Papers submitted to the Conference "Applications of Physics in Mechanical and Material Engineering"

Influence of the Vertex Corrections to the Electron–Phonon Interaction on the Value of the Critical Temperature of YH_{10}

M. Kostrzewa*

Quantum Optics and Engineering Division, Institute of Physics, University of Zielona Góra, Prof. Z. Szafrana 4a, 65-516 Zielona Góra, Poland

Doi: 10.12693/APhysPolA.142.149 *e-mail: m.kostrzewa@if.uz.zgora.pl

Theoretical studies available in the literature suggest that the compound YH_{10} is a promising candidate for a high-temperature superconductor with a phase transition temperature T_C close to room temperature. Numerical solutions of the classical Eliashberg equations at 250 GPa led to the critical temperature of about $T_C = 326$ K. As expected, YH_{10} belongs to the group of superconductors with strong electron–phonon coupling, similar to others with T_C above 200 K, for example, H_3S, LaH_{10}, or YH_6. In 2018, a series of experiments were conducted, and the experimental verifications confirming the existence of a high-temperature superconducting state in LaH_{10} turned out to be groundbreaking. At the time, it seemed that such confirmation concerning YH_{10} would come very quickly. Unfortunately, so far there have been no successful experimental measurements on the high-temperature YH_{10} superconducting phase. The aim of this work is to show the effect of the vertex corrections to the electron–phonon interaction on the value of the critical temperature of YH_{10} at 250 GPa. Thus, it was shown that by including more complex equations into the calculations (the formalism of Eliashberg equations with the vertex corrections), the estimated value of the metal-superconductor phase transition temperature lowers significantly to $T_C = 245.75$ K. Furthermore, we point out that the influence of temperature on the effective electron mass exhibits a similar tendency as that concerning the LaH_{10} superconductor we studied earlier.

topics: YH_{10}, high-temperature superconducting state, vertex corrections

1. Introduction

In recent years, both theoretical and experimental research has been intensively carried out in order to discover a material that will exhibit superconducting properties at room temperature and at a pressure acceptable from the point of view of practical applications. Currently, hydrogen-rich systems are of great interest. Many experiments are performed, and some of them are showing promising results [1–7]. The possibility of the existence of a superconducting state in this type of compounds was first pointed out by Ashcroft in his paper published in *Phys. Rev. Lett.* in May 2004 [8]. The author suggested that hydrogen-rich compounds may exhibit the properties of high-temperature superconductors. In addition, he noted that the achievement of metallic states should occur at pressures much lower than necessary for hydrogen itself (in 1968 he predicted the existence of a high-temperature superconducting state in metallic hydrogen under the influence of pressure above 60 GPa [9]). Although more than a century has passed since Kamerlingh Onnes discovered the phenomenon of superconductivity [10], today we know that there is still no reliable experimental data confirming the existence of a superconducting state in pure hydrogen. There are also studies that exclude the possibility of induction of a superconducting phase in hydrogen with a transition temperature comparable to room temperature [11]. In turn, it was not until 2020 that scientists at Rochester University in New York announced that they had successfully obtained a hydrogen-rich superconductor at a temperature of 287.7 ± 1.2 K under a pressure of 267 ± 10 GPa [6]. Obtaining superconductivity in the carbon–sulfur–hydrogen system at such a high temperature is undoubtedly a great success. However, the results of the experiment, published in the journal *Nature* [6], show the need to keep the material under very high pressure.

It is worth mentioning that theoretical studies previously carried out by other scientists suggest that the compound YH_{10}, which is the main subject of this publication, is a promising candidate for a high-temperature superconductor with a phase transition temperature T_C close to room temperature. According to estimates based on solutions of classical Eliashberg equations (CEE) [12] carried out by Liu et al., $T_C \in 305$–326 K at 250 GPa [13].

The value of the given critical temperature depends on the adopted value of the Coulomb pseudopotential, 0.13 or 0.1, respectively. The Heil's group reported a slightly lower temperature of $T_C = 310$ K at 300 GPa [14]. Meanwhile, the results of other research groups suggest that for YH_{10} the critical temperature is only 250 K, but at an even higher pressure 425 GPa [15]. Following the groundbreaking experimental verifications done in 2018 confirming the existence of a high-temperature superconducting state in a system formed by the combination of hydrogen and lanthanum (LaH_{10}), it seemed that such confirmation for YH_{10} should come very quickly. However, only $T_C = 224$ K for YH_6 [5] and $T_C = 262$ K for YH_9 [7] have been confirmed so far in 2020. It should be noted that the value of T_C for YH_6 is unexpectedly lower than the previous theoretically predicted value — in 2014, the team of Li et al. suggested T_C of 251–264 K at 120 GPa [16], and in 2019 the team of Heil et al. predicted $T_C = 290$ K at 300 GPa [14].

The aim of this work is to show the effect of the vertex corrections to the electron–phonon interaction on the value of the critical temperature of YH_{10} subjected to the pressure of 250 GPa. The continued lack of experimental results suggests that such extensive research should be carried out.

2. Results and discussion

When analyzing the results obtained from the calculations carried out by Liu et al. [13], it can be concluded that YH_{10} belongs to the group of superconductors for which strong electron–phonon coupling is present, as in H_3S, LaH_{10}, and YH_6. The value of the electron–phonon coupling constant for YH_{10} is 2.56 [13]. Although yttrium is a lighter element than lanthanum, both have the same electron configuration on the valence shell. According to the study by Liu and coworkers [13], YH_{10} conforms to the same structure in a pressure range as LaH_{10}. Additionally, these researchers predict the energetic phase stability of the compound YH_{10} from 250 to 300 GPa. Due to the above in this paper for YH_10, the computational methods successfully used to analyze the thermodynamic parameters of the LaH_10 superconductor were used. So far, the influence of the vertex corrections of the electron–phonon interaction on the properties of the superconducting state has not been fully determined. Therefore, we discuss the importance of vertex corrections to the electron–phonon interaction for a promising candidate for a high-temperature superconductor, like YH_{10}. The most interesting case from the point of view of the height of the estimated critical temperature was chosen, namely the system subjected to the pressure of $p = 250$ GPa. So far, the literature on this subject has not presented such results for the system with stoichiometry YH_{10}.

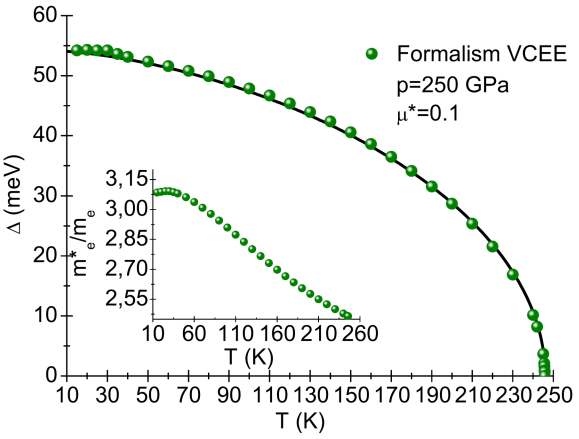

Fig. 1. The dependence of the order parameter on temperature of YH_{10}. The influence of the temperature on the value of effective electron mass to the band electron mass ratio is depicted in the inset.

In these calculations, we use the equations of Frericks et al. [17], which are a generalization of Eliashberg equations included lowest-order vertex correction — the scheme VCEE (vertex corrected Eliashberg equations). In particular, the following values of input parameters were adopted for further calculations: $\lambda = 2.56$, $\mu^\star = 0.1$, $\omega_0 = 100$ meV, and $\Omega_C = 1$ eV. The quantity λ is the electron–phonon coupling constant, $\mu^\star$ — Coulomb pseudopotential, ω_0 denotes the characteristic phonon frequency, and Ω_C represents the cut-off frequency. The function

$$\mu^\star(\omega_m) = \mu^\star\,\theta\big(\Omega_C - |\omega_m|\big) \tag{1}$$

models the repulsion between electrons, θ is the Heaviside function. The pairing kernel is defined by

$$K\,(\omega_n - \omega_m) = \frac{\Omega_C^2}{(\omega_n - \omega_m)^2 + \Omega_C^2}\;\lambda. \tag{2}$$

Eliashberg's equations were solved numerically for a sufficiently large number of Matsubara frequencies. The stable solutions of Eliashberg equations were obtained for $T \geq T_0$=15 K. Based on the analytical continuation method [18] and the solutions of Eliashberg equations on the imaginary axis, we determined the order parameter function on the real axis $\Delta(\omega)$, which in turn allowed us to determine the physical values of the order parameter were determined according to the formula

$$\Delta\,(T) = \mathrm{Re}\Big[\Delta\Big(\omega = \Delta\,(T)\Big)\Big]. \tag{3}$$

The full dependence of the order parameter on temperature depicts Fig. 1. In the inset, the temperature dependence of m_e^*/m_e is presented. The symbol m_e^* represents the effective mass of the electron and m_e means the electron band mass. For the VCEE scheme, the value of this ratio can be estimated from

$$\frac{m_e^*}{m_e} = Z_{n=1}(T), \tag{4}$$

where $Z_n = Z(\mathrm{i}\omega_n)$ represents the wave function renormalization factor, which describes the renormalization of the thermodynamic parameters of the superconducting state by the electron–phonon interaction. The symbol ω_n is the Matsubara frequency as defined by

$$\omega_n = \pi k_{\mathrm{B}} T \left(2n + 1\right), \tag{5}$$

where k_{B} is the Boltzmann constant and n is the integer.

The thermodynamics of the superconducting state of the tested system fully determines the dependence of the order parameter on temperature. In Fig. 1, the spheres represent numerical results. The line, on the other hand, is responsible for the analytical solution obtained on the basis of

$$\Delta\left(T\right) = \Delta\left(T_0\right)\sqrt{1 - \left(\frac{T}{T_C}\right)^{\Gamma}}, \tag{6}$$

where parameter Γ is 1.6, $\Delta(T_0) = 54.213$ meV. As we have shown in the range of analyzed temperatures, vertex corrections affect the values of the order parameter defined as the quotient of ϕ_n and Z_n (ϕ_n is the order parameter function), where the function $\Delta(T) \simeq 0$ we expect a metal-superconductor phase transition. It can be easily seen that the value of the estimated critical temperature for YH_{10} in the VCEE scheme is close to 250 K (245.75 K exactly), which is much lower than that in CEE scheme at the same value of the Coulomb pseudopotential. This result suggests that the inclusion of more complex equations in the calculations has a significant impact on the estimated value of the metal-superconductor phase transition temperature. This in turn indicates that the tested system will unfortunately not be a superconductor with T_C comparable to room temperature. As shown by Liu et al. [13], taking into account the higher value of the Coulomb pseudopotential in the calculations does not benefit the critical temperature value. We came to the same conclusion by analyzing the results obtained from numerical solutions of the classical Eliashberg equations for the YH_6 system, where increasing $\mu^\star$ from 0.1 to 0.1226 led to a decrease in T_C from 236.8 to 224 K [19].

By analyzing the data presented in the inset in Fig. 1, it seems that the vertex corrections to electron–phonon interaction have a significant impact on the value of the effective mass of the electron. One can see that $[m_e^\star]_{T_0}$=3.085 m_e and $[m_e^\star]_{T_C}$=2.466 m_e. Summing up, we believe that vertex corrections noticeably lower the value of $m_e^\star$ (the ratio $m_e^\star/m_e$ decreases with increasing temperature). Moreover, let us note that the influence of temperature on the effective mass of the electron shows a similar tendency as in the case of the LaH_{10} superconductor, previously studied in [19]. It should be emphasized that the results obtained for LaH_{10} were based on experimental measurements. Both these systems, YH_{10} and LaH_{10}, have a comparable structure, so it can be concluded that the results obtained in this paper are reliable.

3. Conclusions

To summarize, the system YH_{10} is a good material for a potential candidate of a high-temperature superconductor characterized by a high value of the electron–phonon coupling constant. It should be noted that, in fact, all hydrogen-rich compounds, in which the existence of a superconducting phase has been experimentally confirmed and for which T_C exceeds 200 K, are characterized by a high value of the electron–phonon coupling constant.

The presented numerical calculations show that the compound YH_{10} does not belong to the group of superconductors with a value of T_C comparable to room temperature. From the discussion in Sect. 2 it follows that the thermodynamic properties of YH_{10} can be correctly reproduced within the Eliashberg formalism in the VCEE scheme. In particular, it was shown that the inclusion of more complex equations than the CEE scheme in the calculations has a significant effect on the estimated value of the metal-superconductor phase transition temperature. The calculations previously performed by Liu et al. [13], based on the classical Eliashberg equations greatly overestimate the value of the critical temperature for the YH_{10} system subjected to a pressure of 250 GPa. For the analyzed system, based on the results obtained in the framework of VCEE, it can be predicted that the value of T_C is close to 250 K (245.75 K to be exact). Furthermore, it has been shown in this paper that the vertex corrections to the electron–phonon interaction have a significant impact on the value of the effective mass of electron, i.e., these corrections noticeably lower the value of the $m_e^\star$. The $m_e^\star/m_e$ ratio has the highest value for the temperature T_0 and the lowest at the critical temperature T_C. Moreover, it should be emphasized that the influence of temperature on the effective electron mass exhibits a similar tendency as in the case of the LaH_{10} superconductor with similar stoichiometry, which we studied earlier [19].

Acknowledgments

The author acknowledge the support of the program of the Polish Minister of Science and Higher Education under the name “Regional Initiative of Excellence” in 2019–2022, project no. 003/RID/2018/19.

References

[1] A.P. Drozdov, M.I. Eremets, I.A. Troyan, V. Ksenofontov, S.I. Shylin, *Nature* **525**, 73 (2015).

[2] A.P. Drozdov, V.S. Minkov, S.P. Besedin, P.P. Kong, M.A. Kuzovnikov, D.A. Knyazev, M.I. Eremets, arXiv:1808.07039, 2018.

[3] A.P. Drozdov, P.P. Kong, V.S. Minkov et al., *Nature* **569**, 528 (2019).

[4] M. Somayazulu, M. Ahart, A.K. Mishra, Z.M. Geballe, M. Baldini, Y. Meng, V.V. Struzhkin, R.J. Hemley, *Phys. Rev. Lett.* **122**, 027001 (2019).

[5] I.A. Troyan, D.V. Semenok, A.G. Kvashnin et al., *Adv. Mater.* **33**, 2006832 (2021).

[6] E. Snider, N. Dasenbrock-Gammon, R. McBride, M. Debessai, H. Vindana, K. Vencatasamy, K.V. Lawler, A. Salamat, R.P. Dias, *Nature* **586**, 373 (2020).

[7] E. Snider, N. Dasenbrock-Gammon, R. McBride, X. Wang, N. Meyers, K.V. Lawler, E. Zurek, A. Salamat, R.P. Dias, *Phys. Rev. Lett.* **126**, 117003 (2021).

[8] N.W. Ashcroft, *Phys. Rev. Lett.* **92**, 187002 (2004).

[9] N.W. Ashcroft, *Phys. Rev. Lett.* **21**, 1748 (1968).

[10] H.K. Onnes, in: *Through Measurement to Knowledge*, Eds. K. Gavroglu, Y. Goudaroulis, Vol. 124, Springer, Dordrecht 1991, p. 261.

[11] M. Kostrzewa, A.P. Durajski, R. Szczęśniak, *J. Supercond. Nov. Magn.* **34**, 2281 (2021).

[12] G.M. Eliashberg, *Sov. phys. JETP* **11**, 696 (1960).

[13] H. Liu, I.J. Naumov, R. Hoffmann, N.W. Ashcroft, R.J. Hemley, *PNAS* **114**, 6990 (2017).

[14] C. Heil, S. di Cataldo, G.B. Bachelet, L. Boeri, *Phys. Rev. B* **99**, 220502 (2019).

[15] A.M. Shipley, M.J. Hutcheon, M.S. Johnson, R.J. Needs, C.J. Pickard, *Phys. Rev. B* **101**, 224511 (2020).

[16] Y. Li, J. Hao, H. Liu, J.S. Tse, Y. Wang, Y. Ma *Sci. Rep.* **5**, 9948 (2015).

[17] J.K. Freericks, E.J. Nicol, A.Y. Liu, A.A. Quong, *Phys. Rev. B* **55**, 11651 (1997).

[18] K.S.D. Beach, R.J. Gooding, F. Marsiglio, *Phys. Rev. B* **61**, 5147 (2000).

[19] I.A. Wrona, M. Kostrzewa, K.A. Krok, A.P. Durajski, R. Szczęśniak, *J. Appl. Phys.* **131**, 113901 (2022).