

Transport in Quantum Systems: Insights from LinReTraCe

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Electrical, thermoelectrical and thermal transport are among the most direct probes of a material's electronic structure. Yet most simulations rely on semi-classical Boltzmann theory, where the scattering rate enters merely as a prefactor. This is not a harmless simplification: in gapped systems it makes the resistivity and coefficients of Hall and Seebeck diverge as $T \rightarrow 0$, the latter in violation of the third law of thermodynamics.

We present LinReTraCe [1], the Linear Response Transport Centre, an open-source package for simulating transport in materials and model systems. Its central innovation is to treat thermal broadening and the finite lifetime of charge carriers on an equal footing. Crucially, the resulting Kubo kernels are obtained in closed form. This semi-analytical character does more than make the quantum treatment as cheap as a semi-classical one: because the answer is a formula rather than a number, its limits can be taken analytically and the energy scales controlling each regime can be identified explicitly; prototypical behaviours (saturation, sign changes, crossing points, universal values) can be extracted rather than merely observed. Crucially, the scattering rate is not a scaling factor but a genuine energy scale shaping the temperature profile of every transport observable. In correlated narrow-gap semiconductors, finite carrier lifetimes reproduce the measured low-temperature saturation of resistivity and Hall coefficient and the linear vanishing of the Seebeck and Nernst coefficients [2,3], without invoking extrinsic impurity states.

The same formalism yields a striking result at a two-dimensional band-tuned metal-insulator (Lifshitz) transition [4]. An exact expression for the conductance of a parabolic band with finite lifetime—valid from the ballistic to the diffusive regime—describes measurements on a field-tuned $\text{MoTe}_2/\text{WSe}_2$ moiré bilayer across the full temperature range, and explains why the established one-parameter scaling breaks down: close to the transition, the scattering rate becomes a second relevant energy scale, broadly beyond the Mott-Ioffe-Regel limit. Exactly at the Lifshitz point the critical resistance is independent of scattering, carrier density and band mass, taking the universal value $R_L = 2\pi\hbar/e^2$ per spin, band and valley. Beyond its universality, this value is a useful classifier. We argue that R_L bounds the critical resistance R_c of a predominantly disorder-driven, Anderson-type transition from above, so that $R_c > R_L$ signals a (Mott/Wigner) transition driven chiefly by interactions—a sufficient criterion that we confront with a range of experimental 2D systems.

LinReTraCe accepts input from electronic-structure codes, Wannier constructions or model Hamiltonians, and accommodates self-energies, including from dynamical mean-field theory. Its modular structure makes further scattering channels straightforward to add; interfaces with first-principles electron-phonon coupling and with disorder-derived scattering rates are under development.

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