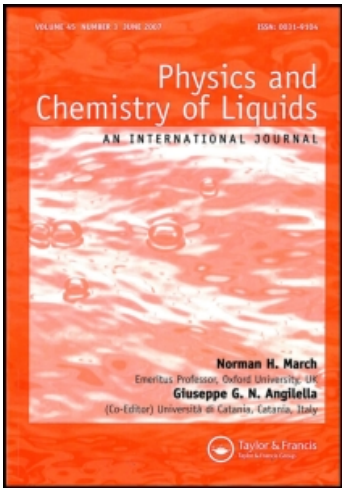

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DIAGONAL DISORDER EFFECTS IN THE MEAN FREE PATH OF LIQUID METALS

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In this work we take account of Fermi level broadening in Bardeen's disorder scattering model. This effect is included in our calculation of the electronic density matrix. We discuss the importance of considering an energy dependent mean free path and we conclude by calculating the Dirac density matrix in the presence of these new ingredients.

KEY WORDS: Density matrix, Fermi level broadening.

1 INTRODUCTION

In the presence of a disordered array of scatters the mean free path l of a conduction electron is certainly finite if it has a wave number of the order of the Fermi wave number. A finite l smears the Fermi surface and introduces an uncertainty in the k values of these electrons. This means in other words that in the presence of disordered scattering the wave number is not necessarily a good quantum number.

We take no attempt in this work to determine the exact density matrix of an electron in a random field produced by disordered centres in a metal. We shall turn our attention instead to a much simpler model put forward long ago by Bardeen[1] which, when combined with inverse transport theory, develops into a self-consistent generalization of Ziman's formula for the electrical resistivity. The resulting theory makes full consideration of Fermi surface relaxation[2,3]. We develop this model a bit further showing how to take explicit account of the energy levels broadening and of the energy dependence of the mean free path.

2 SIMPLE DISORDER SCATTERING MODEL FOR EXTENDED STATES

Supposing that all the scattering centres of the metal are distributed randomly in a slab of finite width, Bardeen calculated the energy derivative $\sigma(\mathbf{r},\mathbf{r}'; E_f)$ of the Dirac density matrix at the Fermi surface. Using free electron states and taking into account

the fact that collision destroys the plane wave's coherence, he was able to show that scattering plus configurational averaging turns σ into

$$\sigma(\mathbf{r}, \mathbf{r}'; E_f) = \sum_i e^{i\mathbf{k}_i \cdot (\mathbf{r}-\mathbf{r}')} \delta(E_f - E_i) e^{-|\mathbf{r}-\mathbf{r}'|/2l}$$

$$= \sigma_0(\mathbf{r} - \mathbf{r}'; E_f) e^{-|\mathbf{r}-\mathbf{r}'|/2l} \tag{1}$$

where E_f is the Fermi energy, l is the electronic mean free path at the Fermi surface, and σ_0 is its free electron value:

$$\sigma_0(\mathbf{r} - \mathbf{r}'; E_f) = \frac{\sqrt{2E_f}}{\pi^2} \frac{\sin(\sqrt{2E_f}|\mathbf{r} - \mathbf{r}'|)}{\sqrt{2E_f}|\mathbf{r} - \mathbf{r}'|} \tag{2}$$

The Bardeen density matrix $n(\mathbf{r}, \mathbf{r}'; E_f)$ can be obtained directly from Eq. (1) if we neglect the mean free path's energy dependence. Using standard theory it then follows that

$$n(\mathbf{r}, \mathbf{r}'; E_f) = \int_0^{E_f} dE\, \sigma(\mathbf{r}, \mathbf{r}'; E_f)$$

$$= n_0(\mathbf{r} - \mathbf{r}'; E_f) \exp(-|\mathbf{r} - \mathbf{r}'|/2l), \tag{3}$$

where

$$n_0(\mathbf{r} - \mathbf{r}'; E_f) = \frac{(2E_f)^{3/2}}{\pi^2} \frac{j_1(\sqrt{2E_f}|\mathbf{r} - \mathbf{r}'|)}{\sqrt{2E_f}|\mathbf{r} - \mathbf{r}'|} \tag{4}$$

is the free electron density matrix, with j_1 being the spherical Bessel function of order 1. The finite mean free path effect, in Bardeen's approximation, is only basically manifest in the off-diagonal density matrices.

As a result if we take the limit $\mathbf{r} \to \mathbf{r}'$ in $n(\mathbf{r}, \mathbf{r}'; E_f)$ it then follows that

$$\lim_{\mathbf{r} \to \mathbf{r}'} n(\mathbf{r} - \mathbf{r}'; E_f) = \frac{k_f^3}{3\pi^2} \tag{5}$$

indicating that there is no shift in the Fermi wave number for a finite l. The existence of a damping factor $e^{-|\mathbf{r}-\mathbf{r}'|/2l}$ guarantees the absence of any discontinuity in the occupation number $n(k)$ at $k = k_f$. However since in Bardeen's model all one-electron states are equally attenuated the mean free path effect is overestimated in the low k region[4]. It is therefore essential to transcend Bardeen's approximation to improve on these two aspects of the theory.

3 DIAGONAL DISORDER EFFECT

The mean free path is essentially the distance over which the electronic wave loses its coherence. When l is finite the uncertainty principle introduces a spread in the k values of all the scattered electrons. Thus, for a short mean free path this spread is larger and the probability that the particle suffers the collision is higher. Let us then assume that the electrons most likely to take part in the scattering process are related to one-

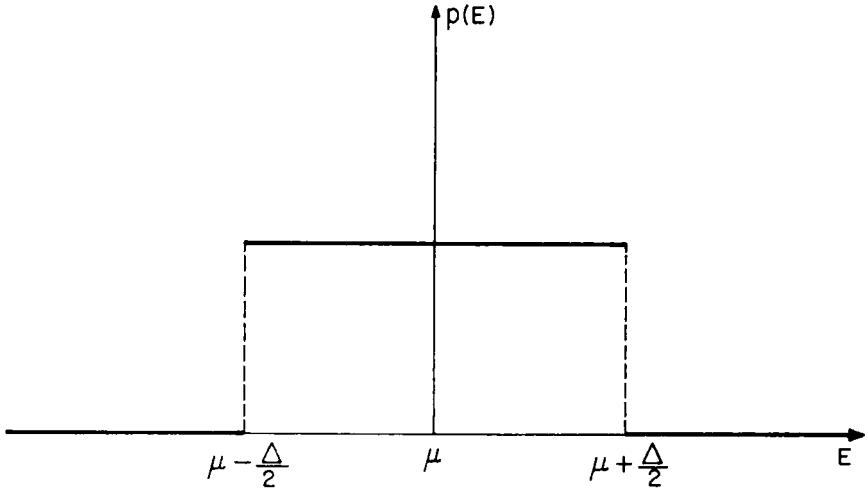

Figure 1

electron states which belong to a continuum of energies of width $\Delta \cong \sqrt{2\mu}/l$, around $E \cong \mu$, with μ being the new chemical potential. Let $p(E)$ be the probability that the scattered particle has a particular energy E value in this continuum of finite width. If, for simplicity, we suppose that all these one-election levels relate to particles with equal probability of being scattered, $p(E)$ takes the simple form below which is displayed in Figure 1.

$$p(E) = \begin{cases} \dfrac{l}{\sqrt{2\mu}} & \mu - \dfrac{\Delta}{2} \leq E \leq \mu + \dfrac{\Delta}{2} \\ 0 & \text{for any other } E \text{ values} \end{cases} \tag{6}$$

Using $p(E)$ we can now argue that the density matrix $\langle \sigma(\mathbf{r}, \mathbf{r}'; \mu) \rangle$ which makes explicit consideration of the Fermi level broadening is the energy average

$$\begin{aligned} \langle \sigma(\mathbf{r}, \mathbf{r}'; \mu) \rangle &= \int_{-\infty}^{\infty} p(E)\sigma(\mathbf{r}, \mathbf{r}'; E)dE \\ &= \frac{l}{\sqrt{2\mu}} \int_{\mu - \Delta/2}^{\mu + \Delta/2} l(E) \frac{\sqrt{2E}}{\pi^2} \frac{\sin(\sqrt{2E}R)}{\sqrt{2E}R} e^{-R/2l(E)}\, dE, \end{aligned} \tag{7}$$

with $R = |\mathbf{r} - \mathbf{r}'|$

If we suppose that $l(E) \cong l$ for the energy region of width Δ around $E \cong \mu$, the previous integral can be easily evaluated to give

$$\begin{aligned} \langle \sigma(R; k_\mu) \rangle = \frac{l e^{-R/2l}}{\pi^2 k_\mu R} &\left\{ \left(k_\mu^2 + \frac{k_\mu}{l} \right) j_1 \left[\left(k_\mu^2 + \frac{k_\mu}{l} \right)^{1/2} R \right] \right. \\ &\left. - \left(k_\mu^2 - \frac{k_\mu}{l} \right) j_1 \left[\left(k_\mu^2 - \frac{k_\mu}{l} \right)^{1/2} R \right] \right\} \end{aligned} \tag{8}$$

with $k_\mu = \sqrt{2\mu}$. Note that if we take the limit $l \to \infty$, $\langle \sigma(R; k_\mu) \rangle$ reduces correctly to the free electron result. In order to complete this discussion we need to establish how the wave number k_μ relates to both k_f and l^{-1}. As we show next this problem is easily solved if we construct the averaged Dirac density matrix $\langle n(R; k_\mu) \rangle$.

4 AVERAGED DIRAC DENSITY MATRIX AND MEAN FREE PATH-ENERGY DEPENDENCE

The averaged density matrix $\langle n(R; k_\mu) \rangle$ can be obtained in principle from the integral

$$\langle n(R; k_\mu) \rangle = \int_0^{k_\mu} \mathrm{d}k \, k \langle \sigma(R; k) \rangle \tag{9}$$

with $k = \sqrt{2E}$. If we then use Eq. (8) to replace $\langle \sigma(R; k) \rangle$ it follows that

$$\langle n(R; k_\mu) \rangle = \frac{1}{\pi^2 R} \int_0^{k_\mu} \mathrm{d}k \, l(k) \left\{ \left(k^2 + \frac{k}{l(k)} \right) j_1 \left[\left(k^2 + \frac{k}{l(k)} \right)^{1/2} R \right] - \left(k^2 - \frac{k}{l(k)} \right) j_1 \left[\left(k^2 - \frac{k}{l(k)} \right)^{1/2} R \right] \right\} e^{-R/l(k)} \tag{10}$$

Due to the their long wave numbers the low energy one-particle states are expectedly insensitive to the random field produced by the disordered array of scatterers. These

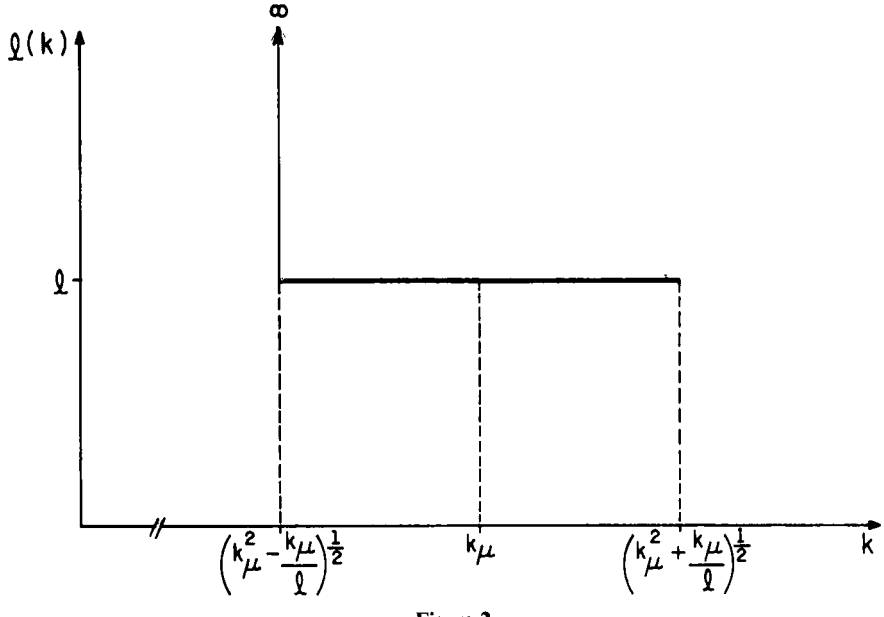

Figure 2

particles will rarely suffer any collision. It is therefore reasonable to consider them as nearly stationary. If we take this assumption further a natural approximation for $l(k)$ is

$$l(k) = \begin{cases} \infty & k \leq \left(k_\mu^2 - \dfrac{k_\mu}{l}\right)^{1/2} \\ l & \left(k_\mu^2 - \dfrac{k_\mu}{l}\right)^{1/2} \leq k \leq k_\mu \end{cases} \tag{11}$$

where l is the electronic mean free path to be determined self-consistently by the transport theory. The simple form of $l(k)$ is shown in Figure 2. If we substitute this last result in Eq. (10) it follows immediately that

$$\begin{aligned} \langle n(R; k_\mu)\rangle = {} & \frac{(k_\mu^2 - k_\mu/l)\, j_1[(k_\mu^2 - k_\mu/l)^{1/2} \cdot R]}{\pi^2 R} \\ & + \frac{l e^{-R/2l}}{\pi^2 R} \int_{(k_\mu^2 - k_\mu/l)^{1/2}}^{k_\mu} \left\{ \left(k^2 + \frac{k}{l}\right) j_1\left[\left(k^2 + \frac{k}{l}\right)^{1/2} R\right] \right. \\ & \left. - \left(k^2 - \frac{k}{l}\right) j_1\left[\left(k^2 - \frac{k}{l}\right)^{1/2} R\right] \right\} \end{aligned} \tag{12}$$

Evaluating this last integral $\langle n(R; k_\mu)\rangle$ becomes

$$\begin{aligned} \langle n(R; k_\mu)\rangle \cong {} & \frac{(k_\mu^2 - k_\mu/l)}{\pi^2} \frac{j_1[(k_\mu^2 - k_\mu/l)^{1/2} R]}{R} \\ & + \frac{l e^{-R/2l}}{\pi^2 R} \left\{ \frac{2}{R^3} \left[2 \sin\left(\frac{R}{2l}\right) \left(\sin k_\mu R - \sin\left(k_\mu - \frac{1}{2l}\right) R \right) \right. \right. \\ & + \left(k_\mu - \frac{1}{2l}\right) R \left(\sin k_\mu R - \cos(R/2l) \sin\left(k_\mu - \frac{1}{2l}\right) R \right) \\ & \left. - k_\mu R \sin\left(\frac{R}{2l}\right) \cos k_\mu R - \frac{R}{2l} \sin k_\mu R \cos\left(\frac{R}{2l}\right) \right] \\ & + \frac{1}{4l^2 R^2 k_\mu^2} \left[k_\mu \sin\left(\frac{R}{2l}\right) \left(\cos k_\mu R - \cos\left(k_\mu - \frac{1}{2l}\right) R \right) \right. \\ & \left. \left. \left. + \frac{1}{2l} \sin k_\mu R\,(1 - \cos(R/2l)) \right] \right] \right\} \end{aligned} \tag{13}$$

Note that the first term of the averaged density matrix is simply the free electron result with k_f shifted to $(k_\mu^2 - k_\mu/l)^{1/2}$. Again in the limit $l \to \infty \langle n(R; k_\mu)\rangle$ reduces correctly to $n_0(R; k_f)$.

In order to establish how k_μ relates to both k_f and $1/l$ it is sufficient to invoke the conservation of the total number of conduction electrons. This implies that, in the

Table 1 Chemical potential wave number, Fermi wave number and empirical mean free path for some liquid metals.

Element	k_μ	k_f	l
Na	0.920×10^8 cm^{-1}	0.920×10^8 cm^{-1}	147×10^{-8} cm
Li	1.116	1.12	35.7
Al	1.74	1.75	18
Hg	1.35	1.37	6.8
Pb	1.61	1.64	5

lim $R \to$ O, $\langle n(R; k_\mu)\rangle$ satisfies the condition.

$$\lim_{R\to O} \langle n(R; k_\mu)\rangle \cong \frac{k_\mu^3}{3\pi^2}\left[1 + \frac{3}{8}\frac{1}{k_\mu l} + O(l^{-2})\right]$$

$$\cong \frac{k_\mu^3}{3\pi^2}\Big|[1 - 3/(8k_\mu l)] = \frac{k_f^3}{3\pi^2} \tag{14}$$

In Table 1 we display the calculated k_μ together with the corresponding k_f and $1/l$ values for some liquid metals. For short mean free path k_μ is slightly shifted with respect to k_f.

5 CONCLUSION

In this work we generalized Bardeen scattering model to take explicit account of the Fermi level broadening. We argued that, in liquid metals, it is more appropriate to consider all one-electron states, which are far below the blurred Fermi surface region, as nearly stationary. For this reason we considered an energy dependent mean free path.

In order to show how large the Fermi level broadening is we display, in Table 2, Δ values, together with the corresponding Fermi energy, for several liquid metals. For alkaline metals, Δ/E_F is quite small. However, for short mean free path liquids such as Pb, this broadening is considerable. Naturally, we need a transport theory to calculate the mean free path self-consistently. If we use the theory of inverse transport coefficients, l is given in terms of the force-force correlation function F. An important ingredient in this theory is precisely the function $\Gamma(k, k_\mu, l)$ which is the Fourier transform of $|\sigma(R; k_\mu)|^2$. The numerical results which show how the new features discussed in this work affect the mean free path calculation will be presented in a later stage.

Table 2 Broadening width Δ, Fermi energy and Δ/E_f ratio.

Element	Δ	E_f	Δ/E_f
Na	6.26×10^{13} cm^{-2}	0.42×10^{16} cm^{-2}	0.015
Li	31.3	0.63	0.049
Al	96.7	1.53	0.063
Hg	198	1.87	0.11
Pb	322	1.34	0.24

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