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A note on the possible mechanisms of high-temperature superconductivity

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Abstract. Possible mechanisms of high-temperature superconductivity are briefly discussed. In particular, a recent paper by P W Anderson on this problem is criticized as containing a number of incorrect and unfounded statements. One of these — that the static dielectric function $\varepsilon(\mathbf{q}, 0)$ cannot be negative — is discussed in detail, as is its consequence, a strong limit on the transition temperature T_c. Proofs are given that $\varepsilon(\mathbf{q}, 0)$ not only can but indeed must be negative in many stable systems, including most of the conventional metals. Various types of electron – electron interaction in superconducting cuprates are discussed. The role of the electron – phonon interaction in cuprates is highlighted.

Since the publication of paper [1] by Bardeen, Cooper, and Schrieffer (BCS), most physicists have come to believe that the superconducting state is due to the electron (Cooper) pairs that occur near the Fermi surface and form a correlated system somewhat similar to the Bose condensate. For two electrons to form a Cooper pair, an attractive force between them is needed. The BCS paper implies that the electrons are 'glued' together in pairs by the attractive force due to the electron – phonon interaction (EPI). The BCS theory, as well as the more detailed description of the EPI given by Eliashberg [2], shows that a critical temperature of superconducting transition T_c can be expressed as

$$T_c \sim \omega_{ph} \exp\left(-\frac{1}{\lambda}\right). \tag{1}$$

Here, ω_{ph} is an average phonon frequency and λ is the electron – phonon coupling constant. According to formula (1), a relatively low T_c in standard superconducting metals is explained by the smallness of both the prefactor, that is the average phonon frequency, and the EPI constant λ.

In the 1960s and 1970s, after the publication of papers by Ginzburg [3] and Little [4], several (mostly theoretical) attempts were made to involve a higher-energy 'glue' into the superconductivity mechanism for the Cooper pairs to form. For some metallic systems, excitons, plasmons, and a number of other electron excitations with energies considerably higher than the phonon frequencies have been proposed as such a glue (see Ref. [5]).

Recently, P W Anderson has published the paper "Is There Glue in Cuprate Superconductors?" [6], in which he has questioned the existence of any glue responsible for the pairing of electrons. In our opinion, this paper contains a number of inaccurate and ungrounded statements. One of these is related to an old discussion between Anderson and a group of theorists at the Lebedev Physical Institute. It concerns the possible sign of static dielectric constant. Previously, Cohen and Anderson used the simple expression for the electron – electron interaction in metals [7]:

$$V(\mathbf{q}, \omega) = \frac{4\pi e^2}{q^2 \varepsilon_{tot}(\mathbf{q}, \omega)}, \tag{2}$$

where $\varepsilon_{tot}(\mathbf{q}, \omega)$ is the momentum- and frequency-dependent total dielectric function of the metal. This function includes a screening due to the Coulomb electron – electron interaction and a contribution of the electron – phonon interaction. The authors of Ref. [7] considered the positivity of the static dielectric constant

$$\varepsilon_{tot}(\mathbf{q}, 0) > 0 \tag{3}$$

as a condition for system stability. They demonstrated that inequality (3) results in a strong limitation on possible values of the critical temperature of superconducting transition T_c. This limitation is due to the interrelation between the Coulomb repulsion constant μ and the electron – phonon coupling constant λ, which can be written as

$$\mu - \lambda = \int d\mathbf{q} \, \frac{4\pi e^2}{q^2 \varepsilon_{tot}(\mathbf{q}, 0)}. \tag{4}$$

It follows from formulas (3) and (4) that

$$\mu > \lambda. \tag{5}$$

Formula (5) means that in this case an effective electron – electron interaction responsible for superconductivity would be repulsive and superconductivity cannot occur in such a system.

Tolmachev has shown [8] that because of electron rescattering at high energies, a renormalization of the Coulomb repulsion occurs, which leads to its 'pseudization', i.e., to the replacement of the constant μ with a Coulomb pseudopotential μ^*, and to a noticeable decrease in the Coulomb repulsion

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contribution to the superconducting pairing:

$$\mu^* = \frac{\mu}{1 + \mu \ln(\varepsilon_F/\omega_{ph})}\,, \tag{6}$$

where ε_F is the Fermi energy. Thus, the effective interaction can become attractive, $\lambda - \mu^* > 0$. The term $\lambda - \mu^*$ appears in various approximate expressions for T_c. For instance, in a simple approximation, the constant λ in exponent (1) can be replaced with $\lambda - \mu^*$. In this case, the maximum value of T_c^{max}, as follows from expressions (1)–(6), satisfies the inequality

$$T_c^{max} \lesssim \varepsilon_F \exp\left(-\frac{1}{\lambda}\right) \lesssim 10\ \text{K}\ (!)$$

even at $\lambda = \mu$. The above arguments are mostly repeated in paper [6], where, as in the earlier paper [7], the electron–phonon (as any other) glue is stated to be ineffective for electron pairing. Furthermore, according to Anderson, the concept of a specific glue binding the Cooper pairs even in conventional superconductors is nothing more than 'folklore': one can equally well believe the Cooper pairs occur because of electron–phonon attraction or the Coulomb repulsion pseudization.

Kirzhnits has strictly proved [5] that inequality (3) has nothing to do with the stability condition of the system, since the function $\varepsilon_{tot}(\mathbf{q}, \omega)$ is not a response to an external action. The stability condition imposes a limitation on the inverse dielectric constant:

$$\frac{1}{\varepsilon_{tot}(\mathbf{q}, 0)} \leqslant 1\,. \tag{7}$$

This inequality is fulfilled if either of the following inequalities is valid: $\varepsilon_{tot}(\mathbf{q}, 0) > 1$ or $\varepsilon_{tot}(\mathbf{q}, 0) < 0$, i.e., negative values of the dielectric constant are acceptable in stable systems.

We discussed the sign problem in detail in our review [9]. Here, in order to solve at least this issue once and for all, we briefly repeat our previous results that demonstrate the existence of negative values of $\varepsilon(\mathbf{q}, 0)$ in many simple systems just in their stability region. One of simple systems with $\varepsilon(\mathbf{q}, 0)$ negative at any momentum $\mathbf{q}$ is the Wigner crystal. The dielectric function $\varepsilon(\mathbf{q}, \omega)$ of the classical Wigner crystal has been thoroughly considered by Bagchi [10], who showed that

$$\frac{1}{\varepsilon(\mathbf{q}, \omega)} = 1 - \frac{\omega_{pl}^2}{q^2} \sum_{\nu} \frac{(\mathbf{q}\mathbf{e}_{\mathbf{q}\nu})^2}{\omega^2(\mathbf{q}, \nu) - \omega^2}\,. \tag{8}$$

Here, ω_{pl} is the plasma frequency of charged particles

$$\omega_{pl}^2 = \frac{4\pi n e^2}{m}\,, \tag{9}$$

where m and n are the mass and density of the particles, respectively, $\mathbf{e}_{\mathbf{q}\nu}$ is the polarization vector of phonons, and $\omega(\mathbf{q}, \nu)$ is the phonon frequency.

A cubic Wigner crystal with one atom per unit cell possesses three phonon modes, two transversal modes with acoustic dispersions at small $\mathbf{q}$ vectors and one longitudinal mode whose frequency $\omega(\mathbf{q}, \nu)$ approaches ω_{pl} at $q \to 0$. The sum rule

$$\sum_{\nu} \omega^2(\mathbf{q}, \nu) = \omega_{pl}^2 \tag{10}$$

is valid for those frequencies. In the static case, expression (8) can be rewritten as

$$\frac{1}{\varepsilon(\mathbf{q}, 0)} = \sum_{\nu} \left\{ (\mathbf{n}\mathbf{e}_{\mathbf{q}\nu})^2 \left[1 - \frac{\omega_{pl}^2}{\omega^2(\mathbf{q}, \nu)}\right]\right\}, \tag{11}$$

where $\mathbf{n} = \mathbf{q}/|q|$. Here, we took into account that

$$\sum_{\nu} (\mathbf{n}\mathbf{e}_{\mathbf{q}\nu})^2 = 1\,. \tag{12}$$

Taking into account the sum rule (10), one can easily see that the right-hand side of expression (11) is always negative at any $\mathbf{q}$ vector. Notice that, according to expression (11), the inequality $\varepsilon(\mathbf{q}, 0) < 0$ is valid just in the stable phase of the Wigner crystal, where all the quantities $\omega^2(\mathbf{q}, \nu)$ are positively defined, i.e., $\omega^2(\mathbf{q}, \nu) > 0$.

It follows from the above that in the Wigner crystal, the negative values of $\varepsilon(\mathbf{q}, 0)$ occur because the single mode of the plasma oscillations, which exists in gaseous and liquid states, is split into three modes in the solid state. This is due to the localization of charges and strong local-field effects in the crystal. Furthermore, as has been shown in Ref. [11], the negative values of $\varepsilon(\mathbf{q}, 0)$ occur in the classical one-component plasma if the interaction parameter $\Gamma = e^2/aT$ [here, $a = (4n/3)^{-1/3}$] is considerably smaller than its value $\Gamma \approx 170$ at which the Wigner crystallization takes place. As is shown in paper [11], the static dielectric function $\varepsilon(\mathbf{q}, 0)$ is negative virtually at all $\mathbf{q}$ vectors in the density range corresponding to $\Gamma > 40$. It is intriguing that at $\Gamma > 40$ the plasma oscillations have a negative dispersion $\omega_{pl}^2(\mathbf{q}) = \omega_{pl}^2(0) - \alpha q^2$ and a finite linewidth. It is also shown in Ref. [11] that the negative values of $\varepsilon_{tot}(\mathbf{q}, 0)$ exist not only in model systems, but also in real systems, e.g., in melted table salt.

The above-considered systems possessing the negative static dielectric function $\varepsilon(\mathbf{q}, 0)$ have, of course, nothing to do with high-temperature superconductivity (HTSC) and with superconductivity in general. Within the 'folklore' approach, the negative values of $\varepsilon(\mathbf{q}, 0)$ ensure that the inequality $\lambda > \mu$ is fulfilled, which favors high T_c values. Expression (2), however, can be applied as it is only for a hypothetical highly-compressed metal where the Coulomb interaction parameter r_s satisfies the condition $r_s \ll 1$. Here, $r_s = (3n/4\pi a_B^3)^{1/3}$, and n and a_B are the density and the Bohr radius of the electrons, respectively. In this case, the dielectric function $\varepsilon_{tot}(\mathbf{q}, 0)$ can be written in the form [5, 9]

$$\frac{1}{\varepsilon_{tot}(\mathbf{q}, 0)} = \frac{4\pi e^2}{q^2 \varepsilon_{el}(\mathbf{q}, 0)} \sum_{\nu} \left\{ (\mathbf{n}\mathbf{e}_{\mathbf{q}\nu})^2 \left[1 - \frac{\omega_{Je}^2(\mathbf{q})}{\omega^2(\mathbf{q}, \nu)}\right]\right\}. \tag{13}$$

Here, $\varepsilon_{el}(\mathbf{q}, 0)$ is the static dielectric function of the electron gas, which can be expressed within the random phase approximation as

$$\varepsilon_{el}(\mathbf{q}, 0) = 1 + \frac{\chi^2}{q^2}\,, \tag{14}$$

$\omega(\mathbf{q}, \nu)$ is the phonon frequency, and $\omega_{Je}(\mathbf{q})$ is the plasma frequency of the jelly-like model:

$$\omega_{Je}^2(\mathbf{q}) = \frac{\omega_{pl}^2}{\varepsilon_{el}(\mathbf{q}, 0)}\,. \tag{15}$$

It is straightforward to show [5, 9] that for a stable phase of the highly-compressed metal the inequality

$$\omega_{\mathrm{Je}}(\mathbf{q}) \geqslant \omega(\mathbf{q}, v) \tag{16}$$

is valid. This inequality guarantees that the static dielectric function of highly-compressed metal is negative at all $\mathbf{q}$ vectors and the inequality $\lambda - \mu > 0$ is satisfied, hence, such metal is superconducting. Certainly, at $r_s \ll 1$ the EPI constant λ is small and T_c is low, but this does not cancel the fact that in this system the total static dielectric function is negative at any $\mathbf{q}$ vector and superconductivity is due to the EPI. Surprisingly, paper [7] contains the expression for the electron–electron interaction and the inverse dielectric constant, which is very close to formula (13). This means that the authors of Ref. [7] have actually given an example of a system with a negative dielectric constant, but overlooked this fact and have yet to notice it. In our early paper [12] the function $\varepsilon_{\mathrm{tot}}(\mathbf{q}, 0)$ was calculated for a few simple metals (K, Al, Pb) and for hypothetical metallic hydrogen. We demonstrated [12] that in potassium $\varepsilon_{\mathrm{tot}}(\mathbf{q}, 0)$ is positive at any $\mathbf{q}$ vector, while in lead and metallic hydrogen it is negative for all $\mathbf{q}$.

Even for many conventional metals the electron–electron interaction that describes the superconducting state has a more complex form than formula (2) [5]. The main challenge here is the successive calculation of the contribution of Coulomb interaction μ to the effective electron–electron interaction. As for the electron–phonon coupling constant λ, there are highly efficient density-functional methods (see, e.g., [13, 14]) for calculating λ, at least for conventional metals. Numerous calculations and tunneling measurements show that in many conventional metals and their compounds, $\lambda \gtrsim 1$. Moreover, as has been shown in Ref. [15], the coupling constant λ in metallic hydrogen can reach a value of about 6. In all these metals, the relation $\lambda \gtrsim 1$ is valid at average electron densities corresponding to $r_s \approx 1$. In a homogeneous electron gas at $r_s < 1$, the Coulomb electron–electron interaction constant μ can be written as [5]

$$\mu = \frac{r_s}{2\pi} . \tag{17}$$

This means that even at $r_s \approx 1$, the inequality $\mu < 1$ is still valid. We notice that the maximum value of μ, as is said in Ref. [7], does not exceed $1/2$. In conventional metals, the Coulomb electron–electron interaction is only weakly affected by the crystal lattice. This is evident, for example, from the good coincidence of the electron plasma energy in a homogeneous electron gas and in a conventional metal with the same average electron density. In addition, the dispersion of plasma oscillations in the both systems is positive:

$$\omega_{\mathrm{pl}}^2(\mathbf{q}) = \omega_{\mathrm{pl}}^2(0) + \alpha q^2 , \tag{18}$$

where $\alpha > 0$.

Contrary to the Coulomb electron–electron interaction, the EPI in crystals is essentially different from the case of a simple homogeneous jelly-like model. In such a model, both the electron–electron and electron–phonon interactions are defined by the ordinary Coulomb interaction, hence $\lambda \approx \mu$, which is easy to understand from formulas (4) and (11), considering that the jelly-like model assumes the single phonon mode with $\omega(\mathbf{q}, v) = \omega_{\mathrm{Je}}(\mathbf{q})$. In the simple approximation, the EPI constant for a standard metal can be expressed as [5]

$$\lambda = \frac{3.01}{r_s} \overline{V_{\mathrm{ie}}^2}(\mathbf{q}) \left\langle \frac{\Omega_{\mathrm{pl}}^2}{\omega^2} \right\rangle . \tag{19}$$

Here, $\overline{V_{\mathrm{ie}}^2}(\mathbf{q})$ is the average square of the electron–ion pseudopotential, ω is the phonon frequency, and Ω_{pl} is the ion plasma frequency:

$$\Omega_{\mathrm{pl}}^2 = \frac{4\pi N Z^2 e^2}{M} . \tag{20}$$

The average phonon frequencies in metals are considerably lower than the ion plasma frequency. This results in relatively high values of λ as compared to μ. As is noticed above, the reason for this is correlations and local-field effects in the ion system, as well as an additional (relative to the Wigner crystal) screening of ion vibration frequencies by the conduction electrons. In many cases, for instance in alkali metals, the smallness of the average square of the electron–ion pseudopotential $\overline{V_{\mathrm{ie}}^2}(\mathbf{q})$ is an essential factor that lowers the coupling constant λ.

It follows from our analysis that the static dielectric constant not only can be negative, but must necessarily be negative in a number of systems, namely in their stable state. In some model metallic systems, for example, in highly-compressed metals with $r_s \ll 1$, the EPI constant λ certainly exceeds the Coulomb electron–electron interaction constant μ. There are, however, less rigorous, but quite plausible, arguments [5, 9, 14, 16] in favor of the fact that in many conventional metals, λ is actually larger than μ and the pseudization of Coulomb contribution, i.e., the conversion μ to μ^* is not important for the existence of the superconducting state.

Recently, after the discovery [17] of superconductivity with $T_c \approx 40$ K in MgB_2, great interest has been shown in searching for new superconductors with strong EPI and relatively high T_c. In this regard, compounds of metals with light elements hold much promise. Besides borides, these are hydrides [18, 19], as well as carbides and nitrides [20]. Such compounds exhibit high frequencies $\omega_{\mathrm{op}} \sim 1/M^{1/2}$ (M is the atomic mass) of the optical phonons, associated with vibrations of the light atoms H, B, C, and N, which leads to a high value of prefactor in expression (1) for T_c. It is this fact that accounts for the high critical temperature of MgB_2, since the coupling between electrons and the optical vibrations of light boron atoms mainly contribute to the occurrence of its superconducting state [21–23]. For a high T_c value to be realized, not only high phonon frequencies, but also large coupling constants between electrons and these phonons are needed. Recently, in order to study this problem, a quantum-mechanical analysis has been performed of the possibility of high λ values being reached in hydrides [19] and carbides [20]. There are also the studies [24–26] of how the strong EPI affects the phonon spectra of metals, namely, the authors of Refs [24–26] have considered the possibility of the existence of large λ together with relatively high phonon frequencies, as well as the role of lattice instability in such systems. This problem is far from new. It had been repeatedly discussed earlier (see, e.g., Refs [5, 16]). In the new studies [20, 24–26] a more rigorous treatment at the quantitative level is given; nevertheless, these papers theoretically predict the possibility of increasing T_c up to 50–200 K in superconductors with a strong EPI. Noteworthy are papers [16, 27], in which the EPI

role is discussed in detail not only for hypothetical HTSC compounds, but also for real superconducting cuprates.

In this respect we are doubtful of some other statements in paper [6], which concern the nature of superconductivity in HTSC-cuprates. In particular, we mean classifying the interactions in superconducting cuprates into 'mammoths, elephants, and mice' in Ref. [6]. The EPI and the electron coupling with low-energy spin excitations are deemed 'mice'. Based on describing cuprates within the Hubbard model, Andersen believes that the electron repulsive interaction U at one site is the strongest and considers it a 'mammoth'. In the framework of this model, an attractive exchange interaction with the coupling constant J occurs between the electrons at neighboring sites. Within a first-order perturbation theory in $1/U$, the constant $J \sim t^2/U$, where t is the overlap integral. This exchange interaction is designated as an 'elephant' in Ref. [6]. The total potential of electron–electron interaction, which occurs if only U and J are taken into account, is represented as a strong short-range repulsion of electrons (at one site) and a long-range attraction (at neighboring sites). It is similar to potentials in the nuclear matter and in He^3. More than four decades ago, superfluidity in these systems was considered [28, 29] and the Cooper pairing of Fermi particles was shown to occur not in the isotropic s-channel, but in the p- or d-channel, depending on the pair spin structure. Generally speaking, it is widely believed (and, perhaps, with some justice) that the Cooper pairs in superconducting cuprates are just of a d-character. On this basis Anderson proposes not to take an interest in the role played by the remaining 'mice' in cuprates, because, in his opinion, superconductivity can be considered within the $t-J$ model, taking into account only the repulsion of electrons at one site and their exchange attraction at neighboring sites.

Indeed, the exchange attraction is sufficient for the antiferromagnetic ordering of spins. In the framework of the simple Hubbard model, only with the repulsion of electrons at one site, the attractive exchange interaction is also sufficient for the superconducting state to occur, although discussions on possible T_c values within this model continue [30]. In reality, however, there is also the Coulomb repulsion of electrons at neighboring sites. As the ARPES measurements [31] show, holes in the CuO_2-plane form, at least for optimally doped samples, a system of strongly interacting Fermi particles. In all likelihood, this system is impossible to describe as a Fermi gas of weakly interacting quasi-particles. As is well known, in a system of strongly interacting Coulomb particles the interaction between them at average distances is comparable, in the order of magnitude, to their kinetic energy. Thus, the Coulomb repulsion between holes at neighboring sites $V \sim t$, i.e., it is much stronger than the exchange interaction. Of course, there is no reason for V to be considerably less than t. We do not know any publications indicating such a reason. Certainly, in a uniform and isotropic system of Fermi particles the d-pairing is unaffected by the s-component of the direct Coulomb repulsion, but this is hardly valid for the Hubbard model accounting for the Coulomb interaction at neighboring sites. In particular, evidence is given by the calculation of superconductivity within the $t-J-V$ model, which shows [30] that in this case a tendency for the superconducting state to form is significantly weakened because the Coulomb repulsion V at neighboring sites is taken into account. Similarly, there is no reason for the EPI in cuprates to be considerably weaker than the exchange interaction or the direct Coulomb repulsion at neighboring sites. The available first-principles calculations of the EPI in cuprates give contradictory results on the EPI constant value, but they produce no indication that the EPI is weaker than the exchange interaction (see Ref. [16]). Furthermore, there is strong evidence that the EPI in cuprates is strong and should be accounted for in the construction of any consistent theory for these systems [16, 32, 33].

Doubts are also cast upon Anderson's attempt to relate low-energy peculiarities in the electron spectra of high-T_c materials to the strong electron scattering caused by large Hubbard repulsion U. The issue here is the existence of so-called 'kinks' in the single-particle excitation spectra of cuprates at 0.03 – 0.09 eV. These peculiarities are usually ascribed to electron coupling with bosonic modes. As follows from the ARPES experiments [31] and optical measurements [34], the coupling constants of electrons with these modes are not small, they are of the order of unity. The physical nature of these bosonic modes has long been under discussion. Two possible candidates for these bosons are usually discussed, namely the phonons and the spin fluctuations. Sometimes this discussion looks curious. For example, in two recent papers [35, 36] the coupling constant between electrons and spin fluctuations has been calculated. In Refs [35, 36], the same $t-J$ Hamiltonian and the same experimental data are used, but the obtained coupling constants differ by three orders of magnitude! However, the ARPES data [37] and tunneling measurements [38] have demonstrated that these bosonic modes are not related to the spin fluctuations. In those experiments, anomalies in the electron spectrum were observed at various doping levels. Positions of the anomalies should coincide with the energies of either phonons, or spin fluctuations. The spin fluctuation energies are known to strongly depend on the doping level, while the phonon frequencies have only a weak dependence on it. As the experiments [37, 38] clearly evidence, the anomaly positions are scarcely affected by the doping level, hence, the spin fluctuations are certainly not responsible for the anomalies under discussion. More recently, peculiarities have also been observed [39] in the cuprate electron spectra at 0.3 – 0.5 eV. These high-energy anomalies are likely due to the Hubbard repulsion U and to the exchange-correlation effects.

To conclude, we note that it is necessary to explore in more detail what the 'high-T_c refrigerator' [6] contains in terms of mammoths, elephants, and mice. We believe that there are still many other unanswered questions concerning high-T_c materials.

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