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INSTABILITY OF METALLIC HYDROGEN STRUCTURE TO SMALL CHANGES IN THE ALLOWANCE FOR THE ELECTRON-ELECTRON INTERACTION

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The binding energy of metallic hydrogen at zero pressure is calculated numerically in second and third order perturbation theory. It is shown that small changes in the allowance for the electron-electron interaction can lead to the vanishing of the metastable "metallic" minimum of the total energy.

The question of the existence of metastable metallic hydrogen is of considerable interest and is discussed in a number of papers [1 - 3].

The most fundamental calculations of the possible metastable structure at zero pressure were performed in [2] and led to the unexpected conclusion that there exists a metastable filamentary structure in which the protons lie close together along parallel filaments, which intersect a perpendicular plane in a lattice made up of regular triangles.

The binding energy was calculated in [2] with inclusion of second and third order perturbation-theory terms in the electron-proton interactions. A number of approximations were made, due to the inaccuracy in the allowance for the interaction of the electrons with one another. In the second-order term, this reduces to an inaccuracy of the employed formula for the dielectric constant of a homogeneous electron gas. In the third-order terms there are also correlation corrections, which have not been taken into account at all in [2].

The second source of errors is the discarding of the higher orders of perturbation theory. In fact, however, it is impossible to calculate the fourth-order terms with present-day computers.

The purpose of the present paper is to ascertain the influence of small corrections, connected with allowance for electron-electron correlations in second and third order of perturbation theory on the qualitative statements made concerning the character of the metastable structure of metallic hydrogen.

The simplest diagrams that take into account the correlation corrections to the energy of the ground state of an electron gas in the external field of the lattice protons are shown in Fig. 1a for the second-order term and in Fig. 1d for the third-order terms. The corresponding integrals can be obtained only numerically. The most widely used method of taking such diagrams into account is to replace in the first diagram the Coulomb potential, which corresponds to the internal wavy line, by a certain effective mean value $V_{eff} = V_c(k^2 + p_F^2)^{1/2}$, where p_F is the Fermi

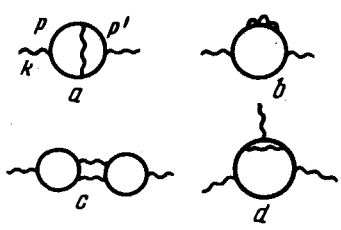

Fig. 1

momentum and λ is a constant.

The corresponding approximation is called the Hubbard approximation [4]. In the present paper, just as in [2], we calculate the energy E2 in second order of perturbation theory, by using the corresponding expression for the polarization operator with $\lambda = 2$:

$$\Pi(k) = \Pi_0(k)\left[1 - \frac{2\pi}{k^2 + \lambda k_F^2}\Pi_0(k)\right]^{-1} \qquad (1)$$

($\Pi_0(k)$ is the polarization operator for the free electrons).

Computer calculations have shown that the summary contribution of diagrams of type 1a, 1b, and 1c leads to a somewhat larger value of $\Pi(k)$ than given by formula (1) [5].

In this paper, by way of an estimate, we used the Hubbard approximation also to calculate diagrams of type 1d. We summed the ladders corresponding to each vertex, and this leads to a third-order term E3 in the binding energy:

$$E3 = \sum_{k_1+k_2+k_3=0} \Pi_3^0(k_1, k_2, k_3)\,\Gamma(k_1)\Gamma(K_2)\Gamma(k_3) \qquad (2)$$

(summation over the vectors of the reciprocal lattice). The quantity Π_3^0 corresponds to the Hartree approximation with allowance for the screening of the Coulomb field of the lattice (an expression for Π_3^0 is given in [2]). The factors Γ take into account the correlation corrections to the vertices:

$$\Gamma(k) = \left(1 - \frac{2\pi}{k^2 + \Lambda p_F^2}\Pi_0(k)\right)^{-1}. \qquad (3)$$

The quantity Λ was varied in the calculations from 2 to ∞ ($\Lambda = \infty$ corresponds to neglecting the correlation corrections to E3, as was done in [2]).

We calculated the binding energy of a primitive hexagonal lattice as a function of the variables c/a (the ratio of the period along the sixfold axis to the period in the basal plane) and the quantity r_s, which is connected with the density, $(4/3)\pi r_s^3 = n^{-1}$. The total binding energy is given by the sum

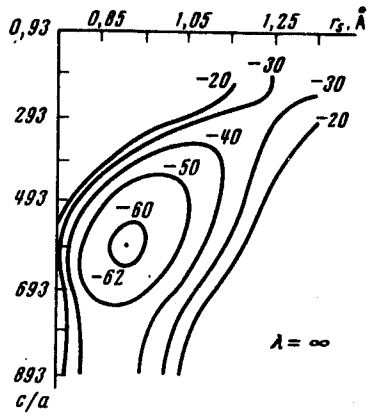

Fig. 2

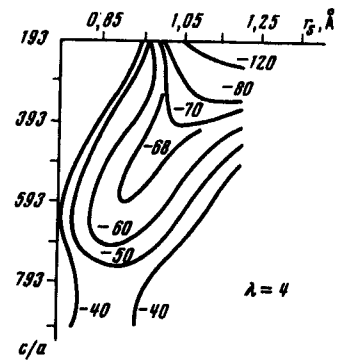

Fig. 3

$$E_{tot} = E_0 + E_{PR} + E2 + E3,$$

where E_{PR} is the electrostatic energy of the lattice and E_0 is the energy of the homogeneous electron gas. E_0 was taken into account in the Nozieres-Pines approximation, as was done in [2].

Figure 2 shows the level lines of the binding energy at $\Lambda = \infty$. The numbers indicate the values of $(1 + E_{tot}) \times 10^3$ Ry. We note the presence of a saddle point that separates the minimum obtained in [2] from the region where the energy begins to decrease noticeably with increasing density; this can be identified with a transition into the region of "molecular" hydrogen, which has a low density at zero pressure.

At $\Lambda = 2$ there is neither saddle point nor "metallic minimum" with high density. A stable state exists only somewhere in a region of low density and small c/a. In this region of the values of the parameters, perturbation-theory calculations are utterly unreliable ($E3/E2 \sim 1$). It is important to note that the absolute change of E2 + E3, due to the deviation of Λ from ∞, amounts according to the table to about 4% of the value of E2 + E3 itself, meaning an exceedingly high sensitivity of the very existence of the "metallic" minimum of the total energy to small changes in the calculation. Calculations show that the critical value of Λ, at which the minimum with high density vanishes, lies in the range $6 > \Lambda_{cr} > 4$. Figure 3 shows the level lines for $\Lambda = 4$.

Energy in Ry/atom, $r_s = 0.903$ Å

c/a	E2	E3		E_{PR}	E_{tot}	
		$\Lambda = \infty$	$\Lambda = 2$		$\Lambda = \infty$	$\Lambda = 2$
0.393	-0.2920	-0.1224	0.1534	-0.7428	-1.0339	-1.0648
0.493	-0.2115	-0.0779	0.0930	-0.8902	-1.0562	-1.0713
0.593	-0.1616	-0.0555	0.0636	-0.9682	-1.0619	-1.0700
0.693	-0.1275	-0.0424	0.0468	-1.0102	-1.0566	-1.0611

Thus, the results of perturbation-theory calculations with allowance for second and third order terms do not indicate unambiguously the existence of metastable metallic hydrogen, since we do not know with sufficient accuracy the polarization operator and the irreducible three-point diagram for a homogeneous electron gas. Allowance for the correlations only in the second-order term, after Hubbard, apparently underestimates the electron energy and it is quite probable that the metastable filamentary minimum for metallic hydrogen at zero pressure does not exist.

It is of interest to verify these statements outside the framework of perturbation theory by directly calculating the band structure.

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SOUND PROPAGATION IN SOLUTIONS OF TWO SUPERFLUID LIQUIDS

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The hydrodynamic equations for solutions of two superfluid liquids were derived in [1], where it was also indicated that undamped sound oscillations of three types should propagate in such solutions. It can be regarded now as established that a phase transition to the superfluid state occurs in liquid He^3 at a temperature on the order of several millikelvin [2]. There can be no doubt that a similar transition can occur in solutions of He^3 in He^4. At sufficiently low temperatures, Cooper pairing of the He^3 atoms should set in and they should go over into the superfluid state. We wish, in this connection, to return to the question of the hydrodynamic properties of a mixture of two superfluid liquids, and investigate, in particular, the propagation of sound in such mixtures.

We write down the hydrodynamic equations of a mixture of two superfluid liquids [1]. The system of equations includes:

a) the continuity equation (ρ is the density and c the concentration)

$$\dot{\rho}_1 + \operatorname{div}(\rho_{s1}\mathbf{v}_{s1} + \rho_{n1}\mathbf{v}_n) = 0; \quad \dot{\rho}_2 + \operatorname{div}(\rho_{s2}\mathbf{v}_{s2} + \rho_{n2}\mathbf{v}_n) = 0 \tag{1}$$

$$\rho_1 = \rho c = \rho_{s1} + \rho_{n1}, \quad \rho_2 = \rho(1-c) = \rho_{s2} + \rho_{n2}$$

($\vec{v}_{s1}$ and $\vec{v}_{s2}$ are the velocities of the superfluid motion of components 1 and 2, respectively, and $\vec{v}_n$ is the velocity of the normal motion[1]);

b) the continuity equation for the entropy

$$\dot{S} + \operatorname{div} S\mathbf{v}_n = 0; \tag{2}$$

c) the equations of the superfluid motions

$$\begin{aligned} \dot{\mathbf{v}}_{s1} + \nabla\left(\mu_1 - \frac{\mathbf{v}_n^2}{2} + \mathbf{v}_n\mathbf{v}_{s1}\right) &= 0, \\ \dot{\mathbf{v}}_{s2} + \nabla\left(\mu_2 - \frac{\mathbf{v}_n^2}{2} + \mathbf{v}_n\mathbf{v}_{s2}\right) &= 0, \end{aligned} \tag{3}$$

where μ_1 and μ_2 are the chemical potentials defined by the following relation for the energy ε:

[1] The normal density $\rho_{n1} = \rho c - \rho_{s1}$ determines the number of normal atoms of the Fermi component, and differs from the normal density ρ_{nF} of the Fermi excitation by a factor m^*/m, where m^* is the effective mass. The normal density ρ_{n2} therefore includes not only the normal density ρ_{nB} of the Bose excitations (phonons) but also part of the normal density of the Fermi excitations $\rho_{n1}(m^*/m - 1)$, i.e., $\rho_{n2} = \rho_{nB} + \rho_{n1}(m^*/m - 1)$.