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Summary of the doctoral dissertation entitled
Analysis of superconducting state beyond the standard Eliashberg scheme

The superconducting state is a phenomenon that has amazed and fascinated scientists from its discovery in 1911 [1] to the present day. Theories describing the superconducting state, such as the Bardeen-Cooper-Schrieffer mean-field theory (BCS) [2, 3] and its generalization, the standard Migdal-Eliashberg theory [4], were a great achievement in solid-state physics. These models made it possible to describe the properties of many superconductors. This fact is due to the fact that a very large group of materials has a relatively simple structure, which leads to a comparatively simple description of their electronic, phonon and electron-phonon properties. Therefore, in order to show how many different physical systems can be described by the standard (isotropic) Migdal-Eliashberg theory, in my doctoral dissertation I presented an analysis of the superconducting state in three materials: $BaGe_3$ [5, 6], HfH_2 [7, 8] i Cr_3RhN [9, 10, 11]. These superconductors differ in many aspects, such as the electron and phonon crystal structure, the electron-phonon coupling constant (λ) and the value of the critical temperature (T_C). In my doctoral dissertation, I showed that these systems can be described very accurately using the isotropic Migdal-Eliashberg theory, i.e. one in which the self-reconciliation of solutions to Eliashberg equations occurs only in relation to electron and phonon energy.

However, not all superconductors fit into the isotropic description framework. There are materials for which the theoretically determined properties of the superconducting state do not agree with the experimental results. This may be caused by too far-reaching approximations used in the standard Eliashberg formalism, such as: assuming a constant electron density of states [12, 13], omitting the dependence of the Elishberg equations on the electronic wave vector ($\mathbf{k}$) [14, 15], taking into account the Coulomb pseudopotential ($\mu^{\star}$) [16, 17] - parameter, which for low values is interpreted as the effective Coulomb interaction between electrons. It is also worth mentioning the approximation of the infinitely wide electron band and the assumption of a half-filled electron band [17]. It is also of considerable importance to take into account the theorem of Migdal [18], which assumes that the vertex corrections to the electron-phonon interaction are negligible. Many of these approximations can significantly affect the properties of the superconducting state of unconventional superconductors.

There are many approximations in the standard Migdal-Eliashberg theory, and omitting them all is an extremely difficult and complicated task. Therefore, in my dissertation, I presented the first steps to go beyond the standard Eliashberg scheme, namely I presented a self-consistent analysis of the properties of the superconducting state, taking into account the electron and phonon wave vector in the calculations and the non-adiabatic effects resulting from the vertex corrections of the electron-phonon interaction.

In the first step, I derived the Eliashberg equations dependent only on the electron momentum, investigating the anisotropic properties of the superconducting state [19]. In this case, I analyzed the superconducting state for a different number of electron band fills $\langle n\rangle \in \langle 0{,}2; 1\rangle$. Then I presented the analysis of the superconducting state taking into account the independent variables in Eliashberg's theory: the electron and phonon wave vector and the Matsubara frequency [20]. In this case, due to the higher complexity of the system of equations, I assumed a half-filled electron band. The difficulty in studying both types of the discussed equations is to take into account all the anisotropic properties of the tested materials. Therefore, I analyze a relatively simple physical system: a two-dimensional square lattice. This allowed for a very detailed study of the anisotropic properties of the superconducting state. The most important and unprecedented result of this analysis in the literature is the information about the existence of an unbalanced superconducting state when the dependence of the equations on the wave vector is taken into account. An unbalanced superconducting state is a state for which the value of the coupling constant in the diagonal self-energy channel is different from the value of the coupling constant in the Cooper channel (non-diagonal self-energy channel). In my doctoral dissertation, I showed that the wave vector-dependent solutions of Eliashberg's equations are characterized by significant heterogeneity in the momentum space. This fact is very often overlooked in the discussion of the superconducting state induced by the linear electron-phonon interaction. However, it may be particularly important in a situation when the vertex corrections to the electron-phonon interaction are large, because their significance is determined by the momentum dependence of the functions $\Delta_{\mathbf{k}}$, $Z_{\mathbf{k}}$ and $\chi_{\mathbf{k}}$, which are solutions to the Eliashberg equations [21, 22, 23, 24].

In the next stage, I took into account the commonly used theorem of Migdal [18], justifying the omission of contributions from the vertex corrections of the electron-phonon

interaction in the Eliashberg equations. This theorem states that if the characteristic energy of phonons in the examined physical system is much lower than the characteristic energy of electrons, then the non-adiabatic effects are insignificant. However, studies of the superconducting state show that there are systems such as fullerene systems [25, 26], the high-T_C cuprates [27, 28, 29], the heavy fermion compounds [30], the superconductors under high magnetic fields [31] and low-dimensional materials [32, 33, 34, 35, 36, 37], which do not meet the above condition, due to the relatively low energy of electrons in relation to the energy of phonons, or a high value the electron-phonon coupling constant. An example of a low-dimensional material in which a non-adiabatic superconducting state is induced is the Li-hBN bilayer - a system composed of two hexagonal planes consisting of boron and nitrogen atoms intercalated by lithium atoms [38]. Analysis of electron and phonon structures showed that this material has Fermi energy and Debye frequency of $\varepsilon_F = 417.58$ meV and $\omega_D = 165.56$ meV, respectively [39, 40]. The coupling between electrons and phonons reaches the value of $\lambda = 1.17$ [41]. Consequently, this leads to a high value of the Migdal dimensionless ratio: $\lambda\omega_D/\varepsilon_F \sim 0.46$. This result made me decide to investigate the non-adiabatic superconducting state of Li-hBN using the generalized isotropic Eliashberg equations available in the literature, taking into account the vertex corrections to the electron-phonon interaction in the lowest order [42]. I compared the obtained results with the the standard Eliashberg's formalism, showing that the properties of the superconducting state in this type of materials should be determined with the use of formalism explicitly taking into account the vertex corrections, due to the risk of a significant overestimation of the critical temperature [43]. Besides, I proved on the example of the discussed compound that taking into account the successive, higher orders of vertex corrections for the electron-phonon interaction is redundant due to insignificant changes in the critical temperature.

The results obtained during the analysis of the non-adiabatic superconducting state prompted me to go beyond the standard Eliashberg scheme, namely to determine the full Eliashberg equations depending on momentum and energy and taking into account the vertex corrections of the electron-phonon interaction in the lowest order. To derive the aforementioned system of equations, I used the formalism of the thermodynamic Green functions, in this case developing the Green matrix function with respect to the equations of motion of the Matsubara type in the second order. These calculations led to a coherent, self-consistent model of a non-adiabatic superconducting state, not present in the literature so far. The analysis of the presented equations shows that omitting Migdal theorem not only causes the existence of additional terms in Eliashberg equations, corresponding to taking into account the next order of vertex corrections, but also modifies the standard terms of the equations under consideration. This result was not included in the isotropic Eliashberg equations [4], which makes this result original and unconventional.

Literatura

[1] H. K. Onnes. The resistance of pure mercury at helium temperatures. *Communications Physical Laboratory of the University of Leiden*, 12:120, 1911.

[2] J. Bardeen, L. N. Cooper, and J. R. Schrieffer. Microscopic theory of superconductivity. *Physical Review*, 106:162, 1957.

[3] J. Bardeen, L. N. Cooper, and J. R. Schrieffer. Theory of superconductivity. *Physical Review*, 108:1175, 1957.

[4] G. M. Eliashberg. Interactions between electrons and lattice vibrations in a superconductor. *Soviet Physics JETP*, 11:696, 1960.

[5] E. Zurek and Y. Yao. Theoretical predictions of novel superconducting phases of $BaGe_3$ stable at atmospheric and high pressures. *Inorganic Chemistry*, 54:2875, 2015.

[6] K. A. Szewczyk, E. A. Drzazga-Szczęśniak, M. W. Jasrosik, K. M. Szczęśniak, and S. M. Binek. The characteristic of the s-wave symmetry superconducting state in $BaGe_3$ compound. *Symmetry*, 11:977, 2019.

[7] Y. Liu, X. Huang, D. Duan, F. Tian, H. Liu, D. Li, Z. Zhao, X. Sha, H. Yu, H. Zhang, B. Liu, and T. Cui. First-principles study on the structural and electronic properties of metallic HfH_2 under pressure. *Scientific Reports*, 5:11381, 2015.

[8] A. M. Duda, K. A. Szewczyk, M. W. Jarosik, K. M. Szczęśniak, M. A. Sowińska, and D. Szczęśniak. Characterization of the superconducting state in hafnium hydride under high pressure. *Physica B: Condensed Matter*, 536:275, 2018.

[9] B. Wiendlocha, J. Tobola, S. Kaprzyk, and D. Fruchart. Electronic structure, superconductivity and magnetism study of Cr_3GaN and Cr_3RhN. *Journal of Alloys and Compounds*, 442:289, 2007.

[10] H. M. Tütüncü and G. P. Srivastava. Phonons and superconductivity in the cubic perovskite Cr_3RhN. *Journal of Applied Physics*, 112:093914, 2012.

[11] K. M. Szczęśniak, R. Szczęśniak, D. Szczęśniak, K. A. Szewczyk, A. M. Duda, and I. A. Domagalska. Study of superconducting phase in cubic anti-perovskite Cr_3RhN. *Physica C*, 442:289, 2017.

[12] P. B. Allen and B. Mitrović. Theory of superconducting T_C. *Solid State Physics*, 37:1, 1993.

[13] F. Jutier, G. A. Ummarino, J.-C. Griveau, F. Wastin, E. Colineau, J. Rebizant, N. Magnani, and R. Caciuffo. Possible mechanism of superconductivity in $PuCoGa_5$ probed by self-irradiation damage. *Physical Review B*, 77:024521, 2008.

[14] M. L. Kulić. Interplay of electron–phonon interaction and strong correlations: the possible way to high-temperature superconductivity. *Physics Reports*, 338:1, 2000.

[15] E. G. Maksimov, M. L. Kulić, and O. V. Dolgov. Bosonic spectral function and the electron-phonon interaction in HTSC cuprates. *Advances in Condensed Matter Physics*, 2010:423725, 2010.

[16] P. Morel and P. W. Anderson. Calculation of the superconducting state parameters with retarded electron-phonon interaction. *Physical Review*, 125:1263, 1962.

[17] F. Marsiglio. Eliashberg theory of the critical temperature and isotope effect. Dependence on bandwidth, band-filling, and direct Coulomb repulsion. *Journal of Low Temperature Physics*, 87:659, 1992.

[18] A. B. Migdal. Interaction between electrons and lattice vibrations in a normal metal. *Soviet Physics JETP*, 34:996, 1958.

[19] K. A. Szewczyk, R. Szczęśniak, and D. Szczęśniak. Unbalanced superconductivity induced by the constant electron–phonon coupling on a square lattice. *Annalen der Physik*, 530:1800139, 2018.

[20] K. A. Szewczyk, M. W. Jarosik, A.P. Durajski, and R. Szczęśniak. The unbalanced phonon–induced superconducting state on a square lattice beyond the static boundary. *Physica B: Condensed Matter*, 600:412613, 2021.

[21] R. Combescot. Critical temperature of superconductors: Exact solution from eliashberg equations on the weak-coupling side. *Physical Review B*, 42:7810, 1990.

[22] K. S. D. Beach, R. J. Gooding, and F. Marsiglio. Reliable Padé analytical continuation method based on a high-accuracy symbolic computation algorithm. *Physical Review B*, 61:5147, 2000.

[23] O.V. Dolgov and V.V. Losyakov. Renormalization factor and odd-ω gap singlet superconductivity. *Physics Letters A*, 190:189, 1994.

[24] J. Cai, X. L. Lei, and L. M. Xie. Vertex correction to the Eliashberg equation for the superconducting critical temperature. *Physical Review B*, 39:11 618, 1989.

[25] L. Pietronero. Superconductivity mechanism in doped C_{60}. *Europhysics Letters*, 17:365, 1992.

[26] W. E. Pickett. *in Solid State Physics, edited by H. Ehrenreich and F. Spaepan.* Academic, New York, 1993.

[27] Y. J. Uemura, L. P. Le, G. M. Luke, B. J. Sternlieb, W. D. Wu, J. H. Brewer, T. M. Riseman, C. L. Seaman, M. B. Maple, M. Ishikawa, D. G. Hinks, J. D. Jorgensen, G. Saito, and H. Yamochi. Basic similarities among cuprate, bismuthate, organic, chevrel-phase, and heavy-fermion superconductors shown by penetration-depth measurements. *Physical Review Letters*, 66:2665, 1991.

[28] Y. J. Uemura, L. P. Le, G. M. Luke, B. J. Sternlieb, W. D. Wu, J. H. Brewer, T. M.

Riseman, C. L. Seaman, M. B. Maple, M. Ishikawa, D. G. Hinks, J. D. Jorgensen, G. Saito, and H. Yamochi. Basic similarities among cuprate, bismuthate, organic, chevrel-phase, and heavy-fermion superconductors shown by penetration-depth measurements [phys. rev. lett. 66, 2665 (1991)]. *Physical Review Letters*, 68:2712, 1992.

[29] N D'Ambrumenil. An unconventional family tree. *Nature*, 352:472, 1991.

[30] R. J. Wojciechowski. On the validity of the Migdal's theorem in the heavy fermion systems. *paper from: International Centre For Theoretical Physics*, 28:1, 1996.

[31] H. Goto and Y. Natsume. A theoretical approach to strong-coupling superconductivity in ultra-high fields in consideration of vertex corrections to Eliashberg-Migdal equations. *Physica B*, 216:281, 1996.

[32] G. Profeta, M. Calandra, and F. Mauri. Phonon-mediated superconductivity in graphene by lithium deposition. *Nature Physics*, 8:131, 2012.

[33] J. Pešić, R. Gajić, K. Hinger, and M. Belić. Strain-enhanced superconductivity in Li-doped graphene. *Europhysics Letters*, 108:67005, 2014.

[34] W. Wan, Y. Ge, F. Yang, and Y. Yao. Phonon-mediated superconductivity in silicene predicted by first-principles density functional calculations. *Europhysics Letters*, 104:36001, 2013.

[35] J. Liao, Y. Zhao, H. Xud, and X. Yang. Phonon-mediated superconductivity in Mg intercalated bilayer borophenes. *Physical Chemistry Chemical Physics*, 19:29237, 2017.

[36] Y. Ge, W. Wan, F. Yang, and Y. Yao. The strain effect on superconductivity in phosphorene: a first principles prediction. *New Journal of Physics*, 17:035008, 2015.

[37] D. F. Shao, W. J. Lu, H. Y. Lv, and Y. P. Sun. Electron-doped phosphorene: A potential monolayer superconductor. *Europhysics Letters*, 108:6, 2014.

[38] B. Altintas, C. Parlak, C Bozkurt, and R. Eryiğit. Intercalation of graphite and hexagonal boron nitride by lithium. *The European Physical Journal B*, 79:301, 2011.

[39] J. Wang, F. Ma, and M. Sun. Graphene, hexagonal boron nitride, and their heterostructures: properties and applications. *Royal Society of Chemistry*, 7:16801, 2017.

[40] A. Nagashima, N. Tejima, Y. Gamou, T. Kawai, and C. Oshima. Electronic structure of monolayer hexagonal boron nitride physisorbed on metal surfaces. *Physical Review Letters*, 75:3918, 1995.

[41] N. H. Shimada, E. Minamitani, and S. Watanabe. Theoretical prediction of phonon-mediated superconductivity with $T_C \approx 25$ K in Li-intercalated hexagonal boron nitride bilayer. *Applied Physics Express*, 10:093101, 2017.

[42] J. K. Freericks, E. J. Nicol, A. Y. Liu, and A. A. Quong. Vertex-corrected tunne-

ling inversion in electron-phonon mediated superconductors: Pb. *Physical Review B*, 55:11651, 1997.

[43] K. A. Szewczyk, I. A. Domagalska, A. P. Durajski, and R. Szczęśniak. Nonadiabatic superconductivity in Li-intercalated hexagonal boron nitride bilayer. *Beilstein Journal of Nanotechnology*, 11:1178, 2020.

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