METALLIC HYDROGEN: A HIGH-TEMPERATURE SUPERCONDUCTOR?

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Application of the BCS theory to the proposed metallic modification of hydrogen suggests that it will be a high-temperature superconductor. This prediction has interesting astrophysical consequences, as well as implications for the possible development of a superconductor for use at elevated temperatures.

It is well known that the alkali metals $(3.2 \leq r_S \leq 5.7)$ are thought to have no superconducting transition, at least within the range of low temperatures currently available. In the standard weak-coupling BCS¹ expression for the transition temperature,

$$T_c = 0.85\Theta_{\rm D} \exp(-1/N_0 V),$$

the parameter N_0V in Na and K (for example) is found to be nearly zero. The cancellation between electron-phonon- and electron-electronderived terms is almost complete (and in some cases overcomplete), and combined with their low Debye temperatures (Θ_D) this leads to near vanishing transition temperatures. Now in terms of the parameter $\lambda^2 = 1/\pi a_0 k_F = 0.166 r_S$ we may write N_0V for a metal of valence Z as

$$N_{0}V = \frac{1}{2}\lambda^{2} \left[\frac{1}{\alpha^{2}} \left\{ 1 + \frac{\lambda^{2}}{(1/4Z)^{2/3}} \ln \frac{\lambda^{2} + 1}{\lambda^{2}(1/4Z)^{2/3}} - \frac{\lambda^{2}}{(1/4Z)^{2/3}(\lambda^{2} + 1)} \right\} - \ln \frac{\lambda^{2} + 1}{\lambda^{2}} \right], \quad (1)$$

where the actual sound velocity has been written $v_s = \alpha (Zm/3M)^{1/2} v_F$ for metals with ionic mass M and Fermi velocity v_F . In (1) the term arising from electron-phonon coupling includes normal and umklapp processes and both have been calculated in the rigid-ion approximation with Thomas-Fermi screened point-ion potentials.² The umklapp contribution to (1) follows from a suggestion by Pines³ and is probably an underestimate. Cancellation of the screened electron-electronand electron-phonon-derived terms in N_0V for the monovalent (Z = 1) metals is largely a result of their r_s range in combination with the fact that the observed α values are close to 1.

The (so far hypotheical) metallic phase of hydrogen⁴ has a zero-pressure density⁵ corresponding to an r_S value of about 1.6. Its compressibility at this density has been calculated by the methods of Ashcroft and Langreth,⁶ and yields a value for the longitudinal sound velocity $v_S = 1.6$ $\times 10^6$ cm/sec; this compares reasonably well with the Bohm-Staver result $v_S = (m/3M)^{1/2}v_F$ = 3.5×10⁶ cm/sec, thereby giving for α the value 0.45. For the sake of comparison, values of α for Na, K, Al, and Pb are, respectively,⁷ 0.82, 1.00, 0.51, and 0.53.

The sound velocity in metallic hydrogen is substantial: Coupled with a light ionic mass the corresponding Debye temperature is $\Theta_D = 3.5 \times 10^3 \,^{\circ}$ K. Substitution of the various quantities involved into (1) gives 0.25 as a reasonable lower limit on $N_0 V.^8$ We note that if metallic hydrogen exists in a close-packed phase (e.g., hcp or fcc) the screened point-ion potential is large enough for significant zone contact with the Fermi surface to occur. This will increase the umklapp contribution already underestimated in (1). In any case the value of T_c is substantial: Calculations of the K value indicate that if metallic hydrogen remains a superconductor for $r_s < 1.6$, it probably becomes of the type-II class.⁹ It is also worth pointing out that a form of metallic hydrogen¹⁰ based on the known stable chemical entity H_2^+ (as metallic ion) is metastable at an $r_{\rm S}$ value of about 3.2. This is probably not superconducting for the reasons mentioned above, although the Debye temperature (about 1.25×10^3 °K) is considerably higher than those found in tha alkali metals.

If the BCS prediction is correct¹¹ then two important consequences follow. First, in the field of astrophysics interest immediately centers on stars and planets whose composition is predominantly hydrogen. Jupiter is an example in the latter category and in addition it is known¹² to have a low temperature (100-200°K) and a substantial magnetic field. Calculations of De Marcus^{4,12} show the intensity of hydrogen to range from about 0.1 at the surface to about 5 g/cm³ ($r_s \sim 0.8$) near the center. This suggests that if indeed the bulk of the planet is composed of hydrogen in the metallic state, part of it may also be in a superconducting state, and the association of magnetic fields with, for example, persistent currents may be of some significance.

Second, because of uncertainties in the equation of state of molecular hydrogen at high densities, estimates of the pressure required to obtain metallic hydrogen are varied.¹³ However, pressures somewhat less than a megabar are typical of these estimates and we remark that pressures in the 600-kbar range are presently available in the laboratory. The range will no doubt be increased and this presents the possibility of developing a high-temperature superconductor stable in the practical sense¹⁴ near atmospheric pressure. An estimate of the possible upper bound on T_C will hinge, of course, on a more detailed estimate of the umklapp contributions to N_0V .

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²When applied to metallic hydrogen, whose ions are point charges, this approximation becomes exact.

³D. Pines, Phys. Rev. <u>109</u>, 280 (1958).

⁴E. Wigner and H. B. Huntington, J. Chem. Phys. <u>3</u>, 764 (1935); R. Kronig, J. deBoer, and J. Korringa, Physica <u>12</u>, 245 (1946); W. C. De Marcus, Astron. J. <u>63</u>, 2 (1958); A. A. Abrikosov, Astron. Zh. <u>31</u>, 112 (1954).

⁵This is strictly a metastable phase. Calculation of

the barrier between metallic and molecular phases shows it to be about 0.2 eV/electron.

⁶N. W. Ashcroft and D. C. Langreth, Phys. Rev. <u>155</u>, 682 (1967).

⁷Notice that for Al, $\alpha^2 = 1$ predicts $N_0 V < 0$.

⁸If we take $\alpha^2 = 0.3$, then $N_0V = 0.25$. Note that $\alpha^2 = 0.2$ in metallic hydrogen.

⁹As r_s decreases, Θ_D increases roughly as r_s^{-1} . This partly compensates the accompanying decrease in $N_0 V$.

 10 This assumes that the screening of the conduction electrons does not alter the bonding on the ${\rm H_2}^+$ by the σ orbital.

 $^{11}\mathrm{Notice}$ that the r_S value of 1.6 is not far outside the value 2.07 (corresponding to metallic Al) for which the BCS theory is successful. Corrections arising from possible strong-coupling effects should not seriously alter the conclusions.

¹²For a summary of the data, see G. M. Michaux, <u>Handbook of the Physical Properties of the Planet Ju-</u><u>piter</u>, National Aeronautics and Space Administration Publication No. SP-3031 (U. S. Government Printing Office, Washington, D. C., 1967). The inner core of Jupiter is thought to be composed of helium. This may also be metallic under high pressure, first with He⁺ ions and subsequently with He⁺⁺. At corresponding r_s values the latter has a lower Debye temperature than H⁺, but being polyvalent, its N_0V value is higher and superconductivity in high-density He⁺⁺ is also a possibility.

¹³The transition pressure is found from the common tangent to the energy-density curves for metallic and molecular hydrogen. The curve for the metal has a minimum (at a density lower than that of the contact point on the tangent) and the metal is metastable here at zero pressure.

¹⁴See Ref. 5. The question of long-term stability at zero pressure is open at the moment.

STRESS-INDUCED ORDERING OF POINT DEFECTS IN COPPER NEAR 10°K*

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An anelastic process near 10°K has been found in proton-irradiated copper. It is tentatively identified as the result of stress-induced ordering of the interstitial member of a close pair. The reorientation occurs without annealing being observed. The thermal activation energy for reorientation is 0.015 eV; the strain symmetry axis is in the $\langle 111 \rangle$ direction.

The low-temperature behavior of point defects produced in copper by irradiating with energetic particles has been extensively studied in recent years.¹⁻⁵ These investigations have yielded much information concerning the annealing of these defects but have left clouded the issue of the atomic configuration of certain defects. By studying the mechical response of a sample to an alternating stress, one can in principle observe the stressinduced ordering of those defects with a strain field whose symmetry is lower than that of the lattice. By observing the effect of applying the stress along different crystallographic directions in single-crystal samples, any preferred orientation of the defect strain field may be investigated.

These measurements have been performed dur-

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¹J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. <u>108</u>, 1175 (1957).