Divergent Thermopower without a Quantum Phase Transition

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A general principle of modern statistical physics is that divergences of either thermodynamic or transport properties are only possible if the correlation length diverges. We show by explicit calculation that the thermopower in the quantum XY model $d = 1 + 1$ and the Kitaev model in $d = 2 + 1$ can 1) diverge even when the correlation length is finite and 2) remain finite even when the correlation length diverges, thereby providing a counterexample to the standard paradigm. Two conditions are necessary: 1) the sign of the charge carriers and that of the group velocity must be uncorrelated and 2) the current operator defined formally as the derivative of the Hamiltonian with respect to the gauge field does not describe a set of excitations that have a particle interpretation, as in strongly correlated electron matter. The recent experimental\textsuperscript{[1]} and theoretical\textsuperscript{[2]} findings on the divergent thermopower of a 2D electron gas are discussed in this context.

A truism in modern statistical mechanics is that divergences (or more generally non-analyticities) in a thermodynamic quantity or a transport property always signal a transition to a new state of matter. In fact, the very notion of adiabatic continuity is based on the intuition that non-analyticities resulting from tuning some system parameter cannot emerge without the crossing of a phase boundary. More precisely, as long as the correlation length remains finite, then no divergences are possible because both transport and thermodynamic properties are governed by the singular part of the free energy. We present here a counter example to this rule. To establish our result, we consider the quantum XY model in 1D and the Kitaev\textsuperscript{[3]} model in 2D, both of which can be solved\textsuperscript{[4–6]} exactly using a mapping to fictitious fermionic degrees of freedom. In both cases, we show exactly that the thermopower, appropriately defined, diverges at fillings that have nothing to do with the quantum phase transition in these models. At the spurious divergences, no thermodynamic quantity experiences a non-analyticity. As we will see, the heart of this problem is a breakdown of the particle interpretation of the current-carrying degrees of freedom.

This work is motivated by recent measurements\textsuperscript{[1]} on the thermopower in a dilute 2D electron gas. These experiments are the latest in a series of remarkable observations\textsuperscript{[7]} that a dilute 2D electron gas exhibits a resistivity that decreases as the temperature is lowered with no apparent upturn (as is expected from the scaling theory\textsuperscript{[8]}), thereby providing evidence for a low-temperature metallic state. Mokashi et al. reported\textsuperscript{[1]} that the thermopower on the metallic side of the transition diverges exhibiting scaling of the form

$$S(T, n) = eTs(n) = T(n - n_c)^{-\mu}$$  \hspace{1cm} (1)

with $\mu = 1.0 \pm 0.1$. Consequently, if the thermopower were to be measured on the insulating side, it should change sign. As a result, they interpreted\textsuperscript{[1]} such a critical divergence, based on a simple appeal to the adiabatic continuity principle, as definitive evidence that the transition to the metallic state represents a true $T = 0$ quantum phase transition. This would then represent the most important finding since the initial discovery paper in 1996\textsuperscript{[9]}. More recently, Kirkpatrick and Belitz\textsuperscript{[2]} argued that the divergence of the thermopower holds crucial implications for the scaling of the specific heat as the exponent $\mu$ determines the product of dynamical and correlation length exponents, $z$ and $\nu$, respectively.

Hence, while explaining the experimental data is certainly of interest, our focus is on whether alternative mechanisms exist for a divergent thermopower other than a quantum phase transition. Although the models in the counterexamples we construct are not directly applicable to the experiments, the mechanism for the divergence of the thermopower is. We find that in strongly correlated systems, the thermopower can diverge simply because the current does not have a particle interpretation.

We treat at first the quantum XY model in 1D. This model can be fermionized\textsuperscript{[4]} \textsuperscript{[10]}

$$H = - \sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i + \Gamma c_i^\dagger c_{i+1} + \Gamma c_{i+1} c_i$$

$$+ h(1 - 2c_i^\dagger c_i)), \hspace{1cm} (2)$$

using the Jordan-Wigner transformation scheme with $c_i$ a canonical fermionic annihilation operator for site $i$. The hopping between two sites is set to 1 in the unit of $J = \frac{1}{2}(J_x + J_y)$, $\Gamma = \frac{J_x - J_y}{\sqrt{2}}$ is a measure of the exchange anisotropy and $h = \frac{\Delta}{2J}$ is the effective magnetic field or in the fermionic model $-2h$ is a dimensionless chemical potential. Although $\Gamma \neq 0$ im-
plies an effective particle non-conservation, thereby making it possible to fix only the average number of particles, we have shown\textsuperscript{11} that a unique expression exists for the thermopower defined as a response to a longitudinal field. We calculated the exact expression for the thermopower\textsuperscript{11} and showed that it diverges at the phase transition, $h = \pm 1$. However, this analysis is far from complete as we will show below. There are additional divergences away from $h = \pm 1$ at which the thermodynamics is completely smooth.

To analyze the thermopower, we Fourier transform the Hamiltonian and diagonalize it using a Bogoliubov transformation. The diagonalized Hamiltonian,

$$
H = \sum_k \varepsilon_k c_k^\dagger c_k,
$$

(3)

contains the new fermionic operators, $\gamma_k = u_k c_k - iv_k c_{-k}^\dagger$ and $\gamma_k^\dagger = u_k c_k^\dagger + iv_k c_{-k}$, whose energies are $\varepsilon_k = \pm 2\sqrt{(h - \cos k)^2 + \Gamma^2 \sin^2 k}$ with $u_k = 2 \cos \frac{\theta_k}{2}$ and $\nu_k = 2 \sin \frac{\theta_k}{2}$ and the angle $\theta_k$ defined through $\sin \theta_k = (\Gamma \sin k)/\varepsilon_k$ and $\cos \theta_k = (h - \cos k)/\varepsilon_k$. We will be analyzing the properties of this model as a function of the average particle density,

$$
x = \langle c_i^\dagger c_i \rangle = \frac{1}{2\pi} \int_0^\pi dk \left( 1 - \cos \theta_k \tanh \left( \frac{\beta \varepsilon_k}{2} \right) \right).
$$

(4)

The thermodynamic quantity of interest is the heat capacity,

$$
\frac{C}{N} = \frac{k_B}{4\pi} \int_0^\pi \varepsilon_k \left( \frac{\varepsilon_k}{k_B T} \right)^2 \text{sech}^2 \left( \frac{\beta \varepsilon_k}{2} \right).
$$

(5)

However, our main focus is the thermopower. To this end, we write the charge ($\hat{J}_x$) and thermal currents ($\hat{J}_Q$) along the $x$-direction in terms\textsuperscript{12} of the responses to an electric field and a temperature gradient,

$$
\frac{1}{\Omega} \langle \hat{J}_x \rangle = L_{11} E_x + L_{12} \left( - \frac{\nabla_x T}{T} \right) \quad (5)
$$

and

$$
\frac{1}{\Omega} \langle \hat{J}_Q \rangle = L_{21} E_x + L_{22} \left( - \frac{\nabla_x T}{T} \right) \quad (6)
$$

uses the Onsager coefficients, $L_{ij}$. In these expressions, $\Omega$ is the volume of the system. The thermopower\textsuperscript{12},

$$
Q = \frac{L_{12}}{TE_{11}},
$$

(7)

is the ratio of the voltage generated per gradient of temperature. An explicit calculation of $L_{ij}$ is possible in frequency and momentum space for the models we consider here. The transport or fast limit corresponds to $\lim_{\omega \rightarrow 0} \lim_{q_x \rightarrow 0}$. For the quantum XY model in 1D, the exact expression\textsuperscript{11} for the thermopower,

$$
\lim_{\omega \rightarrow 0} \lim_{q_x \rightarrow 0} \frac{eQ}{k_B} = \frac{\int_{-\pi}^\pi dk \frac{\varepsilon_k}{k_B T} \sin \frac{dn}{dk}}{\int_{-\pi}^\pi dk (\varepsilon_k^2 + \nu_k^2) \sin \frac{dn}{dk}}.
$$

(8)

involves a simple integral over the first Brillouin zone with an integrand determined by the coherence factors and the fermionic occupation, $n = 1/(e^{\varepsilon/k_B T} + 1)$. The numerator of this expression is bounded over integration in the first Brillouin zone. Consequently any divergence arises entirely from the denominator. We display the results for $\Gamma = 0.8$ and $t = 0.1$ in the first panel of Fig. (1(a)), where $t$ is the dimensionless temperature and defined as

\textsuperscript{1} Although 4 expressions (Eqs. (6a-6d)) are derived in Ref. [11] for the thermopower, Eqs. (6c) and (6d) are valid only for a transverse field, while Eqs. (6a) and (6b) apply strictly for a longitudinal field. (6a) follows from (6b) from the continuity equation which is not valid here. Since the thermopower experimentally is the response to a longitudinal field, only Eq. (6b) is valid in this context and hence the thermopower has a unique definition.
\[ t = k_B T / J. \]

For these parameters, the particle density at the phase transition, \( h = \pm 1 \), is \( x \approx 0.15 \) or the particle-hole complement, \( x \approx .85 \). Fig. 1(a) shows that indeed the thermopower does diverge at these values of \( x \) as we reported earlier. However, there are other divergences, for example at \( x \approx 0.4, 0.6 \) in Panel 1(a) away from the critical value of the filling. The full phase diagram for this model in terms of the total number of divergences is catalogued in Fig. 2. There are a total of five regions: a) no divergences (blue), b) four divergences (red, Panel 1(a)), c) three divergences (yellow), d) two divergences (green), and e) one divergence (purple). Fig. 2 illustrates that only at the phase transition does the heat capacity display the characteristic peak-like feature which turns into a non-analyticity at \( T = 0 \). Hence, non-analyticities in thermodynamics need not affect transport properties and conversely divergences in transport properties are not necessarily accompanied by singularities in the thermodynamics. Before we analyze the origin of these results, we first show that our findings are not an artifact of 1-dimensional (d=1+1) physics. To this end, we consider the Kitaev model,

\[
H = -J_x \sum_{\text{x-bonds}} \sigma_R^x \sigma_{R'}^x - J_y \sum_{\text{y-bonds}} \sigma_R^y \sigma_{R'}^y - J_z \sum_{\text{x-bonds}} \sigma_R^z \sigma_{R'}^z,
\]

on a honeycomb lattice in which the summations are over all links between site \( R \) and \( R' \). This Hamiltonian can be fermionized by the Jordan-Wigner transformation. The result is a model of Dirac fermions,

\[
H = J_x \sum_i (c_i^\dagger + c_i)(c_{i+\hat{x}}^\dagger - c_{i+\hat{x}}) + J_y \sum_i (c_i^\dagger + c_i)
\]

\[
\times (c_{i+\hat{y}}^\dagger - c_{i+\hat{y}}) + J_z \sum_\alpha \alpha_i(2c_i^\dagger c_i - 1),
\]

on a square lattice. At every lattice site there is one conserved quantity, \( \alpha_i \), which has the value of -1 or 1. The ground state of this system corresponds to having \( \alpha_i \) equal to 1 everywhere. So we choose all \( \alpha_i \) to be 1. This Hamiltonian can be solved exactly in the same way as the quantum XY model. The energy spectrum is given by

\[
\epsilon_k = 2\sqrt{(J_x - \sum_i J_i \cos \theta_i)^2 + (\sum_i J_i \sin \theta_i)^2}
\]

and the coherence factors defined through the parameters \( u_k \) and \( v_k \) in the Bogoliubov transformation satisfy

\[
\cos \theta_k = u_k^2 - v_k^2 = \frac{2(J_x - J_y \cos \theta_x - J_z \cos \theta_y)}{\epsilon_k},
\]

\[
\sin \theta_k = 2u_k v_k = \frac{2(J_x \sin \theta_x + J_y \sin \theta_y)}{\epsilon_k}.
\]

The sum on \( i \) in the energy spectrum above is over \( x \) and \( y \). The analogous expression for the thermopower,

\[
\frac{eQ}{k_B} = \frac{\pi}{-\pi} \frac{\int dk_x \int dk_y \frac{e\hbar}{k_B T} \sin k_x \frac{dn}{dk_x} }{\int dk_x \int dk_y (u_k^2 - 2v_k^2 \cos k_x \sin k_y \frac{dn}{dk_x})}.
\]

obtained from an exact calculation of \( L_{ij} \) in the fast limit, is precisely the 2D generalization of Eq. [8].

For the Kitaev model, the thermopower, \( Q = Q(J_x, J_y, J_z, t) \), depends on the average particle density \( x = x(J_x, J_y, J_z, t) \). We write \( J_y \) and \( J_z \) in units of
of $J_x$ (by setting $J_x = 1$). So for a fixed value of $J_y$ and $t$, we can plot thermopower versus particle density by varying $J_x$. Figs. 1(b) and 4 demonstrate that the behaviour is identical to that of the quantum XY model. Hence, our results are not an artifact of 1-dimensional physics. Note that this model also exhibits regions in which no divergence obtains although the quantum phase transition is present.

The origin of this physics is tied to the denominators of the expressions for the thermopower because $L_{12}$ is a completely bounded function for all values of $k$ inside the first Brillouin zone. Consider the denominator, in the case of the XY model

$$\text{XY} \rightarrow \int_{-\pi}^{\pi} dk (u_k^2 - v_k^2) \sin k \frac{dm}{dk},$$

the Kitaev model being the direct 2D analogue. The $\sin k$ factor arises from the momentum dependence of the local current operator, $J_j = -i(c_j^\dagger c_{j+1} - c_{j+1}^\dagger c_j)$. The quantity $q_k = u_k^2 - v_k^2 = \cos \theta_k \propto h - \cos k$ is the effective charge of the quasiparticles, which is even with respect to $k$. It is instructive then to rewrite the denominator,

$$I = \int_{-\pi}^{\pi} dk J(k)n_{k+v_d},$$

in a form which lays plain that it is no more than the current in response to the applied field with $v_d = q_k E_x \tau$, the drift velocity, and $J(k)$ the momentum dependence of the current operator. In the absence of the drift velocity, $I = 0$. Taylor expanding around $v_d = 0$ yields Eq. (13). Herein lies the crux of the problem. In a non-interacting system, the local definition of the current operator used here and that arising from the continuity equation both yield the same result, namely that $J(k) = q_k dE_k/dk = dH/dk$, in which case the integrand is positive definite and cannot integrate to zero. However, for the problem at hand, the current operator arising from the continuity equation, namely $q_k dE_k/dk$, is non-local in space, possessing sink and source terms, and hence is not tenable. Such non-locality typifies most strongly correlated systems because the entities which carry the current are not simply determined by the kinetic part of the Hamiltonian. Consequently, the current operator, defined from the continuity equation is non-local and lacks a particle interpretation. In such cases, $I$ can vanish. The vanishing of $I$ here takes place because the group velocity, $dE_k/dk$, is an odd function of $k$, while $q_k$ is even. Consequently, the momenta at which $q_k$ and $dE_k/dk$ change sign need not be correlated. Because the overall integrand is an even function of $k$, it will have positive and negative contributions on the interval $[0, \pi]$, which for certain system parameters could yield a cancellation as illustrated in Fig. 4.

Classic examples in which the operators in the local current operator do not coincide with the charge carriers are the insulating state of the Hubbard model at half-filling for sufficiently large $U$. In this problem, there is no divergent length scale as there is no order parameter for the Mott insulating state. It is entirely likely that the insulator in the dilute 2D electron gas is induced by the correlations as well as it obtains in the large $r_e$ regime. Hence, caution must be taken in using standard scaling arguments to relate the thermopower to divergent correlation lengths as has been done recently. Unless the charge carriers are local degrees of freedom,
naive scaling with the correlation length is insufficient to describe transport properties such as the thermopower.

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