most intriguing challenges of contemporary physics. It claims that canonical coordinates $x_i$ and $p_i$, satisfying $[x_i, p_j] = i\hbar \delta_{ij}$, do not necessarily preserve their ordinary full meanings at the Planck scales, and they should be replaced by generalized coordinates $X_i$ and $P_j$ for which $[X_i, P_j] \neq i\hbar \delta_{ij}$. See also [12] for recent review. In this manner, Heisenberg uncertainty principle (HUP) is generalized as

$$(\Delta X)(\Delta P) \geq \frac{\hbar}{2}(1 + \beta(\Delta P)^2 + ...), \quad (1)$$

where $\beta$ is called the GUP (generalized uncertainty principle) parameter, and a non-zero minimum (comparable to the Planck length) is obtained for $\Delta x$ as $\hbar \sqrt{\beta}$. Bearing quantum mechanics in mind, it is obvious that replacing HUP with GUP affects everything such as classical systems and orbit problem [4-8], Schrödinger equation [1, 6, 11], cosmological as well as astrophysical scenarios [12], high energy physics [13, 15] and optics [16]. In this regard, Eq. [11] implies the relations $X_i = x_i$, and $P_i = p_i(1 + \beta p^2)$ (up to the first order of $\beta$) which are valid between different mentioned coordinates that come from the commutation relation $[X_i, P_j] = i\hbar(1 + \beta P^2)\delta_{ij}$ [1].

Addressed works and other similar attempts such as [17, 18] have at least two achievements i) they study the effects of existence of a non-zero minimum length on different physical scales, and ii) they give us an estimation on the power and usefulness of different setups for testing $\beta$ parameter and quantum features of gravity in different experiments. Despite all these efforts, there is still a great difference between theoretical predictions and hypothetical experimental constraints on the value of $\beta$ parameter [18]. Of course, it seems that the light twisted by rotating black holes may help us find considerable upper bounds on $\beta$ values compared with those proposed by quantum mechanics [18, 19]. The latter means that it is still a problem to find a quantum mechanical system which assists us to verify GUP within Earth-based labs.

Moreover, it seems that there is a deep connection between quantum features of gravity and generalized statistics [20], where the latter has been investigated in condensed matter systems such as electrons in metals [21]. On the other hand, the application of GUP in ideal gas, as the simplest many-body system, has been investigated in detail in [22], however, the GUP effects have not been studied for a non-ideal gas. The above arguments motivate us to study the effects of GUP (the existence of a non-zero minimum uncertainty in position) on the behavior of electrons within metals. This helps us go beyond ideal gas model and makes a new insight to find the minimal length effects for a more realistic model within the interacting many body systems. It is therefore expectable that one could figure out more details of quantum gravity effects in condensed matter physics.

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Hartree-Fock method \[^{24, 25}\] is one of the most important theories in physics, especially in metals, in which the \(N\)-body wave function is often approximated by the Slater determinant of \(N\) single-particle wave functions. This self consistent method can be considered as a single particle method and the inter-particle interaction is studied as a mean field potential. In spite of good and accurate results and the applicability of this method in metals, there are two important deficiencies: divergence of velocity at the Fermi surface and prediction of some values of bandwidth that are not confirmed by experiments \[^{29, 30}\]. However, motivated by the remarkable achievements of Hartree-Fock approach which includes interaction as well, our aim in the present work is to investigate the influences of GUP on this method with the hope of finding a test bed for GUP within similar experimental systems. This could possibly shed some light on the footprints of GUP in laboratory studies. The current paper is then organized as follows: In sections \[^{IV}\] and \[^{III}\] a brief discussion on GUP formalism along with Hartree-Fock method will be presented, respectively. The effects of minimal length on HF are investigated in Sec. \[^{V}\] and subsequently, the Lindhard screening theory will be examined in the GUP formalism in the section \[^{VI}\]. Finally, a summary and conclusion will be presented.

II. GENERALIZED UNCERTAINTY PRINCIPLE

As mentioned previously, GUP relation Eq. (1) takes the following form,

\[
[X_i, P_j] = i\hbar(1 + \beta P^2)\delta_{ij}.
\]

Defining the general transformation as

\[
(x_i, p_i) \rightarrow (X(x_i, p_i), P(x_i, p_i)),
\]

and after doing some algebra, one can get the \(N\)-dimensional density of state as \[^{26}\],

\[
a(\varepsilon)d\varepsilon = \frac{1}{N} \frac{d^N X d^N P}{\hbar(1 + \beta P^2)^N}.
\]

Therefore, GUP changes the structure of phase space with a greater volume element. On the other hand, following \[^{27}\] and references therein, we can consider

\[
P = \frac{\tan(\sqrt{\beta}p)}{\sqrt{\beta}},
\]

as a consequence of GUP relation. Hence, the Schrödinger equation can be written as,

\[
H = H_0 + \sum_{n=3}^{\infty} \frac{(-1)^{n-1}2^{2n}(2^{2n} - 1)(2n - 1)B_{2n} \beta^{n-2}p^{2(n-1)}}{2m(2n)!},
\]

where \(H_0 = p^2/2m + V(x)\) and \(B_n\) is the \(n\)th Bernoulli number. It can be shown that in the presence of \(n \geq 3\) terms, there is a positive shift within the energy spectrum of particles. It is worth mentioning that a similar procedure can be applied to the Dirac equation and more details can be found in \[^{28}\].

III. HARTREE FOCK APPROXIMATION

The Schrödinger equation governing the behavior of electrons in metals is given as follows

\[
H_0 \Psi(r_1, \ldots, r_N) = E \Psi(r_1, \ldots, r_N),
\]

with

\[
H_0 = \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m} \nabla_i^2 - Z \sum_{R} \frac{e^2}{|r_i - R|} \right) + \frac{1}{2} \sum_{i \neq j}^{N} \frac{e^2}{|r_i - r_j|},
\]

where the first and the second terms are kinetic energy and ionic interaction potential energy, respectively and the last term deals with the electron-electron interaction. Hartree-Fock method \[^{24, 25}\] is one of the most important approaches to obtain the effects of electron-electron interactions within metals. In this approximation all correlations are neglected except that of the Pauli exclusion principle and the 3rd term in the Hamiltonian is converted to a single particle form considering the effect of other electrons as a smooth negative charge distribution. Consequently, utilizing the Slater determinant of single-particle wave functions, the Hamiltonian will be rewritten as a set of \(N\) one-body problems, one of them for each one-electron level. More details can be found in \[^{25}\]. Considering then the plane wave as the single-electron wave function, the energy takes the following form

\[
\varepsilon(k) = \frac{\hbar^2 k^2}{2m} - \frac{1}{V} \sum_{k'} \frac{4\pi e^2}{|k - k'|},
\]

where \(\frac{4\pi e^2}{|k - k'|}\) is the Fourier transform of the exchange energy. Now using

\[
\sum_{k} \rightarrow \frac{V}{(2\pi)^3} \int dk,
\]

the expression for energy can be rewritten as

\[
\varepsilon(k) = \frac{\hbar^2 k^2}{2m} - \frac{2e^2}{\pi} k_F \frac{F_0 \left( \frac{k}{k_F} \right)}{k_F},
\]

where

\[
F_0(x) = \frac{1}{2} + \frac{1}{4x} \ln \left| \frac{1 + x}{1 - x} \right|.
\]
over $k \leq k_F$ along with using Eq. (9). We therefore get

$$
\frac{E}{N} = \frac{\varepsilon^2}{2a_0} \left[ \frac{3}{5} (k_F a_0)^2 - \frac{3}{\pi} (k_F a_0)^3 \right]
$$

$$
= \left[ \frac{2.21}{(r_s/a_0)^2} - \frac{0.916}{(r_s/a_0)^3} \right] \text{Ry},
$$

where $a_0$ is the Bohr radius and $r_s$ is defined as $r_s = \left( \frac{1}{4\pi n} \right)^{1/3}$ where $n = k_F^3 / (3\pi^2)$ and $k_F = \left( \frac{3.63}{r_s/a_0} \right) A^{-1}$.

**IV. MINIMAL LENGTH EFFECTS ON HARTREE-FOCK ENERGY**

In order to calculate the effects of minimal length on the energy of the electron liquid in metals, we use, firstly, Eq. (5) up to the first term in the summation. Therefore, we have, instead of Eq. (8) the following equation for the Fourier transform of single particle energy,

$$
\varepsilon(k) = \frac{\hbar^2 k^2}{2m} + \frac{\beta \hbar^4 k^4}{3m} - \frac{1}{V} \sum_{k'} \frac{4\pi \varepsilon^2}{|k - k'|},
$$

where $k$ and $k'$ are ordinary momenta. Therefore, after integrating over all $k$ states, we obtain

$$
\frac{E}{N} = \frac{2.21}{(r_s/a_0)^2} - \frac{0.916}{(r_s/a_0)^3} + \frac{20.03}{(r_s/a_0)^4} \text{Ry},
$$

where we have used Eq. (9). As it is clear from Eq. (12), by considering the perturbed Hamiltonian, Eq. (5) and $d^3 x d^3 p$ as the phase space volume (where $x$ and $p$ are canonical coordinates), the GUP correction has no contribution in the interaction and exchange energy and the minimal length affects only the kinetic energy as an $x^4$ term. This term is a high density term (small $r_s$) due to the power of $r_s/a_0$.

In order to get more details and for a complete investigation, one must use Eq. (5) together with $d^3 x d^3 p$ as the generalized phase space volume. Therefore, up to the first order of $\beta$ parameter, the Hamiltonian gets the following form,

$$
\hat{H} = H_0 + \sum_i \frac{\beta}{3m} p_i^4 + O(\beta^2) + \ldots,
$$

To proceed one must use [23, 27]

$$
\sum_{\mathbf{p}} \ldots \rightarrow \frac{V}{(2\pi)^3} \int \ldots (1 + \beta P^2)^{-3} d\mathbf{P}.
$$

Considering the first order of $\beta$ parameter in Eq. (11), we have,

$$
P = p \left( 1 + \frac{1}{3} \beta p^2 \right).
$$

Therefore, Eq. (8) must be replaced by

$$
\varepsilon(k) = \frac{\hbar^2 k^2}{2m} + \frac{\beta \hbar^4 k^4}{3m} - \frac{4\pi \varepsilon^2}{(2\pi\hbar)^3} \int \frac{(1 + \beta P^2)^{-3}}{|p - p'|} d\mathbf{P}.
$$

Expanding $(1 + \beta P^2)^{-3}$ together with Eq. (17) and $d\mathbf{P} = dp + \beta p^2 dp$ as well as $P^2 = p^2 + 2/3 \beta p^2$ (up to the first order of $\beta$), we get

$$
\int \ldots \frac{d\mathbf{P}}{(1 + \beta P^2)^3} = \int \ldots \left(1 - 4/3 \beta^2 p^2\right) dp.
$$

After some algebra, we have

$$
\frac{\varepsilon(k)}{\varepsilon_F^0} = x^2 + \beta (4.843 (r_s/a_0)^{-2}) x^4
$$

$$
- 0.663 (r_s/a_0) F_0 (x)
$$

$$
+ \beta 2.42 (r_s/a_0)^{-1} F_1 (x)
$$

$$
+ C_2 \beta^2 (r_s/a_0)^{-3} F_2 (x) + O(\beta^3) + \ldots,
$$

where $C_2$ is a real constant and $\varepsilon_F^0$ is the Fermi energy of the ideal electron gas. One can write Eq. (20), for simplicity, as follows,

$$
\tilde{\varepsilon}(k) = \varepsilon^{\text{HF}}(k) + \varepsilon^{\text{GUP}}(k),
$$

where $\tilde{\varepsilon}(k) = \varepsilon(k)/\varepsilon_F^0$, $\varepsilon^{\text{HF}}(k)$ is that of Eq. (10) scaled by $\varepsilon_F^0$ and

$$
\varepsilon^{\text{GUP}}(k) = \beta (-2.42 (r_s/a_0)^{-1} F_1 (x) + (4.843 (r_s/a_0)^{-2}) x^4),
$$

is the GUP corrections on the exchange energy. The correction factors $F_i (x)$ ($i$ refers to the order of correction) are given by

$$
F_1 (x) = \frac{1}{3} + x^2 + \frac{1 - x^4}{2x} \ln \left| \frac{1 + x}{1 - x} \right|
$$

$$
F_2 (x) = \frac{1}{5} + x^2 + x^4 + \left( \frac{1 - x^6}{2x} \right) \ln \left| \frac{1 + x}{1 - x} \right|
$$

$$
F_3 (x) = \frac{1}{45} + x^2 + x^4 + \left( \frac{1 - x^{10}}{2x^4} \right) \ln \left| \frac{1 + x}{1 - x} \right|
$$

$$
\ldots
$$

These factors are plotted in Fig. (11). It is clear from this figure that the value of correction factors assumes a significant difference with respect to the zeroth order of $\beta$ parameter. Moreover, at higher values of $x$, the difference decreases and tends to a minimum value so that all these factors are nearly in the same order.

In order to investigate the contribution of these corrections to the total energy of the $N$-particle system, we must add up these corrections to all values of wave vectors which are below the Fermi wave vector i.e., $k \leq k_F$. 
Considering GUP summation rule i.e., Eq. (19) together with making sum of Eq. (20) and after some algebra, the total energy per particle, up to the first order of \( \beta \) parameter, can be written as

\[
\frac{E}{N} = \frac{2.21}{(r_s/a_0)^3} - \frac{0.928}{(r_s/a_0)^2} - \frac{20.04}{(r_s/a_0)^2} + \beta \left( \frac{1.0829}{(r_s/a_0)^3} + \frac{3.92}{(r_s/a_0)^2} - \frac{20.04}{(r_s/a_0)^2} \right) R_y, \tag{24}
\]

whence we get GUP-HF-exchange energy as follows

\[
\frac{E^{\text{GUP-HF}}}{N} = \beta \left( \frac{1.0829}{(r_s/a_0)^3} + \frac{3.92}{(r_s/a_0)^2} - \frac{20.04}{(r_s/a_0)^2} \right). \tag{25}
\]

Using the above equation together with Eq. (20) and setting the coefficients of Logarithmic terms to zero, after a little algebra we have

\[
\beta = 0.06849 \times (r_s/a_0)^2 = O \left( (r_s/a_0)^2 \right).
\]

Hence, we get the following Fermi velocity in the GUP form of the Hartree-Fock model

\[
v_F = (4.55 (r_s/a_0)^{-2} - 1.01) \times 10^8 \text{ cm/s},
\]

which is in complete agreement with experimental values \[24\]. Now this value of \( \beta \) parameter is used to calculate the bandwidth and the exchange energy contribution. The bandwidth is defined as the energy difference between the energy at the Fermi level and zero momentum energy

\[
\varepsilon_B = \varepsilon_{k_F} - \varepsilon(0). \tag{27}
\]

As a result, one can plot the exchange energy using the above value for \( \beta \) parameter. Figure (3) represents the GUP-HF energy for \( \beta = 0.068498 \times (r_s/a_0)^2 \). The results show that considering this value of \( \beta \) parameter leads to decreasing the bandwidth to its HF value. Besides, this bandwidth can be eliminated using the effect of minimal length, which is concordant to the experiment. To this end, the energy at points \( x \to 1 \) and \( x = 0 \) is required which can be calculated through Eq. (20). A straightforward calculation then gives

\[
F_0(0) = 1 \quad F_0(x \to 1) = 1/2, \quad F_1(0) = 4/3 \quad F_1(x \to 1) = 4/3,
\]

Substituting these values back into Eq. (20) and assuming the bandwidth energy is equal to zero in Eq. (27), we reach

\[
\varepsilon_B = 1.0 + 0.3315(r_s/a_0) + 4.84(r_s/a_0)^{-2} \beta^2 = 0.
\]

This equation can again has a solution in second order of \( (r_s/a_0) \) with an appropriate constant.

V. GUP EFFECTS ON LINDHARD THEORY

Another method to eliminate the divergence of Fermi velocity is the screening theory. In order to consider the screening effect, we can refer to Thomas-Fermi theory and the Lindhard theory of screening \[24, 27\]. In this manner, we find the charge density in the presence of the total potential \( \phi(r) \) by solving the one-body Schrödinger equation,

\[
\frac{\hbar^2}{2m} \nabla^2 \psi_i(r) - e\phi(r)\psi_i(r) = \varepsilon_i \psi_i(r). \tag{28}
\]

Since the Thomas-Fermi theory of screening has been previously investigated in the GUP formalism \[27\], we here evaluate the minimal length effects on the Lindhard
the induced density is linearly proportional to potential \( \phi \). In terms of Fourier transform, the problem is to find

$$\rho^{\text{ind}}(\mathbf{q}) = \chi(q) \phi(q),$$

(29)

where \( \rho^{\text{ind}}(\mathbf{q}) \) and \( \phi(q) \) are the Fourier transform of induced charge density and screening potential, respectively. Calculations show that the dielectric function is related to the response function as well as charge density in the following from

$$\epsilon(q) = 1 - \frac{4\pi}{q^2} \chi(q) = 1 - \frac{4\pi}{q^2} \rho^{\text{ind}}(\mathbf{q}),$$

(30)

and through a straightforward procedure [24], we get

$$\chi_L = e^2 \sum_k \frac{f^{(0)}(k) - f^{(0)}(k + q)}{\epsilon(k) - \epsilon(k + q)}.$$ 

(31)

Therefore, the dielectric function is found as follows

$$\epsilon(q) = 1 - \frac{4\pi e^2}{q} \sum_k \frac{f^{(0)}(k) - f^{(0)}(k + q)}{\epsilon(k) - \epsilon(k + q)}.$$ 

(32)

After some algebra we get

$$\chi_L(q) = -\frac{k_F}{\pi^2} \left[ \frac{1}{2} + \frac{1 - 4x^2}{4x} \ln \left( \frac{1 + x}{1 - x} \right) \right],$$ 

(33)

where \( x = \frac{q}{2k_F} \) and therefore the static dielectric constant in Lindhard theory becomes

$$\epsilon(q) = 1 + \frac{4\pi k_F}{q^2} \left[ \frac{1}{2} + \frac{4k_F^2 - q^2}{8k_Fq} \ln \left( \frac{2k_F + q}{2k_F - q} \right) \right].$$ 

(34)

Consequently the screen parameter, \( \lambda_L \) can be shown by

$$\lambda_L(q) = 4\pi \frac{k_F}{\pi^2} \left[ \frac{1}{2} + \frac{4k_F^2 - q^2}{8k_Fq} \ln \left( \frac{2k_F + q}{2k_F - q} \right) \right].$$ 

(35)
where \( \delta \rho \) is that of normal screening (Eq. (39)) and \( \delta \rho^{(1)} \) is the first order correction of minimal length that can be calculated as follows

\[
\delta \rho^{(1)} = -\frac{4e}{3\pi^2} \sum_l \left[ (2l + 1) \frac{1}{r^4} \int_0^{k_F} \frac{k^2}{r^3} \left( \sin^2(kr - \frac{l\pi}{2} + \delta_l) - \sin^2(kr - \frac{l\pi}{2}) \right) dk \right].
\]

Performing integration along with applying some simplifications, one gets

\[
\delta \rho^{(1)} = -\frac{e}{3\pi^2} \sum_l \left[ (2l + 1) \left( -\frac{2k_F}{r^3} \cos^2(2k_Fr - l\pi + \delta_l) + \frac{2k_F}{r^3} \sin(2k_Fr - l\pi + \delta_l) \sin \delta_l + 2 \cos \delta_l \sin \delta_l \right) \right].
\]

It is clear from this equation that there are some additional oscillating terms within the potential.

**VI. CONCLUSION**

In this paper, the Hartree-Fock model has been formulated considering the effects of minimal length. The minimal length modifies the minimal volume, and density of states in the phase-space. Our results showed that the Hartree-Fock energy is affected by the minimal length significantly, and the effect is even considerable at lower momenta. In the Hartree-Fock model we encounter two important problems; the Fermi velocity divergence, and the bandwidth increases, depending on density. We presented an efficient approach to overcome these deficiencies by considering the minimal length effects. Our calculations showed that considering the value of \( \beta \) parameter as \( O(\tau_s/a_0^2) \) with an appropriate constant, the problems of the Hartree-Fock model will be controlled.

We also found out that minimal length (GUP) modifies the Schrödinger equation with some extra terms corresponding to different orders of \( \beta \) parameter and \( \sqrt{\beta} = \sqrt{\beta_0} l_{pl} \). Therefore, in spite of physical significance, we can modify the many-electron Schrödinger equation by considering \( l_{pl} \sim O(\tau_s/a_0) \) adjusted by appropriate values of \( \sqrt{\beta} \). Therefore, regarding GUP formalism and its consequences particularly in the form of Eq. (5), we can write the Schrödinger equation up to the first order of GUP corrections, as Eq. (15).

On the other hand, although the contribution of the relativistic motion of electrons in the strong attractive field and near the nucleus are small, they cannot be ignored (32). Accordingly, due to the order of magnitude of \( v_F \), we may expect to have more terms in the expansion of kinetic energy, meaning that the \( O(p^4) \) terms in Eq. (15) can also be justified by the relativistic corrections. Therefore, a many-body Hamiltonian like

\[
H = H_0 + \sum_i \alpha_i p_i^4,
\]
where $\alpha_i$ are coefficients appeared in theory, is generally acceptable. We obtained that, in our model, the HF problems can mathematically be solved. Although, we considered the effects of GUP on both the system Hamiltonian and its phase space, our results indicate that the HF problems are solved, if only the phase space changes are considered. Indeed, the phase space modifications play a very impressive and dominant role below the Fermi surface, and also in eliminating the HF problems compared to that of the Hamiltonian correction.

Another approach to overcome the HF infinite velocity at Fermi surface is to consider the screening potential and the Linhardth theory of screening as well. In this approach, the effect of minimal length on the screen potential has been also investigated in the light of Lindhard theory. We showed that in the minimal length formulation, one must modify the screening length and parameter as well as the long range Friedel oscillations. Our investigation indicates that the effects of minimal length on screening adds more oscillating terms to the induced density.

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