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Many-body energy invariant for T-linear resistivity

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The description of dynamics of strongly correlated quantum matter is a challenge, particularly in physical situations where a quasiparticle description is absent. In such situations, however, the many-body Kubo formula from linear response theory, involving matrix elements of the current operator computed with many-body wavefunctions, remains valid. Working directly in the many-body Hilbert space and not making any reference to quasiparticles (or lack thereof), we address the puzzle of linear in temperature (T-linear) resistivity seen in non-Fermi liquid phases that occur in several strongly correlated condensed matter systems. We derive a simple criterion for the occurrence of T-linear resistivity based on an analysis of the contributions to the many-body Kubo formula, determined by an energy invariant "f-function" involving current matrix elements and energy eigenvalues that describes the DC conductivity of the system in the microcanonical ensemble. Using full diagonalization, we test this criterion for the f-function in the spinless nearest neighbor Hubbard model and in a system of Sachdev-Ye-Kitaev dots coupled by weak single particle hopping. We also study the f-function for the spin conductivity in the 2D Heisenberg model and arrive at similar conclusions. Our work suggests that a general principle, formulated in terms of many-body Hilbert space concepts, is at the core of the occurrence of T-linear resistivity in a wide range of systems, and precisely translates T-linear resistivity into a notion of energy scale invariance far beyond what is typically associated with quantum critical points.

Introduction: How do strongly correlated materials (eg. the high T_c superconducting cuprates, heavy fermions and more recently, twisted bilayer graphene [1–8]) conduct electricity at finite temperature? This is a fundamental question that has existed since the realization of these materials, and the inception of this field decades ago. Experiments have helped build an intricate picture of the phases that occur, both from the point of their static and dynamical properties at finite temperature, but much remains to be accomplished in order to have a definitive theoretical understanding of these materials. For example, at and close to optimal doping, the superconducting phase transitions to the "non Fermi liquid" (nFL) or "strange metal" phase which is characterized by an electrical resistivity that scales linearly with temperature (T-linear) over a wide range of T [2–7, 9]. This is in sharp contrast to Fermi liquid (FL) theory which predicts that the electrical resistivity of a metal scales as T^2 [10].

nFLs, in contrast to FLs, are characterized by a lack of quasiparticles, leading to a concerted effort to find models and mechanisms by which T-linear resistivity can occur. Prominent among these is the Sachdev-Ye-Kitaev (SYK) model and its variants [11–13] which are analytically solvable in a large N limit and exhibit T-linear resistivity (when multiple SYK dots are coupled) [14, 15]. However, the connection of this model to a realistic microscopic model remains to be established. Recent experiments with cold atoms [16] have shown the existence of T-linear resistivity in the Hubbard model which has been supported by dynamical mean field theory [17–21] and exact diagonalization [17, 22] calculations.

We address the question of T-linear resistivity, circumventing the issue of quasiparticles (or lack thereof) completely. We work directly with the full set of quantum many-body wavefunctions (which contain information about the resistivity at all temperature scales), and appeal to a direct analysis of the many-body Kubo formula [23]. This is valid within linear response, which is sufficient given that the experimentally applied electric fields are small perturbations to the full electronic Hamiltonian. The expression for the longitudinal conductivity (*i.e.* the inverse of the electrical resistivity ρ_α) is given by,

$$\sigma_\alpha(\omega, T) = \pi \frac{1 - e^{-\beta\omega}}{\omega Z} \sum_{n,m} \frac{|I^\alpha_{nm}|^2}{e^{\beta E_n}} \delta(E_n + \omega - E_m) \quad (1)$$

where ω is the energy of interest (the DC limit corresponds to $\omega \to 0$), E_n, E_m are eigenenergies of the n^{th} and m^{th} eigenstates respectively, Z is the partition function, α is a label for the spatial direction (x or y in two dimensions) and $I^\alpha_{nm} \equiv \langle n|I^\alpha|m\rangle$ are matrix elements of the current operator, and β is the inverse temperature.

At extremely high T (higher than the many-body bandwidth), Ref. [24] stated a straightforward reason for T-linear resistivity. In this limit, the thermal factors $\exp(-\beta E_n)$, occurring in the numerator and the partition function in the denominator, all become one. At high temperature and vanishing frequency, $\beta \to 0$ and $\omega \to 0$, the factor of $(1 - \exp(-\beta\omega))/\omega \to \beta$, which yields the linear in β conductivity and hence T-linear resistivity. Though mathematically appealing, this argument alone does not explain why T-linear resistivity remarkably survives to lower T. Studies of the high T limit by Refs. [25–27] also suggested that many aspects of T-linear behavior can be understood from high temperature expansions.

Our key contribution is to establish a criterion for T-linear resistivity at finite temperature and to test its general validity.

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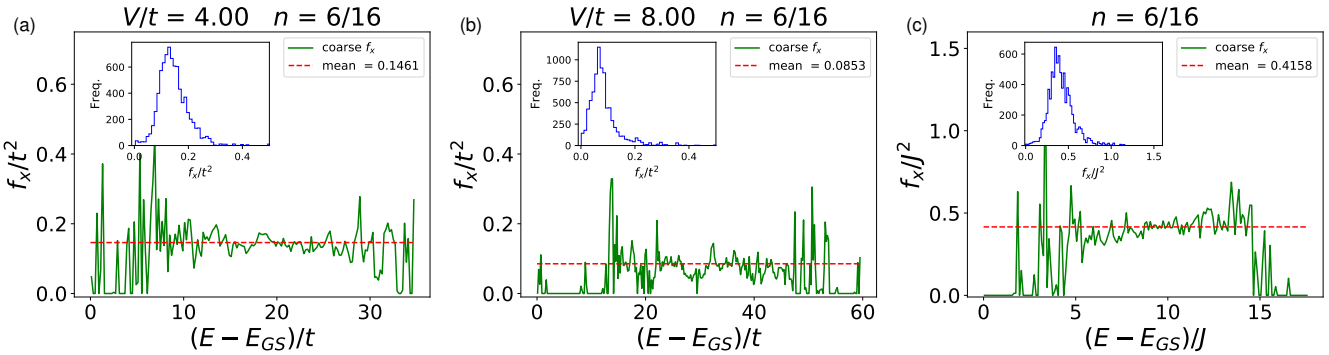


FIG. 1. (a), (b) $f_x(E)$ for the charge conductivity, using $\eta = 0.20t$, as a function of the energy E (in units of t) for the 4×4 2D square lattice nearest neighbor spinless Hubbard model for $V/t = 4, 8$ and for a filling of $n = 6/16$. In each case, the ground state energy E_{GS} has been subtracted out. The insets show histograms of $f_x(E)$ values with the bin width set to 0.01. (c) $f_x(E)$ for the spin conductivity,using $\eta = 0.10J$, of the 2D spin $1/2$ nearest-neighbor Heisenberg model (mapped to a hardcore-bosonic model) on a 4×4 square lattice with (bosonic) filling $n = 6/16$.

We note that the Kubo formula can be rewritten as,

$$\sigma_\alpha(\omega, T) = \Big(\frac{1 - e^{-\beta\omega}}{\omega}\Big)\Big(\frac{\sum_n e^{-\beta E_n} f_\alpha(E_n, |n\rangle, \omega)}{\sum_n e^{-\beta E_n}}\Big), \tag{2}$$

where we have introduced the f-function, defined as,

$$f_\alpha(E_n, |n\rangle, \omega) \equiv \pi \sum_m |I^\alpha_{nm}|^2 \delta(E_n + \omega - E_m) \tag{3a}$$

$$\equiv \lim_{\eta\to 0} \sum_m \frac{\eta |I^\alpha_{nm}|^2}{\eta^2 + (E_n + \omega - E_m)^2}, \tag{3b}$$

where η is a broadening parameter whose use is necessitated by the discreteness of the many-body spectrum in numerical computations on a finite sized system. Once again for $\omega \to 0$, the prefactor outside the summation yields the desired factor of β. This means that the remaining terms must conspire to *perfectly* cancel out to have no temperature dependence. This can happen for an arbitrary range of T, if $f(E_n, |n\rangle) \equiv f(E_n, |n\rangle, \omega \to 0)$ is constant, *i.e.* independent of the energy of the eigenstate and the eigenstate itself. Since there is a continuum of many-body energies and eigenstates in the thermodynamic limit, it is meaningful to coarse grain the f-function by simple averaging within a narrow energy window, as long as the energy window over which the averaging is done is significantly smaller than the lowest temperature scale of interest:

$$f_\alpha(E) \equiv \frac{1}{g(E)} \sum_n \delta(E_n - E) f_\alpha(E_n, |n\rangle), \tag{4}$$

where $g(E) \equiv \sum_n \delta(E_n - E)$ is the many-body density of states ($f_\alpha(E_n, |n\rangle) = f_\alpha(E_n)$ follows from the eigenstate thermalization hypothesis (ETH) [28], but the coarse-grained function is well-defined even in situations where ETH does not hold). The definition in Eq. (4) is also equivalent to the structure factor of the total current operator at $\omega = 0$ in the microcanonical ensemble.

For this averaged $f_\alpha(E)$, we show [28] that its energy invariance is the only generic possibility for T-linear resistivity at arbitrary temperature. This condition must hold in situations where the slope $d\rho_\alpha/dT$ has been found to be invariant with temperature [29]. Furthermore, for resistivity scaling as other powers of T, there does not appear to be any such generic invariant that is defined in the microcanonical ensemble, which indicates that exact T-linear resistivity is somehow "special".

The f-function recasts the complex finite temperature problem into an analysis of the quantum mechanical energies and matrix elements of the current operator. In realistic models, we may expect only *approximate* T-linear resistivity, in which case the conditions on the f-function can be somewhat relaxed: we then expect $f(E)$ to be constant only in energy regimes corresponding to temperatures where the T-linear contribution to the resistivity dominates. At low energies we may expect to see physics associated with antiferromagnetism, superconductivity or FL behavior, and the f-function can not be constant in these regimes.

To test our assertions, we carry out a systematic numerical investigation of the f-function in the spinless Hubbard and SYK models. We also pose and answer an analogous question about spin conductivity in the two dimensional spin-1/2 square lattice Heisenberg model.

Spinless nearest neighbor Hubbard model: Consider a nearest neighbor (nn) spinless Hubbard model on the 2D square lattice,

$$H = -t \sum_{\langle i,j\rangle} c_i^\dagger c_j + \text{h.c.} + V \sum_{\langle i,j\rangle} n_i n_j, \tag{5}$$

where $\langle i, j\rangle$ refer to nn pairs, t is the nn hopping (which we set to 1 for our calculations), V is the strength of the nn repulsion and $c_i^\dagger$ and c_i are the usual electron creation and destruction operators. $n_i = c_i^\dagger c_i$ is the number operator. The current operator is defined as,

$$I^{x(y)} = \frac{it}{\sqrt{N_s}} \sum_{j=1}^{N_s} (c^\dagger_{j+\hat{x}(\hat{y})} c_j - c_j^\dagger c_{j+\hat{x}(\hat{y})}), \tag{6}$$

where N_s is the total number of sites. We simulate an isotropic lattice (4×4 torus i.e. periodic boundary conditions in both directions), and plot only f_x (computed from I^x), since f_y (computed from I^y) is identical.

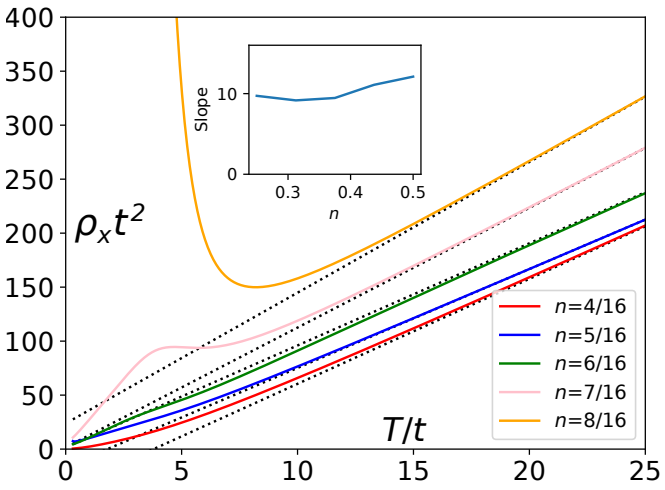


FIG. 2. Resistivity ($\rho_x t^2$), using $\eta = 0.10t$, for the spinless Hubbard model for a representative value of interaction $V/t = 8$ and various fillings. The high temperature part of the curves ($T = 30t$ to $70t$, not shown) is fit to a linear function, the corresponding slope is shown in the inset. The low temperature physics is characterized by metallic or insulating phases which show clear deviations from T-linear resistivity.

Fig. 1 (a) and (b) show plots of $f_x(E)$, for representative values of V/t at a filling of $n = 6/16$. The ground state energy in each case has been subtracted out on the energy axis. A broadening parameter of $\eta = 0.2t$ is used.Additionally, the energy axis is split up into bins of size η and the coarsened value of $f_x(E)$ is obtained by simple averaging over all the eigenstates with eigenenergies that lie in a given bin, as in Eq. (4). The mean value of $f_x(E)$ averaged over the entire eigenspectrum is also shown as a guide to the eye.

If one focuses on the center of the many-body spectrum, $f_x(E)$ does appear to be remarkably flat for all the cases shown. To quantify the degree of flatness of the f-function, we plot the histogram of $f_x(E_k, |k\rangle)$ values for all eigenstates $|k\rangle$ in the spectrum (assigning degenerate states the same f_x-value) in the inset. We observe that the f-value is indeed peaked around a typical value. (In the Supplementary Material (SM) [28] we also show the f-function for other fillings, interaction strengths and broadening parameters.)

Fig. 2 shows a representative set of resistivity curves for $V/t = 8$ and different particle fillings. For small fillings and low temperature, one has a dilute gas of well defined electronic quasiparticles, the f-function is high at low energies, correspondingly the resistivity shows deviation from T-linear behavior that is present at large T. At half filling, one has insulating behavior at low temperature expected of the charge density wave phase. The slope of the T-linear portion (obtained by biasing the fit to include only high T) is shown in the inset and is approximately (but not exactly) constant with filling.

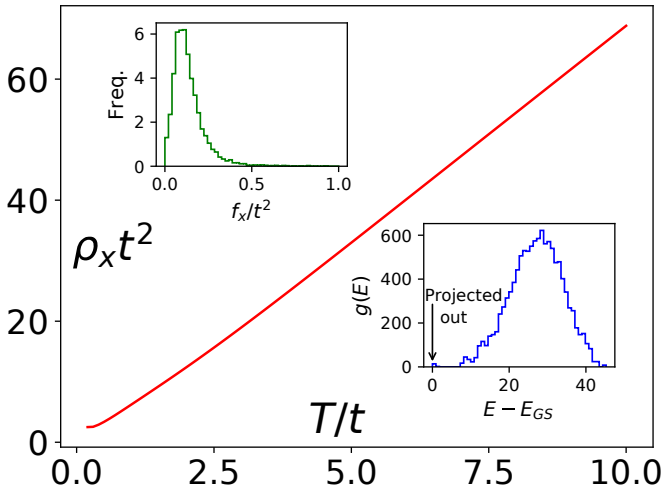


FIG. 3. Resistivity ($\rho_x t^2$), using $\eta = 0.10t$, for the spinless Hubbard model for $V/t = 4.3$ and filling 7/16, after the lowest energy manifold of 16 states is projected out of the calculation. The inset at the bottom right shows the density of states $g(E)$. The inset at the top left shows the histogram of f_x values (normalized histogram) for the remaining $11440 - 16 = 11424$ eigenstates.

We now demonstrate that the operative mechanism behind f-invariance in the spinless nearest neighbor Hubbard model stems from an incoherent quantum liquid of states that extends across energy scales. To do this, we consider the model near half-filling, where the incoherent quantum liquid is separated from the low energy manifold of states $|L_n\rangle$ by a gap in the many-body spectrum. We proceed to project out this low energy manifold by redefining $H \to H + \infty \sum_n |L_n\rangle\langle L_n|$ [30] (Fig. 3). Doing so makes the incoherent quantum liquid extend all the way down to low energies [31]. Then, in the strongly correlated regime $V/t \gtrsim 1$, we find that T-linear resistivity extends from high T down to nearly $T = 0$ without a slope change (Fig. 3), and the resistivity at low T is not much larger than $1/t^2$, *i.e.* not bad metallic. Consequently, f-invariance now extends across the energy spectrum in the modified model.

This projection procedure also causes the transfer of single-particle spectral weight from the upper Hubbard bands down to low frequencies (for a detailed discussion, see SM). The resulting UV-IR mixing in the local single-particle spectral function [32, 33] therefore results in energy scale invariant behavior with respect to the addition or removal of a single particle. Our calculations suggest that an analogous situation arises with the current operator; under projection it also redistributes the UV spectral weight down to low energies, which in turn extends the T-linear regime to low T.

Heisenberg model: The fermionic nature of the constituents has no particular relevance in our Hilbert space viewpoint. This motivates an investigation of a very different model, the 2D spin-1/2 Heisenberg model on a square lattice with the Hamiltonian,

$$H = J \sum_{\langle i,j \rangle} \mathbf{S_i} \cdot \mathbf{S_j}, \tag{7}$$

from the point of view of its spin conductivity. ($\mathbf{S_i}$ represent the usual spin-1/2 operators on site i). The spin current is defined as $I_S^{x(y)} = iJ\sum_{j=1}^{N_s}(S^+_{j+x(y)}S^-_j - S^+_j S^-_{j+x(y)})/\sqrt{N_s}$. [34] (We set $J = 1$ in our calculations.) The model maps to one of hardcore bosons with $t = -J/2$ and $V = J$; a previous investigation by Ref. [26] using high temperature expansions showed that such particles also show T-linear resistivity.

We evaluate the f function for the 4×4 torus in different magnetization sectors, equivalent to different fillings of hardcore bosons. We find that the f-function is indeed flat when viewed at intermediate energy (see Fig. 1 (c) for a representative calculation), paralleling our observations for the fermionic case. These findings hint at the diminished role of particle statistics at high temperature, which we find remarkable yet consistent with recent experiments that have suggested the occurrence of a "bosonic strange metal" [35] with robust T-linear resistivity. It remains to be seen if this effect can be observed for the "spin-resistivity" in insulating magnetic materials.

SYK model: Finally, we discuss our results for the zero-dimensional SYK model of spinless complex fermions c_i [12, 13]. Its Hamiltonian is,

$$H = \frac{1}{(2N)^{3/2}} \sum_{i,j,k,l=1}^{N} J_{ijkl} c_i^\dagger c_j^\dagger c_k c_l, \tag{8}$$

where J_{ijkl} are independent random complex numbers chosen from a Gaussian distribution with standard deviation J, and the model is defined in the limit of large N.

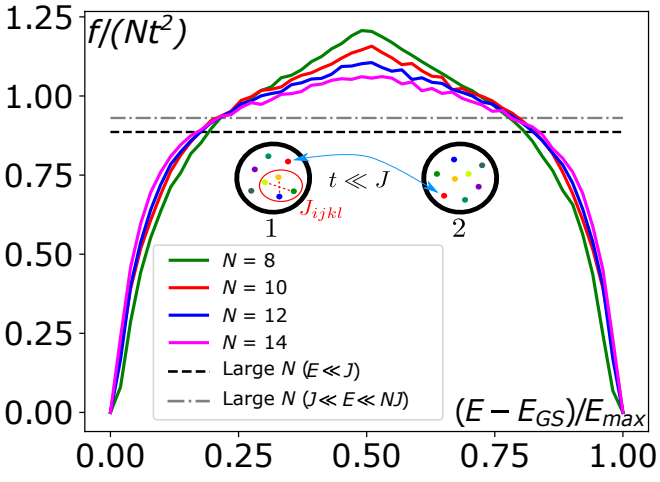


FIG. 4. f-function computed for a two SYK dot system (each having N sites) using exact diagonalization for various values of N, averaged over 128 realizations each. The many-body bandwidth is $E_{\rm max}$, and the ground state energy $E_{\rm GS}$ has again been subtracted out (for each disorder realization). The dashed lines indicate f derived from the large N results for $\rho(T)$ obtained in previous work [29], where we take $f \approx \rho(T)/T$ [28]. The curves will end up within the region between the dashed lines as N is made large.

Owing to the high amount of frustration, the model inhibits the formation of ordered states [11] in the limit of $N \to \infty$ Moreover, the fully random interactions and the absence of single particle hopping also means that there is no Fermi liquid or glassy phase down to zero energy (zero temperature) [12, 36–38]. Thus, the SYK model is one of the simplest known models where nFL physics persists all the way down to $T = 0$.

The concept of charge transport is not well defined for a single zero-dimensional SYK dot. However, one can weakly couple SYK dots (labeled $1, 2$) with infinitesimal single-particle hopping t (Fig. 4), and define an appropriate current operator $I = it\sum_{j=1}^{N}(c^\dagger_{j,1}c_{j,2} - c^\dagger_{j,2}c_{j,1})$, we drop the direction label α here. Field theoretic calculations in the large N limit, where $T \ll NJ$ by definition, have revealed that the resistivity ρ is linear in T [14, 15], and its slope $d\rho/dT$ is nearly invariant [29], *i.e.* it does not depend on the temperature scale (with respect to J) that the system is at, even though the temperature dependences of other physical quantities change drastically as T is increased past J [29] (such as the compressibility, which changes from $\sim T^0$ to $\sim T^{-1}$).

We compute the f-function of the two dot system as follows: since the hopping t is infinitesimal, the dots are effectively decoupled, and the many body states $|n\rangle = |n_1\rangle|n_2\rangle$ are therefore (fermionic) product states of the states on the individual dots. We exactly diagonalize the Hamiltonians for the two dots individually, which have uncorrelated realizations of J_{ijkl}. We then have $(E_m, Q_m \equiv E_{m_1}, Q_{m_1} + E_{m_2}, Q_{m_2})$

$$f(E) = \frac{2\pi t^2}{g(E)} \sum_{n_1,n_2} \sum_{m_1,m_2} \delta(E_m - E)\delta(E_n - E)\delta_{Q_m,Q} \times \delta_{Q_n,Q} \left| \sum_{i=1}^{N} \langle n_1|c_{i,1}|m_1\rangle\langle n_2|c^\dagger_{i,2}|m_2\rangle(-1)^{Q_{m_1}} \right|^2, \tag{9}$$

where $g(E)$ is the many-body density of states of the two dot system, and the total charge on the two dots is Q.

Fig. 4 shows the results of our calculations at $Q = N$ for $N = 8$ to $N = 14$, which were obtained after averaging over 128 realizations of J_{ijkl} for each N. We find that in the middle of the spectrum, the f-function tends to get flatter with increasing N, approaching the large N result. Towards the edges, the f-values are smaller, but increase towards the large N result with increasing N: thus, the profile of the f-function appears to be asymptoting towards the nearly invariant large N result as N is increased. Remarkably, the f-invariance also appears to extend to energy scales $E \sim NJ$ in the middle of the band, far higher than those accessed in the large N field theory calculations, where $E \ll NJ$ by definition.

Discussion: We conclude by discussing the implications of the energy invariance of the f-function, which is a purely microcanonical quantity. For this energy invariance to occur, a subtle interplay between the average size of the matrix element of the current operator and the available number of many-body states at a given energy density is required. The energy invariance of the f-function encodes a notion of energy scale invariance across the many-body spectrum, which is far beyond the purview of low energy effective field theories. Importantly, when viewed in terms of the many-body Hilbert space, different models suggest a universal mechanism behind T-linear resistivity.

Certain correlated electron materials display "perfect" T-linear resistivity across multiple decades of temperature [39–42], which is often associated with the presence of a quantum critical point [43, 44]. This resistivity goes from $\rho \ll h/e^2$ at low T, to a "bad metal" regime where $\rho \gg h/e^2$ at high T, in which the classical mean free path of the electrons becomes comparable to a lattice spacing [45]. This suggests very different physics in the two regimes [16, 46], yet f-invariance must hold across the crossover between them, indicating that they are still related. To probe this physics further, larger system sizes are required: it would be interesting to construct variational wavefunctions [47] or matrix product states for excited states in models of quantum critical metals [48] that could capture this crossover, and see how f-invariance can manifest in terms of the physical parameters used to define these wavefunctions. Also, other computational strategies based on shift-invert based algorithms that target states at a given energy density could be used for calculation of the f-function for larger system sizes, and thus shed further light on the problem of T-linear resistivity.

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