
ON SOME HELIUM METALLIZATION PARAMETERS**V.T. SHVETS, S.V. KOZYTS'KYI, T.V. SHVETS**PACS 72.10.-d, 72.15.-v,
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A density minimum of 5 g/cm^3 , at which the insulator–metal phase transition in helium can take place, has been calculated. The corresponding temperature of this transition of about 9000 K has been estimated. For this purpose, the effective pair ion-to-ion interaction and the electrical resistivity in liquid helium in a vicinity of the transition point into the metallic state are studied in the framework of a nearly free electron model. As a small parameter of the theory, the ratio between, on the one hand, the energy of interaction between conduction electrons and a singly ionized helium atom and, on the other hand, the Fermi energy of electrons was used. The interaction between electrons is taken into account in the framework of the diffraction model of metal, i.e. considering the screening of the electron-to-ion interaction. The exchange interaction and correlations between conduction electrons are taken into account in the local field approximation.

1. Introduction

The existence of metallic hydrogen was predicted for the first time by Wigner and Huntington in 1935 [1]. At high pressures, hydrogen was supposed to transform from the two-atomic molecular insulator state into the one-atomic state with the metallic conductivity. The first report concerning the experimental discovery of metallic hydrogen is dated 1978 [2]. The authors of work [2] informed the community about the discovery of metallic hydrogen with an electrical resistivity of $1000 \mu\Omega \cdot \text{cm}$ at a pressure of 2 Mbar.

It is adopted that the most reliable experimental results concerning metallic hydrogen were obtained in 1996, in work [3], where the dependences of the electrical resistance of this substance on the pressure and the temperature were also studied in detail. Liquid molecular hydrogen was subjected to a shock compression to pressures in the range 0.93–1.80 Mbar at temperatures of 2200–4000 K. At a pressure of 1.4 Mbar, a density of

0.64 g/cm^3 , and a temperature of 3000 K, the insulator–metal phase transition with an electrical resistivity of $500 \mu\Omega \cdot \text{cm}$ in the metal phase was observed. Among the thermodynamic parameters of hydrogen, only the transition pressure was measured in that experiment, but with a high accuracy of 1%. The electrical resistivity was also measured experimentally, but with rather a low accuracy of 25–50%. The values quoted above for the hydrogen density and temperature at the point of metal–insulator phase transition were obtained by the authors with the use of computer-assisted simulations in the framework of the molecular dynamics method. The accuracy of those calculations was not discussed. Actually, it was low, because the expression selected for the potential of the effective ion-to-ion interaction was cumbersome and approximate.

The situation with the helium metallization is much more complicated. Till now, there has been no information concerning the production of helium in the metallic state under terrestrial conditions. The reason evidently consists in that, despite the growing experimental capabilities aimed at achieving high pressures, densities, and temperatures, the conditions needed for the helium metallization have not been reached yet. Note that a similar problem was successfully solved experimentally, e.g., for oxygen [4, 5]. The situation for helium becomes even more complicated, because the magnitudes of thermodynamic parameters necessary for the helium metallization are unknown till now.

This work is aimed at determining some of those parameters. Namely, these are the temperatures and the densities, at which the metal–insulator transition in helium can be observed. For this purpose, we analyze two parameters of metallic helium: the effective pair ion-to-ion interaction and the electrical resistivity. The dependence of the latter on the density is strong. While

using the model of nearly free electrons, the relevant expression diverges, when approaching the metal–insulator phase transition point from the metal side. From our viewpoint, just this circumstance gives a possibility to determine the density at the phase transition point. The electrical resistivity depends rather weakly on the temperature, so that an estimation error for the transition temperature practically does not affect the density value found at this point. In turn, the effective pair ion-to-ion interaction depends on the density of the system only. Knowing the parameters of the pair potential and making a comparison with the corresponding values for the potential in metallic hydrogen, for which the temperature of the phase transition is known, allow this temperature to be evaluated for metallic helium as well.

2. Metal Model

The most popular model of metal is the diffraction one. This model is usually based on the theory of pseudopotentials [6, 7], in which the relatively strong potential of the electron-ion interaction is substituted by a weaker pseudopotential. Such a substitution improves the convergence in the perturbation theory series for various characteristics of metals. Instead, however, we obtain the nonlocality and the nonlinearity of the pseudopotential, as well as the impossibility to carry out calculations with a satisfactory accuracy for disordered systems. In such a case, if needed, calculations can be carried out in higher orders of perturbation theory with the use of ordinary potentials.

In the framework of the approach based on the theory of pseudopotentials, the local model pseudopotentials possessing at least two fitting parameters are usually applied. The latter are selected on the basis of a suitable experimental information. The unique metal, for which such a problem does not exist, is metallic hydrogen. It is so, because, owing to the absence of internal electron shells, the corresponding potential, being the Coulomb one, and the pseudo-potential coincide in this case. For instance, there is no more such a coincidence for metallic helium. In this work, since the experimental information concerning helium is confined, we refuse the pseudopotential concept in favor of the electrostatic potential created by a singly ionized helium atom. Taking the exact solution for an isolated helium ion [8] as a wave function for the ground state of a helium ion, it is easy to obtain the following expression for the Fourier

transform of the sought electrostatic potential:

$$w_0(q) = -\frac{4\pi e^2}{q^2} \left(2 - \frac{16^2}{(16 + q^2)^2} \right). \quad (1)$$

A characteristic dimensionless parameter of the problem is the ratio between the potential of the electron-ion interaction and the Fermi energy. This ratio is not less than 1 for all wave vectors. However, it is important that, for the wave vectors, the magnitudes of which are close to $2k_F$ and which play a substantial role while calculating various properties of disordered metals [6, 7, 9, 10], this ratio is really small for the majority of simple metals. The hydrogen and helium behave similarly practically within the whole range of wave-vector values. Therefore, a similar behavior should be expected for the convergence of the perturbation theory series obtained for various properties of those metals. Those expansions, at least for hydrogen, converge rather well, if not too close to the transition point metal–insulator [11–13].

The fundamental principle of the diffraction model for metals is the exact consideration of the electron-electron interaction by making allowance for the screening of the electron-ion interaction potential. On the one hand, this approximation is compelled, because it is impossible to match the theory of pseudopotentials with the exact account of the electron-electron interaction. On the other hand, owing to the momentum conservation law for the electron subsystem, the electron-electron scattering in disordered metals does not influence the electron transfer phenomena, and this approximation turns out good. In our approach, we leave this principle untouched.

3. Effective Pair Ion-to-Ion Interaction

To calculate the effective pair ion-to-ion interaction, we use the known result [6, 7, 9, 14], which corresponds to the second order of perturbation theory with respect to the potential of the electron-ion interaction in the framework of the diffraction model of metal,

$$U_{\text{ef}}(R) = \frac{z^2 e^2}{R} - \frac{e^2}{2\pi^2} \int_0^\infty w_0^2(q) \frac{\pi_0(q)}{\varepsilon(q)} \frac{\sin(qR)}{qR} q^2 dq. \quad (2)$$

Here, R is the distance between ions, $\pi_0(q)$ the polarization function of the noninteracting degenerate electron gas, and $\varepsilon(q)$ its dielectric permittivity. The effective pair interionic interaction depends only on the electron gas density. When comparing this interaction among various substances, the specific value of density turns

out to be not crucially important. Therefore, assuming these densities to be identical for metallic hydrogen and metallic helium and equal to the known density of hydrogen at the point of the metal–insulator transition, provided that all hydrogen atoms are ionized, we obtain the dependences for the effective pair ion-to-ion interaction on the interionic distance, which are depicted in Fig. 1.

The effective pair interaction between ions is rather sensitive to the choice of an approximation made while taking the exchange interaction and correlations between conduction electrons into account. For some approximations, even the potential well does arise, similarly to what takes place in the random phase approximation, which completely neglects this interaction. In our opinion, this fact can serve as an important criterion for the estimation of the quality of approximations made for the exchange interaction and correlations between conduction electrons. It is of importance, however, that the ratio between the potential well depths for various metals – e.g, for hydrogen and helium – remains almost constant, if the character of approximations for the local potential changes. Therefore, we showed the plots of pair potentials only for one choice of an approximation for the exchange interaction and correlations between conduction electrons, namely, for the dielectric permittivity used in classical works by E.G. Brovman and Yu.M. Kagan dealing with a many-particle model of metal, including metallic hydrogen. Their review is contained in work [15]. In the works discussed, the dielectric permittivity of the electron gas proposed by Geldart and Vosko [16] was used. In this case, the potential well depth is about 178 K for hydrogen and about 488 K for helium. The potential well depth is usually associated with the boiling and critical temperatures of the metal. In particular, for metals with deeper potential wells, those temperatures are higher [6, 7, 14]. Since, for the majority of metals, the metal–insulator transition occurs in a vicinity of the corresponding critical point, this circumstance may serve as a certain guide in the cases where the actual temperature of this transition is unknown. And so it is for helium! Quite reasonable seems the assumption that the helium metallization temperature is approximately three times as high as the corresponding temperature for hydrogen. For hydrogen, it equals 3000 K. Therefore, for helium, it should amount to 9000 K.

As numerical calculations of the effective three-particle interaction in metallic hydrogen show, its contribution to such parameters of the two-particle interaction as the depth and the position of a potential well can be rather considerable under certain conditions [15, 17]. It

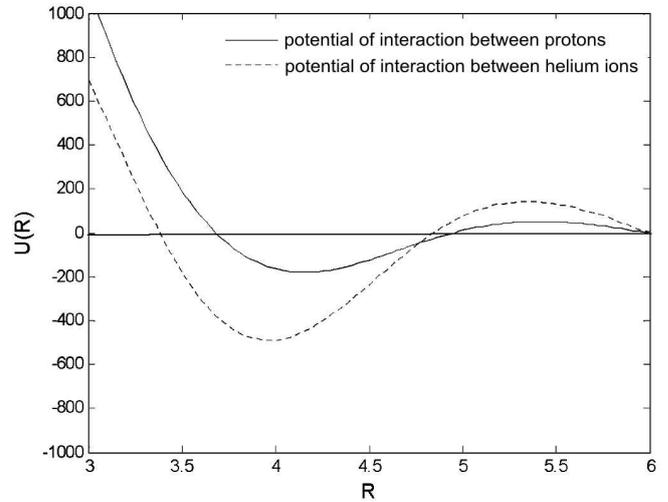


Fig. 1. Effective pair ion-to-ion interaction potentials for hydrogen and helium. The distance between ions is expressed in terms of atomic units, and the potentials in Kelvin degrees

is evident that such a situation can arise in the case of metallic helium as well. This circumstance demands to be analyzed separately.

4. Electrical Resistivity

For simple disordered metals with a relatively high conductivity, the electrical resistivity is determined by the known Drude formula, which is a direct consequence of the nearly free electron model,

$$R = \frac{m}{ne^2} \tau^{-1}. \quad (3)$$

Here, n is the electron gas density, and τ is the relaxation time of the electroconductivity process. The perturbation theory for the resistance in liquid metals was developed in a considerable number of works [18–28]. Below, we use the results of work [18] for specific calculations.

In the framework of the Kubo linear response theory and the method of two-time retarded Green’s functions [28], the reciprocal relaxation time can be presented in the form of the following series in either the electron-proton or electron-ion interaction:

$$\tau^{-1} = \sum_{n=2}^{\infty} \tau_n^{-1}. \quad (4)$$

The general term of this expansion looks like

$$\tau_n^{-1} = \frac{N}{V^n} \times$$

$$\times \sum_{\mathbf{q}_1, \dots, \mathbf{q}_n} W(\mathbf{q}_1) \dots W(\mathbf{q}_n) S(\mathbf{q}_1, \dots, \mathbf{q}_n) \Gamma(\mathbf{q}_1, \dots, \mathbf{q}_n). \quad (5)$$

The idea of this representation and the corresponding notations were taken from the expansion of the ground state energy of an electron gas in simple crystalline metals in a series in the electron-ion interaction parameter [15]. Here, $S(\mathbf{q}_1, \dots, \mathbf{q}_n)$ is the n -particle structure factor of the ionic subsystem, N the number of ions in the system, and $\Gamma(\mathbf{q}_1, \dots, \mathbf{q}_n)$ the electron multipole describing the process of electroconductivity.

The second-order contribution to the reciprocal relaxation time in simple disordered metals has been studied in detail for rather a long time. It looks like

$$\tau_2^{-1} = \frac{m}{12\pi^3 \hbar^3} \int_0^{2k_F} W^2(x) S(x) x^3 dx. \quad (6)$$

Therefore, let us proceed at once to the consideration of the third-order term. It reads

$$\tau_3^{-1} = \frac{N}{V^3} \times \sum_{\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3} W(\mathbf{q}_1) W(\mathbf{q}_2) W(\mathbf{q}_3) S(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) \Gamma(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3), \quad (7)$$

$$\begin{aligned} \Gamma(\mathbf{k}_1 - \mathbf{k}_2, \mathbf{k}_2 - \mathbf{k}_3, \mathbf{k}_3 - \mathbf{k}_1) = \\ = \frac{\pi \hbar}{3mNk_B T} (\mathbf{k}_1 - \mathbf{k}_2)^2 n(\mathbf{k}_1) [1 - n(\mathbf{k}_1)] \frac{\delta(\varepsilon_{\mathbf{k}_2} - \varepsilon_{\mathbf{k}_1})}{\varepsilon_{\mathbf{k}_2} - \varepsilon_{\mathbf{k}_3}}, \quad (8) \end{aligned}$$

where T is the absolute temperature, k_B the Boltzmann constant, and $n(k)$ the Fermi–Dirac distribution function for electrons. After a number of transformations [28], the expression for the third-order contribution can be reduced to the integral

$$\tau_3^{-1} = \frac{m^2}{24\pi^5 \hbar^5 k_F^2} \int_0^\infty \frac{f(k)}{k_F - k} dk. \quad (9)$$

The main problem that arises when considering the third-order contribution to the electric resistance is the three-particle structure factor of the ionic subsystem. Usually, the geometrical approximation is applied to it [28–30],

$$S(\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) = S(\mathbf{q}_1) S(\mathbf{q}_2) S(\mathbf{q}_3). \quad (10)$$

A consequence of this approximation is the following expression for the function $f(k)$:

$$f(k) = \frac{1}{k_F + k} \sum_{n=0}^{\infty} (2n+1) A_n B_n^2(k),$$

where

$$A_n = \int_0^{2k_F} W(q) S(q) P_n \left(\frac{2k_F^2 - q^2}{2k_F^2} \right) q^3 dq,$$

$$B_n(k) = \int_{|k-k_F|}^{k+k_F} W(q) S(q) P_n \left(\frac{k^2 + k_F^2 - q^2}{2kk_F} \right) q dq,$$

and $P_n(x)$ is the Legendre polynomial of the n -th order.

While calculating the electrical resistivity in disorder metals, it is sufficient to take only the terms of the second and third orders in the majority of practically important cases. However, in a vicinity of the metal–insulator transition point, the whole series of perturbation theory has to be summed up. Nowadays, this task cannot be realized. Therefore, we confine the consideration to the calculation of contributions of the second and third orders, depending on the density. The approach to the transition point, where the perturbation theory series diverges, will be monitored by the approach of the third-order-correction magnitude to the value of the second-order contribution to the electrical resistivity.

The expression obtained for the electrical resistivity contains only two key functions governing the accuracy of numerical calculations. These are the form factor of either the proton or ion potential and the pair structure factor for the ionic subsystem. Note that the results of calculations of the electrical resistivity are little sensitive to the choice of the dielectric permittivity function for the electron gas. In particular, the consideration can be confined to the random phase approximation. For hydrogen in the metallic state, the form factor is known precisely. It is the Coulomb potential of a point charge. For a singly ionized helium ion, the form factor can also be calculated with a high accuracy. Therefore, all we need to do is to calculate the pair structure factor of the ionic subsystem.

Unlike the comprehensive body of experimental data concerning liquid metals in a vicinity of their melting temperature, including the data on the pair structure factor, there is the lack of such data for hydrogen in the metallic state. Helium has not been obtained yet in the metallic state. The only probable version is to use a

model expression for the indicated structure factor. The most popular model, which is applied to the determination of the pair structure factor, is the hard-sphere one [31]. This model includes a single fitting parameter, the hard-sphere diameter which cannot be calculated in the framework of the model itself. According to the results of work [32], the hard-sphere diameter is determined from a condition that the kinetic and potential energies of protons or ions at their maximum rapprochement should be equal to each other. This algorithm is based on the application of the effective pair proton-proton or ion-ion interaction, which was considered in the previous sections.

As was marked above, the metal-insulator transition for hydrogen is observed at a density of 0.64 g/cm^3 . However, the electron density, at which the terms of the second and third orders in the perturbation theory series are equal to each other, is by 40% lower than the density in the case of the complete hydrogen ionization. The experimental confirmation of this conclusion was obtained in work [33], where a wider spectrum of measured parameters for metallic hydrogen was presented in comparison with work [3]. In particular, the share of ionized hydrogen atoms was measured as well, with the corresponding value being of about 40%. The theoretical substantiation of this experimental fact was obtained for the first time in work [34]. More exact calculations evidently demand that the scattering of conduction electrons by neutral atoms should be taken into consideration as well, which was done in the cited work. However, it does not affect the divergence. Such a coincidence between the divergence in the electrical resistivity calculated in the nearly free electron model and the metal-insulator transition point is not accidental and allows one to predict, e.g., the density of conduction electrons on the basis of the electrical resistance behavior in the case where this density is not realized experimentally.

In Fig. 2, the plot of the dependence of the electrical resistivity of helium in the metallic state in a vicinity of the metal-insulator transition point at a temperature of 9000 K is depicted. One can see that the density is approximately equal to 5 g/cm^3 at the metal-insulator transition point, provided that all helium atoms are ionized. If the transition density is measured in terms of g/atom units, it is approximately twice as high as the density in the case of hydrogen metallization. It should be noticed that the analysis of the electroconductivity enables only the lower limit for the transition density to be obtained. It is so, because, in the case of the partial ionization of helium atoms, the density of the sys-

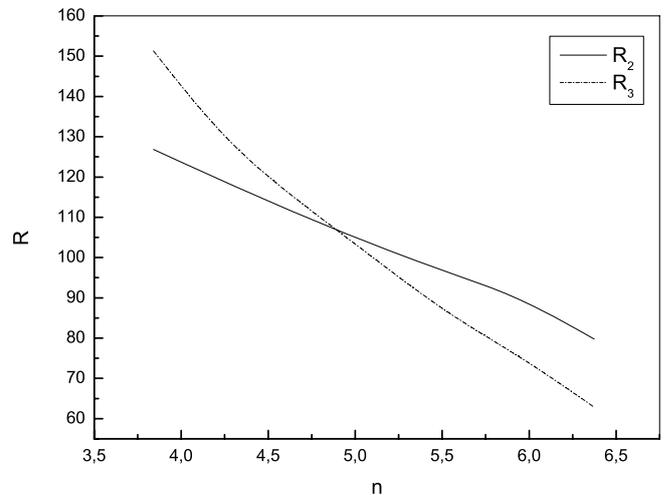


Fig. 2. Dependences of the electrical conductivity of metallic helium (in units of $\mu\Omega \cdot \text{cm}$) on the density (in units of g/cm^3) in the second (R2) and third (R3) orders of perturbation theory

tem consisting of ionized and nonionized helium atoms is higher. As was already marked above, the density of conduction electrons, which corresponds to the metal-insulator transition point, is almost independent of the temperature. As the numerical calculations show, the density of conduction electrons in helium remains the same at a temperature twice as high.

5. Conclusions

Since the potential well depth for helium is approximately three times as large as that for hydrogen, we suppose that the temperature of the transition into a metallic state is higher for helium in approximately the same proportion. That is this temperature must be not lower than 9000 K at the density concerned. Such a high temperature of the transition into the metallic state may probably be one of the reasons that prohibited metallic helium to be obtained under terrestrial conditions till now.

The divergence in the electrical resistivity of helium in a vicinity of the 5-g/cm^3 density evidences a high density of helium at the metal-insulator transition point, provided that every helium atom is singly ionized. Being recalculated in terms of g/atom units, this density turns out to be twice as high as the corresponding density of metallic hydrogen at its transition point. Higher density values would correspond to a partial ionization of helium atoms. This circumstance is one of the reasons why metallic helium has not been obtained yet under terrestrial conditions.

To determine the pressure needed for helium to become a metal, it is necessary to use the equation of state for metallic helium similar to the equation of state for metallic hydrogen [12]. This task will be a subject of our subsequent researches.

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ОЦІНКА ПАРАМЕТРІВ МЕТАЛІЗАЦІЇ ГЕЛІЮ

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Резюме

Розраховано мінімальну густину, за якої гелій переходить у металічний стан. Вона становить приблизно 5 г/см^3 . Оцінено також температуру переходу метал-діелектрик. Вона становить приблизно 9000 К . З цією метою досліджували парну ефективну міжйонну взаємодію в гелії та його електричний опір в околі точки переходу в металічний стан. Розгляд ґрунтувався на моделі майже вільних електронів. У ролі малого параметра використовували відношення потенціалу взаємодії електронів провідності з одноразово іонізованими атомами гелію до енергії Фермі. Взаємодію між електронами враховували відповідно до дифракційної моделі металу, тобто через екранування електрон-іонної взаємодії. Обмінну взаємодію і кореляції електронів провідності враховували у наближенні локального поля.