Thomas–Fermi Screening Length in q-Deformed Statistical Mechanics

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The q-deformed statistical mechanics for fermions has been used to investigate the Thomas–Fermi screening length at finite temperature. Considering linear response, the calculations have been made in a weakly nondegenerate regime. The results show that q-deformation has significant effects on screening length at higher temperatures. The results also show that the q-deformation effects vanish at zero temperature limit and that more correction terms of deformation have more effects on screening length. The behavior of screening length is different for different values of q.

topics: Thomas–Fermi, screening length, q-deformed fermions

1. Introduction

The Thomas–Fermi model is a semi-classical model created to investigate many-body effects in quantum systems. It is applicable in metals, solid-state physics, atomic physics, and astrophysics [1, 2]. In spite of its crudity, because of creating qualified views, this model is used in many fields of modern physics, some of which are regarded as its generalization, e.g., Nozari et al. [3] firstly considered the quantum gravity effects on the condensed matter physics using Thomas–Fermi (TF) theory and showed the importance of quantum gravity in many-body physics. After that, the TF model has been considered in the generalized uncertainty principle context to investigate the minimal length effects on Thomas–Fermi length in relativistic and non-relativistic regimes [4, 5]. Also, in order to obtain a modified Thomas Fermi equation, the effects of non-commutative space-time have been considered in [6].

In this model, briefly, electrons are considered as a homogeneous, uniform electron gas with charge density $-n_0e$, obeying Fermi–Dirac statistics, superimposed on a background of positive charge density n_0e. Considering a point charge Q in a sea of such electrons, the Thomas–Fermi model leads to screening in the Coulomb potential ϕ expressed by the Thomas–Fermi equation [7]

$$\nabla^2\phi(\boldsymbol{r}) = 4\pi e\big(n(\boldsymbol{r})-n_0\big) - 4\pi Q\delta(\boldsymbol{r})\,. \qquad (1)$$

The Thomas–Fermi screening length, λ_F, is a characteristic length scale that describes how quickly the electron density, as well as the associated electrostatic potential, decay away from a charged object or within a material. It quantifies the range over which the electron density screens the electrostatic potential due to the presence of other charged particles.

On the other hand, it has been found that there are some classes of systems for which ordinary quantum statistical mechanics, known as Gibss–Blotzman statistical mechanics, may not be appropriate [8–10], and a kind of extension is needed to describe these systems. Regarding this issue, two principal methods have been proposed for intermediate statistics, namely the nonextensive statistics [11] and q-deformed theory [12, 13]. Because of its possibility to apply in different fields of physics, such as anyon physics [14, 15], thermodynamics of ideal Fermi gas [16–18], and references therein regarding other fields of physics, the q-deformed statistics has attracted great interest last decade. In this regard, it has been shown that the application of q-deformation in fermion systems changes its thermodynamic properties. The q-deformed algebra emerging from statistical mechanics has also been used to formulate quantum mechanics, and the parameter "q" plays the role of experimental fitting [19]. Some applications of this kind of quantum mechanics deformation can be found in [20].

Upon the foregoing discussion, the effect of q-deformed Fermi–Dirac statistics on the Thomas–Fermi screening length has been investigated in this paper. The paper is organized as follows. In the next section, q-deformed algebra and statistical mechanics are briefly introduced. Then, this intermediate statistics is used in the Thomas–Fermi equation to investigate the effect of q-deformation on the screening length. Finally, results and discussion are presented.

2. The q-deformed algebra and statistical distribution function for fermions

The symmetric q-deformed fermion algebra is defined as follows [17]

$$\left[\hat{N}, \hat{a}^\dagger\right] = \hat{a}^\dagger, \qquad [\hat{N}, \hat{a}] = -\hat{a}, \tag{2}$$

and

$$\hat{a}^\dagger \hat{a} = [\hat{N}], \qquad \hat{a}\,\hat{a}^\dagger = [1 - \hat{N}], \tag{3}$$

where $\hat{a}^\dagger$, $\hat{a}$, and $\hat{N}$ are creation, annihilation, and number operator, respectively, and the q-basic number $[x]$ is defined as

$$[x] = \frac{q^x - q^{-x}}{q - q^{-1}}. \tag{4}$$

Here, q is the deformation parameter. The Hilbert space of q-deformed fermions with the basis $|n\rangle$ is defined as [17, 18]

$$\begin{aligned} &\hat{N}|n\rangle = n|n\rangle, \\ &\hat{a}\,|0\rangle = 0, \\ &\hat{a}^+|n\rangle = [1-n]^{1/2}|n+1\rangle, \\ &\hat{a}\,|n\rangle = [n]^{1/2}|n-1\rangle. \end{aligned} \tag{5}$$

The eigenvalues of number operator $\hat{N}$ take only values 0 and 1, and the Pauli principle is satisfied in q-deformed fermions. The mean value of the q-deformed occupation number is defined by [17, 18]

$$[f_{k,q}] = \frac{1}{\Xi}\ \mathrm{Tr}\left\{\exp(-\beta\hat{H})\left[\hat{N}_k\right]\right\}, \tag{6}$$

where $\beta = 1/(k_{\mathrm{B}}T)$, $\hat{H}$ is the Hamiltonian

$$\hat{H} = \sum_k (\varepsilon_k - \mu)\,\hat{N}_k, \tag{7}$$

and k is a state label, $\hat{N}_k$ and ε_k are the number operator and energy associated with state k, respectively, and μ is the chemical potential. Following [17, 18], the statistical distribution function of the q-deformed fermions can be derived as

$$f_{k,q} = \frac{1}{2\ln(q)} \ln\left(\frac{z^{-1}\exp(\beta\varepsilon_k) + q}{z^{-1}\exp(\beta\varepsilon_k) + q^{-1}}\right), \tag{8}$$

where $z = \exp(\beta\mu)$ is the fugacity of the system. One important property of this distribution function is $f_{k,q} = f_{k,1/q}$. One can simply prove that when $q = 1$, we have the standard Fermi–Dirac distribution, and the q-deformed fermions are the same as ordinary fermions,

$$f_{k,q} = \frac{1}{z^{-1}\exp(\beta\varepsilon_k) + 1}. \tag{9}$$

According to (8), the total number of particles, N, and the total energy of the system, U, can be, respectively, given by

$$N = \sum_k \frac{1}{2\ln(q)} \ln\left(\frac{z^{-1}\exp(\beta\varepsilon_k) + q}{z^{-1}\exp(\beta\varepsilon_k) + q^{-1}}\right) \tag{10}$$

and

$$U = \sum_k \frac{\epsilon_k}{2\ln(q)} \ln\left(\frac{z^{-1}\exp(\beta\varepsilon_k) + q}{z^{-1}\exp(\beta\varepsilon_k) + q^{-1}}\right). \tag{11}$$

In the large particle number limit, the sum over k is replaced by integration, and therefore (10) and (11) can be rewritten as

$$N = \frac{g}{h^3}\int \frac{\mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{x}}{2\ \ln(q)} \ln\left(\frac{z^{-1}\exp(\beta\varepsilon(p)) + q}{z^{-1}\exp(\beta\varepsilon(p)) + q^{-1}}\right) = \frac{gV}{\lambda^3}\, h_{3/2}(z,q) \tag{12}$$

and

$$U = \frac{g}{h^3}\int \frac{\mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{x}\ \varepsilon(p)}{2\ \ln(q)} \ln\left(\frac{z^{-1}\exp(\beta\varepsilon(p)) + q}{z^{-1}\exp(\beta\varepsilon(p)) + q^{-1}}\right) = \frac{3}{2}\ k_{\mathrm{B}}T\frac{gV}{\lambda^3}\ h_{5/2}(z,q), \tag{13}$$

where V is the volume, $\varepsilon(P) = p^2/(2m)$ and λ is thermal wavelength,

$$\lambda = \frac{h}{\sqrt{2\pi m\, k_{\mathrm{B}}T}}. \tag{14}$$

In (12) and (13), $h_n(z,q)$ is the generalized Fermi integral of q-fermions

$$h_n(z,q) = \frac{1}{\Gamma(n)}\int_0^\infty \frac{\mathrm{d}x\ x^{n-1}}{2\ \ln(q)} \ln\left(\frac{z^{-1}\exp(x) + q}{z^{-1}\exp(x) + q^{-1}}\right), \tag{15}$$

and $\Gamma(x) = \int_0^\infty \mathrm{d}t\ \exp(-t)t^{x-1}$ is the gamma function. It can be found that when $q = 1$, (15) is just the standard Fermi integral

$$h_n(z,q) = \frac{1}{\Gamma(n)}\int_0^\infty \frac{\mathrm{d}x\ x^{n-1}}{z^{-1}\exp(x) + 1}. \tag{16}$$

3. Thomas–Fermi screening length in the q-deformed statistical mechanics

In order to investigate the q-deformation effects on the Thomas–Fermi screening length, the fugacity, $z = \exp(\beta\mu)$, is considered as $\tilde{z} = \exp(\beta(\mu - e\phi))$. Therefore, the number density n in (1) is as follows

$$n = \frac{g}{h^3}\int \frac{\mathrm{d}\boldsymbol{p}}{2\ \ln(q)} \ln\left(\frac{\mathrm{e}^{-\beta(\mu - e\phi)}\exp(\beta\varepsilon(p)) + q}{\mathrm{e}^{-\beta(\mu - e\phi)}\exp(\beta\varepsilon(p)) + q^{-1}}\right) = \frac{g}{\lambda^3} h_{3/2}(\tilde{z},q). \tag{17}$$

Hence, (1) is rewritten as

$$\nabla^2\phi(\boldsymbol{r}) = 4\pi e\frac{g}{h^3} = \int \frac{\mathrm{d}\boldsymbol{p}}{2\ \ln(q)}\left[\ln\left(\frac{\mathrm{e}^{\beta(\mu - e\phi)}\exp(\beta\varepsilon(p)) + q}{\mathrm{e}^{-\beta(\mu - e\phi)}\exp(\beta\varepsilon(p)) + q^{-1}}\right) - \ln\left(\frac{\mathrm{e}^{-\beta(\mu - \varepsilon(p))} + q}{\mathrm{e}^{-\beta(\mu - \varepsilon(p)} + q^{-1})}\right)\right] - 4\pi Q\delta(\boldsymbol{r}). \tag{18}$$

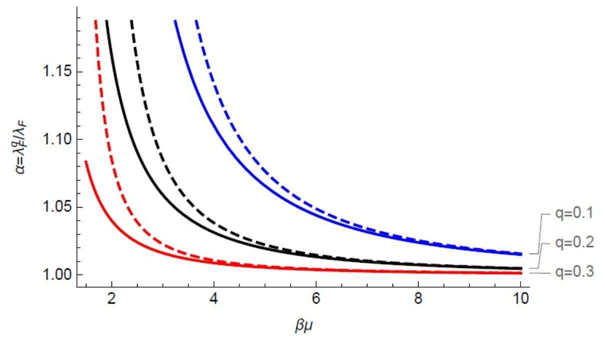

Fig. 1. The ratio of $\alpha = \lambda_F^q/\lambda_F$ for $q = 0.1, 0.2$, and 0.3. The dashed curve shows α up to $\gamma_1(q)$ corrections, and the solid curve shows the value up to $\mathcal{O}(\beta\mu)^{-4}$ because of $\gamma_3(q)$ correction.

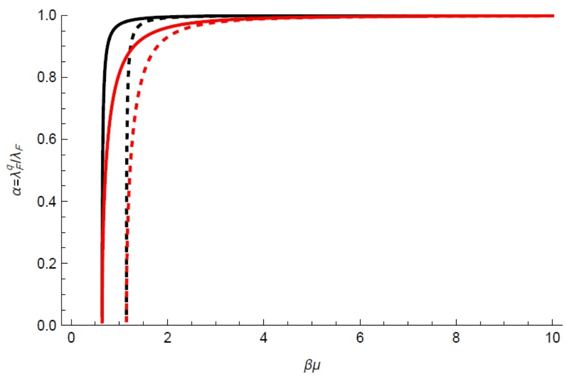

Fig. 2. The ratio of $\alpha = \lambda_F^q/\lambda_F$ for $q = 0.4$ (black curves) and $q = 0.6$ (red curves). The solid (dashed) curves are related to $\gamma_3(q)$ ($\gamma_1(q)$) corrections.

Now, using (12), the Thomas–Fermi model takes the following form

$$\nabla^2\phi(\boldsymbol{r}) = \frac{4\pi e\, g}{h^3\lambda^3}\left[h_{3/2}(\tilde{z},q) - h_{3/2}(z,q)\right] - 4\pi Q\delta(\boldsymbol{r}). \tag{19}$$

In the weakly nondegenerate case, i.e., $|\beta\tilde{\mu}| = |\beta(\mu - e\phi)| \gg 1$ as well as $|\beta\mu| \gg 1$, the generalized Fermi integral (of q-fermions) can be written as

$$h_n(z,q) = \frac{(\ln(z))^n}{\Gamma(n)} + 1 + n(n-1)\frac{\pi^2}{6}\gamma_1(q)\frac{1}{(\ln(z))^2} + n(n-1)(n-2)(n-3)\frac{7\pi^4}{360}\gamma_3(q)\frac{1}{(\ln(z))^4} + \cdots, \tag{20}$$

where

$$\gamma_n(q) = \frac{\int_0^\infty \mathrm{d}x\, \dfrac{x^n}{2\ln(q)} \ln\left(\dfrac{\exp(x)+q}{\exp(x)+q^{-1}}\right)}{\int_0^\infty \mathrm{d}x\, \dfrac{x^n}{\exp(x)+1}}, \tag{21}$$

and it can be proven that $\gamma_n(q) > 1$ when $q \neq 1$ and $\gamma_n(q) = 1$ for $q = 1$.

Substituting the expansion of (21) to (19) leads to

$$\begin{aligned}\nabla^2\phi(\boldsymbol{r}) = \\ 4\pi e\frac{g}{h^3\lambda^3}\Bigg[\Bigg(&\frac{(\ln(\tilde{z}))^n}{\Gamma(n)} + 1 + n(n-1)\frac{\pi^2}{6}\gamma_1(q)\frac{1}{(\ln(\tilde{z}))^2} \\ &+ n(n-1)(n-2)(n-3)\frac{7\pi^4}{360}\gamma_3(q)\frac{1}{(\ln(\tilde{z}))^4} + \cdots\Bigg) \\ &- \Bigg(\frac{(\ln(z))^n}{\Gamma(n)} + 1 + n(n-1)\frac{\pi^2}{6}\gamma_1(q)\frac{1}{(\ln(z))^2} \\ &+ n(n-1)(n-2)(n-3)\frac{7\pi^4}{360}\gamma_3(q)\frac{1}{(\ln(z))^4} + \ldots\Bigg)\Bigg] \\ &- 4\pi Q\delta(\boldsymbol{r}),\end{aligned} \tag{22}$$

where $\ln(\tilde{z}) = \beta(\mu - e\phi)$.

Let us assume that the charge produces only a linear response, meaning that $|e\phi/\mu| \ll 1$. One can therefore expand different powers of $\ln(\tilde{z})$ up to linear terms of ϕ in (22). This leads to

$$\nabla^2\phi(\boldsymbol{r}) = \frac{3}{2}\left[\lambda_F^{(q)}\right]^{-2}\phi - 4\pi Q\delta(\boldsymbol{r}), \tag{23}$$

whose solution is

$$\phi = \frac{Q}{r}\exp\left(-\sqrt{\frac{3}{2}}\frac{r}{\lambda_F^{(q)}}\right), \tag{24}$$

where

$$\left[\lambda_F^{(q)}\right]^{-2} = \frac{4\pi n_0 e^2(\beta\mu)^{3/2}\left(1 - \frac{1}{3}\vartheta_1^q(\beta\mu) - \frac{5}{3}\vartheta_2^q(\beta\mu)\right)}{\mu}, \tag{25}$$

where ${\lambda_F}^{(q)}$ is the modified Fermi length. Here, we have

$$\begin{aligned}n_0 &= \tfrac{1}{3\pi^2}\left(\tfrac{2m\mu}{\hbar^2}\right)^{\frac{3}{2}}, \\ \vartheta_1^q(\beta\mu) &= \tfrac{\pi^2}{8}\gamma_1(q)\beta^{-2}\mu^{-2}, \\ \vartheta_2^q(\beta\mu) &= \tfrac{7\pi^4}{960}\gamma_3(q)\beta^{-4}\mu^{-4}.\end{aligned} \tag{26}$$

In order to investigate the q-deformation effects on the Thomas–Fermi screening length, the quantity of α is defined as

$$\alpha = \frac{\lambda_F^q}{\lambda_F} = \sqrt{\frac{1 - \frac{1}{3}\frac{\pi^2}{8}(\beta\mu)^{-2}}{1 - \frac{1}{3}\vartheta_1^q(\beta\mu) - \frac{5}{3}\vartheta_2^q(\beta\mu)}}, \tag{27}$$

where λ_F is the screening length for the ordinary fermions [7].

In Fig. 1, α has been plotted for values of $q = 0.2, 0.3$, and 0.4. In this figure, the solid curves consider the $\mathcal{O}(\frac{\mu}{k_\mathrm{B}T})^{-2}$ related to the $\gamma_1(q)$ term, and dashed curves show the $\mathcal{O}(\frac{\mu}{k_\mathrm{B}T})^{-4}$ related to the $\gamma_3(q)$ correction. Figure 2 is the same as Fig. 1, but higher values of q are considered. As it is clear from these figures, the q-deformation has more effects on the screening length at higher temperatures, and decreasing temperature decreases the effect of q-statistics. On the other hand, one can see that considering $\gamma_3(q)$ corrections is significant at lower temperatures and decreases the effects of q-deformation.

As an interesting result, our calculations also show that, at higher temperatures, the behavior of q-screening length in the Thomas–Fermi model is different for various values of q, namely q-deformation leads to an increase in screening length ($\alpha > 1$) at $q \lesssim 0.3$. The results also show that the q-deformed screening length is smaller than the ordinary one at higher values of q (for $q > 0.3$, $\alpha < 1$), and it is clear from the figures that the ratio of q-screening length and ordinary one tends to 1 at sufficiently low temperatures. This means that all q-corrections therefore vanish at zero temperature. It should be mentioned that $q > 1$ values were not considered here because of the symmetry property of the q-deformed distribution function, $f_{k,q} = f_{k,q^{-1}}$.

4. Conclusions

The Thomas–Fermi screening length has been investigated using q-deformed statistics. The calculations have been made based on the q-deformed generalized Fermi integral at finite temperature. We found that the screening length of q-fermions is greater than that of ordinary fermions for some values of the deformation parameter. Some other values of q, on the other hand, decrease the screening length. The results show that deformation effects vanish at zero temperature limit. It has been found that considering higher correction terms of q-deformation, along with temperature dependence, leads to more effects on q-screening.

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