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ANHARMONICITY AS AN EXPLANATION FOR ANOMALOUS RESISTANCE OF HIGH-$T_c$ SUPERCONDUCTORS

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Experimental evidence about the temperature dependence of phonon frequencies in $V_3Si$ is used to demonstrate that anharmonicity is a major factor in causing the resistance anomalies recently observed in many high-$T_c$ superconductors.

FISK and collaborators$^1$ have recently pointed out that the electrical resistance of high temperature superconductors (generally intermetallic compounds with both $s$–$p$ and $d$-band constituents) deviates strongly from the Bloch–Gruneisen$^2$ behavior generally found in other metals. A typical example is $V_3Si$ for which the data$^3$ are shown in Fig. 1. Usually the Bloch–Gruneisen theory is interpreted to mean that the difference between the resistivity $\rho(T)$ for $T \gg \theta_D$ from the limiting (impurity dominated) resistivity for $T \to 0$ is linear in temperature, i.e.

$$\rho(T) - \rho_0 = \rho_{s-p}(T)$$

$$= (2nmk_B/n^2\hbar)\lambda_{tr}T, \quad \text{for} \quad T \gg \theta_D, \quad (1)$$

where $(n/m)$ is the effective ratio of electron density to mass, and $\rho_{s-p}(T)$ is a complicated integral over the phonon distribution which simplifies at high temperatures to a linear power of $T$. The strength of the electron–phonon coupling is measured by the dimensionless number$^4 \lambda_{tr}$ which is closely related to the coupling constant $\lambda$ of superconductivity theory.$^5$ It is immediately clear that the data of Fig. 1 cannot satisfy equation (1) because the high temperature resistivity is not really linear. If we denote by $\rho^*(T)$ the extrapolated resistivity at zero temperature from the slope at temperature $T$, then $\rho^*(T) > \rho_0$ for $T \gtrsim 150$ K. (For $V_3Si\theta_D \approx 300$ K.) The quantity $\zeta(300) \equiv [\rho^*(300) - \rho_0]/[\rho(300) - \rho_0]$ can be estimated from the data to be about 0.5. The data in Fig. 1 is taken from a published paper$^3$ and the drawing of slopes is hazardous. We can be in error in estimating $\zeta(300)$ by as much as 50% in either direction.

Many possible explanations for this discrepancy have been given.$^6$ In this note we present evidence for a particularly simple explanation, namely that $\lambda_{tr}$ in equation (1) is temperature dependent because of an anomalously strong temperature dependence of the phonon frequencies. Following McMillan,$^5$ we write $\lambda_{tr}$ as

$$\lambda_{tr} = \frac{n_{tr}}{M(\omega^2)} \quad (2)$$

where $n_{tr}$ is a purely electronic factor involving the electron density of states and matrix elements averaged over the Fermi surface, $M$ is an averaged atomic mass, and $\langle \omega^2 \rangle$ is a mean square phonon frequency calculated with a weight factor $F(\omega)/\omega$ where $F(\omega)$ is the phonon density of states. (This involves an assumption that the coupling factor $a^2_{tr}(\omega)$ is roughly independent of $\omega$, an approximation which probably only fails at small $\omega$.) If we assume the validity of equation (1) at high temperatures, then we can write

$$\zeta(T) = \frac{[\rho^*(T) - \rho_0]/[\rho(T) - \rho_0]}{\rho_{s-p}(T)/\rho_{s-p}(0)}$$

$$= \frac{d \log (\omega^2)}{d \log T} - \frac{d \log (n/m)n_{tr}}{d \log T} \quad (3)$$

A close approximation to the phonon density of
Table 1. Experimental mean squared phonon frequencies and interpolated value of \( d \log (\omega^2)/d \log T \) compared with experimental resistance \( R(300) = [R(300) - \rho_0]/[\rho(300) - \rho_0] \) for four A-15 structure superconducting compounds.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Superconductive ( T_c (K) )</th>
<th>( \omega^2 ) (meV²)</th>
<th>( \omega^2 ) (meV²)</th>
<th>Fractional anharmonicity ( 1 - c )</th>
<th>( d \log (\omega^2) )/d ( \log T )</th>
<th>( \lambda(300) )</th>
<th>Experimental</th>
</tr>
</thead>
<tbody>
<tr>
<td>V₃Si</td>
<td>17</td>
<td>763</td>
<td>642</td>
<td>0.16</td>
<td>0.31</td>
<td>0.5⁵, 0.3⁷</td>
<td></td>
</tr>
<tr>
<td>V₃Ga</td>
<td>15</td>
<td>456</td>
<td>408</td>
<td>0.072</td>
<td>0.17</td>
<td>0.45, 0.3⁷</td>
<td></td>
</tr>
<tr>
<td>V₃Ge</td>
<td>6</td>
<td>572</td>
<td>532</td>
<td>0.06</td>
<td>0.12</td>
<td>0.3⁷</td>
<td></td>
</tr>
<tr>
<td>Nb₃Sn</td>
<td>18</td>
<td>331</td>
<td>287</td>
<td>0.072</td>
<td>0.21</td>
<td>0.6⁸</td>
<td></td>
</tr>
</tbody>
</table>

* Reference 7. b \( T = 4.2 \, K \).,c \( T = 77 \, K \). d \( T = 5.58 \, K \). e Reference 3.


Fig. 1. Experimental values of electrical resistance \( \rho \) as a function of temperature \( T \) for V₃Si (from reference 3). The value \( \rho(296) - \rho_0 = 35 \, \mu\Omega\cdot\text{cm} \) found by linear extrapolation deviates significantly from the Bloch–Gruneisen value of 0.

Fig. 2. Experimental values of \( \log(\omega^2) \) (calculated from the phonon densities of states of reference 7) plotted vs \( \log T \). The solid line is an empirical fit using equation (6).
only about 60% of the effect we are looking for. However, as already mentioned our deduction of \(\Omega(300)\) from the data is quite uncertain. So is the deduction of \(\langle \omega^2(T) \rangle = \frac{1}{2} \frac{d \log \langle \omega^2 \rangle}{d \log T}\) at room temperature from the data which extends only to room temperature. More precise knowledge of resistivity as well as measurements of \(\omega^2\) at higher temperatures are required to see whether mechanisms other than the one discussed here contribute significantly to the resistivity anomaly.

Reichardt and collaborators at Karlsruhe have also sent us unpublished data for \(F(\omega)\) in \(V_3Ga\), \(V_3Ge\), and \(Nb_3Sn\) at two different temperature each. The moments \(\langle \omega^2 \rangle\) are shown in Table 1. For the varadium compounds, an incoherent scattering method was used, while for \(Nb_3Sn\), an average of several scattering angles was taken with a polycrystalline target. The interpolated values of \(\frac{d \log \langle \omega^2 \rangle}{d \log T}\) at room temperature are smaller than in \(V_3Si\), but still fairly large, and tend to scale with \(T^\alpha\), in agreement with Fisk's observations\(^1\) about resistance anomalies. As can be seen from Table 1, anharmonic effects can account for 30% of the anomaly in \(Nb_3Sn\).

Previous attempts\(^8\) to explain the resistivity anomaly have mainly invoked a temperature dependence of \((m/n)_{\pi r}\), which arises from having the electronic density of states vary rapidly with energy over a range \(kT\). It is hard to estimate the magnitude of this effect since no reliable knowledge of the density of states near the Fermi surface to this accuracy is available.

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4. See for example, GRIMVALL G., Phys. Kond. Mat. 11, 279 (1970). The factor \((\tilde{1} - \cos \theta)_{el-ph}\) of that paper is \(\lambda_{\mu r}\) of the present paper.