

Sum rule for thermal conductivity and dynamical thermal transport coefficients in condensed matter

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We display an interesting sum rule for the dynamical thermal conductivity for many standard models of condensed matter in terms of the expectation of a thermal operator. We present the thermal operator for several model systems of current interest, which enable an evaluation of the sum rule and the Lorentz number, the thermoelectric figure of merit as well as the thermopower at high frequencies. As a by-product, we present exact formulas for the $T=0$ chemical potential $\mu(0)$ for charged many-body systems, including the Hubbard model, in terms of expectation values of extensive operators. Simple estimates are provided for the thermopower of an infinitely correlated band model on the triangular lattice, modeling the physics of the sodium cobalt oxide system. The present result goes beyond the Heikes-Mott formula for the thermopower, and contains an additional transport correction that is sensitive to the lattice topology as well as the sign of hopping.

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I. INTRODUCTION

A problem of considerable current interest is the evaluation of the thermal response functions: κ the thermal conductivity and S the thermoelectric response function (Seebeck coefficient) for complex systems. These include strongly correlated matter, where the role of interactions is profound and impossible to capture within perturbative formulations, and also materials with complex unit cells, such as the skutterudites,¹ and negative thermal expansion systems where geometrical frustration plays a major role.² One major motivation for these efforts is from the requirements of the thermoelectric industry, where a large thermoelectric figure of merit [defined in Eq. (39)] is desirable, and it is important to understand the material characteristics that promote a large figure of merit. The standard tool, namely the Boltzmann equation approach, is overly restrictive in that it is tied down to the concept of long-lived and weakly interacting quasiparticles, which are less useful in these contexts.

In this paper, we present a new formalism for computation of the thermal response functions, by considering the response to *dynamical* temperature gradients, i.e., a frequency dependent problem. This yields the frequency dependent thermal conductivity $\kappa(\omega)$ as well as the thermopower $S(\omega)$. The frequency dependence of $\kappa(\omega)$ is of relevance theoretically and also practically: a silicon chip operating at several gigahertz clock speed in a computing processor needs to transport the ac Joule dissipation. The relevant transport parameter in this context is the dynamical $\kappa(\omega)$, which can be much smaller than the static κ for $\omega \sim 100$ GHz.³

Although studying the dynamical conductivity looks at first sight like further complicating an already intractable problem, in fact it turns out that several simplifications arise in the limit of high frequencies. These have a close counterpart in our fairly successful theory of the Hall constant of strongly correlated matter.⁴ In brief, the problem of transport may be decomposed into the following conceptually distinct but technically intertwined aspects: (a) transport proper, (b) single particle description, and (c) interactions. The single

particle aspect determines such variables as the density of states and its derivatives, the transport aspect involves the elastic and inelastic scattering rates usually modeled by a relaxation time, and the interaction aspect involves the influence of correlations. While none of these are trivial, the last one, namely interactions, is conceptually as well as computationally most difficult. For example, in Mott-Hubbard systems, the very notion of the hole is nontrivial in the context of, say, the Hall constant, where one knows that near half filling, the momentum space definition can give opposite results in certain cases to the real space picture for the sign of the Hall constant.⁴

In this context, going to high frequencies is a great advantage if one can isolate combinations of thermal response functions that are relatively less frequency dependent. In the Hall constant problem, the Hall resistivity ρ^{xy} is quite benign, being ω independent at least in the Drude theory, as opposed to the Hall conductivities σ^{xy} and σ^{xx} , which are serious functions of ω *individually* but *not* in the combination leading to ρ^{xy} . Moreover the high frequency limit is the starting point of the Mori-type treatment of transport quantities, as seen in the example for the Hall constant.⁵ In a similar spirit, we identify several variables in this work, and write down the operators that need to be evaluated. We stress that the expectation values of the objects computed here are equilibrium values, and while quite nontrivial in detail, are conceptually much easier than the transport objects; this is the advantage of disentangling dynamics from interactions as in other contexts. While our approach is not exact either, as it depends on the assumption of weak frequency dependence of such combinations, it is quite distinct from the Boltzmann approach and provides a useful counterpoint to the latter, treating the effect of interactions more respectfully. In simple examples, we show that the weak ω dependence is an excellent assumption, and further our results should provide a stimulus for experimental investigation of the frequency dependence of thermal transport constants.

We present an interesting sum rule for the real part of the dynamical thermal conductivity. The sum rule is in terms of

the expectation of an operator (the thermal operator) that is presented for several models of condensed matter physics, and while the task of evaluating it is nontrivial in detail, it is quite feasible to estimate it from other considerations that we present. The situation is akin to the well-known plasma or the f -sum rule; the Thomas-Ritchie-Kuhn sum rule gives the integral of the real conductivity in terms of easily measurable variables in the continuum $4\pi nq_c^2/m$, whereas *on a lattice*, it is [see Eq. (A11)] the expectation of essentially the kinetic energy.⁶ Such an expectation is nontrivial, but several numerical techniques lend themselves to this task quite effectively, such as exact diagonalization and quantum Monte Carlo methods. This new sum rule should be of considerable interest in many situations, including the case of nonlinear lattices, where the classical counterpart is already interesting, since it is the expectation of a single extensive operator, and apparently equally unknown.

Our paper has a twofold purpose. We present the formalism for the thermal transport variables in some detail with the hope of returning to calculate some of them in a later work, and the other is somewhat pedagogical in nature. Existing literature is quite focused on specific issues, and many subtleties receive less mention than their due. It is my impression that a detailed description of the formalism might be useful to some workers. The results of computations based on the formalism presented here should shed light on currently interesting issues, such as the departure from Wiedemann-Franz ratio for the case of strongly correlated systems as seen in experiments, where the Lorentz number departs from the free electron value at low T .⁷

An interesting by-product of our work is the exact formula for the chemical potential $\mu(T)$ at $T=0$ for charged many-body systems in terms of the expectation of an extensive operator. In general the only way of computing $\mu(T)$, including in the ground state, is from the thermodynamic formula $\mu(T)=[\partial F(T,N)]/\partial N$. However at $T=0$, our result shows an alternate and potentially widely useful method. This arises from the physical requirement of the vanishing of thermopower *at all frequencies* in the ground state, being related to entropy transport, and since the high frequency formulas explicitly involve the chemical potential, these yield the alternate formulas for the zero temperature chemical potential of all charged many body systems. We comment on this further in the discussion section (Sec. X). The plan of the paper is as follows.

(a) In Secs. II and III, we derive the complete expressions for the finite frequency thermal conductivity and thermopower, using standard linear response theory, and obtain a sum rule for the dynamical thermal conductivity. It is expressed in terms of a new extensive object Θ^{xx} that we term the “thermal operator.”

(b) Section IV makes a connection with the “standard” Kubo formulas. Our results contain corrections to the Kubo formulas for the case of nondissipative systems such as superconductors, and it might be of interest to see the origin of these in the fine tuning of the standard derivations, as provided in Sec. IV.

(c) In Sec. V, we identify the high frequency observables that are suitable for study being less sensitive to ω . The high frequency Seebeck coefficient is among these, and is ex-

pressed in terms of another new extensive object Φ^{xx} that we denote the “thermoelectric operator.”

(d) The thermal and thermoelectric operators have a dependence on the interactions as well as the details of the specific model systems. Hence it is important to compute these operators for standard models, which is accomplished in the latter sections. In Sec. VI, we present the thermal operator Θ^{xx} for the anharmonic disordered lattice vibration problem, and make a connection with the classical limit. Illustrative examples from harmonic lattice are given to provide a feel for the nature of the operators encountered.

(e) In Sec. VII, we study the intermediate coupling models of current interest, namely the Hubbard model, the homogeneous electron gas, and the periodic Anderson lattice, for which we present the thermal and thermoelectric operators, and also indicate the role of disorder in modifying these variables. We establish the essential correctness of this approach for the case of zero coupling, where the standard Boltzmann-Drude results for the Lorentz number and the thermopower are reproduced.

(f) In Sec. VIII, we study the thermal and thermoelectric operators for the strong coupling models: the Heisenberg model and the infinite U Hubbard model.

(g) In Sec. IX we apply the results of Sec. VIII to the currently interesting case of the triangular lattice Na_xCoO_2 , a metallic thermoelectric material. Our theory yields a formula for the high T limit of the Seebeck coefficient for this system, which contains the Heikes-Mott formula and provides a transport correction to the same. The large transport correction highlights the role of the lattice topology.

(h) In Sec. X, we discuss the special nature of the thermal-type operators, namely the vanishing of its expectation in the ground state. We also comment on the exact formulae for the chemical potential at $T=0$ for charged Fermi systems that our approach yields.

(i) The appendix contains the already well-known results for the electrical conductivity for completeness.

II. THERMAL CONDUCTIVITY AT FINITE FREQUENCIES

For models involving particle flow, we recall that the heat current is defined as the energy current minus μ times the particle current. Therefore to generate the linear response equations, we write the grand canonical ensemble Hamiltonian in the presence of a temperature variation as ($\omega_c = \omega + i0^+$)

$$K = K_0 + K_1 e^{-i\omega_c t}, \quad (1)$$

with adiabatic switching from the infinitely remote past $t = -\infty$ as usual, and $K_0 = \sum_{\vec{r}} K(\vec{r}) = \sum_{\vec{r}} [H(\vec{r}) - \mu n(\vec{r})]$. Here $H(\vec{r})$ is the energy density, and since we are mainly dealing with lattice models, we sum over r . The operator

$$K_1 = \sum_{\vec{r}} \psi(\vec{r}) K(\vec{r}), \quad (2)$$

where $\psi(\vec{r})$ is a small (pseudo) gravitational field with some spatial variation such that its average is zero. This expression follows the conceptually important work of Luttinger.⁸ Alter-

nate schemes such as the Kadanoff-Martin method⁹ lead to the same results. Here $\psi(r)$ is not quite a gravitational field since it couples to $K(r)$ rather than to $H(r)$, but serves the same purpose, it is a *mechanical field* as opposed to the true spatially dependent temperature, which is a *thermodynamic field*. The latter is more subtle, and ensuring that such a varying field is established in a given system is in general a very hard thing to achieve rigorously, requiring as it does a detailed understanding of the equilibration processes that operate on a microscopic and inhomogeneous level. Luttinger's idea reorganizes and subdivides this complication into logically separate parts, and allows us to deal with a mechanical field with an arbitrary spatial variation. The connection with true temperature variation is the next logical step, where Luttinger showed that we may essentially regard $\nabla\psi(\vec{r}) = [\nabla T(\vec{r})]/T$. Here we denote the local temperature by $T(\vec{r})$, and $\beta(\vec{r}) = 1/[k_B T(\vec{r})]$. A formal discussion is provided by Luttinger,⁸ who drew an analogy with the Einstein relation. The latter relates the response to the (mechanical) electrical field to the observed concentration gradient, which in turn is related to its conjugate, namely the (thermodynamic) chemical potential gradient. The resulting frequency dependent linear response functions are understood as responses to this mechanical force. Relating these to the thermodynamic response functions is the other part of the issue, and may be proved only under certain standard assumptions;⁸ we are content to assume the same in this work. A simple qualitative argument to help motivate the identification $\nabla\psi(\vec{r}) = [\nabla T(\vec{r})]/T$, is that the temperature profile varies in such a way as to annul the variation of the added energy fluctuation; therefore, if locally $\psi(\vec{r})$ increases, so does $T(\vec{r})$ so as to maintain the local constancy of the action $\sum_{\vec{r}}\beta(\vec{r})K(\vec{r})$.

Let \mathcal{L} be the number of sites, or equivalently the volume of the system (by setting the lattice constant as unity). We next Fourier transform Eq. (2) by introducing

$$\psi(\vec{r}) = \sum_{\vec{k}} \hat{\psi}(\vec{k}) \exp(-i\vec{k} \cdot \vec{r}), \quad (3)$$

$$K(\vec{r}) = \frac{1}{\mathcal{L}} \sum_{\vec{k}} \hat{K}(\vec{k}) \exp(-i\vec{k} \cdot \vec{r}), \quad (4)$$

so that

$$K_1 = \sum_{\vec{k}} \hat{K}(-\vec{k}) \hat{\psi}(\vec{k}). \quad (5)$$

The heat current operator is Fourier decomposed as $\vec{J}^Q(\vec{r}) = 1/\mathcal{L} \sum \exp(-i\vec{k} \cdot \vec{r}) \vec{J}^Q(k)$. The induced heat current in response to the k th mode with can be computed from linear response theory. We will assume a "temperature" gradient along the unit vector \hat{x} , so that $\nabla T(\vec{r}) = T \nabla \psi(\vec{r}) = T \sum (-ik_x \hat{x}) \hat{\psi}(k_x) \exp(-ik_x x)$. Then

$$\kappa(\omega_c) = \lim_{k_x \rightarrow 0} \kappa(k_x, \omega_c),$$

with

$$\kappa(k_x, \omega_c) = \frac{e^{i\omega_c t}}{\mathcal{L}} \left\{ \frac{\langle \hat{J}_x^Q(k_x) \rangle}{i T k_x \hat{\psi}(k_x)} \right\}. \quad (6)$$

The expectation $\langle \hat{J}_x^Q(k_x) \rangle$ is given by standard linear response theory^{10,8,11} and using Eq. (6) we find

$$\begin{aligned} \kappa(k_x, \omega_c) &= \frac{1}{\hbar T k_x \mathcal{L}} \int_{-\infty}^t e^{i\omega_c(t-t')} dt' \langle [\hat{J}_x^Q(k_x, t), \hat{K}(-k_x, t')] \rangle \\ &= \frac{-i}{\hbar \omega_c T k_x \mathcal{L}} \left(\langle [\hat{J}_x^Q(k_x), \hat{K}(-k_x)] \rangle \right. \\ &\quad \left. + i \int_0^{\infty} e^{i\omega_c t'} dt' \langle [\hat{J}_x^Q(k_x, t'), [\hat{K}(-k_x, 0), K]] \rangle \right). \end{aligned} \quad (7)$$

We integrated by parts to get the second line from the first. In the limit of almost uniform variation, $k_x \rightarrow 0$, we show that

$$\langle [\hat{J}_x^Q(k_x), \hat{K}(-k_x)] \rangle \sim -k_x \langle \Theta^{xx} \rangle, \quad (9)$$

where Θ^{xx} is the thermal operator, to coin a name. In the uniform (i.e., $k_x \rightarrow 0$) operator \hat{J}_x^Q is not a constant of motion, and yet the average is of $O(k_x)$, this is so since the uniform term vanishes by noting that the thermal average

$$\langle [\hat{J}_x^Q, K] \rangle \equiv \frac{1}{\mathcal{Z}} [\text{Tr } e^{-\beta K} \hat{J}_x^Q K - \text{Tr } e^{-\beta K} K \hat{J}_x^Q] = 0 \quad (\text{Identity I}),$$

with $\mathcal{Z} = \text{Tr } e^{-\beta K}$, the last identity following from the cyclicity of trace. Therefore we can write an equation for the *thermal operator* directly as

$$\Theta^{xx} = - \lim_{k_x \rightarrow 0} \frac{d}{dk_x} [\hat{J}_x^Q(k_x), \hat{K}(-k_x)], \quad (10)$$

and thus it is straightforward if tedious to compute it, given the explicit forms of the current and energy operators.

The heat current is obtained from the continuity equation for heat density, written in momentum space as

$$\lim_{k_x \rightarrow 0} \frac{1}{k_x} [\hat{K}(-k_x), K] = \hbar \hat{J}_x^Q, \quad (11)$$

where $\hat{J}_x^Q = \hat{J}_x^Q(k)/k_{x \rightarrow 0}$, so that the thermal conductivity at finite frequencies is

$$\kappa(\omega_c) = \frac{i}{\hbar \omega_c T \mathcal{L}} \left[\langle \Theta^{xx} \rangle - i \int_0^{\infty} e^{i\omega_c t'} dt' \langle [\hat{J}_x^Q(t'), \hat{J}_x^Q(0)] \rangle \right]. \quad (12)$$

It is worth making a comment on the difference between this calculation and that of $\sigma(\omega)$, the electrical conductivity at this point. A calculation of $\sigma(\omega)$, as in the Appendix, is in close parallel to this one for $\kappa(\omega)$, with the electrical current and charge density fluctuation operators (defined in the Appendix) replacing the heat current and the energy density as in $\hat{J}_x^Q(k_x) \rightarrow \hat{J}_x(k_x)$ and with $\hat{K}(-k_x) \rightarrow \rho(-k_x)$. In that case, the commutator $[\hat{J}_x(k_x), \rho(-k_x)]$ explicitly vanishes as $k_x \rightarrow 0$, and hence the analog of the first term inside the round

bracket of Eq. (8) automatically begins as $O(k_x)$, with a coefficient $\propto \langle \tau^{xx} \rangle$ [defined in Eq. (A4)]. In the present case, Eq. (9) together with Eq. (11) again leads to a cancellation of k_x between the numerator and the denominator, leading to a finite result in the uniform limit. Thus the thermal conductivity calculation is somewhat disguised by the noncommutation of the uniform operators i.e., $[\hat{J}_x^Q, K] \neq 0$, which is luckily immaterial, since the *expectation of this object vanishes* due to the Identity I.

We perform a Lehmann representation¹¹ to write Eq. (12) with $p_n = 1/Z \exp(-\beta \epsilon_n)$ as

$$\kappa(\omega_c) = \frac{i}{\hbar \omega_c T \mathcal{L}} \left[\langle \Theta^{xx} \rangle - \hbar \sum_{n,m} \frac{p_n - p_m}{\epsilon_n - \epsilon_m + \hbar \omega_c} |\langle n | \hat{J}_x^Q | m \rangle|^2 \right]. \quad (13)$$

Using the partial fractions identity (for any Δ)

$$\frac{1}{\hbar \omega_c (\hbar \omega_c + \Delta)} = \frac{1}{\Delta} \left(\frac{1}{\hbar \omega_c} - \frac{1}{\hbar \omega_c + \Delta} \right),$$

we obtain

$$\kappa(\omega_c) = \frac{i}{\hbar \omega_c T} D_Q + \frac{i\hbar}{T \mathcal{L}} \sum_{n,m} \frac{p_n - p_m}{\epsilon_m - \epsilon_n} \frac{|\langle n | \hat{J}_x^Q | m \rangle|^2}{\epsilon_n - \epsilon_m + \hbar \omega_c}, \quad (14)$$

where

$$\begin{aligned} D_Q &= \frac{1}{\mathcal{L}} \left[\langle \Theta^{xx} \rangle - \hbar \sum_{n,m} \frac{p_n - p_m}{\epsilon_m - \epsilon_n} |\langle n | \hat{J}_x^Q | m \rangle|^2 \right] \\ &= \frac{1}{\mathcal{L}} \left[\langle \Theta^{xx} \rangle - \hbar \int_0^\beta d\tau \langle \hat{J}_x^Q(-i\tau) \hat{J}_x^Q(0) \rangle \right]. \end{aligned} \quad (15)$$

Using the standard identity $1/(\omega_c - E) = P1/(\omega - E) - i\pi\delta(\omega - E)$ for any E , it is instructive to write the real part of the Lehmann representation of Eq. (14) as

$$\text{Re } \kappa(\omega) = \frac{\pi}{\hbar T} \delta(\omega) \bar{D}_Q + \text{Re } \kappa_{reg}(\omega),$$

with

$$\begin{aligned} \text{Re } \kappa_{reg}(\omega) &= \frac{\pi}{T \mathcal{L}} \left(\frac{1 - e^{-\beta \hbar \omega}}{\omega} \right) \\ &\times \sum_{\epsilon_n \neq \epsilon_m} p_n |\langle n | \hat{J}_x^Q | m \rangle|^2 \delta(\epsilon_m - \epsilon_n - \hbar \omega), \end{aligned} \quad (16)$$

$$\bar{D}_Q = \frac{1}{\mathcal{L}} \left[\langle \Theta^{xx} \rangle - \hbar \sum_{\epsilon_n \neq \epsilon_m} \frac{p_n - p_m}{\epsilon_m - \epsilon_n} |\langle n | \hat{J}_x^Q | m \rangle|^2 \right]. \quad (17)$$

Here κ_{reg} is the regular part of thermal conductivity that excludes the delta function at $\omega=0$, and \bar{D}_Q is the weight of the delta function at $\omega=0$. It is seen that the weight of the zero frequency delta function involves a different object than the one in Eq. (15), there is a cancellation of terms with equal energy between the two terms in Eq. (13). We elaborate on this distinction below.

The sum rule for the real part of the thermal conductivity (an even function of ω) follows from Eq. (16) by integration, or equivalently from Eq. (13) and using the Kramers-Kronig relation to identify the coefficient of i/ω at high frequencies in the complex conductivity as the integral of the real part,

$$\int_0^\infty \text{Re } \kappa(\omega) d\omega = \frac{\pi}{2\hbar T \mathcal{L}} \langle \Theta^{xx} \rangle. \quad (18)$$

This interesting sum rule is one of the main formal results of this paper. The extensive thermal operator Θ^{xx} is analogous to the stress tensor τ^{xx} in the sum rule Eq. (A11) for the electrical conductivity $\sigma(\omega)$, and depends in its details upon the underlying model; we present it in the case of several problems of current interest in the following.

We may rewrite Eq. (14) in a more compact form as

$$\kappa(\omega_c) = \frac{i}{T \hbar \omega_c} D_Q + \frac{1}{T \mathcal{L}} \int_0^\infty dt e^{i\omega_c t} \int_0^\beta d\tau \langle \hat{J}_x^Q(-t - i\tau) \hat{J}_x^Q(0) \rangle. \quad (19)$$

The first term in Eq. (19) is $\propto D_Q$, and is in addition to the original Kubo formula¹⁰ for thermal conductivity, namely the second term. It represents a nontrivial correction for nondissipative situations, but vanishes in dissipative cases due to reasons that we elaborate below.

Integrating the second term of Eq. (19) gives an estimate for $\int_0^\infty \text{Re } \kappa(\omega) d\omega$ namely $\pi/(2T \mathcal{L}) \int_0^\beta d\tau \langle \hat{J}_x^Q(-i\tau) \hat{J}_x^Q(0) \rangle$, which has been written in literature earlier in its high temperature limit.¹² However it cannot be viewed as a sum rule, since the estimate is a correlation function of a pair of extensive currents, rather than a direct expectation value of a single extensive operator as in Eq. (18). Further, in nondissipative situations, this estimate misses the contribution from the D_Q term and is thus incorrect. For dissipational systems, it does reduce to Eq. (18), on using the vanishing of D_Q and Eq. (15). Therefore it is clear that in all cases, Eq. (18) stands in complete parallel to the f -sum rule Eq. (A11) for $\sigma(\omega)$ with the thermal operator Θ^{xx} relating the stress tensor τ^{xx} .

We next make a few comments on the object D_Q , which enters into the correct expression for thermal conductivity Eq. (19), and \bar{D}_Q that enters in Eq. (17). Note that the difference between D_Q and \bar{D}_Q lies in the nature of the double sum over the current matrix elements; \bar{D}_Q explicitly excludes terms with equal energy, so that the difference is a sum over all degenerate manifolds (including diagonal matrix elements $n=m$)

$$D_Q - \bar{D}_Q = -\hbar \beta \sum_{\epsilon_n = \epsilon_m} p_n |\langle n | \hat{J}_x^Q | m \rangle|^2. \quad (20)$$

A detailed discussion of the charge stiffness in the similar context of charge transport is given in Ref. 13, where the distinction between zero and finite temperatures is elaborated upon. Our discussion here is along similar lines, except that here we use the term charge stiffness to denote both D_c and \bar{D}_c whereas these are denoted by the terms Meissner stiffness and charge stiffness in Ref. 13. In the case of the thermal conductivity, D_Q and \bar{D}_Q are thus the thermal analogs of the

Meissner stiffness and the charge stiffness of Ref. 13

The value of D_Q is zero for most dissipational situations, i.e., for generic systems at finite temperatures. It is, however, nonzero in general for systems that display macroscopic many body coherence, i.e., either superfluidity or superconductivity. For a superconductor, the analogous object, D_c in the charge conductivity [see Eq. (A7)] is in fact related to the London penetration depth or the superfluid stiffness, and its nonvanishing is the very hallmark of its “super” nature. It is alternately obtainable from the Byers-Yang relation $D_c \propto \lim_{\phi \rightarrow 0} (d^2/d\phi^2)F(\phi)$ where $F(\phi)$ is the free energy of the superconductor in the presence of a hole threaded by a flux ϕ . While there is no obvious parallel to the flux for thermal conductivity, the formal expressions are very similar.

There has been considerable discussion of the corresponding charge stiffness in recent literature¹⁴ for *integrable many-body systems* in low dimensions, such as the Heisenberg or the Hubbard models in one dimension (1D), where the existence of many conservation laws pushes them away from equilibrium with negligible restoring forces, leading to a ballistic rather than diffusive behavior, as first pointed out by Giamarchi.¹⁴ An interesting numerical study of the statistics of the Kubo conductivity in 1D has also given some insights around the zero frequency limit.¹⁵ Very recently the thermal conductivity has also been discussed in literature for integrable models.¹⁶ In general terms, integrable models are akin to the free particle system rather than to superconductors or superfluids, since there is no broken symmetry. In such cases, we expect $D_Q=0$ but it is possible that $\bar{D}_Q \neq 0$, albeit possibly only for finite sized systems. This is analogous to the charge stiffness story,¹³ where D_c is zero for normal metals whereas \bar{D}_c may be nonzero. In this sense the zero temperature limit is singular; \bar{D}_c occurs in both conductivity and in the Byers-Yang-Kohn type formula $\bar{D}_c \propto \lim_{\phi \rightarrow 0} (d^2/d\phi^2)E_0(\phi)$, with $E_0(\phi)$ the ground state energy in the presence of a flux,¹³ whereas at nonzero T there is a distinction as in the rhs of Eqs. (20) and (A13). The object \bar{D}_Q involves matrix elements of the current in states with *distinct energy*, and these are zero if the energy or heat current is conserved, as in the case of the free electron system. More nontrivially, in the case of the exactly integrable Heisenberg model in 1D, the higher conservation laws include the energy current.¹⁶ In such a case, since the heat current is a constant of motion, it follows that $\hat{J}_x^Q(t) = \hat{J}_x^Q(0)$, leading to a simple calculation of $\kappa(\omega)$ using Eq. (12). Here the second term in Eq. (12) vanishes on using $\hat{J}_x^Q(t) = \hat{J}_x^Q(0)$, giving

$$\kappa(\omega_c) = \frac{i}{\hbar \omega_c T \mathcal{L}} \langle \Theta^{xx} \rangle.$$

Thus $\kappa(\omega_c)$ may be computed for integrable models with a conserved energy current directly from a knowledge of $\langle \Theta^{xx} \rangle$.

We will show in Sec. IV that the vanishing of D_Q is natural for generic systems, using an argument based on the Kubo identity, and also pinpoint the possible technical reason

as to why it is nonzero for, say, a clean superconductor. In subsequent sections we provide an evaluation of the thermal operator Θ^{xx} given in Eq. (10) for various models of current interest.

III. THERMOPOWER

We next study the linear response formulation for thermopower. If we define the charge current and its Fourier decomposition as $\vec{J}(\vec{r}) = 1/\mathcal{L} \sum \exp(-i\vec{k} \cdot \vec{r}) \vec{J}(\vec{k})$, then in the presence of an electric field and a temperature gradient,

$$\langle \hat{J}_x \rangle = \sigma(\omega) E_x + \gamma(\omega) (-\nabla T), \quad (21)$$

where $\hat{J}_x = \hat{J}_x(k_x \rightarrow 0)$. The thermopower is defined as

$$S(\omega) = \frac{\gamma(\omega)}{\sigma(\omega)}. \quad (22)$$

We can obtain $\gamma(\omega)$ by linear response theory in parallel to the thermal conductivity, and the answer is

$$\gamma(\omega_c) = \lim_{k_x \rightarrow 0} \left(\frac{\langle \hat{J}_x(k_x) \rangle e^{i\omega_c t}}{iT k_x \hat{\mu}(k_x) \mathcal{L}} \right). \quad (23)$$

The expression for $\langle \hat{J}_x \rangle$ follows the same lines as that for the heat current and we find

$$\gamma(\omega_c) = \frac{i}{\hbar \omega_c T \mathcal{L}} \left[\langle \Phi^{xx} \rangle - i \int_0^\infty e^{i\omega_c t'} \langle [\hat{J}_x(t'), \hat{J}_x^Q(0)] \rangle \right], \quad (24)$$

where we have introduced another important extensive operator, the “thermoelectric operator,”

$$\Phi^{xx} \equiv - \lim_{k \rightarrow 0} \frac{d}{dk_x} [\hat{J}_x(k_x), K(-k_x)]. \quad (25)$$

It is useful to perform its Lehmann representation, so that

$$\gamma(\omega_c) = \frac{i}{\hbar \omega_c T \mathcal{L}} \left[\langle \Phi^{xx} \rangle - \hbar \sum_{n,m} \frac{p_n - p_m}{\epsilon_n - \epsilon_m + \hbar \omega_c} \times \langle n | \hat{J}_x | m \rangle \langle n | \hat{J}_x^Q | m \rangle \right]. \quad (26)$$

We can proceed further as in the case of thermal conductivity by expanding the product using partial fractions and find

$$\gamma(\omega_c) = \frac{i}{\hbar \omega_c T} D_\gamma + \frac{i\hbar}{T \mathcal{L}} \sum_{n,m} \left(\frac{p_n - p_m}{\epsilon_m - \epsilon_n} \right) \frac{\langle n | \hat{J}_x | m \rangle \langle n | \hat{J}_x^Q | m \rangle}{\epsilon_n - \epsilon_m + \hbar \omega_c}, \quad (27)$$

where

$$D_\gamma = \frac{1}{\mathcal{L}} \left[\langle \Phi^{xx} \rangle - \hbar \sum_{n,m} \frac{p_n - p_m}{\epsilon_m - \epsilon_n} \langle n | \hat{J}_x | m \rangle \langle n | \hat{J}_x^Q | m \rangle \right]. \quad (28)$$

Since the two currents involved are not identical, it is not possible to take the real part of this expression readily, and it

is not profitable to seek a sum rule. It is however, interesting to note that by combining various formulae, the thermopower has a high frequency expansion of the type

$$S(\omega) = S^* + O\left(\frac{1}{\omega}\right),$$

where

$$S^* = \frac{\langle \Phi^{xy} \rangle}{T \langle \tau^{xy} \rangle}, \quad (29)$$

and so a knowledge of Φ^{xy} is useful in determining the asymptotic behavior. We can rewrite this equation as

$$\gamma(\omega_c) = \frac{i}{\hbar \omega_c T} D_\gamma + \frac{1}{T \mathcal{L}} \int_0^\infty dt e^{i\omega_c t} \int_0^\beta d\tau \langle \hat{J}_x(-t - i\tau) \hat{J}_x^Q(0) \rangle. \quad (30)$$

We again note that $D_\gamma = 0$ for most dissipational cases.

IV. KUBO-TYPE FORMULA FOR GENERAL NONDISSIPATIVE SYSTEMS

In an earlier section, we derived the linear response theory expressions for the various conductivities Eq. (6), and argued that the usual formulas quoted in literature, e.g., in Ref. 17 following Kubo¹⁰ and others⁸ have extra terms that arise for nondissipative systems, such as superconductors and superfluids. The reader might wonder as to the origin of these extra terms, since the common belief is that the Kubo formulas are complete and exact. In this section we obtain these terms from a careful analysis of the Kubo arguments. We deal with the case of thermal conductivity below, but the arguments apply equally to the electrical conductivity as the reader can easily see. In the case of the electrical conductivity a simpler argument gives the final result using the transverse gauge, i.e., by realizing the electrical field as the time derivative of a vector potential rather than as the gradient of a scalar potential,^{18,19} although the present method is readily generalized to that case as well, as shown in the Appendix.

We begin with Eq. (7) rearranged in the form preferred by Kubo,

$$\kappa(k_x, \omega_c) = \frac{1}{k_x T \mathcal{L}} \int_0^\infty dt e^{i\omega_c t} \text{Tr}([\rho_0, \hat{K}(-k_x, -t)] \hat{J}_x^Q(k_x)), \quad (31)$$

with the density matrix $\rho_0 = e^{-\beta K} / \mathcal{Z}$. From this point onwards one uses three important steps.

(1) The so-called ‘‘Kubo identity’’¹⁰ which is written as $\mathcal{K}[K(-k_x, -t)] = 0$ where

$$\mathcal{K}[A] \equiv [\rho_0, A] - \int_0^\beta \rho_0 [A(-i\tau), K] d\tau, \quad (32)$$

which is easily derived by inserting a complete set of states.

(2) The conservation law

$$\frac{1}{\hbar k_x} [\hat{K}(-k_x, -t), K] = \hat{J}_x^Q(-k_x, -t). \quad (33)$$

(3) The homogeneous or uniform limit $k_x \rightarrow 0$.

These three steps together give the usual stated result Eq. (12) without the first term involving D_Q . These steps lead one to an expression involving the matrix elements of $K(-\hat{k}_x, -t)/k_x$ and it is tempting to replace this with those of $\hat{J}_x^Q(0, -t)$. It is precisely here that one needs to be careful. As long as k_x is finite it is clear that $\hat{K}(-k_x, -t)$ as well as $\hat{J}_x^Q(-k_x, -t)$ have matrix elements between eigenstates of the Hamiltonian K that are at *different energies*, i.e., inhomogeneous excitations cost energy. In the limit of $k_x \rightarrow 0$ this need not be so, the current operator *can have* matrix elements between states of the same energy, whereas by construction the commutator $[\hat{K}(-k_x, -t), K]$ filters out states with the same energy. Thus the operator identity Eq. (33) is potentially in trouble precisely where we need it. What is easier to justify is to use a time derivative to filter out equal energy states so that a good alternative identity to Kubo’s identity is to use

$$\frac{d\mathcal{K}[K(-k_x, -t)]}{dt} = 0. \quad (34)$$

This is the Kubo identity again, but with the operator $(-i) \times [\hat{K}(-k_x, -t), K]$ in place of $\hat{K}(-k_x, -t)$, this extra commutator with K is transferred to $\hat{J}_x^Q(-k_x, -t)$ on using the conservation law, and improves matters. In this form we can take the next two steps safely since $[\hat{J}_x^Q(0, -t), K]$ does not have any matrix elements between equal energy states. We can now integrate Eq. (34) between finite times and get

$$\mathcal{K}[K(-k_x, t)] = \mathcal{K}[K(-k_x, 0)]. \quad (35)$$

This equation tells us that the errors in replacing the matrix elements of $K(-\hat{k}_x, -t)/k_x$ with those of $\hat{J}_x^Q(-t)$ are *time independent*, i.e., relating solely to the matrix elements of current in the manifold of zero energy difference states. Such a manifold of states is statistically significant only in a superconductor, and hence we expect it to be relevant in that context.

Proceeding as before to the uniform limit, we get

$$\kappa(\omega_c) = \frac{i}{\hbar \omega_c T \mathcal{L}} \left\{ \langle \Theta^{xy} \rangle - \hbar \int_0^\beta d\tau \langle \hat{J}_x^Q(-i\tau) \hat{J}_x^Q(0) \rangle \right\} + \frac{1}{T \mathcal{L}} \int_0^\infty e^{i\omega_c t} dt \int_0^\beta d\tau \langle \hat{J}_x^Q(-t - i\tau) \hat{J}_x^Q(0) \rangle. \quad (36)$$

The term in curly brackets is recognized as $\mathcal{L}D_Q$ as in Eq. (19), and hence the two derivations lead to exactly the same answer.

We have seen that D_Q owes its possible nonvanishing to the matrix elements of the current operator in the manifold of zero energy difference states, such as exist in a superconductor. For most dissipative systems, such a manifold is statistically insignificant, and it should be noted that in such instances, D_Q is actually zero.

The only instances where D_Q and analogously D_c of Eqs. (15) and (A7) are nonzero have to do with superfluid or superconducting states. We remind the reader of the change in terminology from Ref. 13 as remarked on earlier below Eq. (20), D_c represents the Meissner stiffness of Ref. 13. In these cases, D_c for example is proportional to the superconducting density of electrons ρ_s , as in the London theory. Traditionally ρ_s is obtained by taking the current current correlator and taking the limit $\vec{k} \rightarrow 0$ for the *transverse* part, i.e., $\vec{J} \cdot \vec{k} = 0$, after having taken the static limit at the outset—this is the classic Meissner effect calculation.²⁰ However, it is also natural to see the superconducting fraction in the conductivity where we first set $\vec{k} \rightarrow 0$ and *then* let $\omega \rightarrow 0$. This is the procedure followed in the well-known Ferrell-Glover-Tinkham sum rule determination of the penetration depth in superconductors from the infrared conductivity.²¹ In this sequence of taking the uniform limit, it should not matter if we have worked with the longitudinal conductivity rather than the transverse one, and our derivation here is the longitudinal counterpart of the transverse derivation first obtained for the Hubbard-type models in Ref. 19. A nice discussion of the various limits is given in Ref. 22. A superconductor would also have a nonzero D_Q if impurities are neglected; however, impurities *do scatter* quasiparticles and hence one expects disorder to make this object tend to vanish, unlike the variable D_c which is less sensitive to disorder by virtue of the Anderson theorem. There is also the similarity of the D_Q term with that of second sound that one expects in a superconductor, namely an undamped energy wave; D_Q then appears as the residue at a second sound pole in the uniform limit of a suitable propagator.

This derivation also indirectly shows that in the normal dissipative cases, when $D_Q=0$, the sum rule Eq. (18) is obtained starting from the conventional Kubo formula, i.e., Eq. (19) without the first term, by integrating the current current correlator over frequency. This is so since such an integral gives the second part of the expression for D_Q which must equal the first for it to vanish.

It is worth mentioning that another independent argument for the vanishing of D_Q and likewise D_c , or in another context, the spin wave stiffness of a fully saturated ferromagnet,²³ uses the notion of a position operator. If a position operator, or a similar one for energy transport such as the boost operator $[\int dr \vec{r} H(r)]$ is allowed in the list of allowed operators, then it is easy to show that D_c type operators are zero, since one can rewrite the current matrix elements in terms of the matrix elements of the position operator, and then the second part of Eq. (A7) becomes the commutator of the current with the position operator and hence cancels exactly the τ^{xx} term. Such a procedure is invalid in general, as explained carefully by Herring and Thouless,²³ the position operator is illegal in the Hilbert space where periodic boundary conditions are used in a continuum field theory. For a lattice field theory of the sort we are considering, we can always force the introduction of a lattice position operator $\mathcal{X} \equiv \sum_{\vec{r}} x_j n_{\vec{r}}$, but now a careful calculation shows that the cancellation is incomplete; while the bulk terms do cancel, the boundary terms do not.

From this line of thought we conclude that D_c and its relatives would vanish, if the nature of the quantum states is

such that the error made in introducing the position operator is negligible; this again is plausible in a highly dissipative system, where phase coherence is lost over some microscopic length scale that is shorter than the system length. For a superconductor such is certainly not the case nor, for that matter, in a ferromagnet (Ref. 23).

V. HIGH FREQUENCY RESPONSE: LORENTZ RATIO AND THERMOELECTRIC FIGURE OF MERIT

Of great interest are the two quantities, the Lorentz ratio

$$\mathbf{L}(\omega) = \frac{\kappa(\omega)}{T\sigma(\omega)} \quad (37)$$

and the thermoelectric figure of merit Z times T (a dimensionless number)

$$\mathbf{Z}(\omega)T = \frac{S^2(\omega)\sigma(\omega)T}{\kappa(\omega)} \quad (38)$$

$$= \frac{\gamma^2(\omega)T}{\sigma(\omega)\kappa(\omega)}. \quad (39)$$

We can readily evaluate these in the high frequency limit as

$$\mathbf{L}^* = \frac{\langle \Theta^{xx} \rangle}{T^2 \langle \tau^{xx} \rangle}, \quad (40)$$

$$\mathbf{Z}^*T = \frac{\langle \Phi^{xx} \rangle^2 T^2}{\langle \Theta^{xx} \rangle \langle \tau^{xx} \rangle}. \quad (41)$$

Let us also note that the thermopower at high frequencies is expressible in terms of the operators we displayed earlier,

$$S^* = \frac{\langle \Phi^{xx} \rangle}{T \langle \tau^{xx} \rangle}. \quad (42)$$

These variables are computable much more readily than their dc counterparts, and since these do capture the effect of interactions, they are of considerable interest.

VI. LATTICE THERMAL CONDUCTIVITY

We consider here the sum rule as applied to the case of the lattice vibrations. This is a field of great current activity,^{24,25} where most studies are in low dimensions and treat classical anharmonic and disordered lattices with a view to study the conditions for existence of a Fourier law, and also for the emergence of a finite conductivity. We consider a general anharmonic disordered lattice with a Hamiltonian

$$H = \sum_j H_j, \quad (43)$$

$$H_j = \left[\frac{\vec{p}_j^2}{2m_j} + U_j \right], \quad U_j = \frac{1}{2} \sum_{i \neq j} V_{j,i},$$

where $V_{i,j} = V_{j,i} = V(\vec{u}_i - \vec{u}_j)$ is a symmetric two-body potential that is an arbitrary function of the displacement variables \vec{u}_i

including possible anharmonicity. Since no particle flow is involved, it suffices to consider the canonical ensemble Hamiltonian. We will denote the equilibrium lattice points by $\vec{R}_j \equiv (X_j, Y_j, \dots)$ and the antisymmetric force vector $\vec{F}_{i,j} = -(\vec{\partial}/\partial \vec{u}_i) V_{i,j}$. In the following, we will need the derivatives of the antisymmetric force vector which will be denoted by $F_{i,j}^{x(n)} = [\partial^n / \partial (u_i^x)^n] F_{i,j}^x$, and have the obvious symmetry property $F_{j,i}^{x(n)} = (-1)^{n-1} F_{i,j}^{x(n)}$. The energy current can be obtained from computing the time evolution of the energy density, and combining it with the conservation law thereby giving

$$J_x^E = \lim_{k \rightarrow 0} \frac{1}{\hbar k_x} [H, H(k)], \quad (44)$$

where $H(k) = \sum_j e^{i\vec{k} \cdot \vec{R}_j} H_j$. This form of the current operator is popular in literature, e.g., Ref. 26 and differs from the one given by Hardy²⁷ in some details, which are not expected to be very significant. To aid the passage to a classical limit we display the dependence on Planck's constant in this section, setting it to unity elsewhere. The current at finite wave vectors can be found from the above as

$$J_x^E(\vec{k}) = \frac{1}{4} \sum_{i,j} \frac{(X_i - X_j)}{m_i} e^{ik_x X_i} \{p_{x,i}, F_{i,j}^x\}, \quad (45)$$

where we have chosen \vec{k} along the x axis. Using the various definitions, we find the thermal operator

$$\begin{aligned} \frac{1}{\hbar} \Theta^{xx} &= \sum_i \frac{1}{4m_i} \left[\sum_{j \neq i} F_{i,j}^x (X_i - X_j) \right]^2 - \frac{1}{8} \sum_{i,j} \frac{(X_i - X_j)^2}{m_i m_j} \\ &\times [4F_{i,j}^{x(1)} p_{x,i} p_{x,j} + 2i\hbar F_{i,j}^{x(2)} (p_{x,i} - p_{x,j}) + \hbar^2 F_{i,j}^{x(3)}]. \end{aligned} \quad (46)$$

This, together with Eq. (18), then gives us the sum rule for thermal conductivity. Note that the classical limit exists and is readily found by dropping terms involving \hbar in this expression. In the classical limit of Kubo's formula Eq. (19), the inner integral over τ collapses to give

$$\kappa_{classical}(\omega_c) = \frac{1}{k_B T^2 \mathcal{L}} \int_0^\infty e^{i\omega_c t} dt \langle \hat{J}_x^Q(-t) \hat{J}_x^Q(0) \rangle_{classical}, \quad (47)$$

and it is clear that we can express the sum rule in terms of the expectation of $\langle \hat{J}_x^Q \hat{J}_x^Q \rangle$. However our formula Eq. (18) provides a slight advantage in this case too: our result implies that

$$\frac{1}{\hbar} \langle \Theta^{xx} \rangle_{classical} = \frac{1}{k_B T} \langle \hat{J}_x^Q \hat{J}_x^Q \rangle_{classical}, \quad (48)$$

a result that is nontrivial since the lhs involves a single extensive operator whereas the rhs involves the square of an extensive operator, and moreover the only way to prove it seems to be to go back to the inhomogeneous (i.e., k dependent) energy density and perform the steps stated above.

As a simple illustration consider the case of a 1D Harmonic lattice, $H = \sum_i p_i^2 / (2m) + k_s / 2 \sum_i (u_i - u_{i+1})^2$, with $k_s \equiv m\omega_0^2$. In this case, we expect heat transport to be ballistic

rather than diffusive, and hence the static thermal conductivity to diverge. Unlike the case of free electrons (discussed elsewhere in this paper), the current operator is not completely diagonal in the normal mode (phonon) operators, in contrast to the Peierls form of the energy current,²⁸ namely $J^E = \sum \hbar \omega_k v_k n_k$. The integrated conductivity is nontrivial; it gets its weight at finite frequencies from phonon pair creation and destruction processes. The force is linear in the displacements and hence we work out the thermal operator,

$$\Theta^{xx} = (\hbar \omega_0^2 a_0^2) \left[\frac{1}{m} \sum_i p_i p_{i+1} + \frac{k_s}{4} \sum_i (u_{i-1} - u_{i+1})^2 \right]. \quad (49)$$

The expectation of this object can be computed at finite temperatures on using the phonon harmonic oscillator representation as

$$\begin{aligned} \langle \Theta^{xx} \rangle &= \mathcal{L}(\hbar^2 \omega_0^3 a_0^2) \int_0^\pi \frac{dk}{\pi} \\ &\times \left[\left(\frac{1}{2} + \frac{1}{e^{\beta \omega_k} - 1} \right) \left\{ \frac{\omega_k}{\omega_0} \cos(k) + \frac{\omega_0}{\omega_k} \sin^2(k) \right\} \right], \end{aligned} \quad (50)$$

where $\omega_k = 2\omega_0 \sin(ka_0/2)$ is the acoustic phonon energy. At zero temperature, i.e., in the ground state, it can be shown to vanish exactly; this precise cancellation is a characteristic feature of the thermal operators that is in common with most other quantum systems, and we discuss its connection with the vanishing of the specific heat in another section [see discussion near Eq. (89)]. Similar expressions can be worked out in any dimension d . At low temperatures, it is easy to see that $\Theta^{xx} \propto T^{d+1}$ in d dimensions, so that the sum rule Eq. (18) is $\propto T^d$, i.e., similar to the lattice specific heat. At high temperatures, since this model has no scattering of phonons, the sum rule increases linearly with T indefinitely. Through Eq. (18) this implies a T independent behavior at sufficiently high T . The computation for the nonlinear lattice would contain the effects of umklapp as well as normal scattering, and should be numerically feasible as well as interesting.

VII. INTERMEDIATE COUPLING MODELS: FINITE U HUBBARD MODEL, HOMOGENEOUS ELECTRON GAS, AND PERIODIC ANDERSON LATTICE

In this section we will consider the popular intermediate coupling models, namely the Hubbard model and the electron gas as well as the periodic Anderson lattice. We derive for these models the thermal operator Θ^{xx} and the thermoelectric operator Φ^{xx} . We further demonstrate the formalism in the limit of zero interaction, where the Boltzmann-Drude results are reproduced for the specific transport variables mentioned in the earlier sections, namely the Lorentz number and the thermopower. We begin by writing the Hubbard model Hamiltonian in the grand canonical ensemble

$$K = \sum_{\vec{r}} K(\vec{r}), \quad (51)$$

$$K(\vec{r}) = - \sum_{\sigma, \vec{\eta}} t(\vec{\eta}) c_{\vec{r}+1/2\vec{\eta}, \sigma}^{\dagger} c_{\vec{r}-1/2\vec{\eta}, \sigma} - \mu \sum_{\sigma} n_{\vec{r}, \sigma} + U n_{\vec{r}, \downarrow} n_{\vec{r}, \uparrow}. \quad (52)$$

Here $\vec{\eta}$ represents all the neighbors of the site \vec{r} , $t(\vec{\eta})$ is the hopping matrix element, and we have adopted the ‘‘midpoint rule’’ for defining densities of all nonlocal objects such as hopping so as to get convenient expressions for the Fourier transforms of the grand canonical ensemble Hamiltonian $K = H - \mu \hat{N}$,

$$\hat{K}(\vec{k}) = \sum_{\vec{r}} e^{i\vec{k}\cdot\vec{r}} K(\vec{r}) \quad (53)$$

$$= \sum_{\vec{p}, \sigma} (\varepsilon_{\vec{p}} - \mu) c_{\vec{p}+1/2\vec{k}, \sigma}^{\dagger} c_{\vec{p}-1/2\vec{k}, \sigma} + \sum_{\vec{r}} e^{i\vec{k}\cdot\vec{r}} U n_{\vec{r}, \downarrow} n_{\vec{r}, \uparrow}, \quad (54)$$

with $\varepsilon_{\vec{p}} = -\sum_{\vec{\eta}} t(\vec{\eta}) \exp(-i\vec{\eta}\cdot\vec{p})$ the kinetic energy and $n_{\vec{r}} = \sum_{\sigma} n_{\vec{r}, \sigma}$. A more general model, with arbitrary two-body interaction between particles, including the homogeneous electron gas (HEG) model is represented by

$$\hat{K}(\vec{k}) = \sum_{\vec{p}, \sigma} (\varepsilon_{\vec{p}} - \mu) c_{\vec{p}+1/2\vec{k}, \sigma}^{\dagger} c_{\vec{p}-1/2\vec{k}, \sigma} + \frac{1}{2\mathcal{L}} \sum_{\vec{p}, \vec{q}, \vec{l}, \sigma, \sigma'} U(\vec{q}) c_{\vec{p}+\vec{q}+1/2\vec{k}, \sigma}^{\dagger} c_{\vec{p}-1/2\vec{k}, \sigma} c_{\vec{l}-\vec{q}, \sigma'}^{\dagger} c_{\vec{l}, \sigma'}. \quad (55)$$

By specializing to $U(\vec{q}) = U$ and restricting the momenta to the first Brillouin zone we recover the Hubbard model, whereas the electron gas is obtained by letting $U(\vec{q}) = 4\pi e^2 / |\vec{q}|^2$ and letting $\mathcal{L} \rightarrow \Omega$ the box volume. In all cases, the electronic charge density is $\rho(\vec{r}) = q_e n_{\vec{r}}$, where q_e is the charge of the electron ($q_e = -|e|$). The charge current density is given by $\vec{J}(\vec{r}) = i(q_e / \hbar) \sum_{\vec{\eta}, \sigma} \vec{\eta} t(\vec{\eta}) c_{\vec{r}+1/2\vec{\eta}, \sigma}^{\dagger} c_{\vec{r}-1/2\vec{\eta}, \sigma}$, and hence its Fourier transform follows as

$$\vec{J}(\vec{k}) = q_e \sum_{\vec{p}} \vec{v}_{\vec{p}} c_{\vec{p}+1/2\vec{k}, \sigma}^{\dagger} c_{\vec{p}-1/2\vec{k}, \sigma}, \quad (56)$$

where the velocity vector $\vec{v}_{\vec{p}} = (\partial / \partial \hbar \vec{p}) \varepsilon_{\vec{p}} = i / \hbar \sum_{\vec{\eta}} t(\vec{\eta}) \vec{\eta} \exp(-i\vec{\eta}\cdot\vec{p})$. We set the lattice constant $a_0 = 1$ throughout this paper.

A. The thermoelectric operator Φ^{xx}

Let us now work out the thermoelectric term Φ^{xx} defined in Eq. (25). The commutator can be taken and on further carrying out the limiting procedure we find with $\vec{\sigma} = -\sigma$

$$\begin{aligned} \Phi^{xx} = & - \frac{q_e}{2\hbar} \sum_{\vec{\eta}, \vec{\eta}', \vec{r}, \sigma} (\eta_x + \eta'_x)^2 t(\vec{\eta}) t(\vec{\eta}') c_{\vec{r}+\vec{\eta}+\vec{\eta}', \sigma}^{\dagger} c_{\vec{r}, \sigma} \\ & - q_e \frac{\mu}{\hbar} \sum_{\vec{\eta}, \sigma} \eta_x^2 t(\vec{\eta}) c_{\vec{r}+\vec{\eta}, \sigma}^{\dagger} c_{\vec{r}, \sigma} + \frac{q_e U}{4\hbar} \\ & \times \sum_{\vec{r}, \vec{\eta}, \sigma} t(\vec{\eta}) (\eta_x)^2 (n_{\vec{r}, \vec{\sigma}} + n_{\vec{r}+\vec{\eta}, \vec{\sigma}}) (c_{\vec{r}+\vec{\eta}, \sigma}^{\dagger} c_{\vec{r}, \sigma} + c_{\vec{r}, \sigma}^{\dagger} c_{\vec{r}+\vec{\eta}, \sigma}). \end{aligned} \quad (57)$$

This object can be expressed completely in Fourier space as

$$\begin{aligned} \Phi^{xx} = & q_e \sum_{\vec{p}, \sigma} \frac{\partial}{\partial p_x} \{v_{\vec{p}}^x (\varepsilon_{\vec{p}} - \mu)\} c_{\vec{p}, \sigma}^{\dagger} c_{\vec{p}, \sigma} + \frac{q_e U}{2\mathcal{L}} \\ & \times \sum_{\vec{l}, \vec{p}, \vec{q}, \sigma} \frac{\partial^2}{\partial l_x^2} \{ \varepsilon_{\vec{l}} + \varepsilon_{\vec{l}+\vec{q}} \} c_{\vec{l}+\vec{q}, \sigma}^{\dagger} c_{\vec{l}, \sigma} c_{\vec{p}-\vec{q}, \sigma}^{\dagger} c_{\vec{p}, \sigma}. \end{aligned} \quad (58)$$

The more general HEG model yields the result

$$\begin{aligned} \Phi^{xx} = & q_e \sum_{\vec{p}, \sigma} \frac{\partial}{\partial p_x} \{v_{\vec{p}}^x (\varepsilon_{\vec{p}} - \mu)\} c_{\vec{p}, \sigma}^{\dagger} c_{\vec{p}, \sigma} + \frac{q_e}{2\mathcal{L}} \\ & \times \sum_{\vec{l}, \vec{p}, \vec{q}, \sigma, \sigma'} \left[U(\vec{q}) \frac{\partial^2}{\partial l_x^2} (\varepsilon_{\vec{l}} + \varepsilon_{\vec{l}+\vec{q}}) + \frac{\partial U(\vec{q})}{\partial q_x} (v_{\vec{l}+\vec{q}}^x - v_{\vec{l}}^x) \right] \\ & \times c_{\vec{l}+\vec{q}, \sigma}^{\dagger} c_{\vec{l}, \sigma} c_{\vec{p}-\vec{q}, \sigma'}^{\dagger} c_{\vec{p}, \sigma'}. \end{aligned} \quad (59)$$

B. Heat current and the thermal operator Θ^{xx}

We first derive the expression for the heat current; this follows from Eq. (11). Using Eq. (54) and the fact that the $O(U^2)$ term vanishes (both terms are functions of $n_{\vec{r}, \sigma}^{\dagger} n_{\vec{r}, \sigma}$ only), we find

$$\begin{aligned} J_x^Q = & \sum_{\vec{p}} v_{\vec{p}, \sigma}^x (\varepsilon_{\vec{p}} - \mu) c_{\vec{p}, \sigma}^{\dagger} c_{\vec{p}, \sigma} \\ & + \frac{iU}{2\hbar} \sum_{\vec{\eta}, \sigma} t(\vec{\eta}) \eta_x c_{\vec{r}+\vec{\eta}, \sigma}^{\dagger} c_{\vec{r}, \sigma} \{n_{\vec{r}, \vec{\sigma}} + n_{\vec{r}+\vec{\eta}, \vec{\sigma}}\} \\ & = \sum_{\vec{p}, \sigma} v_{\vec{p}}^x (\varepsilon_{\vec{p}} - \mu) c_{\vec{p}, \sigma}^{\dagger} c_{\vec{p}, \sigma} \\ & + \frac{U}{2\mathcal{L}} \sum_{\vec{l}, \vec{p}, \vec{q}, \sigma, \sigma'} \{v_{\vec{l}}^x + v_{\vec{l}+\vec{q}}^x\} \\ & \times c_{\vec{l}+\vec{q}, \sigma}^{\dagger} c_{\vec{l}, \sigma} c_{\vec{p}-\vec{q}, \sigma'}^{\dagger} c_{\vec{p}, \sigma'}. \end{aligned} \quad (60)$$

We also need the current operator at a finite wave vector chosen along the x axis as $\vec{k} \equiv \hat{x} k_x$; this may be written in the case of the more general HEG model as

$$\begin{aligned} J_x^Q(\vec{k}) = & \sum_{\vec{p}, \sigma} v_{\vec{p}}^x (\varepsilon_{\vec{p}} - \mu) c_{\vec{p}+1/2\vec{k}, \sigma}^{\dagger} c_{\vec{p}-1/2\vec{k}, \sigma} + \frac{1}{2\mathcal{L}} \sum_{\vec{l}, \vec{p}, \vec{q}, \sigma, \sigma'} U(\vec{q}) \{v_{\vec{l}}^x \\ & + v_{\vec{l}+\vec{q}}^x\} c_{\vec{l}+\vec{q}+1/2\vec{k}, \sigma}^{\dagger} c_{\vec{l}-1/2\vec{k}, \sigma} c_{\vec{p}-\vec{q}, \sigma'}^{\dagger} c_{\vec{p}, \sigma'}. \end{aligned} \quad (62)$$

We evaluate the thermal operator by a direct calculation

$$\begin{aligned}
\Theta^{xx} = & \sum_{p,\sigma} \frac{\partial}{\partial p_x} \{v_p^x (\varepsilon_p - \mu)^2\} c_{p,\sigma}^\dagger c_{p,\sigma} + \frac{1}{2\mathcal{L}} \sum_{\vec{p},\vec{q},\sigma} U(\vec{q}) \left[\frac{\partial}{\partial p_x} \{ \xi_{\vec{p}} + \xi_{\vec{p}+\vec{q}} \} + \frac{1}{2} (v_{\vec{p}}^x + v_{\vec{p}+\vec{q}}^x)^2 \right] c_{\vec{p}+\vec{q},\sigma}^\dagger c_{\vec{p},\sigma} \rho_{-\vec{q}} + \frac{1}{4\mathcal{L}} \sum_{\vec{p},\vec{q},\vec{l},\sigma,\sigma'} \left[U(\vec{q}) \left\{ (\varepsilon_{\vec{l}-\vec{q}} \right. \right. \\
& - \varepsilon_{\vec{l}}) \frac{\partial}{\partial p_x} (v_{\vec{p}}^x - v_{\vec{p}+\vec{q}}^x) + (v_{\vec{p}}^x + v_{\vec{p}+\vec{q}}^x)(v_{\vec{l}}^x + v_{\vec{l}-\vec{q}}^x) \left. \right\} - 2 \frac{\partial U(\vec{q})}{\partial q_x} (v_{\vec{p}}^x + v_{\vec{p}+\vec{q}}^x)(\varepsilon_{\vec{l}-\vec{q}} - \varepsilon_{\vec{l}}) \left. \right] c_{\vec{p}+\vec{q},\sigma}^\dagger c_{\vec{p},\sigma} c_{\vec{l}-\vec{q},\sigma'}^\dagger c_{\vec{l},\sigma'} + \frac{1}{4\mathcal{L}^2} \sum_{\vec{p},\vec{q},\vec{q}',\sigma} U(\vec{q}) \\
& \times \left[U(\vec{q}') \frac{\partial}{\partial p_x} (v_{\vec{p}+\vec{q}+\vec{q}'}^x + v_{\vec{p}+\vec{q}}^x + v_{\vec{p}+\vec{q}'}^x + v_{\vec{p}}^x) + \frac{\partial U(-\vec{q}')}{\partial q_x'} (v_{\vec{p}+\vec{q}+\vec{q}'}^x + v_{\vec{p}+\vec{q}'}^x - v_{\vec{p}+\vec{q}}^x - v_{\vec{p}}^x) \right] c_{\vec{p}+\vec{q}+\vec{q}',\sigma}^\dagger c_{\vec{p},\sigma} \rho_{-\vec{q}} \rho_{-\vec{q}'}. \quad (63)
\end{aligned}$$

Here we denote $\xi_{\vec{p}} = v_{\vec{p}}^x (\varepsilon_{\vec{p}} - \mu)$ and $\rho_{\vec{q}} = \sum_{k,\sigma} c_{k+\vec{q},\sigma}^\dagger c_{k,\sigma}$. This expression simplifies somewhat in the case of the Hubbard model in real space with $U(\vec{q}) \rightarrow U$, where it may be written as

$$\begin{aligned}
\Theta^{xx} = & \sum_{p,\sigma} \frac{\partial}{\partial p_x} \{v_p^x (\varepsilon_p - \mu)^2\} c_{p,\sigma}^\dagger c_{p,\sigma} \\
& + \frac{U^2}{4\hbar} \sum_{\eta,\sigma} t(\vec{\eta}) \eta_x^2 (n_{\vec{r},\sigma} + n_{\vec{r}+\vec{\eta},\sigma})^2 c_{\vec{r}+\vec{\eta},\sigma}^\dagger c_{\vec{r},\sigma} \\
& - \mu \frac{U}{\hbar} \sum_{\eta,\sigma} t(\vec{\eta}) \eta_x^2 (n_{\vec{r},\sigma} + n_{\vec{r}+\vec{\eta},\sigma}) c_{\vec{r}+\vec{\eta},\sigma}^\dagger c_{\vec{r},\sigma} \\
& - \frac{U}{8\hbar} \sum_{\vec{\eta},\vec{\eta}',\sigma} t(\vec{\eta}) t(\vec{\eta}') (\eta_x + \eta_x')^2 \\
& \times \{3n_{\vec{r},\sigma} + n_{\vec{r}+\vec{\eta},\sigma} + n_{\vec{r}+\vec{\eta}',\sigma} + 3n_{\vec{r}+\vec{\eta}+\vec{\eta}',\sigma}\} \\
& \times c_{\vec{r}+\vec{\eta}+\vec{\eta}',\sigma}^\dagger c_{\vec{r},\sigma} + \frac{U}{4\hbar} \sum_{\vec{\eta},\vec{\eta}',\sigma} t(\vec{\eta}) t(\vec{\eta}') (\eta_x \\
& + \eta_x') \eta_x' c_{\vec{r}+\vec{\eta},\sigma}^\dagger c_{\vec{r},\sigma} \{c_{\vec{r}+\vec{\eta},\sigma}^\dagger c_{\vec{r}+\vec{\eta}+\vec{\eta}',\sigma} + c_{\vec{r}-\vec{\eta}',\sigma}^\dagger c_{\vec{r},\sigma} - \text{H.c.}\}. \quad (64)
\end{aligned}$$

C. Disorder by a site potential

We work out the various sum rules in the presence of site diagonal disorder produced by a (random) potential $K_d = \sum_r V_r n_r$, where we use the subscript d to denote the disorder contribution to various objects. While such a potential disorder does not change the electrical current operator, it does change the heat current, and it is easy to see that

$$\begin{aligned}
(\hat{J}_x^Q)_d = & \frac{i}{2\hbar} \sum_{\eta,\sigma} \eta_x t(\vec{\eta}) (V_{\vec{r}} + V_{\vec{r}+\vec{\eta}}) c_{\vec{r}+\vec{\eta},\sigma}^\dagger c_{\vec{r},\sigma} \\
= & \frac{1}{2} \sum_{\vec{l},\sigma} \hat{V}_{-\vec{l}} (v_{\vec{p}+\vec{l}}^x + v_{\vec{p}}^x) c_{\vec{p}+\vec{l},\sigma}^\dagger c_{\vec{p},\sigma}, \quad (65)
\end{aligned}$$

where we defined the Fourier transform of the potential $\hat{V}_{\vec{k}} = (1/\mathcal{L}) \sum_{\vec{r}} \exp(i\vec{k} \cdot \vec{r}) V_{\vec{r}}$. From these definitions, we find the disorder contribution to the thermopower sum rule

$$\begin{aligned}
(\Phi^{xx})_d = & \frac{q_e}{2} \sum_{\vec{l},\vec{p},\sigma} \hat{V}_{-\vec{p}} \left(\frac{\partial^2 \varepsilon_{\vec{l}+\vec{p}}}{\partial l_x^2} + \frac{\partial^2 \varepsilon_{\vec{l}}}{\partial l_x^2} \right) c_{\vec{p}+\vec{l},\sigma}^\dagger c_{\vec{l},\sigma} \\
= & \frac{1}{2\hbar} \sum_{\eta,\sigma} \eta_x^2 t(\vec{\eta}) (V_{\vec{r}} + V_{\vec{r}+\vec{\eta}}) c_{\vec{r}+\vec{\eta},\sigma}^\dagger c_{\vec{r},\sigma}. \quad (66)
\end{aligned}$$

We compute the disorder contribution to the thermal conductivity sum rule as

$$\begin{aligned}
\hbar(\Theta^{xx})_d = & \frac{1}{4} \sum_{\vec{r},\vec{\eta},\sigma} t(\vec{\eta}) \eta_x^2 (V_{\vec{r}} + V_{\vec{r}+\vec{\eta}})^2 c_{\vec{r}+\vec{\eta},\sigma}^\dagger c_{\vec{r},\sigma} \\
& - \mu \sum_{\vec{r},\vec{\eta},\sigma} t(\vec{\eta}) \eta_x^2 (V_{\vec{r}} + V_{\vec{r}+\vec{\eta}}) c_{\vec{r}+\vec{\eta},\sigma}^\dagger c_{\vec{r},\sigma} \\
& + \frac{U}{2} \sum_{\vec{r},\vec{\eta},\sigma} t(\vec{\eta}) \eta_x^2 (V_{\vec{r}} + V_{\vec{r}+\vec{\eta}}) (n_{\vec{r},\sigma} + n_{\vec{r}+\vec{\eta},\sigma}) c_{\vec{r}+\vec{\eta},\sigma}^\dagger c_{\vec{r},\sigma} \\
& - \frac{1}{8} \sum_{\vec{\eta},\vec{\eta}',\sigma} t(\vec{\eta}) t(\vec{\eta}') (\eta_x + \eta_x')^2 \\
& \times \{3V_{\vec{r}} + V_{\vec{r}+\vec{\eta}} + V_{\vec{r}+\vec{\eta}'} + 3V_{\vec{r}+\vec{\eta}+\vec{\eta}'}\} c_{\vec{r}+\vec{\eta}+\vec{\eta}',\sigma}^\dagger c_{\vec{r},\sigma}. \quad (67)
\end{aligned}$$

This expression can be written in Fourier space as

$$\begin{aligned}
(\Theta^{xx})_d = & \frac{1}{4} \sum_{\vec{l},\vec{p},\sigma} \left\{ 2 \frac{d}{dp_x} (\xi_{\vec{p}} + \xi_{\vec{p}+\vec{l}}) + (v_{\vec{p}}^x + v_{\vec{p}+\vec{l}}^x)^2 \right\} \hat{V}_{-\vec{l}} c_{\vec{p}+\vec{l},\sigma}^\dagger c_{\vec{p},\sigma} \\
& + \frac{1}{4} \sum_{\vec{l},\vec{l}',\sigma} \frac{d}{dp_x} \{v_{\vec{p}}^x + v_{\vec{p}+\vec{l}}^x + v_{\vec{p}+\vec{l}'}^x + v_{\vec{p}+\vec{l}+\vec{l}'}^x\} \\
& \times \hat{V}_{-\vec{l}} \hat{V}_{-\vec{l}'} c_{\vec{p}+\vec{l}+\vec{l}',\sigma}^\dagger c_{\vec{p},\sigma} + \frac{U}{2\mathcal{L}} \sum_{\vec{l},\vec{l}',\vec{p},\vec{q},\sigma} \frac{d^2}{dp_x^2} \\
& \times \{ \varepsilon_{\vec{p}} + \varepsilon_{\vec{p}+\vec{q}} + \varepsilon_{\vec{p}+\vec{l}} + \varepsilon_{\vec{p}+\vec{l}+\vec{q}} \} \\
& \times \hat{V}_{\vec{l}} c_{\vec{q}+\vec{l},\sigma}^\dagger c_{\vec{l},\sigma} c_{\vec{p},\sigma}^\dagger c_{\vec{p}+\vec{l}+\vec{q},\sigma}. \quad (68)
\end{aligned}$$

Here we need to average the final expression over the

disorder potential, either perturbatively or numerically exactly. We save this task for a future work.

D. Free electron limit and comparison with the Boltzmann theory

It is easy to evaluate the various operators in the limit of $U \rightarrow 0$, and this exercise enables us to get a feel for the meaning of these various somewhat formal objects. We note that

$$\begin{aligned}\langle \tau^{xx} \rangle &= 2q_e^2 \sum_p n_{\bar{p}} \frac{d}{dp_x} [v_{\bar{p}}^x], \\ \langle \Theta^{xx} \rangle &= 2 \sum_p n_{\bar{p}} \frac{d}{dp_x} [v_{\bar{p}}^x (\varepsilon_{\bar{p}} - \mu)^2], \\ \langle \Phi^{xx} \rangle &= 2q_e \sum_p n_{\bar{p}} \frac{d}{dp_x} [v_{\bar{p}}^x (\varepsilon_{\bar{p}} - \mu)].\end{aligned}\quad (69)$$

Here $n_{\bar{p}}$ is the Fermi function and the factor of 2 arises from spin summation. At low temperatures, we use the Sommerfeld formula after integrating by parts, and thus obtain the leading low T behavior:

$$\begin{aligned}\langle \tau^{xx} \rangle &= \mathcal{L} 2q_e^2 \rho_0(\mu) \langle (v_{\bar{p}}^x)^2 \rangle_{\mu} \\ \langle \Theta^{xx} \rangle &= \mathcal{L} T^2 \frac{2\pi^2 k_B^2}{3} \rho_0(\mu) \langle (v_{\bar{p}}^x)^2 \rangle_{\mu} \\ \langle \Phi^{xx} \rangle &= \mathcal{L} T^2 \frac{2q_e \pi^2 k_B^2}{3} \left[\rho_0'(\mu) \langle (v_{\bar{p}}^x)^2 \rangle_{\mu} + \rho_0(\mu) \frac{d}{d\mu} \langle (v_{\bar{p}}^x)^2 \rangle_{\mu} \right],\end{aligned}\quad (70)$$

where $\rho_0(\mu)$ is the density of states per spin per site at the Fermi level μ and the primes denote derivatives with respect to μ , the average is over the Fermi surface as usual. These formulas are indeed very close to what we expect from Boltzmann theory. Indeed, replacing $i/\omega \rightarrow \tau$ with a relaxation time τ in the leading (high frequency) terms in the general formulas reproduces the familiar Boltzmann-Drude results²⁹ for the thermal conductivity, thermopower, and the electrical conductivity. We may form the high frequency ratios

$$\begin{aligned}S^* &= T \frac{\pi^2 k_B^2}{3q_e} \frac{d}{d\mu} \ln[\rho_0(\mu) \langle (v_{\bar{p}}^x)^2 \rangle_{\mu}], \\ L^* &= \frac{\pi^2 k_B^2}{3q_e^2}.\end{aligned}\quad (72)$$

It is therefore clear that the high frequency result gives the same Lorentz number as well as the thermopower that the Boltzmann theory gives in its simplest form. Clearly one can get more sophisticated with respect to the treatment of transport issues, such as a k dependent relaxation time in the Boltzmann approach,^{28,30} provided the interesting physics is in that direction. Our approach enables us to provide a more sophisticated treatment of *interactions and disorder* by com-

puting the averages of the more complex operators given above, and this is useful for strongly correlated systems provided the transport relaxation issues are relatively benign.

E. Periodic Anderson lattice

We present the thermoelectric operator for the important case of the periodic Anderson lattice describing conduction electrons c 's that hybridize with a correlated set of localized levels described by f 's as

$$\begin{aligned}K &= - \sum_{\sigma, \tilde{\eta}} t(\tilde{\eta}) c_{\tilde{r}+\tilde{\eta}}^{\dagger} c_{\tilde{r}} - \mu \sum_{\sigma} n_{\tilde{r}\sigma} + (\varepsilon_0 - \mu) \sum_{1 \leq \nu \leq N_f} f_{\tilde{r},\nu}^{\dagger} f_{\tilde{r},\nu} \\ &+ U \sum_{\sigma, \tilde{r}, \nu < \nu'} n_{\tilde{r},\nu}^f n_{\tilde{r},\nu'}^f + \sum_{\sigma, \nu} V(\sigma, \nu) (c_{\tilde{r},\sigma}^{\dagger} f_{\tilde{r},\nu} + \text{H.c.}).\end{aligned}\quad (73)$$

The charge current operator is exactly as it is in the case of the Hubbard model since the f levels are localized, and using the same ideas as before to define an inhomogeneous energy $K(\vec{k})$ and computing the familiar commutator Eq. (25) we find the thermoelectric operator

$$\begin{aligned}\Phi^{xx} &= q_e \sum_{\tilde{p}, \sigma} \frac{\partial}{\partial p_x} \{v_{\tilde{p}}^x (\varepsilon_{\tilde{p}} - \mu)\} c_{\tilde{p},\sigma}^{\dagger} c_{\tilde{p},\sigma} \\ &+ \frac{q_e}{2\hbar} \sum_{\sigma, \nu, \vec{k}} V(\sigma, \nu) \frac{d^2 \varepsilon(\vec{k})}{dk_x^2} (c_{\vec{k},\sigma}^{\dagger} f_{\vec{k},\nu} + f_{\vec{k},\nu}^{\dagger} c_{\vec{k},\sigma}).\end{aligned}\quad (74)$$

At $T=0$ the expectation of this operator should vanish (see the discussion section), whereby we obtain a formal expression for the chemical potential at $T=0$ from the above.

VIII. STRONG COUPLING MODELS: THE HEISENBERG MODEL AND THE $U=\infty$ HUBBARD MODEL

In this section we consider the case of strong coupling, and present the thermal and thermoelectric operators for the case of the Heisenberg model and the infinite correlation limit of the Hubbard model.

A. Heisenberg model

We first obtain the thermal operator for the ever popular Heisenberg model in any dimension described by the Hamiltonian

$$H = \sum_{\vec{r}} H_{\vec{r}}, \quad H_{\vec{r}} = \frac{1}{2} \sum_{\tilde{\eta}} J_{\tilde{\eta}} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}+\tilde{\eta}}.\quad (75)$$

Clearly $H(\vec{k}) = \sum_{\vec{r}} e^{i\vec{k}\cdot\vec{r}} H_{\vec{r}}$ and from the conservation law of local energy we obtain the energy current operator

$$\hat{J}_x^E(k_x) = \frac{1}{4} \sum_{\vec{r}, \tilde{\eta}_1, \tilde{\eta}_2} (\eta_{1,x} - \eta_{2,x}) J_{\tilde{\eta}_1} J_{\tilde{\eta}_2} (\vec{S}_{\vec{r}+\tilde{\eta}_1} \times \vec{S}_{\vec{r}+\tilde{\eta}_2} \cdot \vec{S}_{\vec{r}}) e^{ik_x x}.\quad (76)$$

Using the standard commutators we find the thermal operator to be a four-spin operator in general. It is expressed as

$$\begin{aligned}
\Theta^{xx} = & \frac{1}{8} \sum_{\vec{r}, \vec{\eta}_1, \vec{\eta}_2, \vec{\eta}_3} (\eta_{1,x} - \eta_{2,x}) J_{\vec{\eta}_1} J_{\vec{\eta}_2} J_{\vec{\eta}_3} \\
& \times [\eta_{3,x} (\vec{S}_{\vec{r}+\vec{\eta}_1} \times \vec{S}_{\vec{r}+\vec{\eta}_2}) \cdot (\vec{S}_{\vec{r}} \times \vec{S}_{\vec{r}+\vec{\eta}_3}) \\
& - (2\eta_{2,x} + \eta_{3,x}) (\vec{S}_{\vec{r}+\vec{\eta}_1} \times \vec{S}_{\vec{r}}) \cdot (\vec{S}_{\vec{r}+\vec{\eta}_2} \times \vec{S}_{\vec{r}+\vec{\eta}_3}) \\
& + (2\eta_{1,x} + \eta_{3,x}) (\vec{S}_{\vec{r}+\vec{\eta}_1} \times \vec{S}_{\vec{r}+\vec{\eta}_3}) \cdot (\vec{S}_{\vec{r}+\vec{\eta}_2} \times \vec{S}_{\vec{r}})].
\end{aligned} \tag{77}$$

In this expression $\vec{r}, \vec{r}+\vec{\eta}_1, \vec{r}+\vec{\eta}_2$ are necessarily distinct sites, but $\vec{r}+\vec{\eta}_3$ can coincide with the last two, and hence the order of the products needs to be treated carefully. For simple cubic lattices this expression simplifies a bit, but in essence it involves four-spin correlations.

B. The $U \rightarrow \infty$ Hubbard model

In this section we consider the limit of $U \rightarrow \infty$, and consider the kinetic energy only, i.e., the t part of the t - J model, since this is expected to dominate in transport properties, at least far enough from half filling and for $t \gg J$. The addition of the J part can be done without too much difficulty, but we ignore it here for brevity. In this limit the fermionic commutation relations need to be modified into the Gutzwiller-Hubbard projected operators³¹

$$\tilde{c}_{\vec{r},\sigma} = P_G c_{\vec{r},\sigma} P_G,$$

$$\begin{aligned}
\{\tilde{c}_{\vec{r},\sigma}^\dagger, \tilde{c}_{\vec{r}',\sigma'}^\dagger\} &= \delta_{\vec{r},\vec{r}'} \{\delta_{\sigma,\sigma'} (1 - n_{\vec{r},\sigma}) + (1 - \delta_{\sigma,\sigma'}) \tilde{c}_{\vec{r},\sigma}^\dagger \tilde{c}_{\vec{r},\sigma'}^\dagger\} \\
&= Y_{\sigma,\sigma'} \delta_{\vec{r},\vec{r}'}.
\end{aligned} \tag{78}$$

The presence of the Y factor is due to strong correlations, and makes the computation nontrivial. The number operator $n_{\vec{r},\sigma}$ is unaffected by the projection. We note down the expressions for the charge current and the energy current at finite wave vectors by direct computation

$$\begin{aligned}
\hat{K}(k) &= - \sum_{\vec{r}, \vec{\eta}, \sigma} (t(\vec{\eta}) + \mu \delta_{\vec{\eta},0}) e^{i\vec{k} \cdot (\vec{r}+1/2\vec{\eta})} \tilde{c}_{\vec{r}+\vec{\eta},\sigma}^\dagger \tilde{c}_{\vec{r},\sigma}, \\
\hat{J}_x(k) &= i \frac{q_e}{\hbar} \sum_{\vec{r}, \vec{\eta}, \sigma} \eta_x t(\vec{\eta}) e^{i\vec{k} \cdot (\vec{r}+1/2\vec{\eta})} \tilde{c}_{\vec{r}+\vec{\eta},\sigma}^\dagger \tilde{c}_{\vec{r},\sigma}, \\
\hat{J}_x^Q(k) &= - \frac{i}{2\hbar} \sum_{\vec{r}, \vec{\eta}, \vec{\eta}', \sigma} (\eta_x + \eta'_x) t(\vec{\eta}) t(\vec{\eta}') e^{i\vec{k} \cdot (\vec{r}+1/2(\vec{\eta}+\vec{\eta}'))} \\
&\quad \times Y_{\sigma',\sigma}(\vec{r} + \vec{\eta}') \tilde{c}_{\vec{r}+\vec{\eta}+\vec{\eta}',\sigma'}^\dagger \tilde{c}_{\vec{r},\sigma} - \frac{\mu}{q_e} \hat{J}_x(k).
\end{aligned} \tag{79}$$

We evaluate the thermopower operator as

$$\begin{aligned}
\hbar \Phi^{xx} &= - \frac{q_e}{2} \sum_{\vec{\eta}, \vec{\eta}', \vec{r}, \sigma, \sigma'} (\eta_x + \eta'_x)^2 t(\vec{\eta}) t(\vec{\eta}') \\
&\quad \times Y_{\sigma',\sigma}(\vec{r} + \vec{\eta}) \tilde{c}_{\vec{r}+\vec{\eta}+\vec{\eta}',\sigma'}^\dagger \tilde{c}_{\vec{r},\sigma} - q_e \mu \\
&\quad \times \sum_{\vec{\eta}, \sigma} \eta_x^2 t(\vec{\eta}) \tilde{c}_{\vec{r}+\vec{\eta},\sigma}^\dagger \tilde{c}_{\vec{r},\sigma}.
\end{aligned} \tag{80}$$

Note that if we set $Y \rightarrow 1$, this expression reduces to the $U \rightarrow 0$ limit of the Hubbard result Eq. (58), as one would expect. We next compute the thermal operator (summing over all spin variables)

$$\begin{aligned}
\hbar \Theta^{xx} &= \mu \sum_{\vec{\eta}, \vec{\eta}', \vec{r}, \sigma, \sigma'} (\eta_x + \eta'_x)^2 t(\vec{\eta}) t(\vec{\eta}') Y_{\sigma',\sigma}(\vec{r}) \\
&\quad + \tilde{\eta} \tilde{c}_{\vec{r}+\vec{\eta}+\vec{\eta}',\sigma'}^\dagger c_{\vec{r},\sigma} + \mu^2 \sum_{\vec{\eta}, \sigma} \eta_x^2 t(\vec{\eta}) \tilde{c}_{\vec{r}+\vec{\eta},\sigma}^\dagger \tilde{c}_{\vec{r},\sigma} \\
&\quad + \frac{1}{4} \sum_{\vec{\eta}, \vec{\eta}', \vec{r}, \sigma, \sigma', \sigma''} (\eta_x + \eta'_x + \eta''_x) (2\eta_x + \eta'_x \\
&\quad + \eta''_x) t(\vec{\eta}) t(\vec{\eta}') t(\vec{\eta}'') Y_{\sigma',\sigma'}(\vec{r} + \vec{\eta} + \vec{\eta}') Y_{\sigma',\sigma}(\vec{r}) \\
&\quad + \vec{\eta}' \tilde{c}_{\vec{r}+\vec{\eta}+\vec{\eta}'+\vec{\eta}'',\sigma''}^\dagger \tilde{c}_{\vec{r},\sigma} + \frac{1}{4} \sum_{\vec{\eta}, \vec{\eta}', \vec{\eta}'', \vec{r}, \sigma} (\eta_x + \eta'_x) (-\eta_x \\
&\quad + \eta'_x + \eta''_x) t(\vec{\eta}) t(\vec{\eta}') t(\vec{\eta}'') \\
&\quad \times \{[\tilde{c}_{\vec{r}+\vec{\eta}',\sigma}^\dagger \tilde{c}_{\vec{r}+\vec{\eta}'+\vec{\eta}'',\sigma} \tilde{c}_{\vec{r}+\vec{\eta}'+\vec{\eta}'',\sigma}^\dagger \tilde{c}_{\vec{r}+\vec{\eta}',\sigma} \tilde{c}_{\vec{r}+\vec{\eta}'+\vec{\eta}'',\sigma}^\dagger \tilde{c}_{\vec{r}+\vec{\eta}',\sigma}^\dagger \tilde{c}_{\vec{r},\sigma} \\
&\quad - \{\tilde{c}_{\vec{r}+\vec{\eta}',\sigma}^\dagger \tilde{c}_{\vec{r}+\vec{\eta}'+\vec{\eta}'',\sigma} + \text{H.c.}\} \tilde{c}_{\vec{r}+\vec{\eta}'+\vec{\eta}'',\sigma}^\dagger \tilde{c}_{\vec{r},\sigma}].
\end{aligned} \tag{81}$$

IX. THE TRIANGULAR LATTICE SODIUM COBALT OXIDE: HIGH TEMPERATURE EXPANSION FOR THERMOPOWER

The sodium cobalt oxide Na_xCoO_2 system is of great current interest; the composition $x \sim 0.68$ gives a metal with a high thermopower $\sim 100 \mu\text{V/K}$, which is further highly magnetic field dependent.^{32,33} It is notable in that the underlying lattice is triangular, and it has been modeled by a triangular lattice t - J model with electron doping.³⁴ In this section we give a brief application of our technique to this system, which yields an interesting formula for the high T limit of the thermopower S^* that contains significant correction to the Heikes-Mott formula that is used in the same high T limit. A detailed study is in preparation and will be published separately; here we use the leading high T term to illustrate the advantage of the above formalism in tackling such a problem. We neglect contributions from the exchange part of the t - J model and focus on the kinetic energy which is expected to dominate the transport contributions. Let us compute the thermopower S^* from Eqs. (80), (A4), and (29),

$$S^* = - \frac{\mu}{q_e T} + \frac{q_e \Delta}{T \langle \tau^{xx} \rangle}, \tag{82}$$

where

$$\Delta = - \frac{1}{2\hbar} \sum_{\vec{\eta}, \vec{\eta}', \vec{r}} (\eta_x + \eta'_x)^2 t(\vec{\eta}) t(\vec{\eta}') \langle Y_{\sigma',\sigma}(\vec{r} + \vec{\eta}) \tilde{c}_{\vec{r}+\vec{\eta}+\vec{\eta}',\sigma'}^\dagger \tilde{c}_{\vec{r},\sigma} \rangle. \tag{83}$$

This is a very useful alternate formula to the Heikes formula,^{35,36} where the second term in Eq. (82) is thrown out.

It interpolates very usefully between the standard formulas for low temperature as well as at high temperature. The second term represents the “transport” contribution to the thermopower, whereas the first term is the thermodynamic or entropic part, which dominates at high temperature, as we shall show. In fact for S^* we can actually make a systematic expansion in powers of βt , unlike the dc counterpart, where it is not possible to make such an expansion.

The computation of the different parts proceeds as follows: we show readily that (for the hole doped case) using translation invariance and with n as the number of particles per site at high T ,

$$\hbar \langle \tau^{xy} \rangle = 6 \mathcal{L} q_e^2 t \langle \tilde{c}_1^\dagger \tilde{c}_0 \rangle \sim 3 \mathcal{L} q_e^2 \beta t^2 n (1-n). \quad (84)$$

The structure of the term Eq. (83) is most instructive. At high temperatures, for a square lattice we need to go to second order in βt to get a contribution with $\eta_x + \eta'_x \neq 0$, to the expectation of the hopping $\langle c_{\vec{r}+\vec{\eta}+\vec{\eta}',\sigma'}^\dagger c_{\vec{r},\sigma} \rangle$. For the triangular lattice, on the other hand, we already have a contribution at first order. For the triangular lattice, corresponding to each nearest neighbor, there are precisely two neighbors where the third hop is a nearest neighbor hop, and each of these gives the same factor $(\eta_x + \eta'_x)^2 = 1/4$, hence at high temperatures

$$\Delta \sim -\frac{3}{2\hbar} \mathcal{L} t^2 \sum_{\sigma,\sigma'} \langle Y_{\sigma',\sigma}(\vec{\eta}) \tilde{c}_{\vec{\eta}+\vec{\eta}',\sigma'}^\dagger \tilde{c}_{0,\sigma} \rangle. \quad (85)$$

The spins must be the same to the leading order in βt where we generate a hopping term $\tilde{c}_{0,\sigma}^\dagger \tilde{c}_{\vec{\eta}+\vec{\eta}',\sigma}$ from an expansion of $\exp(-\beta K)$, and hence a simple estimation yields

$$\Delta = -\frac{3}{4\hbar} \mathcal{L} t^3 \beta n (1-n)(2-n) + O(\beta^3). \quad (86)$$

This, together with $\mu/k_B T = \ln[n/2(1-n)] + O(\beta^2 t^2)$, gives us the result for $0 \leq n \leq 1$

$$S^* = \frac{k_B}{q_e} \left\{ \ln[2(1-n)/n] - \beta t \frac{2-n}{4} + O(\beta^2 t^2) \right\}, \quad (87)$$

and

$$S^* = \frac{k_B}{q_e} \left\{ \ln[2(n-1)/(2-n)] + \beta t \frac{n}{4} + O(\beta^2 t^2) \right\} \quad (88)$$

for $1 \leq n \leq 2$ using particle hole symmetry. Thus we can estimate the hopping parameter from the high temperature T dependence of the thermopower. From the temperature dependence of the data of Terasaki *et al.*³² and assuming $S \sim S^*$ one finds that $t = -110^\circ \text{K}$, and with this, $S^* \sim 120 \mu\text{V/K}$, fairly close to the observed value. Thus the sign and rough magnitude of the hopping are as expected from other grounds.³⁴ An interesting corollary of our analysis is that if the sign of hopping t were reversed, i.e., if $t > 0$ for the electron doped case, then the thermopower S^* would approach its high T value from above, and since the low T behavior is fixed to vanish linearly, it implies that S^* (and hence presumably S), must have a maximum, unlike the case $t < 0$. It follows that a material with similar absolute value of hopping as Na_xCoO_2 , but with the opposite sign of hopping,

would have a greater and hence an even more exciting thermoelectric behavior.

Hence, the nature of the high T expansion shows that the triangular lattice is exceptional in that the transport corrections to the entropic part are much larger than for the square lattice; they are of $O(\beta t)$ for the first as opposed to $O(\beta t)^2$ for the latter. Also these are potentially much more sensitive to a magnetic field than the corresponding one for the square lattice since these $O(\beta t)$ terms are themselves functions of the magnetic field $\sim O(B^2)$. In the degenerate limit, it seems quite possible that the field dependence of the transport part might be comparable to the spin entropy contribution.³³

The alternate formula Eqs. (82) and (29) for the thermopower thus has the interesting property that it captures the expected low T Fermi-liquid-type behavior as well as the high T Heikes-type behavior. It should be most interesting to apply numerical techniques to evaluate this for all T , a calculation that seems quite possible with existing techniques, at least for small systems.

X. DISCUSSION

It is curious that the recognition of the sum rule Eq. (18) for the thermal conductivity, has lagged so far behind Kubo's seminal paper in 1957.¹⁰ One of the reasons may be that most later workers followed the method given in Sec. IV following the Kubo identity. This method does give the sum rule as shown here, but only when one dissects the Kubo identity carefully, keeping the possibility of superconductivity in mind. On the other hand, the many-body linear response type method adopted in Sec. II runs into some discouragement, which is relieved only upon recognizing the role of Identity I in leading to a sensible result, as elaborated in the discussion following Eq. (12).

We have shown that the sum rule for thermal conductivity involves the thermal operator Θ^{xx} and the Seebeck coefficient involves Φ^{xx} , which are formally evaluated in this work, for various models of current interest. We plan to return to a numerical evaluation of some of these in the context of strongly correlated matter in a future study. We make some remarks on the nature of the variables and the prospects for their evaluation.

One notable fact is the vanishing with T^2 of the expectation of Θ^{xx} and Φ^{xx} for a Fermi gas; this is seen from the evaluation in Eq. (71) explicitly. This leads to questions such as: What is the origin of this behavior? Is this behavior true in general? The answer is that these variables must vanish at low temperature in a fashion that is dictated by the specific heat. This connection is a deep one and we explain it next.

Let us first recognize that the specific heat (at constant chemical potential) can be written as an energy-energy correlation function,

$$C_\mu = \frac{1}{T} \lim_{k \rightarrow 0} \int_0^\beta d\tau \langle \hat{K}(k, -i\tau) \hat{K}(-k) \rangle, \quad (89)$$

and the T dependence of this correlator is known in various systems in general terms. For metals and other Fermi liquids, the specific heat at constant N , i.e., C_N is the usual measured

one and differs from this by the thermodynamic relation

$$C_\mu = C_N + T \frac{(\partial S / \partial \mu)_T^2}{(\partial N / \partial \mu)_T}, \quad (90)$$

where the correction term is small for a Fermi liquid at low $T \sim O(T^3)$. The thermal operator is expressed as

$$\frac{\langle \Theta^{xx} \rangle}{\hbar T} = \frac{1}{d} C_\mu v_{eff}^2, \quad (91)$$

where d is the spatial dimension, and the above defined effective velocity v_{eff} is given by

$$v_{eff}^2 = \lim_{k \rightarrow 0, t \rightarrow 0} \frac{-d}{k_x^2 T C_\mu} \frac{d^2}{dt^2} \int_0^\beta d\tau \langle \hat{K}(k, t - i\tau) \hat{K}(-k) \rangle \\ = d \frac{\int_0^\beta d\tau \langle \hat{J}_x^Q(0, -i\tau) \cdot \hat{J}_x^Q(0, 0) \rangle}{\int_0^\beta d\tau \langle \hat{K}(0^+, -i\tau) \hat{K}(0^-, 0) \rangle}. \quad (92)$$

Here we have used the relation $D_Q=0$ for generic systems to replace Θ^{xx} by the current current expectation. The above formulas show that the variable Θ^{xx}/T is best thought of as being the specific heat times the square of a velocity, much as in the kinetic theory of thermal conduction where $\kappa = (1/d)Cv^2\tau$, so that the temperature dependence comes predominantly from the specific heat and the effective velocity captures the dynamics, without being very sensitive to T . Of course it must be understood that Θ^{xx} does not contain the scattering rate, which disappears in the sum rule. From a computational point of view, it seems best to use such a decomposition. At any rate, this line of argument gives us a qualitative understanding for the rather ‘‘magical property’’ of the Θ^{xx} operators listed, namely the vanishing of their average at low T in the true ground state.

Our work also yields an interesting exact formula for the zero temperature chemical potential for most metallic many-body systems. Since we expect the thermopower of metals to vanish in the ground state at all frequencies (being related to the entropy), equating the expectation of Φ^{xx} to zero gives us explicit formulas for the ground state chemical potential $\mu(0)$. This approach can be used in most cases, including hard core Bose metallic systems. In the interesting case of the Hubbard model, from Eq. (57), we find a formula for the ground state chemical potential as a ratio of expectation values of two operators

$$\mu(0) = \frac{\mathcal{N}}{\mathcal{D}},$$

$$\mathcal{N} = \frac{U}{4} \sum t(\vec{\eta}) (\eta_x)^2 \langle (n_{\vec{r},\sigma} + n_{\vec{r}+\vec{\eta},\sigma}) (c_{\vec{r}+\vec{\eta},\sigma}^\dagger c_{\vec{r},\sigma} + c_{\vec{r},\sigma}^\dagger c_{\vec{r}+\vec{\eta},\sigma}) \rangle \\ - \frac{1}{2} \sum (\eta_x + \eta'_x)^2 t(\vec{\eta}) t(\vec{\eta}') \langle c_{\vec{r}+\vec{\eta}+\vec{\eta}',\sigma}^\dagger c_{\vec{r},\sigma} \rangle,$$

$$\mathcal{D} = \sum \eta_x^2 t(\vec{\eta}) \langle c_{\vec{r}+\vec{\eta},\sigma}^\dagger c_{\vec{r},\sigma} \rangle, \quad (93)$$

where the denominator is recognized as essentially the stress tensor $\langle \tau^{xx} \rangle$. In the noninteracting case, this reduces to $\mu(0) = \varepsilon_F$, and thus generalizes this familiar relation to the interacting case. Similar formulas result for other models considered in this work, using the same idea. Usually one has to resort to differentiating the ground state energy with respect to the number of particles, and this can be inaccurate in numerical studies. Our formula is exact and a consequence of the vanishing of S^* at $T=0$. It is interesting that standard many-body textbooks^{11,17} do not quote this type of expression, and hence it is interesting to verify this in some cases where exact results are known from other arguments. The Hubbard model on bipartite lattices is a good a check of this result, since the chemical potential at half filling (only) is easily found using particle hole symmetry to be $U/2$. One can manipulate the expression Eq. (93) using the particle hole symmetry, and this result is easily reproduced.

We have presented the detailed form of the thermal and thermoelectric operators Θ^{xx} and Φ^{xx} for the Hubbard model, and also for the strongly correlated limit $U \rightarrow \infty$ above. Results for other models not discussed here can be readily found using the method presented. We have also presented the operators that give the disorder contribution to these variables, these can in principle be evaluated in perturbation theory in the disorder and interaction, and it should be interesting to compute these as well in low dimensions where the effect of disorder is marked. The operators for the lattice thermal conductivity should be interesting in the context of nonlinear lattices, and lend themselves to numerical evaluation rather easily in the classical limit, and the quantum cases also seem to be manageable with existing computational resources.

One set of applications concerns the effect of strong correlations on the thermoelectric power factor and the figure of merit in narrow band systems. These can be evaluated at high frequencies and such calculations should be useful guides to the role of interactions and band filling. We provide in Sec. IX a simple example of this formalism by computing the high temperature thermopower for the triangular lattice. This important and currently popular case models the physics of sodium cobalt oxide.³³ Interestingly the T dependence of the thermopower leads to estimates of the band width that seem comparable to other estimations.

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APPENDIX: ELECTRICAL CONDUCTIVITY

To complete the calculation we summarize the results for the electrical conductivity, which are already well known in literature.^{6,13,18,19,21,22} We note that in parallel to the calculation of the thermal conductivity, the conductivity can be ex-

pressed in terms of the correlations of the current operator \hat{J}_x as

$$\sigma(\omega_c) = \frac{i}{\hbar\omega_c\mathcal{L}} \left[\langle \tau^{xx} \rangle - i \int_0^\infty e^{i\omega_c t'} dt' \langle [\hat{J}_x(t'), \hat{J}_x(0)] \rangle \right], \quad (\text{A1})$$

where the stress tensor

$$\tau^{xx} = \lim_{k_x \rightarrow 0} \frac{1}{k_x} [\hat{J}_x(k_x), \rho(-k_x)] \quad (\text{A2})$$

$$= \frac{q_e^2}{\hbar} \sum_{\vec{r}} \eta_x^2 t(\vec{r}) c_{\vec{r}+\vec{\eta},\sigma}^\dagger c_{\vec{r},\sigma} \text{ or} \quad (\text{A3})$$

$$= \frac{q_e^2}{\hbar} \sum_{\vec{k},\sigma} \frac{d^2 \varepsilon_{\vec{k}}}{dk_x^2} c_{\vec{k},\sigma}^\dagger c_{\vec{k},\sigma}, \quad (\text{A4})$$

assuming a charge q_e for the particles, and $n(\vec{r})$ the particle density at \vec{r} , and the charge fluctuation operator $\rho(\vec{k}) = q_e \sum \exp(i\vec{k} \cdot \vec{r}) n(\vec{r})$. Again performing the Lehmann representation we find

$$\sigma(\omega_c) = \frac{i}{\hbar\omega_c\mathcal{L}} \left[\langle \tau^{xx} \rangle - \hbar \sum_{n,m} \frac{p_n - p_m}{\epsilon_n - \epsilon_m + \hbar\omega_c} |\langle n | \hat{J}_x | m \rangle|^2 \right]. \quad (\text{A5})$$

We can use partial fractions and write

$$\sigma(\omega_c) = \frac{i}{\hbar\omega_c} D_c + \frac{i\hbar}{\mathcal{L}} \sum_{n,m} \frac{p_n - p_m}{\epsilon_n - \epsilon_m} \frac{|\langle n | \hat{J}_x | m \rangle|^2}{\epsilon_n - \epsilon_m + \hbar\omega_c}, \quad (\text{A6})$$

where the charge or Meissner stiffness is given by

$$D_c = \frac{1}{\mathcal{L}} \left[\langle \tau^{xx} \rangle - \hbar \sum_{n,m} \frac{p_n - p_m}{\epsilon_n - \epsilon_m} |\langle n | \hat{J}_x | m \rangle|^2 \right]. \quad (\text{A7})$$

The more familiar superfluid density $\rho_s(T)$ and plasma frequencies $\omega_p, \omega_{p,s}$ for the total and superconducting condensate are defined in terms of D_c and $\langle \tau^{xx} \rangle$ by

$$\omega_{p,s}^2 \equiv \frac{4\pi q_e^2 \rho_s(T)}{m} = \frac{4\pi D_c(T)}{\hbar}, \quad (\text{A8})$$

$$\omega_p^2 = \frac{4\pi}{\hbar\mathcal{L}} \langle \tau^{xx} \rangle,$$

so that Eq. (A7) is just the lattice version of the well-known London decomposition of electronic density into superconducting and normal parts. The real part of the Lehmann rep is

$$\text{Re}\sigma(\omega) = \pi \delta(\hbar\omega) \bar{D}_c + \frac{\pi}{\mathcal{L}} \left(\frac{1 - e^{-\beta\hbar\omega}}{\omega} \right) \times \sum_{\epsilon_n \neq \epsilon_m} p_n |\langle n | \hat{J}_x | m \rangle|^2 \delta(\epsilon_m - \epsilon_n - \hbar\omega), \quad (\text{A9})$$

where

$$\bar{D}_c = \frac{1}{\mathcal{L}} \left[\langle \tau^{xx} \rangle - \hbar \sum_{\epsilon_n \neq \epsilon_m} \frac{p_n - p_m}{\epsilon_n - \epsilon_m} |\langle n | \hat{J}_x | m \rangle|^2 \right], \quad (\text{A10})$$

using a cancellation between the terms with equal energy between the two terms.

The lattice version of the f sum rule for the real part of the conductivity (an even function of ω) follows as

$$\int_0^\infty \text{Re}\sigma(\omega) d\omega = \frac{\pi}{2\hbar\mathcal{L}} \langle \tau^{xx} \rangle. \quad (\text{A11})$$

We may rewrite Eq. (A6) in a more compact form as

$$\sigma(\omega_c) = \frac{i}{\hbar\omega_c} D_c + \frac{1}{\mathcal{L}} \int_0^\infty dt e^{i\omega_c t} \int_0^\beta d\tau \langle \hat{J}_x(-t - i\tau) \hat{J}_x(0) \rangle. \quad (\text{A12})$$

The difference between the two stiffnesses is

$$D_c - \bar{D}_c = -\beta\hbar \sum_{\epsilon_n = \epsilon_m} p_n |\langle n | \hat{J}_x | m \rangle|^2. \quad (\text{A13})$$

Thus if we know that $D_c = 0$ by some independent argument, then this provides us with an alternate expression for \bar{D}_c .¹⁴

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Erratum: A Sum Rule for Thermal Conductivity and Dynamical Thermal Transport Coefficients in Condensed Matter, Phys. Rev. B 73, 085117 (2006)

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We correct three equations below. All related discussion is unchanged.

(i) Equation (41) should read as:

$$\mathbf{Z}^*T = \frac{\langle \Phi^{xx} \rangle^2}{\langle \Theta^{xx} \rangle \langle \mathcal{T}^{xx} \rangle}. \quad (41)$$

(ii) The sentence containing Equations (87 and 88) should read:

This together with $\mu/k_B T = \ln(n/2(1-n)) + O(\beta^2 t^2)$ gives us the result for $0 \leq n \leq 1$

$$S^* = \frac{k_B}{q_e} \left\{ \ln[2(1-n)/n] - \beta t \frac{2-n}{2} + O(\beta^2 t^2) \right\}, \quad (87)$$

and

$$S^* = -\frac{k_B}{q_e} \left\{ \ln[2(n-1)/(2-n)] + \beta t \frac{n}{2} + O(\beta^2 t^2) \right\} \quad (88)$$

for $1 \leq n \leq 2$ using particle hole symmetry $t \rightarrow -t$, $n \rightarrow 2-n$, $q_e \rightarrow -q_e$, with $q_e = -|e|$.