Superconducting and normal properties of the low-dimensional phases of the metallic hydrogen

E A Mazur\textsuperscript{1,2}, R Sh Ikhsanov\textsuperscript{3} and M Yu Kagan\textsuperscript{3,4}

\textsuperscript{1}National Research Nuclear University MEPhI, Kashirskoe sh. 31, Moscow, Russia
\textsuperscript{2}Kurchatov Institute National Research Center, Moscow, Acad. Kurchatov sq. 1, Russia
\textsuperscript{3}National Research University Higher School of Economics, Myasnitskaya st., 20, Russia
\textsuperscript{4}P.L. Kapitza Institute for Physical Problems, Kosygin st., 2, 119334, Moscow, Russia

E-mail: mkagan@hse.ru, eugen_mazur@mail.ru

Abstract. In the first part of the paper we consider properties of a two-dimensional low density \((n = 1)\) electron system with strong onsite Hubbard attraction \(U > W\) (\(W\) is the bandwidth) in the presence of a strong random potential \(V\) uniformly distributed in the range from \(-V\) to \(+V\). In the framework of the Bogoliubov-de Gennes approach we observed an appearance of inhomogeneous state of spatially separated Fermi-Bose mixture of Cooper pairs and unpaired electrons with the formation of bosonic droplets of different size in the unpaired fermionic matrix. Software package to solve the system of Eliashberg equations that describes the transition of a metal to a superconducting state is presented. We use a version of the Eliashberg system of equations written on the imaginary axis. The system is presented in two versions: without taking into account the corrections for the chemical potential of electrons and with taking them into account. The calculations were performed for the I41/amd phase of metallic hydrogen at a pressure of 500 GPa.

1. Introduction

Attractive-U Hubbard model while being very successful [1-4] for analyzing different electronic systems with strong local attraction still has its drawbacks connected with the absence of frequency dispersion and retardation effects in it. The simplest model which catches these effects is the Migdal-Eliashberg model for strong coupling electron-phonon (or more generally electron-boson) superconductivity. The first convincing results in the framework of this model in connection with superconductivity in low-dimensional phases of metallic hydrogen belong to the group of one of the authors of the present paper [5-11]. Note that in the experimental situation [12], hydrides, as well as metallic hydrogen, are synthesized by compression to high pressures, which entails the appearance of regions with a spatially distributed strong random potential. Thus, it is very important to generalize the results of [5-11] on the inhomogeneous case and the presence of impurities [8]. In the present article, we consider two-dimensional attractive-U Hubbard model for an s-wave superconductor at low temperatures \(T\) in a strong random potential [13-14] and analyze this model in detail in the framework of the Bogoliubov-de Gennes (BdG) approach, taking into account both the solutions with positive energy values \(E_n\) and the solutions with negative values of the energy of the electronic system [15]. Our goal is to observe...
how the amplitude of local pairing $\Delta(r)$ changes spatially in the presence of disorder in the parameter ranges which have not been analyzed and correspond to strong Hubbard interaction $|U| > W$ and strong diagonal disorder $V > W$ at low electron densities $n = 0.125 - 0.3$. We also pursue a goal to study the effect of spatial inhomogeneities [16-18] on physically relevant correlation functions.

In the second part of the article, we present the first results on the Eliashberg superconductivity for homogeneous (until now) metallic hydrogen based on the system of equations on the imaginary axis. The Eliashberg approach for the inhomogeneous case will be a subject of future investigations.

### 2. Equations for inhomogeneous case and formulation of the model

We consider two-dimensional Hubbard model for an s-wave type disordered superconductor with a short range (onsite) attraction between carriers, described by the Hamiltonian:

$$H = -t \sum_{i,j,\sigma} \langle c_{j,\sigma}^+ c_{i,\sigma} + h.c. \rangle - |U| \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_i \left( V_i - \mu \right) n_{i\sigma}. \tag{1}$$

Here, the first term describes kinetic energy, where $t$ corresponds to hoppings to the neighboring sites of the square lattice, $U = -|U|$ is the amplitude of the Hubbard attractive potential at one site ($U < 0$), $c_{i\sigma}^+$ ($c_{i\sigma}$) are the creation (annihilation) operators for an electron with spin $\sigma$ at the square lattice site $i$, $n_{i\sigma}$ is the local electron density at site $i$ for one component of the spin and $\mu$ is the chemical potential. The random potential $V_i$ is selected independently for each site and is governed by a uniform distribution in the range $[-V,V]$. Thus, $V$ controls the intensity of diagonal disorder in the system. Introducing the Hartree-Fock shift of the chemical potential $\mu_i = \mu - |U| n_{i\sigma}(r)/2$, which depends on site $i$, we write the BdG equations for the Bogoliubov functions $u_n(r)$, $v_n(r)$ participating in pairing [14]. Namely

$$t \sum_{k} \begin{cases} u_n(r_i \pm \hat{x}, \pm \hat{y}) + (V_i - \mu_i) u_n(r_i) + \Delta_i v_n(r_i) = E_n u_n(r_i) \\ \Delta_i u_n(r_i) + t \sum_k v_n(r_i \pm \hat{x}, \pm \hat{y}) - (V_i - \mu_i) v_n(r_i) = E_n v_n(r_i) \end{cases}, \tag{2}$$

At the same time the pairing potential $\Delta_i$ at the site $r_i$ appearing in system (2), reads [14]:

$$\Delta_i = \Delta(r_i) = |U| \sum_n \langle u_n(r_i)^* v_n(r_i) (1 - 2 f_n) \rangle.$$

Here $E_n$ are the excitation energies in the system, $\mu$ is the chemical potential in the presence of a random diagonal disorder $V$, $U(r_i)$ is the mean-field potential at the site $r_i$ [4]. To take correctly into account both the pairing potential and chemical potential $\mu$ in the system, which requires taking into account states below the Fermi level, we will keep the solutions of the system (2) with both positive energy values $E_n$ and solutions with negative values of the energy of the electronic system, $f_n = 1/\left[ \exp(E_n/kT) + 1 \right]$ is the Fermi-Dirac distribution function for a given value of the excitation energy $E_n$. The chemical potential $\mu$ is determined from the self-consistency condition for the density of particles $n$ (which corresponds to the average number of electrons per site). We can effectively write down the normalization condition in the standard form $\sum_n |u_n(r_i)|^2 + \sum_n |v_n(r_i)|^2 = 1$. In (2) and (3), in addition to the random potential $V_i$, the mean-field potential $U(r_i)$ at the site $r_i$ is included [13]. This yields

$$U_i = U(r_i) = |U| \sum_n \left[ |u_n(r_i)|^2 f_n + |v_n(r_i)|^2 (1 - f_n) \right].$$
3. Calculations for a high degree of disorder in the range of electron concentration from low $n=0.15$ to average values $n=0.32$

This section presents the results of the calculations in the range of electron densities from low $n = 0.15$ to moderate values $n = 0.30$ for the disorder amplitude of $V = 8\tau$ and Hubbard amplitude $|U| = 6\tau$ for a lattice with $24 \times 24$ sites.

Figure 1. Two-dimensional distribution of electron density (left column) and order parameter (right column) for $n = 0.11$, $|U|/t = 6$ on a $24 \times 24$ lattice with a disorder amplitude of $V/t = 8$ (left pair of figures), for $n = 0.17$, $|U|/t = 6$, on a $24 \times 24$ lattice with a disorder amplitude of $V/t = 8$ (right pair of figures).

Figure 2. Two-dimensional distribution of electron density (left column) and order parameter (right column) for $n = 0.30$, $|U|/t = 6$, on a $24 \times 24$ lattice with a disorder amplitude of $V/t = 8$.

As we can see, for the density $n = 0.11$, single pairs or doubled pairs of electrons (quartets) are observed on adjacent cells (figure 1), while at $n = 0.17-0.30$, larger droplets of the order parameter are observed (figures 1-2). Droplets of the order parameter merge into the network of chains resembling the percolating cluster in the form of the tree with a lot of branches (figure 2), which practically do not experience discontinuities along their length.

4. Software tools for the solution of Eliashberg system of equations

We have developed software tools for solving the electron-phonon theory basic equations written on the imaginary axis for isotropic superconductors. For a selected superconductor, the program calculates the superconducting transition temperature $T_c$ and several properties of the superconductor [19]:

- $\xi$ – the electron-phonon mass enhancement parameter,
- $\gamma$ – the Sommerfeld constant,
- $\omega_n$ – the characteristic phonon frequency,
- $\Delta(0)$ – the energy gap at $T = 0\ K$,
- $H_c(0)$ – the upper critical magnetic field at $T = 0\ K$,
- $\Delta C(T_c)$ – discontinuity jump of heat capacity at $T = T_c$,
- $\beta$ – the isotope coefficient.

In this work Eliashberg system of equations is written for a set of dependent variables $\{\varphi_n, Z_n, \chi_n\}_{n=0}^M$ (independent ones are $\{\omega_n\}_{n=0}^M$), where $M$ is the maximum number of the Matsubara
frequencies, $\omega_n = \pi k_n T (2n + 1)$, $n \in [0, M]$, the Matsubara frequencies, $\varphi$ is the order parameter, $Z$ is the electron mass renormalization function, and $\chi$ is the shift of the chemical potential of electrons. The system looks as follows:

$$
\begin{align*}
\varphi_n &= \frac{\pi}{\beta T} \sum_{m=0}^{M} \left\{ \lambda_{nm}^{(1)} - 2\mu^* \theta(\omega_c - \omega_m) \right\} \varphi_m \cdot N_m(\varphi_m, Z_m, \chi_m), \\
Z_n &= 1 + \frac{1}{\beta T} \sum_{m=0}^{M} \lambda_{nm}^{(1)} \omega_m Z_m \cdot N_m(\varphi_m, Z_m, \chi_m), \\
\chi_n &= -\frac{\pi}{\beta T} \sum_{m=0}^{M} \left\{ \lambda_{nm}^{(1)} - 2\mu^* \theta(\omega_c - \omega_m) \right\} \cdot P_m(\varphi_m, Z_m, \chi_m) e_m(\varphi_m, Z_m),
\end{align*}
$$

where $\beta T = 1/k_B T$, $T$ – the absolute temperature, $k_B$ – the Boltzmann constant, $\mu^*$ – the effective Coulomb repulsion, $\theta(\omega)$ – the Heaviside step function, $\omega_c$ – the cutoff frequency, $\lambda_{nm}^{(1)} = \lambda (n - m) \pm \lambda (n + m + 1)$, $\lambda(n) = 2 \int_{0}^{\infty} \frac{\omega \cdot \alpha^2 F(\omega)}{\omega^2 + (2\pi nk_B T)^2} d\omega$; $\alpha^2 F(\omega)$ – the electron-phonon spectral function; $\omega_D$ – the Debye frequency, $N_m(\varphi, Z, \chi) = \pi^{-1} \int_{\infty}^{\infty} \frac{N_0(E)}{(E + \chi^2 + Z^2 \omega_c^2 + \varphi^2)} dE$, $N_0(E)$ – the single-spin density of electronic states, $\mu$ – the chemical potential of electrons; $P_m(\varphi, Z, \chi) = \pi^{-1} \int_{\mu}^{\infty} \frac{N_0(E)}{(E + \chi^2 + Z^2 \omega_c^2 + \varphi^2)} dE$, $e_m(\varphi, Z) = \frac{\omega_c Z}{\sqrt{\omega_c^2 Z^2 + \varphi^2}}$. The superconducting transition temperature $T_c$ is determined as the temperature at which the value of $\Delta_0 = \varphi(\omega_0)/Z(\omega_0)$ goes to zero.

We also present the results of calculations performed for the liquid phase of metallic hydrogen under a pressure of 500 GPa [5] for the following parameters values: $\mu = \mu^* = 0.1$, $\mu = 6.8$ eV, $\omega_c = 0.34$ eV. The results are the following: $T_c = 221$ K, $\zeta = 1.68$, $\gamma = 10.2$ mV/(mole K²), $\Delta_0 = 0.122$ eV, $\psi(0) = 42.5$ meV, $H_e(0) = 61.8$ T, $\Delta C(T_c) = 6.36$ J/(mole K), $\beta = 0.487$.

Until now we considered the system of Eliashberg equations in the homogeneous case. Homogeneous impurity distribution in the superconductor and its influence on the critical temperature within the Eliashberg scheme was considered in [8] by Grebenyev and Mazur. There are two possible approaches for inhomogeneous or granular alloys. One of them can be connected with the compressibility analysis in the equation for the number of particles conservation (one of the equations of the system). Namely, the negative regions of the inverse compressibility $dN / d\mu < 0$ ($\mu$ is a chemical potential) will correspond to the instability of the homogeneous case towards the formation of superconducting (SC) droplets with the nonzero order parameter in the insulating matrix.

Another approach can be connected with the granular case as a starting point for the Eliashberg analysis. Here the first step is to calculate the Eliashberg critical temperature for the finite size granule (for the SC droplet) and then to account for the coherence between granules. We plan to pursue both approaches in an upcoming study.

5. Conclusions

As the disorder grows, the spatial distribution of the local pairing amplitude $\Delta(r)$ first takes the form of individual droplets and then takes the form of individual pairs. Our results show, that when we increase the density, at first the transition from single electron pairs to larger droplets (containing a larger number of pairs) takes place. We can say that effectively we consider here the spatially separated Fermi-Bose mixture with the clusters of (bosonic) paired electron states embedded in the matrix of
unpaired fermionic states [16]. And finally, a large percolating network of paired chains is formed in our system manifesting percolative phase-transition from granular to SC state.

As a natural generalization of the results presented in the second part of our article, we plan to extend our scheme for the Eliashberg equations to take into account coherently the effects of impurities [8], multiband nature of the investigated compounds [20, 21], and the possibility of the formation of the inhomogeneous states (droplets formation in them) especially close to the first-order phase transition between liquid and crystalline metallic hydrogen. The solution of Eliashberg equations in the presence of inhomogeneities will enrich the results based on Bogoliubov-de Gennes equations for dirty superconductors. Beyond the Eliashberg approach, we plan to account also for the quantum nature of properties of the ionic (proton) component and the possibility for the formation of two Bose-condensates in the system – the first one being the Bose condensate of the Cooper pairs embedded in the electron component and the second one – a biproton Bose condensate (as in neutron stars) in an ionic component [22, 23].

Acknowledgments
This work was supported by the Competitiveness Enhancement Project of NRNU MEPhI (contract No. 02.a03.21.0005, 08.27.2013) using the equipment of the collective use center “Complex for modeling and processing data from research facilities of the mega-class” SIC “Kurchatov Institute” (subsidy of the Ministry of Education and Science, work identifier RFMEFI62117X0016), http://ckp.nrcki.ru/. M.Yu.K. thanks for the support HSE Program of Basic Research and expresses his gratitude to the RFBR fund (grant N20-02-00015).

References
[1] Kagan M. Yu. 2013 Modern Trends in Superconductivity and Superfluidity, Lecture Notes in Phys., v. 874 (Springer, Dordrecht)
[2] Kagan M.Yu., Frésard R., Capezzali M. and Beck H. 1998 Phys.Rev. B 57 5995
[3] Kagan M.Yu., Frésard R., Capezzali M. and Beck H. 2000 Physica B 284-288 347
[4] Kagan M.Yu. 2016 Pis’ma v ZHETP 103 822
[5] Kudryashov N.A., Kutukov A.A. and Mazur E.A. 2016 JETP letters 104 460
[6] Degtyarenko N.N., Mazur E.A. and Grishakov K.S. 2017 JETP Letters 105 664
[7] Degtyarenko N.N. and Mazur E.A. 2016 JETP letters 104(5) 319
[8] Grebenev V.N. and Mazur E.A. 1987 Fizika Nizkikh Temperatur 13(5) 478
[9] Degtyarenko N.N., Mazur E.A. and Grishakov K.S. 2017 Solid State Communications 262 33
[10] Degtyarenko N.N. and Mazur E.A. 2018 Journal of Physics: Conference Series 941(1) 012060
[11] Kudryashov N.A., Kutukov A.A. and Mazur E.A. 2017 JETP Letters 105(7) 430
[12] Pickard Chris J., Errea I. and Eremets M.I. 2020 Annual Review of Condensed Matter Physics 11
[13] Kagan M.Yu. and Mazur E.A. 2021 JETP 132(4) 596
[14] Kagan M.Yu. and Mazur E.A. 2021 J. Phys.: Conf. Ser. 1740 012045
[15] De Genes P.-J. 1966 Superconductivity of metals and alloys (Benjamin, New York)
[16] Kagan M.Yu., Menushenkov A.P., Kuznetsov A.V. and Klement’ev K.V. 2001 JETP 93 615
[17] Kagan M. Yu., Kugel K.I. and Rakhmanov A.L. 2021 Physics Reports 916 1
[18] Kagan M.Yu. and Kugel K.I. 2001 Physics Uspekhi 171 577
[19] Carbotte J.P. and Marsiglio F. 2008 Superconductivity (Springer, Berlin, Heidelberg) 73
[20] Mazur E.A. and Dubovik V.M. 2015 The European Physical Journal B 88(6) 150
[21] Mazur E.A. and Dubovik V.M. 2015 JETP letters 101(8) 549
[22] Kagan M.Yu. 2016 Pis’ma v ZHETP 103 822
[23] Kagan M.Yu. and Bianconi A. 2019 Condens Matter (Switzerland) 4 51