

SUPERCONDUCTIVITY IN JELLIUM MODEL REVISITED

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We reanalyze superconductivity in jellium model within the dielectric formalism developed by Kirzhnits, Maksimov, and Khomskii (KMK), which is probably the most reliable approach to this model. The linearized KMK integral equation for superconducting transition temperature is analyzed analytically and solved numerically by direct diagonalization to obtain T_c dependence on Wigner–Seitz radius r_s . As a first systematic extension beyond random-phase approximation (RPA), static Hubbard local-field corrections are incorporated into the dielectric function. Our results in general narrow the interval of possible T_c values in comparison with widely scattered results of some of the previous works. For the case of metallic hydrogen our calculations show $T_c(r_s)$ dependence with characteristic dome with maximum of T_c at $r_s \sim 9.0$ of the order of some fractions of Kelvin only, despite the naive expectations based on the high values of pairing Boson frequency. This is due to the weak-coupling regime of superconductivity in jellium model at all densities.

Keywords: superconducting transition temperature, dielectric formalism, jellium model, metallic hydrogen

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1. INTRODUCTION

Jellium model is the simple (plasma) model of a metal, which consists of electrically neutral (structureless) gas of electrons and ions interacting via Coulomb repulsion. With respect to superconductivity it was popularized by De Gennes [1] and since then it was used in dozens of papers, especially in the context of high-temperature superconductivity [2]. Actually this simple model demonstrates a number of remarkable properties, like the natural emergence of longitudinal oscillations (phonons) due to screening and superconductivity in purely Coulomb system, so that it can be considered as a simplest microscopic model of a metal with emergent properties, characteristic of real metals.

In the following we shall consider only the case of the gas of electrons and protons as a possible model for metallic hydrogen, which is the actively studied topic today since the prediction of high-temperature in it as well as in different hydrides and also in astrophysical objects like white dwarfs and pulsars or Jupiter [3–6]. The optimism with respect to the possible high val-

ues of T_c in these systems was essentially based on rather high values of ion (proton) plasma frequency, playing the role of the phonon coupling cut-off in BCS-like approach [2]. The experimental discovery of high-temperature superconductivity in hydrides [7, 8] has greatly stimulated also the theoretical studies in this field.

Strangely enough the estimates of T_c in all of the cited theoretical papers varied very much, and were only qualitative. There were apparently no attempts to analyze T_c of the jellium model more or less rigorously until recently. The first such attempt was undertaken in an interesting paper by van der Marel and Berthod [9], who analyzed the problem both analytically and numerically solving BCS — like equations with electron–ion interaction described in general form as the dynamically screened Coulomb interaction:

$$V(q, \omega) = \frac{4\pi e^2}{q^2 \varepsilon(q, \omega)}, \quad (1)$$

where all physics is actually contained the general dielectric function $\varepsilon(q, \omega)$ which was taken in the simplest RPA — approximation typically used to describe jellium. Rather unexpectedly their numerical calculations produced rather low values of T_c at any densities, with maximum values not exceeding 30 K. More so,

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their analytical analysis of Eliashberg parameters for the jellium model produced the value of T_c not exceeding 25 mK! For some unclear reason the authors has not discussed this drastic inconsistency of these values at all, though they rightly noticed that these unexpected results were due to a weak-coupling superconductivity in hydrogen jellium.

The present paper returns to the analysis of superconductivity of the jellium model of metallic hydrogen. In our opinion the direct use of (1) as a kernel of BCS gap equation, as was in fact done in Ref. [9] is rather inconsistent. The problem of the use of dielectric formalism in superconductivity theory was analyzed more than 50 years ago in a remarkable paper by Kirzhnits, Maksimov and Khomskii (KMK) [10], where BCS weak-coupling theory was especially reformulated for the use of general interaction of form of (1) with the aim of analyzing most general pairing interactions in solids. At a time it was seen even as an alternative to Migdal–Eliashberg–McMillan theory of superconductivity (for the review of this theory see [11–13]) developed for the case of electron–phonon mechanism of Cooper pairing, which is now state of the art approach in microscopic calculations in most of real superconductors (including hydrides). Unfortunately, up to now the KMK formalism has not been generalized to strong coupling superconductors and to our knowledge was never used in the studies of real materials. However it is still conceptually important in the studies of non-phonon mechanisms of pairing and is ideally fit to analyze model interactions like those in the jellium model. The KMK dielectric formalism provides a natural framework in which retardation and Coulomb screening are treated on equal footing as it uses the dynamically screened Coulomb interaction (1) directly in equations determining T_c . In Appendix A we present a brief derivation of KMK formalism with the special emphasis on jellium model.

Within this framework:

1. retardation emerges dynamically,
2. Coulomb repulsion and attraction are treated simultaneously,
3. no phenomenological pseudopotential is required,
4. the superconducting gap function becomes strongly energy dependent.

In the present work we use this classic approach to analyze T_c in the jellium model of metallic hydrogen with

the aim to settle the remaining theoretical inconsistencies of these model and extending this analysis outside the region of weak correlations.

2. DIELECTRIC FUNCTION AND COLLECTIVE MODES

We adopt the standard form of dielectric function in jellium mode [1]:

$$\varepsilon(q, \omega) = 1 + \frac{k_{TF}^2}{q^2} - \frac{\omega_0^2}{\omega^2}. \quad (2)$$

Here the electronic part is just the simplest static Thomas–Fermi screening derived within RPA approximation. Throughout this work we use atomic units: $\hbar = e = m = 1$ and consider only hydrogen ions (anticipating application to metallic hydrogen), so that the ionic plasma frequency is given by

$$\omega_0 = \sqrt{\frac{3}{Mr_s^3}}, \quad (3)$$

where the ratio of proton and electron mass is

$$M = \frac{m_p}{m} \approx 1836. \quad (4)$$

The list of other parameters fo electronic subsystem is given in Appendix B.

The collective ionic (phonon) mode is determin by

$$\varepsilon(q, \Omega_q) = 0. \quad (5)$$

This gives

$$\Omega_q^2 = \frac{\omega_0^2 q^2}{q^2 + k_{TF}^2}, \quad (6)$$

or equivalently,

$$\Omega_q = \omega_0 \frac{q}{\sqrt{q^2 + k_{TF}^2}}. \quad (7)$$

At small momentum,

$$q \ll k_{TF}, \quad (8)$$

one obtains acoustic behavior:

$$\Omega_q \sim q. \quad (9)$$

At large momentum,

$$q \gg k_{TF}, \quad (10)$$

we obtain saturation:

$$\Omega_q \rightarrow \omega_0. \quad (11)$$

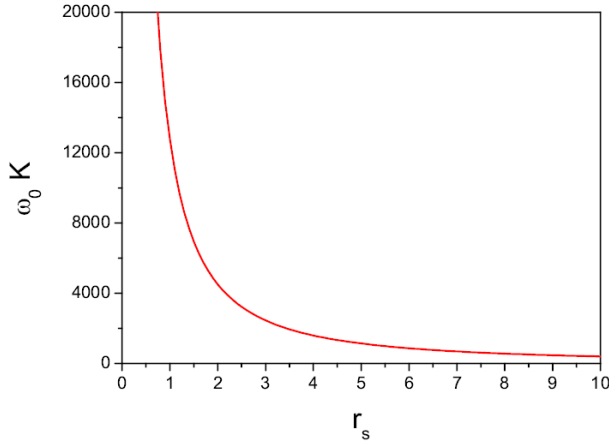


Fig. 1. Ion plasma frequency ω_0 of jellium model as a function of r_s . It is approximately the upper cut-off of phonon spectrum in this model

This is the main property of the jellium model — it explicitly demonstrates the emergence of sound waves (phonons) due to screening in this Coulomb system. In some sense the same mechanism operates in real solids, where fundamentally only Coulomb forces are present, while phonons appear as emergent excitations.

In Fig. 1 we show the r_s dependence of proton plasma frequency ω_0 which is an effective upper cut-off of phonon spectrum in jellium model (an analogue of Debye frequency in solids). We can see that for typical metallic densities corresponding to $r_s \sim 2-3$ it is pretty large. Actually that was the driving idea of a possible high — temperature superconductivity in metallic hydrogen, hydrides and astrophysical objects [3–6].

3. SPECTRAL REPRESENTATION

The spectral density of the inverse dielectric function which is crucial for KMK theory is defined by

$$\rho(q, \Omega) = -\frac{1}{\pi} \text{Im} \frac{1}{\varepsilon(q, \Omega + i0)}. \quad (12)$$

Introduce

$$A_q = 1 + \frac{k_{TF}^2}{q^2}. \quad (13)$$

Then

$$\varepsilon(q, \omega) = A_q \left(1 - \frac{\Omega_q^2}{\omega^2} \right). \quad (14)$$

Therefore

$$\frac{1}{\varepsilon(q, \omega)} = \frac{1}{A_q} \frac{\omega^2}{\omega^2 - \Omega_q^2 + i0}. \quad (15)$$

Thus we immediately obtain

$$\rho(q, \Omega) = \frac{1}{2} \Omega_q \frac{q^2}{q^2 + k_{TF}^2} \delta(\Omega - \Omega_q). \quad (16)$$

This will be used in all calculations which follow.

4. COULOMB COUPLING CONSTANT

The statically screened Coulomb interaction is

$$V_C(q) = \frac{4\pi}{q^2 + k_{TF}^2}. \quad (17)$$

The dimensionless Coulomb coupling is

$$\mu = N(0) \langle V_C(q) \rangle_{FS}, \quad (18)$$

where the averaging is over the momenta on the Fermi surface. The transferred momentum on the Fermi surface satisfies

$$q^2 = 2k_F^2(1 - \cos \theta). \quad (19)$$

The angular integration over the Fermi surface is performed as

$$\langle f(q) \rangle_{FS} = \frac{1}{2} \int_{-1}^1 d \cos \theta f(q(\theta)). \quad (20)$$

Thus

$$\mu = N(0) \frac{1}{2} \int_{-1}^1 d \cos \theta \frac{4\pi}{2k_F^2(1 - \cos \theta) + k_{TF}^2}. \quad (21)$$

Performing the integral gives

$$\mu = \frac{1}{2\pi k_F} \ln \left(1 + \frac{4k_F^2}{k_{TF}^2} \right). \quad (22)$$

Substituting the explicit expressions for k_F and k_{TF} we obtain

$$\mu(r_s) = \frac{r_s}{12.06} \ln \left(1 + \frac{6.03}{r_s} \right). \quad (23)$$

5. KMK PAIRING KERNEL

The linearized superconducting «gap» equation of KMK approach takes the form¹⁾ [10]

$$\Phi(\xi) = - \int_{-\infty}^{\infty} d\xi' K(\xi, \xi') \frac{\tanh(\xi'/2T)}{2\xi'} \Phi(\xi'), \quad (24)$$

¹⁾ Strictly speaking in KMK theory $\Phi(\xi)$ is not a superconducting gap $\Delta(\xi)$, but $\Phi(\xi) \sim \text{Re} \Delta(\xi)$.

where

$$K(\xi, \xi') = \mu(\xi, \xi') - 2 \int_0^\infty d\Omega \frac{\nu(\xi, \xi'; \Omega)}{\Omega + |\xi| + |\xi'|}, \quad (25)$$

and $\mu(\xi, \xi')$ is Coulomb repulsion kernel which can safely be taken as Fermi surface average:

$$\mu(\xi, \xi') = N(0) \langle V_C(q) \rangle_{FS} = \mu. \quad (26)$$

We also have to introduce the usual high-energy cut-off at E_F (which is considered to be of an order of bandwidth, defining the maximum energy in our problem) for ξ, ξ' integration in KMK formalism. The rest may be called an attractive contribution due to effective «phonon» exchange and written as [10]

$$K_{att}(\xi, \xi') = -2 \int_0^\infty d\Omega \frac{\nu(\xi, \xi'; \Omega)}{\Omega + |\xi| + |\xi'|}, \quad (27)$$

where we also slightly simplify the general KMK equations by taking the Fermi surface average of $\nu(\xi, \xi'; \Omega)$ as

$$\nu = N(0) \left\langle \frac{4\pi}{q^2} \rho(q, \Omega) \right\rangle_{FS}, \quad (28)$$

which is explicitly expressed via spectral density $\rho(q, \Omega)$ given by Eq. (16). Substituting this exact spectral density into Eq. (27) we get

$$K_{att}(\xi, \xi') = -4\pi N(0) \left\langle \frac{\Omega_q}{(q^2 + k_{TF}^2)(\Omega_q + |\xi| + |\xi'|)} \right\rangle_{FS}. \quad (29)$$

The total kernel therefore becomes

$$K(\xi, \xi') = N(0) \left\langle \frac{4\pi}{q^2 + k_{TF}^2} \right\rangle_{FS} - 4\pi N(0) \left\langle \frac{\Omega_q}{(q^2 + k_{TF}^2)(\Omega_q + |\xi| + |\xi'|)} \right\rangle_{FS}, \quad (30)$$

which actually determines T_c after solving the KMK integral equation (24).

6. BCS AND ELIASHBERG – McMILLAN APPROXIMATIONS

At low energies $|\xi|, |\xi'| \ll \Omega_q$, performing calculations as above one finds

$$K_{att}(0, 0) \approx -4\pi N(0) \left\langle \frac{1}{q^2 + k_{TF}^2} \right\rangle_{FS} \equiv \lambda, \quad (31)$$

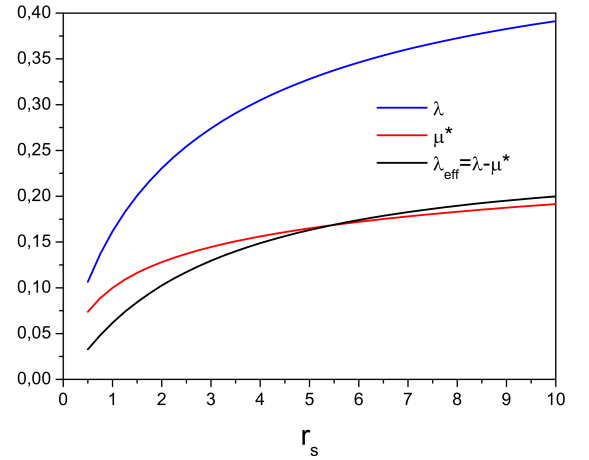


Fig. 2. Effective couplings $\lambda = \mu$ and pseudopotential μ^* in jellium model as functions of r_s , compared with effective pairing constant λ_{eff}

which is the pairing constant of BCS theory. Comparing Eq. (31) with Eq. (18) we immediately see that

$$\lambda = \mu, \quad (32)$$

which is a well known result for the jellium model [9].

In BCS approximation it is usually assumed that

$$K_{att} = \lambda \theta(\omega_0 - \xi) \theta(\omega_0 - \xi'), \quad (33)$$

so that ω_0 acts as an upper energy cut-off for electron-phonon interaction.

Linearized integral equation (24) is then approximately solved [1], assuming

$$\Phi(\xi) = \Phi_{att} \theta(\omega_0 - \xi) + \Phi_C \theta(E_F - \xi) \quad (34)$$

and reducing Eq. (24) to a simple system of two linear equations for Φ_{att} and Φ_C , which acquires nontrivial solution at temperatures $T < T_c$, where T_c is given by the standard BCS expression:

$$T_c = \frac{2\gamma}{\pi} \omega_0 \exp \left(-\frac{1}{\lambda - \mu^*} \right), \quad (35)$$

where $\gamma = 1.78$ is Euler constant, and Coulomb pseudopotential μ^* is given by the usual expression with Tolmachev logarithm:

$$\mu^* = \frac{\mu}{1 + \mu \ln \frac{E_F}{\omega_0}}. \quad (36)$$

Using here the explicit expression for $\mu(r_s) = \lambda(r_s)$ we get $\mu^*(r_s)$ and $\lambda_{eff}(r_s) = \lambda(r_s) - \mu^*(r_s)$ for the effective BCS coupling from Eq. (35). The appropriate

r_s dependencies of all couplings are shown in Fig. 2. Using now these values of coupling constants in (35) we obtain characteristic $T_c(r_s)$ dependence shown at the insert in Fig. 3 [14]. The appearance of the dome is quite natural if you just look at r_s dependence of parameters entering BCS expression. What is actually surprising are the low values of T_c with maximum of 3.28 K only achieved at $r_s = 7.50$, despite large values of the pre-exponential factor of ω_0 . This contradicts optimistic expectations expressed in Refs. [2–6]. But explanation is quite simple — the coupling is always weak in jellium model with λ_{eff} only slightly exceeding 0.1 at for all realistic values of r_s as can be seen from Fig. 2.

The situation becomes even worse, if we use the same coupling parameters in McMillan's expression for T_c [9],

$$T_c = \frac{\omega_0}{1.45} \exp \left\{ -\frac{1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62\lambda)} \right\}, \quad (37)$$

giving even lower values of T_c in milli-Kelvin range, as shown by the blue line in Fig. 3.

Below we shall numerically solve KMK integral equation (24) to obtain more rigorous estimate of T_c in jellium model.

7. NUMERICAL SOLUTION OF THE KMK EQUATION

Standard BCS-like approximation neglects non-trivial dependence of kernel $K_{att}(\xi, \xi')$ (27) on ξ and ξ' by putting them on the Fermi surface and introducing the sharp integral cut-off at ω_0 in (24). Actually this cut-off is rather smooth and fully determined by attractive kernel dependence on $|\xi|$ and $|\xi'|$. At large energies,

$$|\xi| + |\xi'| \gg \Omega_q, \quad (38)$$

we obtain

$$K_{att}(\xi, \xi') \sim -\frac{\Omega_q}{|\xi| + |\xi'|}. \quad (39)$$

Thus the attractive interaction continuously disappears while Coulomb repulsion remains (up to the large energies of the order of E_F). The superconducting eigenfunction $\Phi(\xi)$ therefore changes sign in energy space. At low energies $\Phi(\xi) > 0$, while at high energies $\Phi(\xi) < 0$. This gives a dynamic mechanism of generating Coulomb pseudopotential.

In the following we directly solve KMK integral equation (24) determining T_c with kernel defined in (30) and determine $T_c(r_s)$ dependence numerically. The numerical implementation proceeds through the following steps.

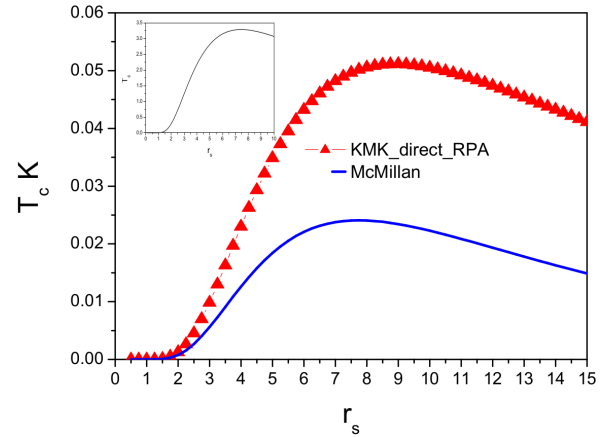


Fig. 3. Critical temperature of superconducting transition T_c in jellium model as a function of r_s . Red triangles — direct numerical solution of KMK integral equation, blue line — McMillan formula for T_c . At the insert: BCS approximation.

7.1. Energy Grid

A logarithmic mesh is used:

$$10^{-10} E_F \leq \xi \leq E_F, \quad (40)$$

which, by the way, introduces abovementioned integration cut-off in Eq. (24).

7.2. Hermitian Symmetrization

Define

$$w_i = \frac{\tanh(\xi_i/2T)}{2\xi_i} \Delta\xi_i, \quad (41)$$

where

$$\Delta\xi_i = \frac{1}{2}(\xi_{i+1} - \xi_{i-1}). \quad (42)$$

The kernel is symmetrized according to

$$\tilde{K}_{ij} = \sqrt{w_i} K_{ij} \sqrt{w_j}. \quad (43)$$

This produces a Hermitian matrix with real eigenvalues.

7.3. Transition Temperature

The superconducting transition temperature is determined from

$$\lambda_{max}(T_c) = 1. \quad (44)$$

The largest eigenvalue is obtained by direct diagonalization.

More details on numerical implementation can be found in Appendix B.

8. NUMERICAL RESULTS WITHIN RPA

First we present the results for the standard jellium model with $\varepsilon(q, \omega)$ defined by Eq. (2) and obtained within RPA. The resulting calculations exhibit a dome-like dependence on the Wigner–Seitz radius shown in Fig. 3 (red triangles). At small r_s the electron gas is weakly interacting and the effective attraction remains extremely small. Increasing r_s enhances the importance of retardation effects and increases the pairing strength. For sufficiently large r_s , however, screening weakens and the assumptions underlying the RPA dielectric function become progressively less reliable.

The maximum of $T_c \approx 0.051\text{ K}$ is achieved at $r_s = 9.0$, which is relatively close to maximum $T_c \approx 0.024\text{ K}$ obtained from McMillan expression at $r_s = 7.75$.

The superconducting eigenfunction exhibits the characteristic sign-changing structure predicted by the KMK formalism, with a positive low-energy sector and a negative high-energy tail (see Appendix C).

Among other features this behavior provides a direct microscopic realization of Coulomb pseudopotential physics of the usual BCS theory without an artificial cut-off at ω_0 .

The obtained maximal T_c is orders of magnitude lower than that obtained by numerical analysis in [9]. Van der Marel–Berthod approach effectively inserts the dynamically screened Coulomb interaction into BCS gap equation using the substitution $\omega \rightarrow \xi - \xi'$. This yields a kernel depending on frequency transfer $V(\xi - \xi')$. Such type of approach was criticized by KMK [10] many years ago. They stressed that the genuine pairing kernel is derived from the spectral density of the inverse dielectric function (12), which depends on positive $|\xi|$ and $|\xi'|$ separately. KMK kernel is smooth, real and automatically retarded. In a sense it justifies the standard BCS-like approach to superconductivity and is much more reliable for calculations of T_c .

Surprisingly our T_c values are also much lower than those obtained from BCS expression (35) and are closer to that following from McMillan’s (37). McMillan’s transition temperature is strongly suppressed in comparison to that of BCS mainly due to mass renormalization term $1 + \lambda$ in the exponent of (37), which is due to strong-coupling effects of Eliashberg theory. KMK theory is usually considered a weak-coupling approximation neglecting mass renormalization effects. We believe that the observed T_c suppression in comparison with BCS is due to combination of nontrivial ξ

dependence of Eigenfuctions $\Phi(\xi)$ of Eq. (24) and those of the kernel $K(\xi, \xi')$ in the same equation. Eigenfuctions of Eq. (24) are discussed in Appendix C.

The main conclusion is that direct solution of the linear integral equation (24) produces the values of T_s of the order of fractions of Kelvins for all reasonable values of r_s .

9. BEYOND RPA: HUBBARD LOCAL-FIELD CORRECTIONS

Strictly speaking all expressions for jellium model were derived within RPA perturbation theory approximation for electron gas, which is valid only for $r_s < 1$. The RPA neglects all exchange — correlation effects in the electronic response, which become important in the region of $r_s > 1$. Thus all the results given above for this region are only of qualitative nature.

There is a long history of theoretical attempts to take correlation effects into account in the theory of interacting electron gas. Here we shall only consider a first extension beyond RPA incorporating the so called static Hubbard local-field corrections, which approximately describes exchange correlation «hole», forming around each electron, which partly suppresses screening at small distances [15]. It is commonly believed that Hubbard local-field correction extends the validity of RPA to the region of $r_s \sim 3\text{--}5$. This local-field correlation factor was chosen by Hubbard in the following form

$$G_H(q) = \frac{1}{2} \frac{q^2}{q^2 + k_F^2}. \quad (45)$$

This expression satisfies the physically desirable limits

$$G_H(q) \rightarrow 0, \quad q \ll k_F, \quad (46)$$

$$G_H(q) \rightarrow \frac{1}{2}, \quad q \gg k_F. \quad (47)$$

Then the dielectric function becomes

$$\varepsilon_H(q, \omega) = 1 + \frac{k_{TF}^2}{q^2} [1 - G_H(q)] - \frac{\omega_0^2}{\omega^2}. \quad (48)$$

The corresponding screening denominator is

$$D_H(q) = q^2 + k_{TF}^2 [1 - G_H(q)]. \quad (49)$$

The collective mode in jellium is modified accordingly:

$$\Omega_H(q) = \omega_0 \frac{q}{\sqrt{D_H(q)}}. \quad (50)$$

The Coulomb contribution becomes now

$$K_C^{(H)} = N(0) \left\langle \frac{4\pi}{D_H(q)} \right\rangle. \quad (51)$$

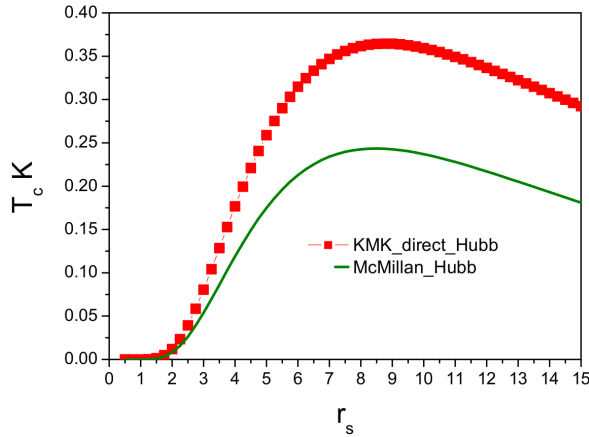


Fig. 4. Critical temperature of superconducting transition T_c in jellium model as a function of r_s with the account of Hubbard local-field correction. Red squares — direct numerical solution of KMK integral equation, green line — McMillan formula for T_c obtained with $\lambda = \mu$ increased due Hubbard local-field correction

Similarly, the attractive contribution becomes

$$K_{\text{att}}^{(H)} = -4\pi N(0) \left\langle \frac{\Omega_H(q)}{D_H(q) [\Omega_H(q) + |\xi| + |\xi'|]} \right\rangle. \quad (52)$$

Equations (49)–(52) constitute the central result of the beyond-RPA extension developed in the present work. Physically, local-field corrections act in two competing ways. First they reduce the effectiveness of long-range screening by decreasing the dielectric denominator. Second, they suppress large-momentum Coulomb scattering through the exchange-correlation hole surrounding each electron. The resulting influence on superconductivity is therefore highly nontrivial.

Because the superconducting instability originates from a delicate cancellation between repulsive and attractive contributions, relatively small local-field corrections may produce substantial changes in the transition temperature.

Our results shown in Fig. 4 demonstrate that T_c is increased several times, as compared to pure RPA case. Also in this Figure we show a comparison with corresponding values obtained from McMillan expression (37) with recalculated couplings $\lambda = \mu$, accounting for Hubbard local-field corrections. Actually their r_s behavior is very similar to that shown in Fig. 2, but the absolute values are slightly increased in comparison to RPA, leading to corresponding increase of T_c . However maximum T_c value remains less than 1K.

More complicated schemes accounting for correlation effects in electron gas may be, in principle, incor-

porated into KMK scheme. But there are no reasons to believe that these will lead to significant further increase of T_c in jellium model.

10. DISCUSSION AND CONCLUSIONS

We have presented a detailed derivation and numerical implementation of the KMK dielectric formalism for superconductivity in jellium. The exact pairing kernel was derived from the spectral representation of the inverse dielectric function. The superconducting instability emerges from delicate cancellation between Coulomb repulsion and retarded ionic attraction, producing the coherent picture of microscopic origin of superconductivity in this simplest possible model with realistic interaction.

Most part of our work was devoted to discussion of contradictions between T_c values obtained in earlier papers. We believe that our use of general KMK dielectric function formalism allowed to settle these inconsistencies. The final conclusion is simple and rather pessimistic — for no reasonable set of jellium model parameters we were not able to obtain T_c larger than fractions of Kelvin.

In general T_c demonstrates a typical dome dependence on r_s which in a simple BSC or Eliashberg–McMillan approaches directly follows from competition between ω_0 dependence on r_s leading to its very large values at small r_s and r_s dependence of coupling constants $\lambda = \mu$ and μ^* . Direct numerical solution of KMK equations fully confirm this picture, solving the problem for microscopic interaction which are determined from dynamically screened Coulomb interaction with dynamic dielectric function $\varepsilon(q, \omega)$ of the jellium model.

Apparently there is no way to change these results significantly within simple generalizations of jellium model, such as more correct account of correlation (local field) effects in electron gas, which we also considered in a simplest possible Hubbard approximation.

In general our results are in agreement with the famous arguments of Anderson and Cohen [16], who showed long ago that in any model with $\lambda \leq \mu$ it is not possible to obtain T_c larger than few Kelvins, no matter how large is an energy of collective excitations leading to pairing. Please note, that these arguments are just inapplicable in a general case due to a possibility of realistic systems with $\lambda > \mu$ [17], especially in the strong coupling limit of Eliashberg theory [18].

The interest to superconductivity in jellium was revived in Ref. [9] in the context of metallic hydrogen and superconductivity in hydrides. Our results (as well as

those of Ref. [9]) clearly show that this model is inappropriate starting point in this field, as the values of T_c obtained are very small, due to realization of weak coupling for all parameters of the model. It is clear from the very beginning that jellium model probably describes some kind of liquid (or even gaseous, plasma-like) state of metallic hydrogen, which has almost nothing to do with predicted solid metallic hydrogen or hydrides with their specific crystal structures, complicated multiple band electron spectra and sometimes rather exotic Fermi surfaces and multiple branches in phonon spectra. These aspects of real hydrides, as well as of possible solid metallic hydrogen are responsible to realization of very strong electron–phonon pairing in these systems in a sense of Allen–Dynes approach to Eliashberg theory [19], which allows to achieve very large values of T_c up to room temperatures [18, 20].

At the same time the toy jellium model is still very interesting as probably the only solvable model, which can fully describe the origin of phonon — ike excitations and superconductivity in microscopic model with only Coulomb interactions. In real solids all spectra of collective excitations are in fact originating only from Coulomb interactions, but we are still very far from full microscopic theory explaining the emergence of these excitations, more so from the real microscopic theory of superconductivity. In this sense jellium model gives us a hope that such theory can be sometimes constructed.

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Codes Availability. All codes used in these calculations are available from the author on a resonable request.

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APPENDIX A. DERIVATION OF KMK KERNEL

Below we present for completeness a short and slightly simplified version of KMK equations with special emphasis on jellium model.

The dielectric formulation of superconductivity developed by Kirzhnits, Maksimov, and Khomskii (KMK) [10] expresses the pairing interaction directly through the frequency-dependent dielectric function of the electron-ion plasma. Unlike Eliashberg theory, where phonons are introduced explicitly, the KMK ap-

proach starts from the exact screened Coulomb interaction

$$W(q, \omega) = \frac{V_C(q)}{\varepsilon(q, \omega)}, \quad (53)$$

where²⁾

$$V_C(q) = \frac{4\pi e^2}{q^2} \quad (54)$$

is the bare Coulomb interaction.

Linearized KMK equation is derived [10] using the spectral representation of $\varepsilon^{-1}(q, \omega)$. Causality implies that is analytic in the upper half-plane of complex ω . Therefore it admits the Kramers–Kronig representation

$$\varepsilon^{-1}(q, \omega) = 1 + \int_0^\infty d\Omega \rho(q, \Omega) \left[\frac{1}{\Omega - \omega} + \frac{1}{\Omega + \omega} \right], \quad (55)$$

and

$$\rho(q, \Omega) = -\frac{1}{\pi} \text{Im} \varepsilon^{-1}(q, \Omega + i0) \quad (56)$$

is the spectral density of the inverse dielectric function.

Substituting Eq. (55) into Eq. (53) gives

$$W(q, \omega) = V_C(q) + V_C(q) \int_0^\infty d\Omega \rho(q, \Omega) \left[\frac{1}{\Omega - \omega} + \frac{1}{\Omega + \omega} \right]. \quad (57)$$

The first term here is instantaneous Coulomb repulsion, while the second contains all retarded effects.

The exact linearized Gor'kov equation in Matsubara representation can be written as

$$\Phi(k, i\omega_n) = -T \sum_m \int \frac{d^3 k'}{(2\pi)^3} W(q, i\omega_n - i\omega_m) \times \\ \times G(k', i\omega_m) G(-k', -i\omega_m) \Phi(k', i\omega_m). \quad (58)$$

Near T_c the normal-state Green's functions are

$$G(k, i\omega_n) = \frac{1}{i\omega_n - \xi_k}. \quad (59)$$

After rather long technical manipulations involving Matsubara frequency summation KMK [10] obtained the following one-dimensional linear integral equation, where $\Phi(\xi)$ is already a function of a single variable ξ :

$$\Phi(\xi) = - \int_0^\infty d\xi' \frac{\tanh(\xi'/2T)}{\xi'} K(\xi, \xi') \Phi(\xi'). \quad (60)$$

²⁾ For clarity here we write down electric charge e explicitly

Here the KMK kernel takes the form

$$K(\xi, \xi') = \mu(\xi, \xi') - 2 \int_0^\infty d\Omega \nu(\xi, \xi'; \Omega) \frac{1}{\Omega + \xi + \xi'}. \quad (61)$$

The spectral function entering pairing is

$$\nu(\xi, \xi'; \Omega) = N(0) \langle V_C(q) \rho(q, \Omega) \rangle_{FS}. \quad (62)$$

The notation $\langle \dots \rangle_{FS}$ denotes Fermi-surface averaging as defined in the main part of our paper above.

For the electron-ion plasma we can take

$$\varepsilon(q, \omega) = \varepsilon_e(q, \omega) - \frac{\omega_i^2}{\omega^2}. \quad (63)$$

The electronic dielectric function is approximated by its static limit,

$$\varepsilon_e(q, \omega) \rightarrow \varepsilon_e(q, 0). \quad (64)$$

Using Thomas–Fermi approximation,

$$\varepsilon_e(q) = 1 + \frac{k_{TF}^2}{q^2}. \quad (65)$$

Thus

$$\varepsilon(q, \omega) = 1 + \frac{k_{TF}^2}{q^2} - \frac{\omega_i^2}{\omega^2}. \quad (66)$$

To shorten expressions we introduce now

$$D(q) = q^2 + k_{TF}^2. \quad (67)$$

Then

$$\varepsilon(q, \omega) = \frac{D(q)}{q^2} - \frac{\omega_i^2}{\omega^2}. \quad (68)$$

Inverting Eq. (66) gives

$$\varepsilon^{-1}(q, \omega) = \frac{q^2 \omega^2}{D(q) \omega^2 - q^2 \omega_i^2}. \quad (69)$$

The collective mode of jellium model can be written as

$$\Omega_q^2 = \omega_i^2 \frac{q^2}{D(q)}. \quad (70)$$

Then

$$\varepsilon^{-1}(q, \omega) = \frac{q^2}{D(q)} \frac{\omega^2}{\omega^2 - \Omega_q^2}. \quad (71)$$

Using

$$\frac{\omega^2}{\omega^2 - \Omega_q^2} = 1 + \frac{\Omega_q^2}{\omega^2 - \Omega_q^2}, \quad (72)$$

one obtains

$$\varepsilon^{-1} = \frac{q^2}{D(q)} + \frac{q^2 \Omega_q^2}{D(q)} \frac{1}{\omega^2 - \Omega_q^2}. \quad (73)$$

Then one one finds

$$\rho(q, \Omega) = \frac{q^2 \Omega_q}{2D(q)} \delta(\Omega - \Omega_q). \quad (74)$$

All spectral weight here resides in the ionic collective mode.

Substituting Eq. (74) into Eq. (62), we obtain

$$\begin{aligned} V_C(q) \rho(q, \Omega) &= \frac{4\pi e^2}{q^2} \frac{q^2 \Omega_q}{D(q)} \delta(\Omega - \Omega_q) = \\ &= \frac{4\pi e^2 \Omega_q}{D(q)} \delta(\Omega - \Omega_q). \end{aligned} \quad (75)$$

Performing the Ω integration gives

$$K_{attr} = -N(0) \left\langle \frac{2\pi e^2 \Omega_q}{D(q)} \frac{1}{\Omega_q + \xi + \xi'} \right\rangle_{FS}. \quad (76)$$

This is precisely the attractive contribution used in practical KMK calculations in the main part of our text.

Using (73), in (53) we can write the total interaction as

$$W(q, \omega) = \frac{4\pi e^2}{q^2 + k_{TF}^2} + \frac{4\pi e^2}{q^2 + k_{TF}^2} \frac{\Omega_q^2}{\omega^2 - \Omega_q^2}. \quad (77)$$

The second term here in KMK equation is transformed into attractive kernel (76), while the first term represents the remaining static Coulomb repulsion:

$$W(q, 0) = \frac{4\pi e^2}{q^2 + k_{TF}^2}. \quad (78)$$

The corresponding dimensionless Coulomb potential is defined as usual

$$\mu = N(0) \left\langle \frac{4\pi e^2}{q^2 + k_{TF}^2} \right\rangle_{FS} \quad (79)$$

and was extensively used above.

The major simplification of our analysis here in comparison with [10] is the reduction of all interactions to their Fermi surface averages. KMK formulation is more general with explicit «off-shell» expressions. We believe that for jellium model the use of these expressions is excessive, though all calculations can also be performed, in principle, also for this general case.

APPENDIX B. MAIN PARAMETERS AND NUMERICAL PROCEDURE

We consider the homogeneous electron gas with density

$$n = \frac{3}{4\pi r_s^3}, \quad (80)$$

where r_s is the Wigner–Seitz radius measured in atomic units. Throughout this work we use Hartree atomic units, so that energies are measured in units of Hartree energy $Hr = mc^2\alpha^2 = 315775.0 \text{ K} \approx 27 \text{ eV}$ ($\alpha = e^2/\hbar c$ is the fine structure constant). All lengths are measured in the values of Bohr radius: $a_0 = \hbar/mc\alpha$ and r_s is just dimensionless. The Fermi momentum is

$$k_F = (3\pi^2 n)^{1/3} = \frac{(9\pi/4)^{1/3}}{r_s}. \quad (81)$$

The free-electron dispersion is

$$\xi_k = \frac{k^2 - k_F^2}{2}. \quad (82)$$

The Fermi energy becomes

$$E_F = \frac{k_F^2}{2}. \quad (83)$$

The density of states per spin projection at the Fermi level is

$$N(0) = \frac{k_F}{2\pi^2}. \quad (84)$$

The Thomas–Fermi momentum is

$$k_{TF}^2 = \frac{4k_F}{\pi}. \quad (85)$$

The linearized superconducting «gap» equation is written as

$$\Phi(\xi) = - \int_{-\infty}^{\infty} d\xi' K(\xi, \xi') \frac{\tanh(\xi'/2T)}{2\xi'} \Phi(\xi'), \quad (86)$$

where the kernel $K(\xi, \xi')$ was defined in (30).

The transferred momentum on the Fermi surface satisfies

$$q^2 = 2k_F^2(1 - \cos \theta). \quad (87)$$

The angular integration over the Fermi surface is performed directly using:

$$\langle f(q) \rangle_{FS} = \frac{1}{2} \int_{-1}^1 d \cos \theta f(q(\theta)). \quad (88)$$

Energy discretization is introduced giving

$$\Phi_i = \sum_j M_{ij} \Phi_j. \quad (89)$$

The matrix elements are

$$M_{ij} = -K_{ij} \frac{\tanh(\xi_j/2T)}{2\xi_j} \Delta\xi_j, \quad (90)$$

where

$$\Delta\xi_i = \frac{1}{2}(\xi_{i+1} - \xi_{i-1}). \quad (91)$$

To obtain a Hermitian eigenvalue problem one introduces

$$w_i = \frac{\tanh(\xi_i/2T)}{2\xi_i} \Delta\xi_i, \quad (92)$$

and defines

$$\tilde{K}_{ij} = \sqrt{w_i} K_{ij} \sqrt{w_j}. \quad (93)$$

The superconducting instability occurs when maximum eigenvalue of Eq. (86)

$$\lambda_{\max}(T_c) = 1. \quad (94)$$

This criterion forms the basis of the numerical calculations presented below.

The numerical solution of the KMK equation presents a nontrivial challenge because the thermal factor

$$W(\xi, T) = \frac{\tanh(\xi/2T)}{2\xi} \quad (95)$$

contains the Cooper singularity

$$W(\xi, T) \sim \frac{1}{2\xi}, \quad \xi \rightarrow 0. \quad (96)$$

A uniform energy mesh would therefore require an impractically large number of points. To resolve both infrared and ultraviolet scales efficiently, we introduce a logarithmic mesh

$$\xi_i = \xi_{\min} \left(\frac{\xi_{\max}}{\xi_{\min}} \right)^{i/(N-1)}, \quad i = 0, \dots, N-1. \quad (97)$$

In the calculations reported here we typically used

$$\xi_{\min} = 10^{-10} E_F, \quad (98)$$

$$\xi_{\max} = E_F \quad (99)$$

with

$$N = 200 - 300. \quad (100)$$

This choice provides accurate resolution of both the Cooper logarithm and the high-energy Coulomb tail and corresponds to sharp cut-off at E_F . Actually our numerics has shown that the value of T_c is very slowly (logarithmically) increasing as we increase this cut-off from E_F to $10^3 E_F$ etc. This is unphysical growth — introducing the smooth cut-off beyond E_F we achieve

full convergence of our results for T_c to the values obtained with sharp E_F cut-off as we increase integration limits to $10E_F$, 10^2E_F and beyond.

The numerical solution proceeds as follows:

1. Construct logarithmic energy grid.
2. Compute angularly averaged kernel.
3. Form thermal weights.
4. Construct Hermitian matrix

$$\tilde{K}_{ij} = \sqrt{w_i} K_{ij} \sqrt{w_j}. \quad (101)$$

5. Determine largest eigenvalue.
6. Solve for

$$\lambda_{\max}(T_c) = 1 \quad (102)$$

by root finding.

This procedure yields the superconducting transition temperature directly without introducing additional fitting parameters.

APPENDIX C. EIGENFUNCTIONS

Our numerical calculations produced eigenfunctions $\Phi(\xi)$ of Eq. (24) with ξ -dependence shown in Fig. 5 and in Fig. 6, presenting it on electron and ion energy scales. This behavior is almost universal with eigenfunctions changing sign at $\xi \sim \omega_0$. This behavior reflects the electron-«phonon» nature of pairing in jellium model.

The node at $\xi \sim \omega_0$ means that below ω_0 attraction dominates, while above ω_0 Coulomb repulsion overwhelms attraction. The eigenfunction automatically separates these two regions. This is essentially the same physics that produces Tolmachev logarithm in BCS and Eliashberg theories. The remarkable point is that KMK seems to generate it directly from the eigenvalue problem without introducing a pseudopotential by hand.

Why KMK T_c is so much lower than BCS? Our numerics are giving a fairly clear answer. The naive BCS estimate assumes $\Phi(\xi) = \text{const}$ through the entire pairing region. The actual KMK solution instead looks schematically like $\Phi(\xi)$ positive³⁾ for $\xi < \sim \omega_0$ and $\Phi(\xi)$ negative for $\xi > \sim \omega_0$. Also for some part

³⁾ Actually the sign here is relative due to linear nature of KMK integral equation, only sign change matters.

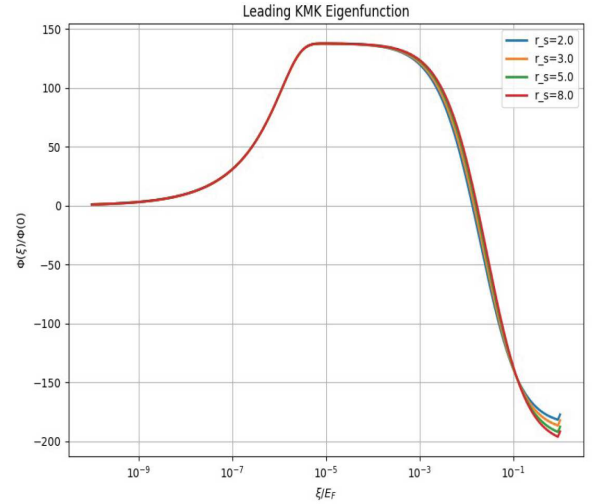


Fig. 5. Eigenfunctions of KMK equation ξ behavior on electronic energy scale for several typical values of r_s

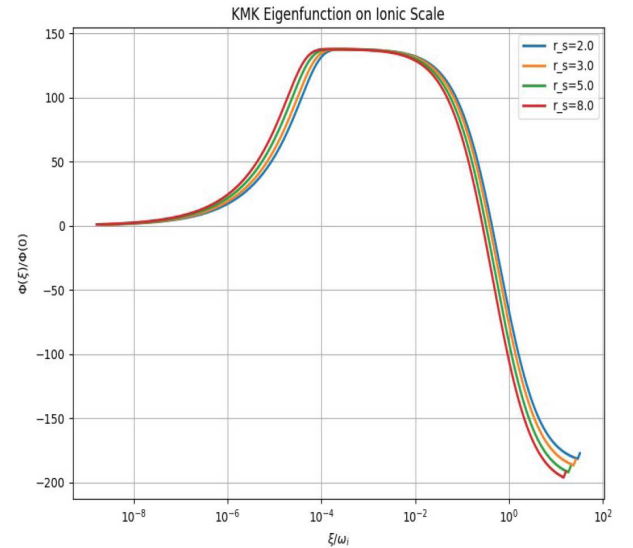


Fig. 6. Eigenfunctions of KMK equation ξ behavior on ion energy scale for several typical values of r_s

of low ξ region $\Phi(\xi)$ is rather small. The entire shape of $\Phi(\xi)$ matters. Our eigenfunctions are not some two-step functions. They are rather smooth objects extending over many decades in energy. Consequently the largest eigenvalue of the kernel is just smaller than one would infer from a simple averaged coupling picture. That naturally lowers T_c .

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