Marginal Fermi liquid in twisted bilayer graphene

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Linear resistivity at low temperatures is a prominent feature of high-Tc superconductors which has been also found recently in twisted bilayer graphene. We show that due to an extended van Hove singularity, the T-linear resistivity can be obtained from a microscopic model of twisted bilayer graphene around the van Hove singularities in the two highest valence bands. The linear behavior is shown to be related to the linear energy dependence of the electron quasiparticle decay rate, which implies the low-energy logarithmic attenuation of the quasiparticle weight. These are distinctive features of a marginal Fermi liquid, which we also see reflected in the respective low-temperature logarithmic corrections of the heat capacity and the thermal conductivity, leading to the consequent violation of the Wiedemann-Franz law.

Introduction. The discovery of a Mott insulating and superconducting state in magic angle twisted bilayer graphene (TBG) has stimulated great interest, both from the theoretical as well as from the experimental side.

One striking and astonishing result of the initial experiments was the similarity of the phase diagram to the one of high-Tc superconductors. This analogy has further been manifested by the observation of a strange metal regime with its linear temperature dependence of the resistivity. Treating the charge fluctuations classically, one may obtain a T-linear resistivity down to some temperature scale, e.g., ∼5–10 K in the case of electron-phonon interaction. However, the linear resistivity observed experimentally extends down to ∼0.5 K for doping levels where no superconducting instability is found. Assuming a dominant role of the electron-phonon interaction, one could not further explain the gate dependence of the resistivity, which in turn seems to rule out also a conventional BCS-pairing scenario.

Recently, we presented a theory for the observed superconductivity in TBG. It is based on the Kohn-Luttinger mechanism, where the strongly anisotropic screening eventually leads to an attractive interaction between electrons around the Fermi surface. Crucial for the relatively high critical temperature of 1 K is the extended van Hove singularity that develops beyond a certain twist angle. In this Letter, we will argue that this property may also explain the linear T-dependence of the resistivity down to the lowest temperatures in the experiment.

More generally, we will show that the electron quasiparticle decay rate is linear in the energy variable and that, consequently, the quasiparticle weight acquires a logarithmic attenuation at low energies. These are the distinctive features of marginal Fermi liquid behavior, which we will see to have a reflection in the respective low-temperature logarithmic corrections of the specific heat and the thermal conductivity, leading to the consequent violation of the Wiedemann-Franz law.

Models. To model TBG, we will use the commensurable tight-binding model (TBM) parametrised by the integer i corresponding to the twist angle \( \cos \theta_i = \frac{3i^2 + 3i + 0.5}{2i^2 + 3i + 1} \). The hopping parameters are taken from Ref. 39 such that the nearest-neighbour intralayer hopping is set to \( t = -2.7 \) eV and the vertical interlayer hopping to \( t_{\perp} = 0.48 \) eV. We will also use the continuous model (CM) first introduced by Lopes dos Santos, Peres, and Castro-Neto to treat the case of long-ranged interaction within the RPA. For a recent review on general bilayer systems, see Ref. 44.

We will focus the discussion on the second highest valence band in the Moiré Brillouin zone of a twisted graphene bilayer with twist angle \( \theta_{28} \approx 1.16^\circ \), showing the Fermi lines for filling levels shifted \(-0.2 \) meV (left) and \(-1.0 \) meV (right) below the level of the saddle points placed along the \( \Gamma K \) lines.

FIG. 1. Energy contour maps of the second highest valence band in the Moiré Brillouin zone of a twisted graphene bilayer with twist angle \( \theta_{28} \approx 1.16^\circ \), showing the Fermi lines for filling levels shifted \(-0.2 \) meV (left) and \(-1.0 \) meV (right) below the level of the saddle points placed along the \( \Gamma K \) lines.
include relaxation effects or slightly different hopping parameters. Remarkably, the same extended van Hove singularities are also found in the CM, as already discussed in Ref. 36.

Resistivity. We can compute the resistivity relying on the quasiclassical formalism of the Boltzmann equation. In this approximation and assuming an on-site Hubbard interaction $U$, the resistivity $\rho$ is given by

\[ \rho = \frac{\rho_0 U^2}{k_B T} \int \frac{d^2k}{(2\pi)^2} \int \frac{d^2k'}{(2\pi)^2} |(k|k')|^2 n_F(\varepsilon_k) (1 - n_F(\varepsilon_{k'})) \times \delta (\varepsilon_{k+k'} - \varepsilon_k + \varepsilon_{k'}) , \]

where $\rho_0 = \hbar/e^2$ and $A$ being the area of the system. This equation can be recast in a way that makes explicit use of the transport scattering rate. We can write

\[ \rho = \rho_0 \frac{1}{T} \sum \frac{n_F(\varepsilon_k)}{\tau_{tr}(k)} , \]

where we have defined

\[ \frac{1}{\tau_{tr}(k)} = U^2 \int \frac{d^2k'}{(2\pi)^2} \int_0^{\varepsilon_K} d\omega |(k|k')|^2 (1 - n_F(\varepsilon_{k'})) \times \delta (\varepsilon_k - \varepsilon_{k'} - \omega) \text{Im} \chi_{tr}(k-k', \omega) \]

with the imaginary part of the susceptibility

\[ \text{Im} \chi_{tr}(q, \omega) = \int \frac{d^2p}{(2\pi)^2} |(p|p+q)|^2 n_F(\varepsilon_p) (1 - n_F(\varepsilon_{p+q})) \times \delta (\varepsilon_{p+q} - \varepsilon_p - \omega) . \]

The values of the resistivity $\rho$ and the transport scattering rate $1/\tau_{tr}(k)$ depend on the shift $\Delta \mu$ of the Fermi level with respect to the vHS as well as on the point chosen along the Fermi line. We illustrate here the transport behavior by taking $\Delta \mu$ in the range from $-0.2$ to $-2.5$ meV. The evolution of the Fermi line below the level of the vHS can be seen in Fig. 1, where the quasi-flat dispersion along the $\Gamma - K$ direction for $|\Delta \mu| \sim 0.2$ meV become apparent.

To show the dependence of the transport decay rate on momentum, we have taken a sequence of points along the Fermi line as shown in Fig. 1. The results obtained for $\Delta \mu = -0.2$ meV and $-0.5$ meV are given in Fig. 2. In the two cases, $1/\tau_{tr}(k)$ shows a dependence which is linear in $T$ to a very good approximation, with a crossover from a larger to a smaller slope at a temperature of a few K.

From the results for the transport decay rate, we obtain the resistivity by applying Eq. (2). At low temperatures, we may assume that only quasiparticles in the energy range of $T$ contribute, so that the resistivity can be computed as an average over the Fermi line

\[ \rho \sim \rho_0 \int d\varepsilon_k \frac{1}{\tau_{tr}(k)} , \]

where $k_\parallel$ is the longitudinal component of the momentum and $v_k$ is the Fermi velocity along the Fermi line.

The resistivity obtained in this way can be seen in Fig. 3, where its temperature dependence for different values of $\Delta \mu$ from $-0.2$ to $-2.5$ meV is shown. There is a clear difference between the behavior of the left and right plots at low temperatures. As seen in Fig. 3, the good approximation to a linear $T$-dependence is lost as soon as the Fermi line departs from the van Hove singularity. When $\Delta \mu$ is between $-0.2$ and $-0.5$ meV, however, the linear $T$-dependence of the resistivity is quite clear, although with different slope above and below a crossover temperature of the order of a few K. Very suggestively, a change in the slope of the resistivity has been also seen in the experimental observations about half-filling of the Moiré unit cell, displaying a larger (smaller) slope of the linear $T$-dependence below (above) a temperature which is $\approx 6$ K in the measurements reported in Ref. 35.

Quasiparticle properties. The linear temperature dependence of the transport decay rate can be traced back to the low-energy behaviour of the electron self-energy $\Sigma(k, \omega)$. Its imaginary part can be most easily computed in terms of the conventional electron-hole susceptibility $\chi(q, \omega)$ as

\[ \text{Im} \Sigma(k, \omega) = - U^2 \int \frac{d^2p}{(2\pi)^2} \int_{-\infty}^{\infty} d\omega_p |(k|p)|^2 \text{sgn}(\omega_p) \times \delta (\omega_p - \varepsilon_p) \text{Im} \chi(k-p, \omega - \omega_p) . \]
The real part of the self-energy can be obtained by making use of the Kramers-Kronig relation, which in this case takes the form

$$\text{Re} \left( \Sigma(k, \omega) \right) = \frac{2\omega}{\pi} \int_0^\infty d\Omega \frac{\text{Im} \left( \Sigma(k, \Omega) \right)}{\Omega^2 - \omega^2}. \quad (7)$$

When the Fermi level is close to the vHS, the imaginary part of the self-energy computed from Eq. (6) has a linear dependence on the frequency \(\omega\) which is similar to the temperature dependence of the transport decay rate represented in Fig. 2. Consequently, the dependence of the real part of the self-energy on \(\omega\) displays a significant deviation from linear behavior, with a logarithmic correction which is another evidence of the departure from Fermi liquid behavior. This is shown on the left of Fig. 4, where the real part of \(\Sigma(k, \omega)/\omega\) is represented for the points on the Fermi line as defined in Fig. 1, when the Fermi level is shifted by \(\Delta \mu = -0.2\) meV with respect to the vHS.

We observe that the real part of the self-energy behaves as \(\Sigma(k, \omega) \sim \omega \log(\omega)\), which amounts to state that the electron quasiparticles are progressively attenuated when approaching the Fermi level. The dressed electron propagator becomes

$$G(k, \omega) = \frac{1}{\omega - \varepsilon_k - \Sigma(k, \omega)} \sim \frac{\Delta}{\omega - \varepsilon_k + i\gamma\omega} \quad (8)$$

after rewriting the self-energy corrections in terms of the quasiparticle weight \(\Delta\) and the imaginary shift \(i\gamma\omega\) of the quasiparticle pole. The quasiparticle weight is suppressed following the low-energy scaling \(\Delta \sim 1/|\log(\omega)|\), which is the hallmark of the marginal Fermi liquid behavior.\(^{46,47}\)

**Heat capacity.** The anomalous behavior of the electron quasiparticles has also a significant impact on the temperature dependence of observables like the heat capacity. This is obtained from the entropy \(S\), which can be expressed as\(^{48}\)

$$S = \frac{i}{\pi} \frac{1}{k_B T} \int \frac{d^2k}{(2\pi)^2} \int_{-\infty}^{\infty} d\omega \frac{\partial n_F(\omega)}{\partial \omega} \log \left( \frac{G_R(k, \omega)}{G_A(k, \omega)} \right), \quad (9)$$

where \(A\) is the area of the system and \(G_R, G_A\) are respectively the retarded and advanced electron Green’s functions. The momentum integral can be performed along the Fermi line by decomposing \(k\) into a longitudinal \(k_\parallel\) and a transverse \(k_\perp\) component which leads to

$$\frac{S}{A} \approx \frac{1}{\pi^2 T^2} \int dk_\parallel \frac{d\varepsilon_k}{v_k} \int_{-\infty}^{\infty} d\omega \frac{\partial n_F(\omega)}{\partial \omega} \times \arctan \left( \frac{\text{Im} \left( \Sigma(k, \omega) \right)}{\omega - \text{Re} \left( \Sigma(k, \omega) \right) - \varepsilon_k} \right) \quad (10)$$

where the integral in \(k_\parallel\) is carried out along the Fermi line.

Given the dependence of the real part of the self-energy on \(\omega\), we see from Eq. (10) that the entropy must have a dominant scaling behavior \(S \sim T \left| \log(T) \right|\).

The heat capacity \(C\) is obtained by taking the derivative of \(S\) with respect to \(T\) and it inherits, therefore, the logarithmic correction that we find in the entropy:

$$C = T \frac{\partial}{\partial T} S \sim T \left| \log(T) \right| \quad (11)$$

We have evaluated the heat capacity in our model by applying the values that we get for the real part of the self-energy to the computation of the expression Eq. (10). The results can be seen on the right of Fig. 4, which displays a clear logarithmic correction on top of the conventional linear \(T\)-dependence of the heat capacity at low temperatures.

**Thermal conductivity.** The logarithmic correction of the heat capacity has also a direct translation into the temperature dependence of the thermal conductivity \(\kappa\). This quantity is related to the heat capacity through the thermal diffusivity \(\alpha\) according to the formula \(\kappa = \alpha C\). The thermal diffusivity is in turn proportional to the mean free path of the energy carriers.\(^{49}\) When the Fermi level is close to the vHS as in the case corresponding to the plot on the left of Fig. 2, we can rely on the linear \(T\)-dependence of the transport scattering rate, which implies that

$$\kappa(T) = \alpha C \sim \left| \log(T) \right|. \quad (12)$$

This behavior should be observable down to the temperature scale at which the transport starts to be dominated by the scattering from disorder (impurities or lattice defects) in the twisted bilayer. Above that scale, we see that the temperature dependence of the thermal conductivity should be dictated by the logarithmic correction present in the heat capacity, thus leading to a modification of the Wiedemann-Franz law.\(^{50}\)
FIG. 5. The scattering rate $\hbar/\tau$ of TBG with $i = 29$ as function of the temperature for various chemical potentials around the vHS and long-ranged interaction with surrounding dielectric material $\epsilon = 5$. $n_k^q$ denotes the number momentum of the first Brillouin zone, indicating the good convergence of the scattering rate. The dashed line indicates the Planckian scattering rate $\hbar/\tau = 0.086\text{meV} \cdot T[K]$.

Long-ranged interaction. So far, we have assumed a strongly screened Hubbard interaction, valid for gates close to the twisted bilayer sample. For gates farther away, we expect also effects from the long-ranged Coulomb potential to become important. In this case, we calculate the scattering rate by incorporating the intrinsic screening effects within the $G_0W$-approximation of the self-energy, starting from the Coulomb potential $v = \frac{e^2}{2\epsilon_0 q}$ with $\epsilon = 5$.

The $G_0W$-approximation requires the knowledge of the real and imaginary parts of the susceptibility and, in order to speed up the calculations, we have made use of the less time-consuming CM. The two lowest VBs of the TBM can only be compared to the CM by combining its lowest VBs from the two $K$-valleys, $E_p^K$ and $E_p^K'$, to give $E_p^\pm = \max(E_p^K, E_p^K')$ and $E_p^- = \min(E_p^K, E_p^K')$. For twist angles $\theta > 1.1^\circ$, the two combined bands only touch at the six $\Gamma K F$-lines for which $E_p^\pm = E_p^K'$ in the CM.

The relaxation time within the $G_0W$-approximation at finite temperature for a quasiparticle (hole) state with $\Delta = E_p^- - \mu$ is given by\cite{35}

$$\frac{1}{\tau(\Delta)} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\omega) \frac{1}{A} \sum_q \frac{v_q}{|\langle p|p+q\rangle|^2} \times \text{Im} \left( \frac{1}{\epsilon(q, \omega)} \right) \delta (\hbar\omega - (E_p^- - E_{p+q}^-))$$

which involves the dielectric function within the RPA

$$\epsilon(q, \omega) = 1 - v_q \chi^-(q, \omega)$$

with the polarisability

$$\chi^-(q, \omega) = \frac{2}{A} \sum_k |\langle k|k+q\rangle|^2 \frac{n_F(E_k^\pm) - n_F(E_{k+q}^\pm)}{\hbar\omega - (E_{k+q}^- - E_k^\pm) + i0^+},$$

and the temperature-dependent weight factor

$$f(\omega) = \frac{\coth(\beta\hbar\omega/2) - \tanh(\beta(\hbar\omega - \Delta)/2)}{1 + e^{-\beta\Delta}}.$$

We further defined the eigenstates $|p\rangle$, the Fermi function $n_F(E) = (e^{\beta E} + 1)^{-1}$, the inverse temperature $\beta = 1/(k_B T)$.

In Fig. 5, we show the resulting scattering rate for different chemical potentials relative to the vHS as function of the temperature. Good convergence is demonstrated by showing the results for different discretizations of the first Brillouin zone (1. BZ), $n_q^2$ being the number of momenta in the 1. BZ. Interestingly, for larger temperature the results are close to the Planckian scattering rate $\hbar/\tau = 0.086\text{meV} \cdot T[K]$ indicated as dashed line which is in good agreement to the experimental findings of Ref.35. The results for small temperatures are thus not be trusted since this model does not incorporate the inter valley coupling crucial for the linear temperature behaviour as discussed in the previous sections.

Summary. Relying on a TBM, we have been able to obtain a linear temperature dependence of the resistivity for filling factors around the vHS in the valence band of TBG, in the framework of a model with on-site Hubbard interaction $U$. The linear behaviour of the resistivity can be traced back to the more general frequency dependence of the electron Green’s function, characterised by a logarithmic correction indicating marginal Fermi liquid behavior. We thus predict that fingerprints of a marginal Fermi liquid should also be present in the heat capacity and the thermal conductivity. Observing these features experimentally would give compelling evidence that the Kohn-Luttinger mechanism is at work in magic angle graphene. Finally, we argue that nearly Planckian resistivity is obtained from our model if long-ranged interaction is included with the $G_0W$-approximation.

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