

Shell correction to the Thomas–Fermi statistical model of plasma with different atomic composition at high and low temperatures

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Abstract. The refined semiclassical method based on the Thomas–Fermi statistical model takes into account the shell effects by means of an additive correction. The method has been verified in the calculations of a plasma equation of state at high temperatures. To expand its application range to low temperatures some assumptions are revised that have been made to obtain the simple formula for a shell correction. The validity of the assumptions is discussed and the results of their refusal are analyzed. As examples, a number of single-particle states in the ideal plasma of a few elements with strongly differing atomic numbers is calculated.

1. Introduction

The modern semiclassical method [1, 2] employs the Thomas–Fermi (TF) statistical model and includes the shell effects by means of an additive correction. It has been successfully used to describe the thermodynamic properties of a classical high-temperature plasma. Last time some papers [3–5] appeared on the subject of the method’s refinement and expansion of its application range. The purpose of our paper is to attract attention to some restraints, which one may be confronted with as using the approach at low temperatures.

The method [1, 2] substantially utilizes a smallness (in comparison with TF-term) and additivity of the corrections. For high temperatures the smallness of the shell correction and efficiency of its application have been verified in the calculations of plasma ionization state and equation of state. However, some additional assumptions were made to obtain a simple formula for the shell correction. The assumptions were confirmed at high temperatures, but they require proving or changing as a temperature decreasing.

The assumptions include:

- (i) result depends only on an energy spectrum behavior near a point of the chemical potential,
- (ii) square-law dependence of a radial action on an orbital momentum,
- (iii) disregard of the discreteness of an orbital quantum number l .

The last assumption means that a summation over l is identically substituted by an integration.

It was shown in our paper [6], that refusal of the last approximation (iii) substantially increases the accuracy of the semiclassical method while calculating ionization potentials of



free ions. However, it turned out that a plasma situation is much more complex and requires a more thorough study.

In the paper we discuss the correctness of assumptions enumerated above as a plasma temperature decreasing and analyze results of their refusal as calculating a number of single-particle states for a few elements with strongly differing atomic numbers.

We use the atomic units: $\hbar = m_e = e = 1$, $[m] = 9.11 \times 10^{-28}$ g, $[L] = a_0 = 5.29 \times 10^{-9}$ cm, $[n] = 6.75 \times 10^{24}$ cm $^{-3}$, $[\rho] = 11.2$ g/cm 3 , $[P] = 294.18$ Mbar, $[E] = [T] = 27.21$ eV.

2. Discrete spectrum contribution into the number of states

We consider a plasma of an element with the atomic number Z and mass M at the temperature T and mass density ρ . We use the Wigner–Zeits spherical neutral cell approach. Volume v and radius R of the cell and the ion concentration n_i are equal to

$$v = \frac{4\pi R^3}{3} = 11.2 \frac{M}{\rho} = 6.75 \times 10^{24} n_i, \quad [\rho] = \text{g/cm}^3, \quad [n_i] = \text{cm}^{-3}.$$

Self-consistent $U(r)$ and chemical μ_{TF} potentials are calculated by the TF-model in the Wigner–Zeits cell. The quantization condition is used to calculate one-electron spectrum ε_{nrl}

$$S_{\varepsilon\lambda} = \int p_{\varepsilon\lambda}(r) dr \equiv \pi \nu_{\varepsilon\lambda} = \pi(n_r + 1/2) = \pi(n - \lambda), \quad (1)$$

where

$$p_{\varepsilon\lambda}(r) = \sqrt{p_{\varepsilon}^2(r) - \lambda^2/r^2}, \quad p_{\varepsilon}^2(r) = 2[\varepsilon - U(r)], \quad \lambda = l + 1/2,$$

n, n_r, l —principal, radial and orbital quantum numbers.

We consider the discrete spectrum contribution into the number of states N_{disc} and pass from the sum over n_r to the integral according to the Poisson formula

$$\sum_{n=a}^b F_n = \sum_{k=-\infty}^{\infty} \int_{a-\epsilon_1}^{b+\epsilon_2} F(n) \cos(2\pi kn) dn, \quad \epsilon_1, \epsilon_2 < 1, \quad (2)$$

$$N_{disc}(\mu) = 2 \sum_{n_r, l} (2l + 1) f\left(\frac{\varepsilon_{n_r l} - \mu}{T}\right) = 2 \sum_{l=0}^{\infty} (2l + 1) \sum_{k=-\infty}^{\infty} \int_{-1/2}^{1/2} \cos(2\pi k n_r) f\left(\frac{\varepsilon_{n_r l} - \mu}{T}\right) dn_r. \quad (3)$$

Here generally $\mu \neq \mu_{\text{TF}}$, $f(x) = (1 + e^x)^{-1}$ is the Fermi distribution function.

Using the results of derivation of the equation (1)

$$\frac{\partial \varepsilon}{\partial n_r} = \frac{\pi}{\tau_{\varepsilon\lambda}}, \quad \tau_{\varepsilon\lambda} = \frac{\partial S_{\varepsilon\lambda}}{\partial \varepsilon} = \int \frac{dr}{p_{\varepsilon l}(r)},$$

the term $k = 0$ in equation (3) can be written as

$$N_{k=0}(\mu) = \frac{2}{\pi} \sum_l (2l + 1) \int_{U_{min}(\lambda)} \tau_{\varepsilon\lambda} f\left(\frac{\varepsilon - \mu}{T}\right) d\varepsilon. \quad (4)$$

Addition the continuous spectrum contribution to the equation (4) leads to the expression

$$N_1(\mu) = \frac{\sqrt{2T}}{\pi} \sum_l (2l + 1) \int_0^R \text{I}_{-1/2} \left(\frac{p_{\mu\lambda}^2(r)}{2T} \right) dr, \quad (5)$$

where

$$I_{-1/2}(y) = \int_0^\infty \frac{x^{-1/2}}{1 + e^{x-y}} dx$$

is the Fermi–Dirac function with the asymptotic forms

$$I_\nu(y \rightarrow -\infty) \rightarrow \Gamma(\nu + 1) \exp(y), \quad I_\nu(y \rightarrow +\infty) \rightarrow \frac{y^{\nu+1}}{\nu + 1}. \quad (6)$$

One can conclude the TF-result

$$N_{\text{TF}}(\mu) = \frac{\sqrt{2}}{\pi^2} T^{3/2} \int I_{1/2} \left(\frac{p_\mu^2(r)}{2T} \right) d\mathbf{r}, \quad d\mathbf{r} = 4\pi r^2 dr, \quad N_{\text{TF}}(\mu_{\text{TF}}) = Z \quad (7)$$

from equation (5) as substituting the sum over l by the integral and changing the integration order over r and l .

The rest sum over k in equation (3) is the shell term. We calculate it by integrating over energy ε by parts. The term outside the integral is zero therefore the shell correction is equal to

$$N_2(\mu) = \frac{2}{\pi} \sum_l (2l + 1) \sum_{k=1}^\infty \frac{1}{k} \int_{-\infty}^\infty \left[-\frac{\partial f(\dots)}{\partial \varepsilon} \right] \sin[2\pi k(\nu_{\varepsilon\lambda} + \lambda)] d\varepsilon. \quad (8)$$

To estimate the integral

$$\int_{-\infty}^\infty \left[-\frac{\partial f\left(\frac{\varepsilon-\mu}{T}\right)}{\partial \varepsilon} \right] \sin[2\pi k(\nu_{\varepsilon\lambda} + \lambda)] d\varepsilon, \quad (9)$$

we take into account the shape of the function $-\frac{\partial f(\dots)}{\partial \varepsilon}$ with the maximum at the point $\varepsilon = \mu$ and oscillating behavior of the multiplier $\sin[2\pi k(\dots)]$. Using the stationary phase method we obtain

$$N_2(\mu) = \frac{2}{\pi} \sum_{l=0}^{l_{\max}} (2l + 1) \sum_{k=1}^\infty \frac{(-1)^k}{k} \sin(2kS_{\mu\lambda}) \frac{2\pi k \tau_{\mu\lambda} T}{\sinh(2\pi k \tau_{\mu\lambda} T)}. \quad (10)$$

Here l_{\max} is calculated from the equation

$$\lambda_{\max}^2(\mu) = \max_r [p_\mu^2(r)r^2], \quad l_{\max} = [\lambda_{\max} - 1/2].$$

So one can see that the shell effects is really determined by the spectrum behavior near the point $\varepsilon = \mu$ (see assumption (i)).

3. Comparison of the different shell term expressions

Now we write out the approximate expression for the shell correction from the papers [1,2]

$$\delta N_{sh}(\mu, T) = \frac{2}{\pi \delta_\mu} \sum_{k=1}^\infty \left[\frac{2\pi^2 k \frac{\partial \lambda_\mu}{\partial \mu} T}{\sinh\left(2\pi^2 k \frac{\partial \lambda_\mu}{\partial \mu} T\right)} \cos(2\pi k \lambda_\mu) - \frac{2\pi k \tau_\mu T}{\sinh(2\pi k \tau_\mu T)} \cos(2k S_\mu) \right] \frac{1}{k^2} \quad (11)$$

and show the relationship between equation (11) and equation (10). Here δ_μ is the integral

$$\delta_\mu = \int_0^{R_\mu} \frac{dr}{r^2} \left[\frac{1}{p_\mu(r)} - \frac{1}{\sqrt{2Z/r}} \right] - \sqrt{\frac{2}{ZR_\mu}},$$

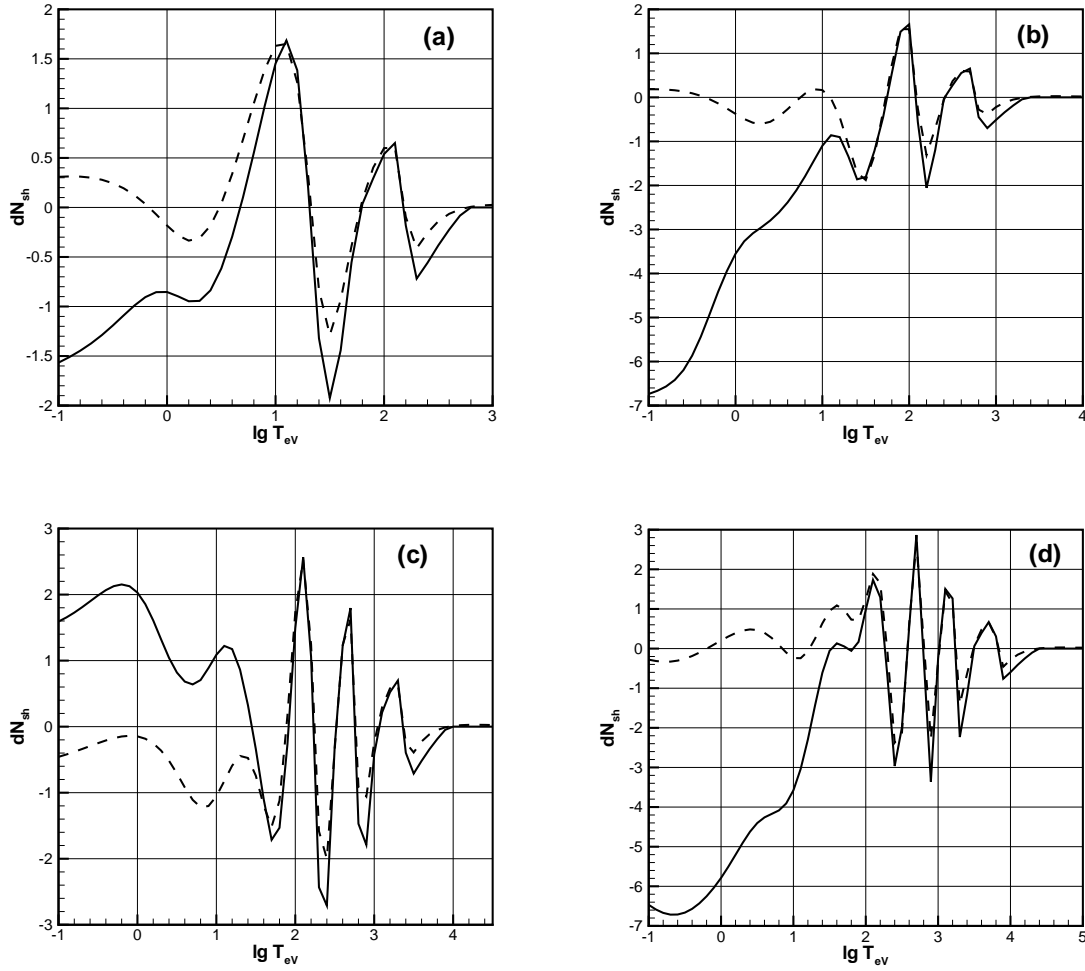


Figure 1. Shell correction to the number of states for the aluminium (a), iron (b), xenon (c), uranium (d) plasma with $n_i = 10^{18} \text{ cm}^{-3}$ as the temperature function, calculated at $\mu = \mu_{\text{TF}}$ according equation (10) (solid line) and according equation (11) (dashed line).

R_μ is the return point.

Taking into account the trivial equations

$$(-1)^k \sin(2kS_{\mu\lambda}) \equiv \sin(2k[S_{\mu\lambda} + \pi\lambda]),$$

since $\lambda = l + 1/2$, l is an integral number, and

$$\tau_{\mu\lambda} = \frac{\partial S_{\mu\lambda}}{\partial \mu} \equiv \frac{\partial(S_{\mu\lambda} + \pi\lambda)}{\partial \mu},$$

equation (10) can be written as

$$N_2(\mu) \equiv \frac{2}{\pi} \sum_{l=0}^{\infty} 2\lambda \sum_{k=1}^{\infty} \frac{\sin(2k[S_{\mu\lambda} + \pi\lambda])}{k} \frac{2\pi k \tau_{\mu\lambda} T}{\sinh(2\pi k \tau_{\mu\lambda} T)}. \quad (12)$$

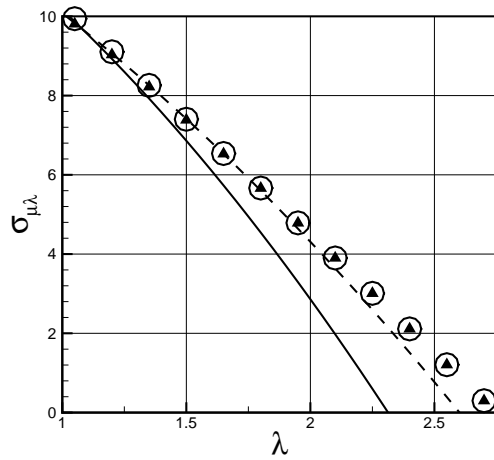


Figure 2. The dependence on λ of the radial action $\sigma_{\mu\lambda} \equiv S_{\mu\lambda}$ (symbols) and square-law equation (15) (lines) at temperatures $\lg T_{eV} = -2$ (open circles and solid lines) and $\lg T_{eV} = -1$ (triangles and dashed lines) for the iron plasma with $n_i = 10^{18} \text{ cm}^{-3}$; $\mu = \mu_{TF}$.

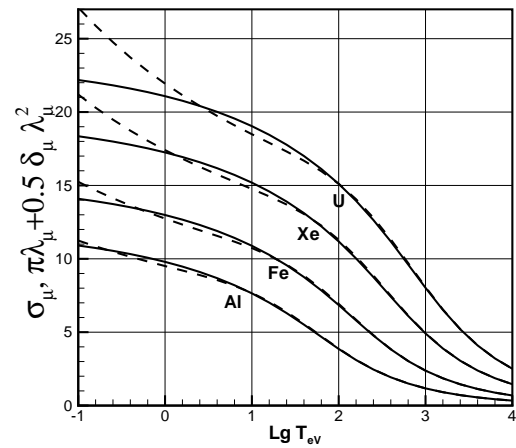


Figure 3. The dependence on a temperature of the action $\sigma_{\mu} \equiv S_{\mu}$ (solid lines) and square-law equation (16) (dashed lines) for the aluminium, iron, xenon, uranium plasma with $n_i = 10^{18} \text{ cm}^{-3}$; $\mu = \mu_{TF}$.

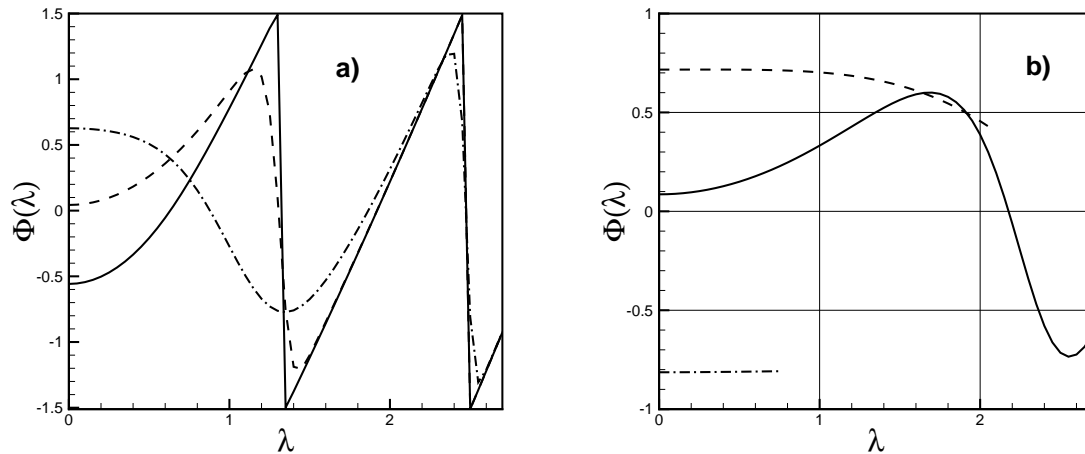


Figure 4. Dependence on λ of the integrand $\Phi(\lambda)$ in equation (14) for the iron plasma with $n_i = 10^{18} \text{ cm}^{-3}$; $\mu = \mu_{TF}$: (a) at low temperatures (— $\lg T_{eV} = -2$, --- $\lg T_{eV} = -1$, — · — $\lg T_{eV} = 0$); (b) at high temperatures (— $\lg T_{eV} = 1$, --- $\lg T_{eV} = 2$, — · — $\lg T_{eV} = 3$).

Let us again use the Poisson formula equation (2) to pass from the sum over l to the integral

$$N_2(\mu) \equiv \frac{2}{\pi} \sum_{s=-\infty}^{\infty} (-1)^s \int_0^{\lambda_{\mu}^2} d\lambda^2 \cos(2\pi s\lambda) \sum_{k=1}^{\infty} \frac{\sin(2k[S_{\mu\lambda} + \pi\lambda])}{k} \frac{2\pi k\tau_{\mu\lambda}T}{\sinh(2\pi k\tau_{\mu\lambda}T)} \quad (13)$$

and restrict ourselves to the term $s = 0$, that means we disregard of the l -discreteness and

substitute the sum over l by the integral, that is the assumption (iii),

$$N_2(\mu, T) \simeq \frac{2}{\pi} \int_0^{\lambda_\mu^2} d\lambda^2 \sum_{k=1}^{\infty} \frac{\sin(2k[S_{\mu\lambda} + \pi\lambda])}{k} \frac{2\pi k \tau_{\mu\lambda} T}{\sinh(2\pi k \tau_{\mu\lambda} T)}. \quad (14)$$

Then using the assumption (ii), that is the square-law dependence of the radial action $S_{\mu\lambda}$ on λ :

$$S_{\mu\lambda} = S_{\mu 0} - \pi\lambda - \delta_\mu \lambda^2/2, \quad 0 \leq \lambda \leq \lambda_\mu, \quad S_{\mu 0} \equiv S_\mu, \quad (15)$$

and integrating the oscillating term solely one can obtain the equation (11) from equation (14).

4. The results of computation

There is a comparison of the calculation results by equation (11) and equation (10) for different elements on figure 1. We can see a rather good fit of the both results at high temperatures and the discrepancy at low ones for all the elements. One can see also a coincidence of wavelike humps and troughs of the both curves and an additive monotone component at low temperatures in the curves according equation (10).

To understand the reason of the discrepancy at low temperatures let us now revise the correctness of our assumptions (ii) and (iii).

The square law equation (15) is true up to the temperature ~ 1 eV. Figure 2 demonstrates the lack of fit at low temperatures and $\lambda > 1$. Having noted that the value δ_μ depends on a temperature, so though there is no dependence of the function $S_{\mu\lambda}$ on a temperature in this area, but the square-law curve depends on it.

Let us use another method of revising the square-law dependence of the function $S_\mu(\lambda)$. If the equation (15) is correct over all the range $0 \leq \lambda \leq \lambda_\mu$, we can write the equation

$$S_\mu = \pi\lambda_\mu + \delta_\mu \lambda_\mu^2/2. \quad (16)$$

Figure 3 demonstrates a rather good fit of this relation up to the temperature ~ 1 eV for the different elements and so the assumption (ii) cannot be a reason of the discrepancy.

As discussing the assumption (iii) we keep in mind that the substitution of a sum over l by the integral in the equation (8) is possible if the integrand $\Phi(\lambda)$ is a rather smooth function of an argument. At high temperatures this condition is true as it can be seen from figure 4b. Figure 4a demonstrates a strongly irregular behavior of the integrand $\Phi(\lambda)$ at low temperatures. So it is just a reason of the discrepancy under consideration.

5. Conclusions

Our analysis clarified:

- The principle reason of discrepancy between results of equation (10) and equation (11) at low temperatures is the substitution of the summation over l by the integration.
- The sum over l at low temperatures includes an appreciable monotone component in addition to the oscillating term.
- The corresponding shell term is not small one that conflicts with the assumptions about smallness of the corrections in the method [1, 2].

Therefore it is impossible to use the different approaches as calculating the terms N_1 and N_2 . If we disregard of the l -discreteness for the term N_1 the same should be done for the term N_2 too.

Acknowledgments

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