Article

Integrability and Ideal Conductance at Finite Temperatures

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Abstract

We analyse the finite temperature charge stiffness $D(T>0)$, by a generalization of Kohn's method, for the problem of a particle interacting with a fermionic bath in one dimension. We present analytical evidence, using the Bethe ansatz method, that $D(T>0)$ is finite in the integrable case where the mass of the particle equals the mass of the fermions and numerical evidence that it vanishes in the nonintegrable one of unequal masses. We conjecture that a finite $D(T>0)$ is a generic property of integrable systems.

Reference

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Integrability and Ideal Conductance at Finite Temperatures

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We analyze the finite temperature charge stiffness $D(T > 0)$, using a generalization of Kohn's method, for the problem of a particle interacting with a fermionic bath in one dimension. We present analytical evidence, using the Bethe ansatz method, that $D(T > 0)$ is finite in the integrable case where the mass of the particle equals the mass of the fermions and numerical evidence that it vanishes in the nonintegrable case of unequal masses. We conjecture that a finite $D(T > 0)$ is a generic property of integrable systems.

This work relates the finite temperature charge transport to the response of energy levels to an infinitesimal flux and proposes a connection to the integrability of quantum systems. Starting with the formulation by Kohn [1], the charge stiffness (or Drude weight) representing the weight of the delta function contribution $D\delta(\omega)$ part in the dynamical conductivity $\sigma(\omega)$ has been investigated as a criterion for a metallic, superconducting, or insulating state [2,3]. The original approach [1] relates D to the response of the ground state energy to a magnetic flux and thus requires only calculation of an equilibrium property, bypassing a complete evaluation of the Kubo formula [4].

A similar concept also appears in the study of the conductance of disordered metallic systems. Starting with the work of Thouless [5] a close relation has also been established between the conductance, the sensitivity on boundary conditions (being equivalent to the introduction of a flux), and the statistical properties of *single-particle* energy spectra [6] of metallic systems.

Recently it has also been observed that the level statistics in *many-particle* correlated systems is closely related to the integrability of the system [7,8]. Still the implications of this fact on transport quantities in correlated fermion systems at finite temperatures $T > 0$, e.g., a nonzero dc resistivity $\rho(T) > 0$ or on the contrary a possible finite charge stiffness $D(T) > 0$, have not been known so far.

In this work we analyze the relation between integrability and transport in the generic problem of a single tagged particle moving in a bath of fermions by a generalization of Kohn's method at finite temperatures.

Kohn's method at $T > 0$.—We consider a general tight-binding Hamiltonian of the form

$$\hat{H} = -t \sum_i (e^{i\phi} d_{i+1}^\dagger d_i + \text{H.c.}) + \hat{H}_{\text{int}} = \hat{T} + \hat{H}_{\text{int}}, \quad (1)$$

representing a one–dimensional (1D) system of length L with periodic boundary conditions pierced by a flux $L\phi$, using the Peierls construction. $\hat{T}$ is the kinetic part and $\hat{H}_{\text{int}}$ is the interaction part of the Hamiltonian. From the Kubo formula [2,9] we can relate the imaginary part of the dynamical conductivity $\sigma''(\omega)$ to the charge stiffness D,

$$D = \frac{1}{2}[\omega \sigma''(\omega)]_{\omega \to 0}$$
$$= \frac{1}{L}\left\{ \frac{1}{2}\langle -\hat{T} \rangle - \sum_{m \neq n} p_n \frac{|\langle n | \hat{j} | m \rangle|^2}{\epsilon_m - \epsilon_n} \right\}, \quad (2)$$

where $\hat{j}$ is the current operator, $\langle \hat{T} \rangle$ is the thermal expectation value of the kinetic energy, and $p_n = e^{-\epsilon_n/T}/Z$ is the Boltzmann weight for an eigenstate $| n \rangle$ of Hamiltonian (1) with energy ϵ_n.

On the other hand [1], we can evaluate, using second order perturbation theory, for $\phi \to 0$ a shift of the level $| n \rangle$:

$$\epsilon_n(\phi) = \langle n | \hat{H}(\phi = 0) | n \rangle - \phi \langle n | \hat{j} | n \rangle$$
$$- \phi^2 \sum_{m \neq n} \frac{|\langle n | \hat{j} | m \rangle|^2}{\epsilon_m - \epsilon_n} - \frac{1}{2}\phi^2 \langle n | \hat{T} | n \rangle. \quad (3)$$

Extracting second order terms in ϕ (the curvature of levels) we see that

$$D = \frac{1}{L} \sum_n p_n D_n = \frac{1}{L} \sum_n p_n \frac{1}{2} \frac{\partial^2 \epsilon_n(\phi)}{\partial \phi^2}. \quad (4)$$

In this demonstration we assumed that the levels $| n \rangle$ are nondegenerate, but the same procedure can be used for degenerate levels after applying first order degenerate perturbation theory to lift the level degeneracy. This expression for $D(T)$ generalizes Kohn's method to $T > 0$ and reduces its evaluation to the calculation of curvature of levels under an external flux. Easier than the complete evaluation of Kubo formula, it can be performed either numerically on finite size systems followed by finite size scaling or in some cases (e.g., integrable systems) analytically [10]. It also provides a basis for analyzing the conditions for the occurrence of ideal conductance.

The ground state of the metal should be characterized by $D_0 = D(T = 0) > 0$ [1–3], where D_0 is a measure

of the charge carriers *coherent* motion. On physical grounds it is commonly assumed [3] that $D(T > 0) = 0$, for generic macroscopic interacting systems (involving umklapp scattering), except in the superconducting phase. This statement, never really proved to our knowledge for interacting fermions, implies according to our Eqs. (2) and (4) that the positive curvature of the ground state D_0 is cancelled by (mostly) negative curvatures of low lying states, a situation reminiscent of the mechanism for phase transitions and the disappearance of long range order.

Model system.—The Hamiltonian describing a particle in a bath of spinless fermions is

$$\hat{H} = - t_h \sum_i (e^{i\phi} d^\dagger_{i+1} d_i + \text{H.c.})$$

$$- t \sum_i (c^\dagger_{i+1} c_i + \text{H.c.}) + U \sum_i d^\dagger_i d_i c^\dagger_i c_i , \quad (5)$$

where $c_i (c^\dagger_i)$ are annihilation (creation) operators for N spinless fermions and $d_i (d^\dagger_i)$ for the (tagged) particle on an L-site chain with periodic boundary conditions. The interaction comes only through the on-site repulsion $U > 0$. The current $\hat{j}$ in (2) refers to the particle only ($\hat{j} = -it_h \sum_i d^\dagger_{i+1} d_i + \text{H.c.}$) and $[\hat{j}, \hat{H}] \neq 0$. The volume normalization $1/L$ in (4) is absent as the current refers only to one particle.

The model (5) is well adapted to our study: It is integrable by the Bethe ansatz method in the case of equal masses, i.e., $t_h = t$ [11] (equivalent to the problem of a Hubbard chain in a nearly polarized state $S^z = S^z_{\max} - 1$) and nonintegrable for unequal masses ($t_h \neq t$). We have also previously studied D_0 [12] of the particle as well as its quasiparticle properties [13].

We first present the results for $D(T)$ from exact numerical diagonalization of the Hamiltonian (5) on finite size systems. We will consider only the $N = L/2$ case, which in this system should be analogous to all other fillings. By numerical calculation of the energy spectrum with and without a small flux ϕ (typically $\phi \simeq 10^{-4}$) we deduce the energy level curvature from

$$D_n = \frac{1}{2} \frac{\epsilon_n(\phi) + \epsilon_n(-\phi) - 2\epsilon(0)}{\phi^2} . \quad (6)$$

In Fig. 1 we present $D(T)$ as a function of t_h/t, for different temperatures T, size systems (from 6 to 14 sites), but fixed $U/t = 2$. We observe (a) a nonmonotonic behavior of $D(T)$ as we sweep through the integrable $t_h = t$ point for $T > 0$, and (b) a very weak dependence of $D(T)$ with system size for the integrable case $t_h = t$ while a rather strong one for the nonintegrable ones.

These observations are the first hints that something particular happens at the integrable point. To further study this behavior, we present in Fig. 2 $D(T)/D_0$ as a function of $1/L$ for $t_h = t$. We indeed observe a scaling in $1/L$, which we also know is the relevant one to recover the ground state D_0 [12]. The circle at $1/L = 0$ indicates
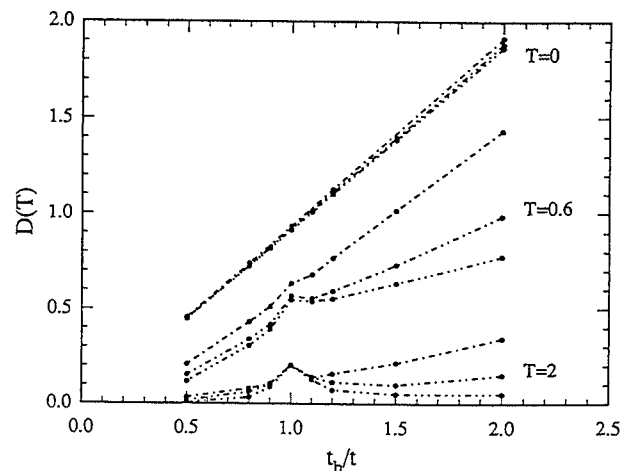

FIG. 1. $D(T)/D_0$ as a function of the t_h/t for $U/t = 2$, different temperatures T, and system sizes L: $(- \cdot -) L = 6$, $(- \cdot \cdot -) L = 10$, and $(- \cdot \cdot \cdot -) L = 14$.

that the result of the Bethe ansatz calculation for $t_h = t$ is in very good agreement with the extrapolated numerical results.

The same plot in Fig. 2 of $\ln D(T)/D_0$ as a function of L^2 for $t_h = 0.5t, 1.2t, 2.0t$ seems to indicate a strong L dependence following a law $D(T) \simeq e^{-\gamma L^2}$ for these nonintegrable cases. This is consistent with a rapid decrease of $D(T)$ for systems larger than the mean free path.

Next, to obtain an impression of the overall behavior of $D(T)$ as function of temperature we present in Fig. 3 $D(T)/D_0$ for $t_h = t, 0.5t$, and different size systems. For $t_h = 0.5t$, $D(T)/D_0$ seems to scale to zero for any $T > 0$ as we have found above, while for $t_h = t$ there is a smooth decrease with T. At high temperatures $D(T) \propto 1/T$, vanishing for $T \to \infty$ which is a general feature of
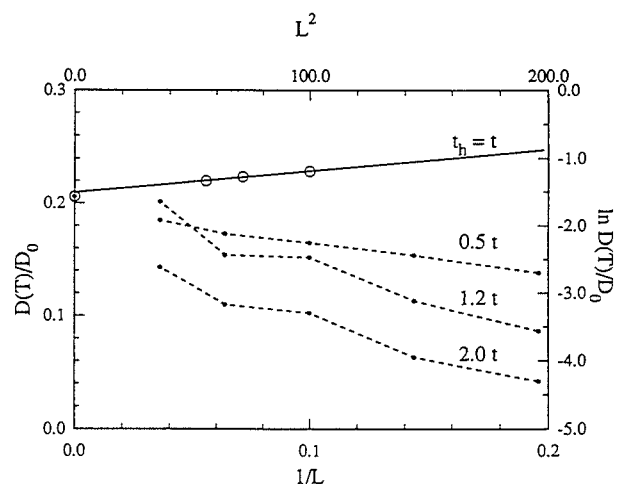

FIG. 2. Lower and left axes: scaling of $D(T = 2t)/D_0$ with system size $1/L$ (circles) for $t_h = t$, $U/t = 2$. The $\odot$ indicates the Bethe ansatz result. The continuous line is a linear fit for $L = 10, 14, 18$ sites. Upper and right axes: scaling of $\ln D(T = 2t)/D_0$ with L^2 (dots) for $U/t = 2$ and $t_h = 0.5t, 1.2t, 2.0t$.
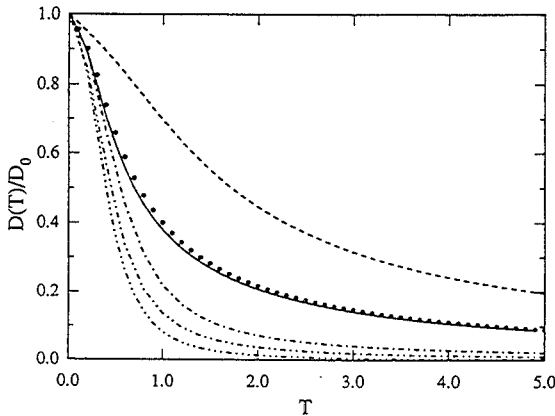
FIG. 3. $D(T)/D_0$ as a function of T for $U/t = 2$. Numerical results are indicated by $(- \cdot -)$ $L = 6$, $(- \cdot \cdot -)$ $L = 10$, $(- \cdot \cdot \cdot -)$ $L = 14$, and $t_h = 0.5t$; points indicate $t_h = t$ and $L = 18$. The continuous line is the Bethe ansatz result and the dashed line $D(T)/D_0$ for a free particle.

systems on a lattice. Finally, the discrepancy from the free particle $D(T)$ indicates that the temperature effects cannot be accounted for by a simple scaling of D_0.

Bethe ansatz analysis.—We present here an analytical approach for the calculation of $D(T)$ for the integrable case using the Bethe ansatz method along the line of reference [12]. The starting point is the Lieb-Wu [14] solution of the Hubbard model adapted for one spin up fermion (the tagged particle) and N spin down fermions. The Bethe ansatz wave functions, in the presence of flux ϕ, are then characterized by $N + 1$ quantum numbers k_j given by the following equations (we take $t_h = t = 1$):

$$Lk_j = 2\pi I_j + \theta(\sin k_j - \Lambda), \qquad j = 1, \ldots, N + 1,$$
(7)

$$\theta(p) = -2\tan^{-1}(4p/U),$$
(8)

$$L \sum_{j=1}^{N+1} k_j = 2\pi \sum_{j=1}^{N+1} I_j + 2\pi J + L\phi.$$
(9)

Every state is characterized by a set of half-odd integers $\{I_j\}$ and the (half-odd) integer J for an (even) odd number of fermions. However, this set of states (regular) does not constitute a complete set; to obtain a complete set we must include states representing bound states of energy of order U. The simplest way to include these states is by considering an electron-hole transformation $[\tilde{c}_i = c_i^\dagger,$ $\tilde{d}_i = (-1)^i d_i]$ and then solving Eq. (7) but for a $L - N$ number of fermions (equal to the number of holes).

The total energy of a regular state is given by

$$E = \sum_{j=1}^{N+1} \epsilon(k_j) = \sum_j (-2\cos k_j),$$
(10)

and, for a bound state,

$$E = U + \sum_{j=1}^{L-N+1} 2\cos k_j.$$
(11)

In the following we present explicitly the analysis for the contribution of regular states only as it is clear how to include the bound ones by the prescription described above [15] (although we include both contributions in the results presented in Figs. 2 and 3).

To order $1/L$ and for $UL \gg 1$ the values of k_j are given by

$$k_j = k_j^0 + \frac{1}{L}\theta(\sin k_j^0 - \Lambda), \qquad k_j^0 = \frac{2\pi I_j}{L}.$$
(12)

To order 1 then the energy and momentum of a state can be written as

$$E = \sum_j \epsilon(k_j^0) + \frac{2}{L}\sin k_j^0 \theta(\sin k_j^0 - \Lambda),$$
(13)

$$\frac{1}{L}\sum_j \theta(\sin k_j^0 - \Lambda) = \frac{2\pi J}{L} + \phi.$$
(14)

In this scheme the interaction between the particle and the fermions is represented through second term in Eq. (13), a correlation energy; the coupling to the flux ϕ is through the collective coordinate Λ. In the thermodynamic limit, defining a density $\rho(k)$ $(-\pi \leq k \leq +\pi)$ we obtain

$$E(\rho(k), \Lambda) = \frac{L}{2\pi}\int dk \, \rho(k)\left(-2\cos k + \frac{2}{L}\sin k \, \theta(\sin k - \Lambda)\right),$$
(15)

$$\frac{1}{2\pi}\int dk \, \rho(k)\theta(\sin k - \Lambda) = P + \phi, \qquad P = \frac{2\pi J}{L}.$$
(16)

To calculate the thermal average of the curvature of energy levels we will work in the grand canonical ensemble for the system plus the one particle. Assuming that the equilibrium distribution of k's is not affected by the presence of the one particle we use the Fermi-Dirac distribution for free fermions $f(k) = 1/(1 + \exp[(\mu - \epsilon(k)]/T)$ (μ is the chemical potential). We then assume that the distribution of Λ's is determined by the average correlation energy $\epsilon_c(\Lambda)$,

$$\epsilon_c(\Lambda) = \frac{1}{2\pi}\int dk \, f(k)2\sin k \, \theta(\sin k - \Lambda),$$
(17)

through a Boltzmann weight $w(\Lambda) = \exp[-\epsilon_c(\Lambda)/T]$.

Finally $D(T)$ is given by

$$D = \frac{1}{2\pi Z_\Lambda}\int_{-\infty}^{+\infty} d\Lambda \, g(\Lambda)w(\Lambda)\frac{1}{2\pi}\int dk \, f(k)D(\Lambda, k),$$
(18)

with $g(\Lambda) = \partial P/\partial \Lambda$ determined from Eq. (16):

$$\frac{\partial P}{\partial \Lambda} = \frac{1}{2\pi}\int dk \, f(k)\frac{\partial \theta(\sin k - \Lambda)}{\partial \Lambda},$$
(19)

$$Z_\Lambda = \frac{1}{2\pi} \int d\Lambda \, g(\Lambda) w(\Lambda) \tag{20}$$

(in the total partition function Z_Λ we add the contribution from both the regular and bound states):

$$D(\Lambda, k) = \frac{1}{2} 2\sin k \left[\frac{\partial^2 \theta}{\partial \Lambda^2} \left(\frac{\partial \Lambda}{\partial \phi} \right)^2 + \frac{\partial \theta}{\partial \Lambda} \frac{\partial^2 \Lambda}{\partial \phi^2} \right]. \tag{21}$$

By successive differentiation of Eq. (16) we can determine $\partial \Lambda / \partial \phi = 1/g(\Lambda)$ and $\partial^2 \Lambda / \partial \phi^2$.

Evaluating the expressions (18)–(21) we obtain the results presented in Figs. 2 and 3 in very good agreement with the numerical results, providing support for our approach [15]. We also verified that the agreement remains (within a couple of percent) for other values of the interaction (e.g., $U/t = 8$).

Comments.—From our formulation of D at *finite temperatures* as a thermal average over level curvatures, we can try to understand the difference in behavior between integrable and nonintegrable systems as an effect of many-body level fluctuations. In nonintegrable cases the level repulsion prevents level crossings, i.e., crossings are statistically negligible for macroscopic systems. Then each level $\epsilon_n(\phi)$ fluctuates on the scale $\Delta\epsilon \propto 1/\mathcal{N}(E)$, where $\mathcal{N}(E)$ is the many-body density of states. Therefore, the curvature D_n averaged over ϕ or over different k vectors in the thermodynamic limit should vanish. On the other hand, in integrable systems levels in general cross, so fluctuations of $\epsilon_n(\phi)$ do not necessarily vanish for $L \to \infty$. Hence there is no restriction on the average $D(T)$, except that $D > 0$. The difference between both cases is intimately related to level statistics.

This connection between integrability and finite temperature charge transport born out of this model calculation, we can conjecture to hold true for other quantum (as well as classical) integrable systems. We can trace it to the existence of a macroscopic number of conservation laws. It is plausible that with respect to transport one should distinguish two types of models within the class of 1D correlated systems where some solvable models [16] are available:

(a) In few (mostly solvable) 1D models the current is a conserved quantity. This is generically the case for models without umklapp scattering, e.g., the Luttinger model, 1D Bose gas, etc., but also for the $U = \infty$ Hubbard model [17]. In these cases one expects at $T > 0$ ideal conductance of the system characterized by $\rho(T) = 0$ or $D(T) > 0$.

(b) Nontrivial answers are expected for models with umklapp scattering, e.g., for the 1D Hubbard model, the t-V model, etc. If our conjecture is correct we expect integrable models as the Hubbard, t-V, or supersymmetric t-$J(J = 2t)$ models to behave as ideal conductors at finite temperatures. We can then argue that even 1D nonintegrable models as the U-V model (with longer range interactions), as they are characterized by the integrable Luttinger liquid Hamiltonian at low energies, should behave as nearly ideal conductors at low T; the δ peak then would broaden to a narrow Drude peak of weight $D(T)$ [18].

We should stress that our study is based on the Kubo linear response theory [4] whose applicability in the context of Luttinger liquids has recently been debated [19]. Further work is necessary on other (one- and eventually higher-dimensional) integrable systems to lend further support for these ideas.

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