Comments and Addenda

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Comments on the Liquid-Metal Model for the Calculated Electrical Resistivity of an Exploding Copper Wire

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It is shown that there is no justification for the recent attempt to treat an exploding wire as a liquid metal in calculating the electrical resistivity. An improved version of this calculation leads to a discrepancy of a factor of 12 between liquid-metal theory and the exploding-wire experiment.

In a recent paper, Ben-Yosef and Rubin[1] (BR) calculated the electrical resistivity ρ of liquid Cu as a function of density and found 10% agreement between their results and exploding-wire measurements[2] over a wide density range. On this basis, they concluded that a liquid metal is a suitable model for calculating the electrical resistivity of an exploding wire. We wish to call attention to a totally unwarranted assumption which is fundamental to their entire calculation. They assumed that the pseudopotential for Cu can be adequately represented by the simple form of a screened Coulomb potential. We shall show that using an improved form for the pseudopotential leads to a result for ρ differing from that of BR by a factor of 12. This eliminates the 10% agreement with experiment found by BR for their calculation of ρ, and calls into question the meaningfulness of their conclusions.

BR calculated the resistivity using the Ziman formula[3]

$$\rho = C\int_0^1 x^3 v^2(x) a(x)\, dx, \qquad (1)$$

where C is a known constant, $x = q/2k_F$, $v(x)$ is the pseudopotential, and $a(x)$ is the static structure factor. For $v(x)$, BR used essentially the form calculated by Harrison,[4] which for Cu turned out to be approximately a screened Coulomb potential. For $a(x)$, BR chose the Ashcroft-Lekner hard-sphere model.[5] BR found that assuming a value of the hard-sphere diameter $\sigma = 3.05$ Å for all densities gave agreement with the data to within 10% over the density range $n = (1.2\text{–}3.3)\times 10^{22}$ cm^{-3}.

Our principal criticism of the BR calculation lies in their choice of a screened Coulomb potential for $v(x)$. This form of $v(x)$ is negative for all x, a result contradicted by band calculations.[6] In Harrison's[4] $v(x)$ for Cu, the repulsive (positive) contribution, represented by his parameter β [$=2.2$ in units of Ry (Bohr radius)^3], turned out to be very small. On this basis, BR set β equal to zero, ignoring entirely the positive contribution to $v(x)$, and obtained a simple screened Coulomb potential. However, Harrison states that he applied his method of calculating the pseudopotential to Cu in a formal way only in order to illustrate how *unsuitable* his method is for the noble metals. As he notes,[4] "The assumption that the core states are the same [in the metal] as in the atom is completely inadequate for copper···. Further, the entire perturbation treatment is questionable." Indeed, Harrison's calculated pseudopotential for Cu, employed by BR, is grossly in error. In particular, this $v(x)$ has a relatively large *negative* value at the first reciprocal-lattice vector, corresponding to $x = 1.11$, whereas all band calculations[6] for Cu demand that $v(x = 1.11)$ be *positive*. Harrison himself points out this discrepancy, emphasizing that "This confirms our misgivings at the start ···."

To illustrate how important it is to use the proper pseudopotential for calculating ρ, we have repeated the calculation of BR using the same $a(x)$ but a much sounder approximation to $v(x)$. We chose the repulsive parameter such that $v(x)$ equals one-half of the band gap[6] ($E_{\text{gap}} = 0.44$ Ry) at the smallest reciprocal-lattice

[1] N. Ben-Yosef and A. G. Rubin, Phys. Rev. Letters **23**, 289 (1969).
[2] A. G. Rubin and C. V. Fish (to be published).
[3] J. M. Ziman, Phil. Mag. **6**, 1013 (1961).
[4] W. A. Harrison, Phys. Rev. **131**, 2433 (1963).
[5] N. W. Ashcroft and J. Lekner, Phys. Rev. **145**, 83 (1966).
[6] See the article by F. M. Mueller, Phys. Rev. **153**, 659 (1967), and references therein.

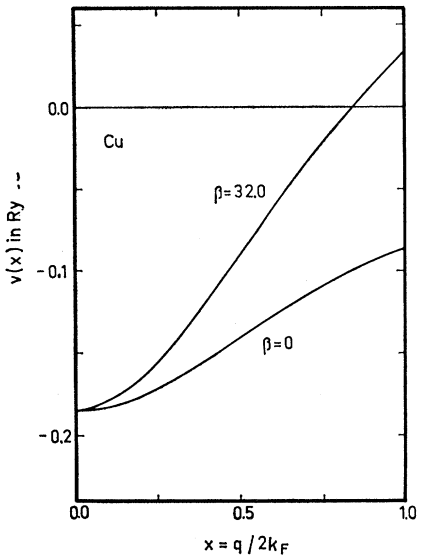

FIG. 1. Pseudopotential for Cu at the density $n=3.3\times10^{22}$ cm^{-3}. The curve with $\beta=0$ corresponds to the choice of Ben-Yosef and Rubin, whereas our choice of $\beta=32.0$ gives a much more realistic estimate.

vector, corresponding to $x=1.11$ at $T=0$°K. The requirement leads to the value $\beta=32.0$, a value quite comparable to the value of β for other metals (see Table III of Ref. 4). Using this improved, more realistic $v(x)$ (see Fig. 1), we repeated the calculation of BR at the density $n=3.3\times10^{22}$ cm^{-3} and obtained a resistivity smaller by a factor of 12. It is easy to understand this large change in ρ. For the potential used by BR, over 80% of the contribution to ρ comes from the region of the integral between $0.8<x<1.0$. A glance at Fig. 1 shows the large percentage change in $v(x)$ between the two pseudopotentials in this important region. If one notes that the square of $v(x)$ appears in the integral for ρ, one is not surprised to find an order of magnitude decrease in ρ.

We wish to emphasize clearly that our choice for $v(x)$, though qualitatively correct, is *not* to be taken as quantitatively accurate. Though our $v(x)$ represents a most reasonable choice within the framework of the single-plane-wave formalism, nevertheless, as is well known, the large *s-d* interaction for Cu requires special handling.

We would also like to comment on BR's choice for the static structure factor $a(x)$. They choose the Ashcroft-Lekner hard-sphere model[5] for $a(x)$ with the hard-sphere diameter $\sigma=3.05$ Å. BR claim that this choice of $a(x)$ with this fixed value for σ at all densities adequately represents the static structure factor over a wide range of density. One should test this assertion by comparing to the measured $a(x)$ data for liquid Cu at ordinary densities, the only density range for which experimental data is available for comparison. However, at ordinary densities ($n\simeq8\times10^{22}$ cm^{-3}), the value $\sigma=3.05$ Å implies the totally unphysical result of a packing fraction which exceeds considerably the value of 0.74 that corresponds to the closest possible packing in the solid phase. In fact, the BR packing fraction of 1.18 even exceeds unity.

In conclusion, we take issue with the BR assertions (a) that an exploding wire can be treated as a liquid metal for calculating the electrical resistivity, (b) that a screened Coulomb potential is an adequate representation for the pseudopotential of Cu, and (c) that the Ashcroft-Lekner hard-sphere model for $a(x)$ with a density-independent hard-sphere diameter of 3.05 Å provides a suitable description of the static structure factor for liquid Cu.