
THERMODYNAMIC PROPERTIES OF METALLIC HYDROGEN

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The internal energy, free energy, and pressure as functions of density and temperature have been calculated for metallic hydrogen. The regions of temperatures and pressure correspond to the conditions of experiments on the formation of metallic hydrogen, as well as to those observed in the cores of giant planets of the Solar system, such as Jupiter and Saturn. Hydrogen is assumed to be in an atomic state, and all its electrons are itinerant. To calculate the thermodynamic potentials of metallic hydrogen, the perturbation expansion in the electron-proton interaction is used. The electron subsystem is considered within the random phase approximation with regard for the exchange interaction and electron correlations within the local field approximation. A proton-proton interaction is taken into account within the rigid sphere approximation. Since the electron-proton interaction for metallic hydrogen is known precisely, the only parameter of the theory is a sphere diameter. For its determination, the effective pairwise proton-proton interaction is used. The zeroth-, second-, and third-order terms of the perturbation expansion are taken into account to perform the numerical calculations of thermodynamic characteristics. The third-order term is found to be important, although it is far smaller than the second-order one over the whole regions of temperature and pressure under consideration. The thermodynamic potentials of metallic hydrogen are the monotonically increasing functions of density and temperature. The pressure values, calculated for the temperatures and densities characteristic of the conditions of obtaining of metallic hydrogen under terrestrial conditions, coincide to a high accuracy with the corresponding values reported by the authors of the discovery of metallic hydrogen.

1. Introduction

The possibility that hydrogen can exist in a metallic state was first predicted in 1935 [1]. However, the actual discovery of metallic hydrogen, together with a detailed study of the dependence of its electric resistance on pressure and temperature, was made in 1996 [2]. In work [2], the molecular hydrogen in a liquid state was subjected to a shock compression to the high values of pressure (0.93–1.80 Mbar) at temperatures 2200–4400 K. Under a pressure of 1.4 Mbar at a temperature of 3000 K, the metal–insulator transition was observed. Actually, a case in point was the metal–semiconductor transition, since the band gap in molecular hydrogen did not disappear

completely, but only decreased from 15 to 0.3 eV, i.e. practically to the temperature of a specimen. It should be noted that the attempts to probe the metallic state of hydrogen, both theoretically and experimentally, had also been made earlier. So, in work [3], the electric resistance of molecular hydrogen was measured under the lower values of pressure (0.1–0.2 Mbar). The authors observed the exponential character of the temperature dependence of the resistance, which is characteristic of the semiconductors with a band gap of 12 eV. The first deep investigation of the equation of state for the metallic hydrogen in a crystalline state at low temperatures dated back to 1971 [4]. The first statement on the discovery of metallic hydrogen was issued in 1978 [5]. The authors reported on the discovery of metallic hydrogen at a pressure of 2 Mbar.

In recent years, the studies of the equilibrium properties of metallic hydrogen have been conducted on a wide front [6–9]. To a great extent, the importance of such studies is based on a fact that, taking into account the extreme conditions of the existence of metallic hydrogen under terrestrial conditions, only a few of its equilibrium characteristics, for example the density or temperature, are measurable. Such an important characteristic of metallic hydrogen as pressure is already a calculable characteristic. An important feature of the theoretical investigation of the equilibrium properties of metallic hydrogen is the use of the approximation of nearly free electrons. It is this approximation that we also use for the calculations of the electric conductivity of metallic hydrogen [10]. In the present work, we also make assumption that hydrogen is in the genuine metallic state with a zero band gap, rather than in the semiconducting state with a band gap of 0.3 eV, as has been observed experimentally. Such a state can be realized either at higher pressures or at higher temperatures. It is noteworthy that the Jupiter core having a radius twice smaller than that of the planet consists of hydrogen that is at pressures of 3–40 Mbar and temperatures of 10000–20000 K.

2. Hamiltonian

Assume that hydrogen is in a disordered atomic state and all its electrons are itinerant. Then the Hamiltonian of the electron subsystem of metallic hydrogen can be chosen in the same form, as that used for the simple liquid metals [11]:

$$H = H_i + H_e + H_{ie}. \quad (1)$$

The Hamiltonian of the proton subsystem reads

$$H_i = \sum_{n=1}^N T_n + \frac{1}{2V} \sum_{\mathbf{q}} V(\mathbf{q}) [\rho^i(\mathbf{q}) \rho^i(-\mathbf{q}) - N]. \quad (2)$$

The first term on the right-hand side describes the kinetic energy of protons, the second one — the Coulomb energy of their interaction. Here, V is the system volume, N — the number of protons, T_n — the kinetic energy of the n -th proton, $V(\mathbf{q})$ — the Fourier transform of the proton-proton, electron-electron, and electron-proton Coulomb interactions, and $\rho^i(\mathbf{q})$ — the Fourier transform of the density of protons. At high temperatures, the proton subsystem can be considered as classical.

For all the temperatures under consideration, the electron gas is strongly degenerated. Therefore, it is expedient to use the representation of the plane wave secondary quantization for its description. Then, the Hamiltonian of the electron subsystem can be written as

$$H_e = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} a_{\mathbf{k}}^+ a_{\mathbf{k}} + \frac{1}{2V} \sum_{\mathbf{q}} V(\mathbf{q}) [\rho^e(\mathbf{q}) \rho^e(-\mathbf{q}) - N]. \quad (3)$$

The first term on the right-hand side describes the kinetic energy of the electron gas, the second one — the Coulomb energy of the electron interaction. Here, $a_{\mathbf{k}}^+$ and $a_{\mathbf{k}}$ are the operators of creation and annihilation, respectively, for the electrons in the state with a wavevector \mathbf{k} , $\varepsilon_{\mathbf{k}}$ — the free electron energy, m — the electron mass, $\rho^e(\mathbf{q})$ — the Fourier transform of the electron density operator, and N is the electron quantity operator.

The Hamiltonian of the Coulomb interaction between electrons and protons reads

$$H_{ie} = \frac{1}{V} \sum_{\mathbf{q}} V(\mathbf{q}) \rho^i(\mathbf{q}) \rho^e(-\mathbf{q}). \quad (4)$$

In the starting expression for the Hamiltonian, the electric neutrality of the system is taken into account through the elimination of the term with $\mathbf{q} = 0$ in each of the sums.

3. Internal Energy

The internal energy of the system can be obtained by means averaging the Hamiltonian over a Gibbs ensemble

$$E = \langle H \rangle = E_i + E_e + E_{ie}. \quad (5)$$

A contribution of the proton subsystem to the energy is

$$E_i = \langle H_i \rangle = N \frac{3}{2} k_B T + N \frac{1}{2V} \sum'_{\mathbf{q}} V(\mathbf{q}) [S^i(\mathbf{q}) - 1]. \quad (6)$$

A prime near the index of summation means the elimination of a summand with $\mathbf{q} = 0$, and T is the absolute temperature of the system. The first and second terms on the right-hand side are the kinetic energy of protons and the Madelung energy, respectively. For the latter, the accuracy of calculations depends on the accuracy of the approximation utilized for a static structure factor of the proton subsystem, $S^i(\mathbf{q})$.

The energies of the electron subsystem and the interaction between the electron and proton subsystems are handy to be considered together. Their sum, i.e. the ground-state energy of the electron gas in the field of protons, can be expanded in a power series in the electron-proton interaction:

$$E_e = \langle H_e \rangle + \langle H_{ie} \rangle = \sum_{n=0}^{\infty} E_n. \quad (7)$$

Each summand obtained on the expansion in the electron-proton interaction should be developed, in turn, in a series in the electron-electron interaction. For the zeroth order term of the electron-proton interaction expansion, this series reads

$$E_0 = E_{0e} + E_{HF} + E_{cor} \quad (8)$$

or, at zero temperature,

$$E_0 = N \left(\frac{1.105}{r_s} - \frac{0.458}{r_s} - 0.058 + 0.016 \ln r_s \right). \quad (9)$$

Here, the first summand in the parentheses, which is the zeroth order term of the expansion in the electron-electron interaction, is the kinetic energy of an ideal electron gas, with r_s being the Brueckner nonideality parameter defined as the radius of a sphere, whose volume equals that shared by one electron in the

system. The second summand is the first-order term of the expansion in the electron-electron interaction or the Hartree–Fock energy [12]. The third and fourth summands are the higher-order terms of the expansion in the electron-electron interaction or the correlation energy, for which the Nozieres–Pines interpolating formula [12,13] is used.

The ground-state energy of metallic hydrogen doesn't contain the first-order term of the expansion in the electron-proton interaction, since this interaction is of the Coulomb type and its zeroth Fourier component doesn't contribute to the energy due to the electric neutrality of the system. The second- and higher-order terms, the so-called band structure energy, read

$$E_n = \frac{N}{V^n} \sum_{\mathbf{q}_1, \dots, \mathbf{q}_n} \Gamma^{(n)}(\mathbf{q}_1, \dots, \mathbf{q}_n) V(\mathbf{q}_1) \dots V(\mathbf{q}_n) \times \times S^i(\mathbf{q}_1, \dots, \mathbf{q}_n) \Delta(\mathbf{q}_1 + \dots + \mathbf{q}_n). \quad (10)$$

Here, $S^i(\mathbf{q}_1, \dots, \mathbf{q}_n)$ is the n -particle structural factor of the proton subsystem, $\Delta(\mathbf{q}_1 + \dots + \mathbf{q}_n)$ — the Kronecker symbol, $\Gamma^{(n)}(\mathbf{q}_1, \dots, \mathbf{q}_n)$ — the so-called n -terminal electron network which formally precisely takes into account the electron-electron interaction. There are a few variants of approximate calculations of the multiterminal electron networks [14–17] and the multiparticle structural factors of the proton subsystem [18]. For the two-terminal electron network, the results obtained by all authors coincide with each other and read

$$\Gamma^{(2)}(\mathbf{q}, -\mathbf{q}) = -\frac{1}{2} \frac{\pi(\mathbf{q})}{\varepsilon(\mathbf{q})}. \quad (11)$$

Here, $\pi(\mathbf{q})$ is the polarization function of the electron gas and $\varepsilon(\mathbf{q})$ is its dielectric permittivity. We choose the latter in the random phase approximation with regard for the exchange interaction and electron correlations in the local field approximation [19]. For the three-terminal electron network, the results obtained by different authors differ appreciably. As follows from our calculations, it is in work [16] that the correct result is obtained for the model of ideal electron gas. It is this result that we use for our calculations:

$$\Gamma^{(3)}(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) = \frac{\Lambda_0^{(3)}(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3)}{\varepsilon(\mathbf{q}_1)\varepsilon(\mathbf{q}_2)\varepsilon(\mathbf{q}_3)}, \quad (12)$$

where $\Lambda_0^{(3)}(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3)$ is the three-terminal electron network of the degenerate ideal electron gas. The

approximation used for the three-terminal network takes into account the electron-electron interaction in the approximation of a self-consistent field, which, in turn, accounts for this interaction through the screening of the external field, i.e. the proton field. After making the substitution of summation by integration in a spherical coordinate system, the second- and third-order terms of the expansion in the electron-proton interaction can be shown to take the form

$$E_2 = N \frac{-1}{4\pi^2} \int_0^\infty \frac{\pi(q)}{\varepsilon(q)} V^2(q) S(q) q^2 dq, \quad (13)$$

$$E_3 = N \frac{1}{4\pi^4} \int_0^\infty dq_1 q_1^2 \int_0^\infty dq_2 q_2^2 F(q_1, q_2), \quad (14)$$

$$F(q_1, q_2) = \frac{1}{2} \int_0^\pi \frac{\Lambda_0^{(3)}(\mathbf{q}_1, \mathbf{q}_2, -\mathbf{q}_1 - \mathbf{q}_2)}{\varepsilon(q_1)\varepsilon(q_2)\varepsilon(|\mathbf{q}_1 - \mathbf{q}_2|)} V(q_1) \times \times V(q_2) V(|\mathbf{q}_1 + \mathbf{q}_2|) S(\mathbf{q}_1, \mathbf{q}_2, -\mathbf{q}_1 - \mathbf{q}_2) \sin(\theta_{12}) d\theta_{12}.$$

Since the electron-proton interaction is known precisely, the principal approximation that we used to calculate the third-order term of the expansion in the electron-proton interaction is the geometric approximation for the three-particle structural factor [18, 20, 21]:

$$S(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) = S(\mathbf{q}_1) S(\mathbf{q}_2) S(\mathbf{q}_3). \quad (15)$$

It is seen from Fig. 1 that, as the density increases, the role of the band structure energy, namely the second- and third-order terms of the expansion in the electron-proton interaction, decreases, i.e. the convergence conditions for the perturbation expansion in terms of this interaction get improved. In addition, over all the regions of densities and temperatures under investigation, the third-order term of the expansion in the electron-proton interaction is smaller than the second-order one. One more circumstance is noteworthy: at the densities greater than that of the transition into the metallic state (0.3 mole/cm³), the internal energy becomes positive and approaches the value characteristic of an ideal gas, as the density grows.

4. Free Energy and Pressure

By definition, the free energy reads

$$F = E - TS, \quad (16)$$

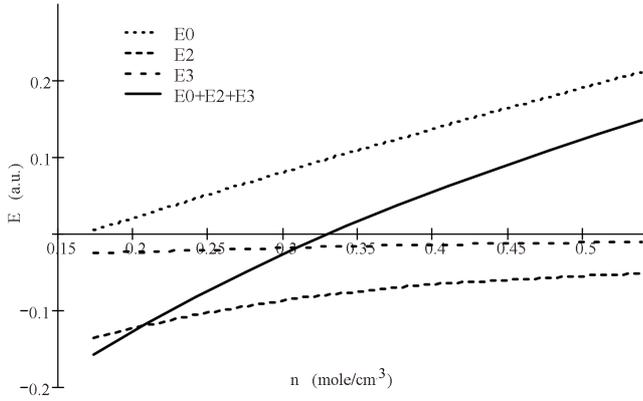


Fig. 1. Internal energy for metallic hydrogen at a temperature of 9000 K. E_0 , E_2 , and E_3 are the zero-, second-, and third-order perturbation terms, respectively

where S is the entropy of the system which consists of the electron and proton terms. For the degenerate electron gas, the electron term can be neglected in comparison with the proton one. The latter can be chosen in the rigid sphere approximation [13,22,23] as

$$S = S_i = S_{r,s} = S_{0i} + S_i(\eta), \quad (17)$$

where

$$S_{0i} = Nk_B \ln \left[\frac{e}{n} \left(\frac{eMk_B T}{2\pi\hbar^2} \right)^{3/2} \right] \quad (18)$$

is the entropy of the ideal proton gas, M the proton mass, n the density of protons, and η their packing density. The contribution originated from the interaction between protons is

$$S_i(\eta) = Nk_B \frac{3\eta^2 - 4\eta}{(1 - \eta)^2}. \quad (19)$$

As is seen from Figs. 2 and 3, the free energy and pressure are the monotonically increasing functions of density. For the case of free energy, this dependence is almost linear.

5. Effective Pairwise Proton-Proton Interaction

The important characteristic of metals is the effective pairwise interionic interaction. The corresponding expression for the pairwise proton-proton interaction in the second-order of the perturbation expansion in the electron-proton interaction, $V_{\text{eff}}(R)$ with R being a distance between protons, is well-known [23]. Its

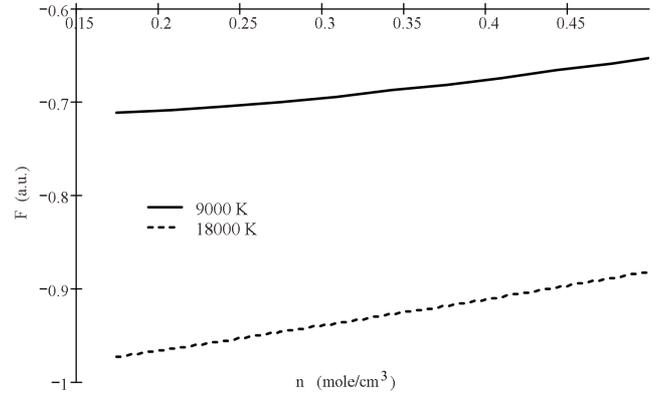


Fig. 2. Density dependence of the free energy for metallic hydrogen at various temperatures

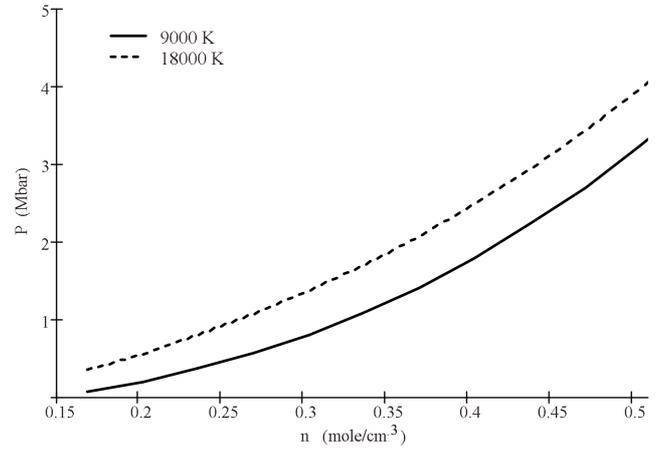


Fig. 3. Pressure dependence of the free energy for metallic hydrogen at various temperatures

important property is that it contains no fitting parameters and depends only on the system density. The only universal approximation used for its derivation is the random phase approximation for the electron subsystem with regard for the exchange interaction and electron correlations in the local field approximation.

We will find a rigid sphere diameter σ , i.e. the minimal distance that protons can approach each other at a given temperature, from the condition of equality of the proton kinetic and potential energies:

$$V_{\text{eff}}(\sigma) = 3k_B T/2. \quad (20)$$

Here, the kinetic energy is counted out from the bottom of a potential well. The character of the effective pairwise proton-proton interaction is seen from Fig. 4.

As follows from the figure, for the hydrogen density corresponding to the transition into metallic state (0.3

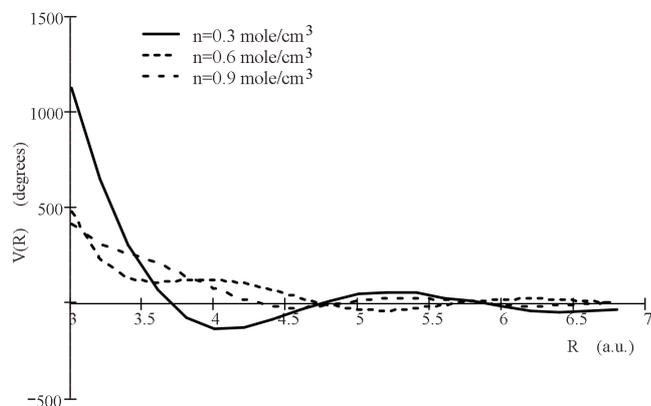


Fig. 4. Effective pairwise proton-proton interaction (in units of Celsius degrees) as a function of the distance between protons for various densities ($T=3000$ K)

mole/cm³), the potential well depth is only a few hundreds of Celsius degrees. At higher densities, the potential well practically disappears. Thus, for metallic hydrogen being at high temperatures, only the repulsion between protons is important. This is unambiguous evidence against the possibility that metallic hydrogen can exist at high temperatures as the external pressure is taken away. Under these conditions, the system is unstable.

6. Discussion of Results

According to the data of the authors who made the discovery of metallic hydrogen [2], the pressure equals 1.4 Mbar at a temperature of 3000 K and a density of 0.3 mole/cm³. As follows from our calculations, the pressure is 1.38 Mbar under the same conditions. From our point of view, such closeness of the pressure values gives the evidence for the similarity of the simplifying assumptions and the methods of calculations of the pressure, rather than indicates the adequacy of the theory to the experiment conditions. A problem concerning the applicability of various models, for example that of nearly free electrons, can be solved within the frames of the theory itself. The dimensionless parameter that characterizes the applicability of the model of nearly free electrons is $\hbar/\varepsilon_F\tau$, where ε_F is the Fermi energy, τ the lifetime of an electron on the Fermi level. This time is close to the relaxation time for the electric and thermal conductivities in metals. The model is applicable when this parameter is less than unity.

Figure 5 shows the density dependence of this parameter for the three values of temperatures. It is seen from the figure that $\hbar/\varepsilon_F\tau$ is close to unity at high

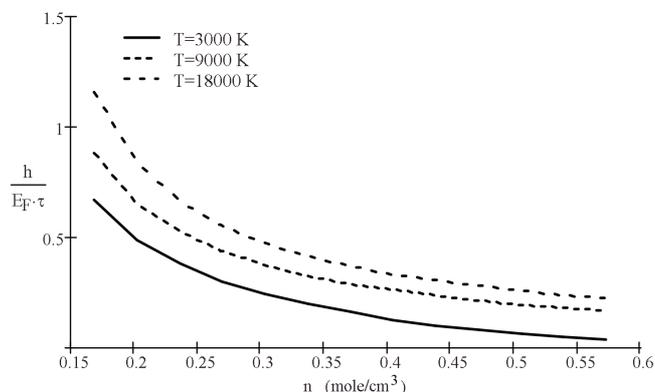


Fig. 5. Density dependence of the dimensionless parameter $\hbar/\varepsilon_F\tau$ at various temperatures

temperatures provided that the densities are low. Thus, under these conditions, the model of nearly free electrons is inapplicable. On the contrary, at low temperatures, the parameter is less than unity for the case of high densities, and therefore, the above model is applicable. In particular, the model is applicable for the density $n=0.3$ mole/cm³, at which metallic hydrogen was obtained for the first time.

The second important feature of the theory is a fundamental role of the electron-proton interaction in the formation of not only the kinetic, but also thermodynamic properties of metallic hydrogen. This follows from the results of numerical calculations. When the electron-proton interaction is not accounted for, the pressure takes on a nonphysical value -0.27 Mbar at a temperature of 3000 K and a density of 0.3 mole/cm³. The account of this interaction in the second-order perturbation theory already results in a pressure of 1.13 Mbar. Further, when the third-order term is taken into account, the pressure becomes equal to 1.38 Mbar. How correct is the use of the perturbation theory for the calculation of the energy of an electron gas in the field of protons is seen from the following estimations. In the first approximation with respect to the electron-proton interaction, the electron gas energy equals 0.45 a.u. The second-order term is equal to -0.076 a.u., and the third-order one -0.17 a.u. Such values of the first terms of the perturbation expansion in the electron-proton interaction allow one to optimistically estimate the convergence of the whole series.

In this respect, the situation with convergence of the series of the perturbation expansion for the energy is better than that, for example, for the electric resistance [10]. In the latter case, as is seen from Fig.

6, the perturbation expansion series which begins with the second-order terms in the electron-proton interaction converges too slowly. It also follows from the figure that, for all the density values under consideration, the third-order term is less than the second-order one only by a few tens of percents. However, the convergence of the perturbation expansion series for the electric resistance improves with increase in the density.

As concerns the pressure (Fig. 3), its value grows with increase in both temperature and density. The corresponding dependences have monotonic and nonlinear character. The reliability of the results obtained is higher at temperatures far exceeding 3000 K, than at the temperature at which metallic hydrogen was obtained under terrestrial conditions. The reason for this consists in the presence of the band gap of 3000 K in width in the electron energy spectrum of metallic hydrogen at a density of 0.3 mole/cm³. This allows one to apply the theory developed, for example, to the estimation of the pressure in the cores of giant planets of the Solar system, where the temperatures are much higher.

At the same time, in the case of high temperatures, it is necessary to take into account the temperature correction terms to both the multiterminal networks and the dielectric permittivity of the electron gas. It can be easily seen that, even within the temperature interval under consideration, the dimensionless parameter $\hbar/\varepsilon_F\tau$ that characterizes the electron gas degeneration is sufficiently great, and its account can noticeably change the results that we obtained.

Returning to the pressure at which metallic hydrogen was discovered, it should be mentioned the following. Both the electric resistance and pressure were calculated by us within the frames of the same model and with the application of the same approximations. The value of electric resistance, measured experimentally, is more than one order higher than that obtained by us as a result of the approximate summation of terms of the perturbation expansion series for the electric resistance. Under these conditions, the pressure values obtained by us theoretically cannot be close to the experimental ones. Most likely, these values are far smaller. Thus, the answer to the question, at which pressure metallic hydrogen was discovered, remains open. The reason for such an uncertainty is not associated with the model of metallic hydrogen that we used. As was noted above, the conditions of the model applicability are fulfilled well enough. One of the reasons can originate from a neglect of the band gap existence in the electron energy spectrum, which, however, is important only at the

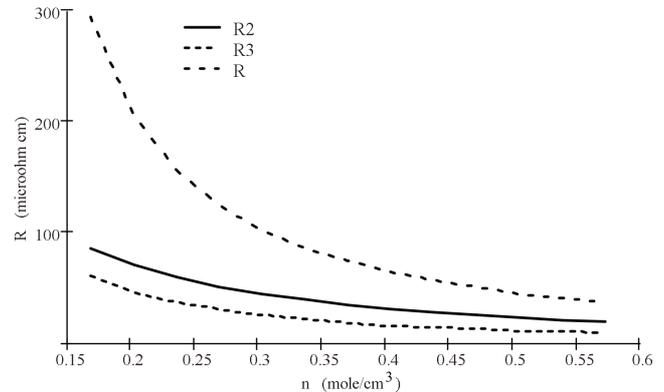


Fig. 6. Electric resistance at 9000 K. R_2 and R_3 are the contributions of the second- and third-order perturbation terms, respectively; R is the result of the approximate summation of the perturbation expansion series

relatively low temperatures and densities. The other reason lies in the uncertainty as to which fraction of hydrogen is in the atomic state. The role of the latter can also be important only at the relatively low temperatures and densities.

Thus, the theory we developed pretends to the quantitative description of both the equilibrium and nonequilibrium properties of metallic hydrogen only in a region of high temperatures and densities. At the same time, if a temperature equals 3000 K, the density should by far exceed 0.3 mole/cm³. Moreover, if the density equals 0.3 mole/cm³, then the temperature should by far exceed 3000 K.

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ТЕРМОДИНАМІЧНІ ВЛАСТИВОСТІ МЕТАЛІЧНОГО ВОДНЮ

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Резюме

Обчислено внутрішню і вільну енергію та тиск металічного водню як функції густини та температури. Досліджений інтервал температур і густин відповідає як умовам експерименту з отримання металічного водню, так і умовам в ядрах планет-гігантів Сонячної системи, таких, як Юпітер і Сатурн. Вважається, що водень перебуває в атомарному стані і всі його електрони колективізовані. Для знаходження термодинамічних потенціалів металічного водню використовується теорія збурень за електрон-протонною взаємодією. Електронна підсистема розглядається у наближенні випадкових фаз із врахуванням обмінної взаємодії і кореляцій електронів у наближенні локального поля. Протон-протонна взаємодія враховується у наближенні твердих сфер. Оскільки для металічного водню електрон-протонна взаємодія відома точно, то, фактично, єдиним параметром теорії є діаметр твердих сфер. Для його обчислення використано парну ефективну електрон-протонну взаємодію. У чисельних розрахунках термодинамічних характеристик металічного водню взято до уваги члени нульового, другого і третього порядків теорії збурень. Член третього порядку виявився досить суттєвим, але в усьому розглянутому інтервалі температур і тисків він значно менший за член другого порядку. Термодинамічні потенціали металічного водню є монотонно зростаючими функціями густини і температури. Значення тиску для температур і густин, характерних для умов отримання металічного водню в земних умовах, з високою точністю збігаються з відповідними значеннями, наведеними авторами відкриття металічного водню.