Metals with Small Electron Mean-Free Path: Saturation versus Escalation of Resistivity

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Abstract
Resistivity of metals is commonly observed either to ‘escalate’ beyond the Ioffe-Regel limit (mean free path \( \ell \) equal to lattice constant \( a \)) or to ‘saturate’ at this point. It is argued that neither behavior is well-understood, and that ‘escalation’ is not necessarily more mysterious than ‘saturation.’

72.15.Eb, 72.15.Lh, 72.15.Rn

During the period 1954-1986, ‘high temperature’ superconductivity occurred primarily in Nb\(_3\)Sn and related materials with the A15 crystal structure. Although peculiar resistivity \( \rho(T) \) had been noticed \cite{1} and modeled (corrected for non-zero \( k_B T/\epsilon_F \)) \cite{2}, it was not until the Fisk-Lawson paper \cite{3} that the general nature of the peculiarity was known. At first the peculiarity seemed to correlate with high \( T_c \) and therefore large electron-phonon coupling, but the Fisk-Webb paper \cite{4} showed that even a low \( T_c \) material had ‘saturating’ resistivity when the resistivity became large enough. Data from these two classic papers is shown in Fig. 1. Fisk and Webb observed that the mean free path \( \ell \) was becoming nearly as small as the lattice constant \( a \). This violation of the condition \( \ell \gg a \) (required for validity of the quasiparticle picture and the Bloch-Boltzmann resistivity theory) seemed from the available data to lead quite generally to ‘saturation’ of resistivity. Unfortunately, correcting theory for non-zero \( a/\ell \) (with values of order 1) is more important, and much more difficult than correcting for non-zero \( k_B T/\epsilon_F \) (which is usually small.)

To strengthen the case, ‘saturation’ could be provoked not only by the thermal disorder of high \( T \) lattice vibrations, but also by static disorder, such as radiation damage \cite{5}. It could also be modelled by a ‘shunt-resistor model’ \cite{6} \( 1/\rho(T) = 1/\rho_{\text{Boltz}} + 1/\rho_{\text{sat}} \). If we take the saturation value \( \rho_{\text{sat}} \) to be the same as the Boltzmann value \( \rho_{\text{Boltz}} \) extrapolated to the Ioffe-Regel point \( \ell = a \), then the ‘shunt-resistor’ formula can be written \( \rho(T) = \rho_{\text{Boltz}}(T)/(1 + a/\ell(T)) \). When \( a/\ell(T) \) is large and the second term dominates the denominator, then \( \ell(T) \) cancels from the formula and \( \rho \) becomes independent of \( T \).

In spite of the explicit warning \cite{4} that no theory of ‘saturation’ existed, it was often assumed that the case was closed. The reasoning \cite{7} was that \( \ell \) cannot sensibly become smaller than \( a \), so one should just use the Boltzmann result with \( \ell \) replaced by \( a \). The fault with this argument \cite{8} that it denies the possibility of Anderson localization under static disorder, was easy to forget. A careful theoretical discussion has to mention that if \( \ell \) is not longer than \( a \), then the concept of a mean free path has to be abandoned. One has no right to take a formula which contains a factor \( 1/\ell \) and replace it with \( 1/a \), because the theoretical framework which provided the formula has already been destroyed.

FIG. 1. Upper panel: resistivity from Ref. \cite{3} normalized to the value at 273 K. The ‘bulge’ in Rh\(_{17}\)S\(_{15}\) was originally correlated with the higher superconducting transition. Lower panel: absolute resistivity from Ref. \cite{4} of a good superconductor (Nb\(_3\)Sn, \( T_c = 18 \) K) saturates at the same final resistivity value as a poor superconductor (Nb\(_3\)Sb). This shows that ‘saturation’ correlates with magnitude of resistivity rather than \( T_c \) or strength of electron-phonon coupling.
In recent years it became possible to calculate resistivity for highly disordered metals (with non-interacting electrons) by the Kubo formula or an equivalent Landauer formulation. The results for the most familiar model are shown in Fig. 2. Rather than saturating, the resistivity escalates. In the center of the band formed by a single s orbital on a simple cubic lattice, Boltzmann theory (in Born approximation, at $T = 0$) gives \[ \rho_{\text{Boltz}} = (\hbar/a^2)(6.94a/\ell), \] and $a/\ell = 0.0283(W/\ell)^2$, where $t$ is the hopping parameter and $\pm W/2$ is the interval of the random on-site disorder potential. Numerically converged results for large disorder are plotted versus $a/\ell$, with $a$ set arbitrarily at 3 Å. Of course, $\ell$ is meaningless over most of the range shown, and the horizontal axis is just an alternate parameterization of $(W/\ell)^2$.

There are three things to notice: (1) Boltzmann theory continues to give a good answer even at $a/\ell = 1$ where it is invalid; (2) there is a very large interval between the Ioffe-Regel point $a/\ell = 1$ and the point where states become all localized, $(a/\ell)_c = 7.71$; (3) rather than saturating, the resistivity escalates toward the scaling region where it diverges as $((a/\ell)_c - a/\ell)^{-\nu}$ with critical exponent $\nu \approx 1.57$.

![FIG. 2. Resistivity of a half-filled s-band on a cubic lattice with random on-site potential fluctuations, plotted versus $a/\ell$. Here $\ell$ is not a physical mean free path, but instead the value given by Boltzmann theory, extended beyond is range of validity. The points were calculated in ref. 9. The solid line is the Bloch-Boltzmann prediction in Born approximation. The dashed line is the expected saturated form, $\rho_{\text{sat}}/(1 + a/\ell)$, and the dot-dashed line is a naive scaling formula $\rho_{\text{sat}}/(1 - \ell_c/\ell)$, with $\ell_c = a/7.71$, the observed point of the Anderson transition.](image)

One of the first indications that ‘saturation’ was not ubiquitous was the observation by Gurvitch and Fiory that resistivity of high $T_c$ superconductors seems to fail to saturate. The failure of ‘saturation’, which I will call ‘escalation’, is probably not rare after all. Emery and Kivelson call such metals ‘bad metals.’ Fig. 3 shows resistivities of several metals. Alkali-doped C$_{60}$ saturates (if at all) only for very short $\ell$ (less than 1 Å.) Among oxide metals, saturation seems rare for simpler compounds like Sr$_2$RuO$_4$, and may occur at very large resistivity values for certain complex oxides like La$_4$Ru$_6$O$_{19}$. Quite likely the mean free path in this last case is also very small.

![FIG. 3. Resistivity versus temperature for various metals. Data are from Ref. 13 (K$_3$C$_{60}$); Ref. 14 (Sr$_2$RuO$_4$); Ref. 16 (La$_4$Ru$_6$O$_{19}$). The error bars represent the error estimated in the geometric normalization for K$_3$C$_{60}$.](image)

There are exotic theories which attribute ‘bad metal’ behavior to quasi-1d electron conduction on fluctuating stripes. One can naively model this by meandering stripes containing metallic electrons whose resistivity is not high. Dilution of the metallic stripes in an intervening non-metallic phase causes an apparent high resistivity and short mean-free path. Arnason et al. reported an interesting experiment where a static real-space model doped C$_{60}$, and Calandra and Gunnarsson use a 3-fold degenerate band to model doped C$_{60}$, and Calandra and Gunnarsson use a 5-fold degenerate band to model Nb$_3$X. These interesting quantum-Monte-Carlo (QMC) calculations find no saturation in the C$_{60}$ model, and saturation in the Nb$_3$X model. The difference apparently is in the form of electron-phonon coupling used (Coulomb inter-
actions were omitted). When phonons were coupled to on-site potential as in Fig. 3, saturation was not found, whereas when coupled to the hopping matrix element, vibrations were found to cause saturating resistivity. In this latter case, theoretical QMC results could be fit by Kubo theory calculated under the assumption that vibrations could be treated adiabatically, i.e., modelled as static disorder. This approximate analysis agrees with qualitative arguments I made with Chakraborty long ago [23], emphasizing the importance of allowing a multi-orbital band structure.

The conclusions to draw from this are: (1) there still is no theory of saturation, although computational results are giving a first outline; (2) it seems no harder to account for escalation than for saturation. Therefore it is perhaps an unproven guess that metals with escalating resistivity are more exotic than metals which show saturation. However, an exotic origin of escalation has been nicely demonstrated in the case of high $T_c$ cuprates. Resistivity versus doping and temperature was re-examined by Ando et al. [24]. They make a very convincing case that the mechanism of transport is intimately related to antiferromagnetic correlations over a wide doping range. A candidate picture by which this can happen is the model of self-organizing stripe inhomogeneities [17].

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