Semiclassical Theory of Thermal Resistivity in Metals

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We extend traditional semiclassical approaches for electrons in metals to include thermal deformation potentials exerting forces on electrons, just as do external fields. The slowly traveling deformations nonperturbatively participate in smooth quasielastic exchange of energy and momentum with electrons. Analytic estimates and numerical simulations reveal an approximate $T^4$ rise in low temperature resistivity in 2D, followed by a rollover to linear in $T$ above the Bloch-Gruneisen temperature. The deformation potential takes the form of a blackbody classical electromagnetic field. Correlations of the same origin as in the Hanbury-Brown-Twiss effect cause non-Gaussian electron momentum diffusion, and suggest deviations from integer power law behavior.

Traditionally, electrons in metals under external electromagnetic fields are treated semiclassically [1, 2]. Band energy is promoted to the status of a Hamiltonian and external classical fields are added. This program is ultimately phenomenological, but very successful.

Since the 1950 paper of Bardeen and Shockley [3] the notion of a deformation potential resulting from phonon induced lattice strain has been firmly established, and used then as now in inelastic single electron-phonon perturbation theory.

Current practice if both deformation potentials and external fields is important is to use a mixed approach, treating the electron-phonon interaction by perturbation theory, and using semiclassical equations for the external fields [4].

Might there be a unified treatment for both, i.e. can the deformation potential be treated semiclassically, as a pseudoelectric field generating a classical force on the electron? The answer seems to be yes.

Semiclassical deformation model. Consider a uniform crystal at 0 Kelvin. For given band energy $E(k)$, the electron group velocity is $d\vec{r}/dt = \partial E(k)/\partial (\hbar k)$. If there are externaly applied electric and magnetic fields, the traditional phenomenological semiclassical model [1, 2] promotes the band energy to the role of the kinetic part of an electromagnetic Hamiltonian, with electric and magnetic fields $\vec{E}$ and $\vec{B}$ giving $d(\hbar k)/dt = -e\vec{E}(\vec{r}, t) - \frac{\hbar}{c} \vec{r} \times \vec{B}(\vec{r}, t)$; $c$ is the speed of light.

Responsibility for resistivity in a pure metal lies mainly with acoustic phonons, with inhomogeneities generated by strain - i.e. deformation potentials. These can be considered to generate pseudoelectric fields and put on a par with external fields. In fact, the thermal equilibrium deformation potential (equation (1), below) considered as an electric potential generates forces on the electron that follow the blackbody Planck radiation law, except for magnitude.

Moreover, electrons are in a semiclassical regime with respect to the deformation potential, with short Fermi level electron wavelengths compared to the scale of the pseudoelectric deformation fields. This supports the idea that the deformation potential can be taken into the semiclassical domain.

The deformation potential arises because band structure is affected locally by strain induced by acoustic phonons. We may take those phonon modes that are active at a given temperature (in the sense of Bose occupation) to be collected into coherent states, so an electron interacts smoothly and quasielastically with well defined, moving inhomogeneous pseudoelectric field gradients. There is an exact prescription for a thermal ensemble of coherent states (that have classical parameters for mean position and momentum) for a harmonic lattice that gives all equilibrium expectation values of operators [5]. This follows the role of the coherent states in classical electromagnetic fields, including blackbody radiation.

When interference effects are important, the full quantum version of the single electron dynamics is an option, as is the semiclassical Van Vleck-Morette-Gutzwiller Green function (the stationary phase version of the Feynman path integral). This is a program laid out for external fields long ago by Lifshitz and Kosevich[6].

The deformation potential. The ingredients for constructing a deformation potential begin with phonon induced lattice displacements. The important parameter is changes in atom-atom distances, i.e. the strain field [7]; rigid movement of groups of atoms are of little consequence.

The deformation potential becomes a time dependent sum over all longitudinal acoustic phonon modes of all propagation directions and with a weighting given by (the square root of) Bose occupations,

$$V_D(\vec{r}, t) = \frac{E_d}{v_s} \sum_k \sqrt{\frac{2\hbar \omega_k \cos (k \cdot \vec{r} - \omega_k t + \phi_k)}{\rho V \sqrt{\exp (\hbar \omega_k/k_B T)} - 1}}$$

where $\phi_k$ is an arbitrary phase shift of each mode, $v_s$
is the longitudinal acoustic sound speed and $\omega_k = v_s |\vec{k}|$, $E_d$ is the deformation potential constant that varies from several eV to tens of eV, $\hbar$ is the reduced Planck constant, and $k_B$ is the Boltzmann constant.

Constructing a random electromagnetic potential implied by Planck’s Law of thermal radiation yields the same form (in 2D and in 3D) as the deformation potential; the strength of the potential and the wave speed are of course different. The classical electromagnetic version of the deformation potential appeared already as a vector potential in Hanbury-Brown-Twiss[8]. Acoustic phonons are also linear dispersion thermally populated harmonic degrees of freedom, so the blackbody electromagnetic potential connection is not surprising, although it seems to have gone unnoticed.

In fact the controversy surrounding the early days of the Hanbury-Brown-Twiss effect involving the success of a classical wave explanation for what seemed manifestly to be a quantum phenomenon is precisely relevant to the present paper. As became clear in that discussion, leading no less than to the birth of quantum optics, quantum optical and classical field results are understood to be fully compatible, within now well understood limitations. The subject of electrical resistivity of metals has so far proceeded entirely within a paradigm analogous to quantum optics. Without any question, it can also cast so far proceeded entirely within a paradigm analogous to blackbody thermal and classical field results are understood to be fully compatible, within now well understood limitations.

We expect the (phenomenological) Hamiltonian equations

$$\frac{d(h\vec{k})}{dt} = -\frac{\partial E(\vec{k},\vec{r},t)}{\partial \vec{r}}; \quad \frac{d\vec{r}}{dt} = \frac{\partial E(\vec{k},\vec{r},t)}{\partial (h\vec{k})}, \tag{2}$$

where $E(\vec{k},\vec{r},t) = E(\vec{k},a(\vec{r},t))$ is a band energy in terms of the local atomic spacing $a(\vec{r},t)$, or better, the local strain field derived from the atomic spacings. We take the spacial dependence of $E(\vec{k},\vec{r},t)$ to be the deformation potential.

**Transparency above the Bloch-Grüneisen temperature.** A key constant in equation (1) is $k_{max}$, which can be $k_{max} \sim 2k_F$ where $k_F$ is the Fermi momentum, or if it comes earlier, $k_{max} \sim k_{Debye}$. In any case, $T_{BG} = 2\hbar v_s k_{max}/k_B$. At low temperature this restriction has no effect since the sum over modes effectively cuts off sooner, but at the Bloch-Grüneisen temperature and above the cut off is important. If $k_{max} \sim k_{Debye}$, undulations in the deformation potential shorter than $\lambda_F = 2\pi/k_F$ have little refractive influence on the electrons at the Fermi level and it is as if there were not present. This is a well known ballistic transparency effect for small scale fluctuations of a medium that are uniform when averaged over a wavelength or so [9], familiar for visible light in clear glass for example.

Figure 1 gives numerical examples demonstrating the transparency specific to short wave components of the deformation potential, uniform on larger scales, but random on small scales.

Above $T_{BG}$, electrons continue to be refracted by the longer wavelength components of the deformation potential, which are getting stronger as temperature increases. In our classical simulations we omitted the short wavelength components of the deformation potential that develop above the Bloch-Grüneisen transition.

**Properties and influence of the deformation potential.** In our semiclassical approach, the deformation potential generates a classical force deflecting electron ray paths. The picture is one of gently curving rays suffering the unruly (but not completely random - see a discussion below) weakly time dependent forces of the deformations. From the phase and coordinate space perspective, the motion is expected to be a branched flow [10–12]. In Fig. 2 we see contour maps of the two dimensional deformation field at the top at two temperatures and the branched flow evolution of the same manifold of trajectories riding over the potential. The trajectories were launched from a point in space over a small range of angles as seen at the left in each panel. There are no hard collisions or defects, but the finite mobility is evident. The mobility of the electrons is proportional to the relaxation time.

**Classical ray path tests.** Now we investigate the ray momentum diffusion numerically. Including screening, we take the electric potential to be proportional to the deformation potential: $E(\vec{k},\vec{r},t) = E(\vec{k}) + \lambda N_D(\vec{r},t)$. Without the screening effect, the proportionality constant will be unity, $\lambda = 1$. For each temperature, we run thousands of trajectories with the same initial kinetic energy, with random initial directions and positions, using several realizations of the random deformation potential. We use $v_s \sim 5 \times 10^3 \text{m/s}$ as the speed of longitudinal acoustic

**FIG. 1.** Quantum wavepacket propagation in refractive (upper left) and ballistically transparent (lower left) random potentials. The potentials on the left are deformation potentials of the same form, differing in horizontal scale but not in height. The same wavepacket is sent into the viewing area from the upper right, starting in a flattened region of the potentials. Wavefront shaping and deflection (leading to branched flow if continued) is clearly seen in the upper right, whereas the wave at the lower right ignores the shorter correlation length potential.
FIG. 2. (Top) Deformation potential contours calculated with equation (1). The peaks and valleys get higher and deeper as temperature increases, and the length scale of potential decreases in proportion to increasing temperature. (Bottom) Semiclassical electron pathways reveal branched flow typical of weak random scattering [10–12].

phonons, \( a \sim 10^{-10} \) m and \( k_F \sim 10^8 \) m\(^{-1}\) as typical values of lattice spacing (length scale) and the Fermi momentum, respectively, for metals. We use a fourth-order symplectic scheme for integration.

The function \( c(t) = \vec{p}(0) \cdot \vec{p}(t) \) measures the correlation between the initial momentum and the momentum at a time \( t \). In a Gaussian random diffusive process we have \( \langle c(t) \rangle = e^{-\frac{t}{\tau}} \); we suppose for now that we can treat the deformation potential as causing random diffusion of momentum, although there may be refinements needed, caused by spatial correlations in the deformation potential. It possesses a nonrandom averaging property: straight sections of trajectories find that the perpendicular forces from the higher frequency modes average to 0. This is easy to show from equation (1).

The results are shown in Fig. 3, showing an approximate \( T^4 \) low temperature rise in resistivity in 2D, rolling over to near \( T_{BG} \) above the Bloch-Grüneisen temperature \( T_{BG} \). The inset of Fig. 3 shows the exponential decay of the correlation as a function of time, revealing an exponential decay for the given time window. The slope of this plot is taken as the relaxation time \( \tau \) and the resistivity was calculated from \( \rho = \frac{n e^2}{m \tau} \); \( m \) is the electron mass. A key experimental paper by Efetov and Kim [13] showed very similar plots in graphene with doping varying the carrier density almost a factor of 10.

random Hanbury-Brown-Twiss correlations in the deformation potential. In fact only for a Markovian Gaussian random process should the sampling time not matter, and our numerical results show a strongly nongaussian momentum distribution for short to moderate times. The concept of a single relaxation time or free path may need re-examining, but this is beyond the scope of this paper. Therefore, it would be surprising if integer power laws for temperature dependence of the resistivity emerged, except in limiting approximations, as derived in the Appendix.

Thermal relaxation and fluctuation. Energy is exchanged because electrons collide quasielastically with moving deformation hills and valleys (the phonon bath is at a fixed temperature). It is neither possible nor necessary to keep track of individual phonons.

The time derivative required for mean squared energy dispersion brings down a factor of \( \omega \sqrt{k_x^2 + k_y^2} \), and on the other hand the spatial derivative for mean squared momentum dispersion brings down a factor of \( k_y \) in 2D, if the trajectory is temporarily moving along \( x \)-direction. Since \( \omega \sqrt{k_x^2 + k_y^2} = v_s \sqrt{k_x^2 + k_y^2} \), the two quantities are very closely related.

Without time dependence of the deformations, we have \( dE/dt = 0 \) (electron energy conserved). However instead \( dE/dt = \partial E/\partial t \) given the \( \omega \sqrt{k_x^2 + k_y^2} \) term in the argument of the cosines. It is reassuring that the semiclassical quasielastic approach thus comes with its own mecha-
The approach suggests a new model of electron-phonon interactions, involving soft quasielastic collisions of electrons with slowly moving (as seen by the electrons) deformation potential hills and valleys.

In the appendix we make approximations tantamount to classical perturbation theory, yielding $T^4$ in 2D and $T^5$ in 3D as limiting low temperature behaviors. Although an approximate $T^4$ low temperature rise in resistivity in 2D appeared numerically, there are strong reasons to believe the temperature rise need not be analytic nor universal. Even the exactness of $T^4$ above the Bloch-Grüneisen temperature is in question, since although the classical perturbation theory gives that power, there are known corrections lying with the exact trajectories. Indeed the experimental rise is typically more like $T^{1.2}$, a significant deviation (see Table 2.1 of Kasap [14]).

The model of electron-phonon interactions has been taken from one phonon inelastic events to smooth quasielastic ones, accounting for both energy and momentum changes with the same forces. The notion of quasi-elastic electron interactions with thermal distributions of phonon coherent states achieves a certain parity with electrons in classical electromagnetic fields—a long overdue development we believe. There are single photon processes but there are also interactions with statistical populations of coherent states of a thermal radiation field (classical blackbody electromagnetic fields). Similarly, there are single phonon processes, but there are also interactions with coherent states of the phonon field. In certain limits, one picture is far more useful than the other.

The semiclassical approach to deformation potential scattering has many implications for future work. Simulations of temperature dependent single particle magnetic- toresistance may now be possible without other assumptions about relaxation mechanisms. Full thermalization theory will however need more work, at the very least to somehow incorporate Pauli blocking effects.

Our approach is compatible with the standard perturbation approach, in the sense that we obtain a $T^4$ resistivity in the Appendix in the weak potential limit.

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APPENDIX: ANALYTIC ESTIMATES

Momentum diffusion can be understood by following the fluctuating force normal to an electron’s instantaneous velocity. We need the decay of the correlation $\langle \vec{p}_0 \cdot \vec{p}_T \rangle \sim |p_0|^2 (1 - \chi^2/2)$ where $\chi \approx v_y/v_x$ and $v_y(t) = \int_0^t f_y(t') dt$ with $\dot{x} = v_x = \partial E(\vec{r}, \vec{k}, t)/\partial k_x$. The procedure is to suppose a weak deformation potential and a straight line trajectory, along $x$ without loss of generality. We compute $f_y(t) = -\partial V_D(x(t), y, t)/\partial y$, integrate it from $t = 0$ up to time $t = t$, take the square, and ensemble average it.

The integrand $f_y(t)$ is a sum over all the cosine $y-$derivative phonon mode contributions, each with a random phase $\phi$, and a propagation direction given by $k_x = k \sin \theta$, $k_y = k \cos \theta$. One term reads

$$\int_0^t dt' k \cos \theta \sin(k \sin \theta \nu_F t' + y k \cos \theta + \phi_j) \frac{\cot \theta}{\nu_F} (\cos(\phi_j) - \cos(k \sin \theta \nu_F t + \phi_j))$$

This is a peculiar function that does not blow up at $\theta = 0$ for any $\phi_j$ in spite of first appearances. The summation over all $k$ can now be done in polar coordinates, integrating over $k$ and $\theta$. The square of the sum of all these terms reduces to the diagonal terms when averaged over realizations of the deformation potential (different $\phi_j$, or now $\phi(k, \theta)$). If we do the integral over $\phi_j$ first, we can get

$$\int_0^{2\pi} d\phi_j \int_0^{2\pi} d\phi_j \left[ \frac{\cot \theta}{\nu_F} \frac{(\cos(\phi_j) - \cos(k \sin \theta \nu_F t + \phi_j))}{\nu_F} \right]^2$$

$$= 2\pi^2 v_F \left[ -2 + v_F k t J_1(v_F k t) - 2 + v_F k t \pi H_0(v_F k t) \right] + J_0(v_F k t) \left[ 2 + 2(v_F k t)^2 - (v_F k t)^2 \pi H_1(v_F k t) \right]$$

where $H$’s and $J$’s are Struve and Bessel functions, respectively. This begins as $k^2 t^2$ for very small $k t$ but rises at larger $k t$ by modestly oscillating around a line of slope 1.

Finally putting back the thermal weighting, we get a Debye integral, which at low temperature may be taken to infinity, and neglecting the modest oscillation,

$$\int_0^{\infty} k^3 dk/\langle e^{Bk}/k^{3/2} e^{-T} - 1 \rangle \sim T^4$$

The factor of $k^3$ has three origins. First there is a $k$ for the density of states in the magnitude of the wavevector; a second factor of $k$ arises from the square of the
\((\sqrt{\omega_k})^2 = v_sk\) in the numerator of equation 1, and finally we just discussed another factor of coming from the ensemble average of the time integrals. The \(T^4\) dependence is easily seen by the change of variable \(k/T \rightarrow u\). At high temperature, the cut-off \(k_{BG}\) matters, and we have

\[
\frac{k_B T}{\hbar v_s} \int_0^{k_{BG}} k^2 dk \sim T^5
\]

(5)

In 3D the straight line trajectory is still one dimensional, and there is an extra factor of \(k\) in the density of states. Then, finally we have

\[
\int k^4 dk/(e^{\hbar v_s/k_BT} - 1) \sim T^5.
\]

(6)

First order quantum perturbation theory misses correlations between successive events. There is indeed such a correlation: the forces on a trajectory from the deformation potential self-average, becoming near vanishing over straight paths. Pushes one way are followed by pushes the opposite; this is not a simple random walk in momentum. The justification of first order quantum perturbation theory and the rule that requires the birth or death of a phonon actually comes from Bragg and diffuse scattering of very fast particles passing through a perfect lattice, where the chance of any collision is small.

Actual classical ray paths are not perfectly straight and the averaging is not complete. However, the averaging encourages nearly linear trajectories, which feeds more averaging.

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