Temperature and voltage measurement in quantum systems far from equilibrium

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We show that a local measurement of temperature and voltage for a quantum system in steady state, arbitrarily far from equilibrium, with arbitrary interactions within the system, is unique when it exists. This is interpreted as a consequence of the second law of thermodynamics. We further derive a necessary and sufficient condition for the existence of a solution. In this regard, we find that a positive temperature solution exists whenever there is no net population inversion. However, when there is a net population inversion, we may characterize the system with a unique negative temperature. Voltage and temperature measurements are treated on an equal footing: They are simultaneously measured in a noninvasive manner, via a weakly-coupled thermoelectric probe, defined by requiring vanishing charge and heat dissipation into the probe. Our results strongly suggest that a local temperature measurement without a simultaneous local voltage measurement, or vice-versa, is a misleading characterization of the state of a nonequilibrium quantum electron system. These results provide a firm mathematical foundation for voltage and temperature measurements far from equilibrium.

I. INTRODUCTION

Scanning probe microscopy revolutionized the field of nanoscience and enabled the measurement of local thermodynamic observables such as voltage and temperature in nonequilibrium quantum systems. The ability to define local thermodynamic variables in a system far from equilibrium is of fundamental interest because it is a necessary step toward the construction of nonequilibrium thermodynamics. Many experiments in mesoscopic electrical transport utilize voltage probes as circuit elements, and scanning potentiometers are now a mature technology, routinely achieving sub-angstrom spatial resolution. In contrast, scanning thermometry has proven significantly more challenging, but is currently undergoing a rapid evolution toward nanometer resolution, leading to important insights into transport and dissipation at the nanoscale. A fundamental challenge for theory is to develop a rigorous mathematical description of such local thermodynamic measurements. Until now, mainly operational definitions have been advanced, leading to a competing panoply of often contradictory definitions of such basic observables as temperature and voltage.

The second law of thermodynamics is one of the cornerstones of physics. The origin of the second law was rooted in empirical observations in the early nineteenth century, and its theoretical explanation emerged with the gradual development of the statistical foundation of thermodynamics. The statistical basis of the second law places it in a league of its own, among the laws of physics. A quote on the subject, at once exalting and to the point, by the famous astrophysicist Sir Arthur Eddington reads as follows: “The law that entropy always increases, I think, the supreme position among the laws of Nature. If someone points out to you that your pet theory of the universe is in disagreement with Maxwell’s equations — then so much the worse for Maxwell’s equations. If it is found to be contradicted by observation — well, these experimentalists do bungle things sometimes. But if your theory is found to be against the second law of thermodynamics I can give you no hope; there is nothing for it but to collapse in deepest humiliation.” Any theory which purports to describe the measurement of temperature, voltage or other thermodynamic parameters, must therefore satisfy this fundamental requirement, and as Eddington notes, regardless of the nature of microscopic interactions.

We examine statements of the second law of thermodynamics, accompanied with mathematical proofs, and their consequences, in the context of local noninvasive measurements of temperature and voltage in nonequilibrium quantum electron systems. We derive our results from very general considerations, i.e., for electron transport in steady state, arbitrarily far from equilibrium, and for arbitrary interactions within the quantum electron system. Our considerations apply to any system of fermions, charged or neutral. While our analyses in this article are presented in a theorem-proof format, their motivation draws from physical principles. We show that the uniqueness of the temperature and voltage measurement is a consequence of the second law of thermodynamics and that, in order to obtain a unique measurement, it is necessary to measure both temperature and voltage simultaneously. Simply put, this is because electrons carry both energy and charge.

In order to have a meaningful definition of temperature, the Hamiltonian must be bounded below \( \langle H \rangle \geq -c \) for some finite \( c \in \mathbb{R} \). By the same token, a system can, in principle, exhibit negative temperatures if the energy averaged over the spectrum is bounded above \( \langle H \rangle \leq c \) for some finite \( c \in \mathbb{R} \). These are well-known results in statistical physics, and we highlight their role in the context of local noninvasive measurements of temperature and voltage. We derive a condition, that is both necessary and sufficient, for the existence of a joint tem-
temperature and voltage measurement. This condition corresponds physically to a nonequilibrium system that does not exhibit local population inversion. We obtain also, as a corollary of the former condition, the result that nonequilibrium systems exhibiting local population inversion can be characterized with a negative temperature which is also unique. Population inversion is the working principle behind important Fermionic devices such as the maser and laser [48, 51].

In this article, we consider a probe that couples exclusively to the electronic degrees of freedom. Out of equilibrium, the temperature distributions of different microscopic degrees of freedom (e.g., electrons, phonons, nuclear spins) do not, in general, coincide, so that one has to distinguish between measurements of the electron temperature [37, 38, 44, 52] and the lattice temperature [53, 54]. This distinction is particularly acute in the extreme limit of elastic quantum transport [55], where electron and phonon temperatures are completely decoupled. It should be emphasized that the electrons within the system are free to undergo arbitrary interactions, e.g., with photons, phonons, other electrons, etc. However, direct heat transport into the probe via black-body radiation, phonons, etc. is excluded. Inclusion of these additional heat transfer processes into the probe leads to a temperature measurement that is simply a combination of the temperatures of the various microscopic degrees of freedom [45].

The article is organised as follows. We outline the formalism in Sec. II and introduce a postulate that helps put our results on sound mathematical footing. In Sec. III we discuss our theory of local thermodynamic measurements, explain the idea behind noninvasive measurements, and also derive some useful expressions for further analysis. In Sec. IV we provide several statements of the second law of thermodynamics and show their relation to the uniqueness of temperature and voltage measurements. In Sec. V we start by defining certain useful quantities and proceed to derive the condition for the existence of a solution. We also discuss here the case of broadband probes in order to further illustrate the physical meaning behind our results, and conclude that probes operating in the broadband limit can be considered to be ideal. We consider the other extreme as well, i.e., narrowband probes and conclude that they are unsuitable for measurements. Our results are illustrated for a two-level system which is detailed in Sec. VI. We conclude with a summary of our central findings in Sec. VII contrasting our approach to prior theoretical work, and discuss possible future directions. Some key results on the local properties of fermions in a nonequilibrium steady state are presented in Appendix A which are needed in our analysis of the measurement problem.

II. FORMALISM

We use the nonequilibrium Green’s function formalism (NEGF) for describing the motion of electrons within a quantum conductor. A general expression for the nonequilibrium steady-state electrical current \(\nu = 0\) [50] and the electronic contribution to the heat current \(\nu = 1\) [57] flowing into a macroscopic electron reservoir \(P\), can be written in a form analogous to the two-terminal Landauer-Büttiker formula [13]:

\[
I_p^{(\nu)} = \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega (\omega - \mu_p) \nu T_{ps}(\omega) \left[ f_s(\omega) - f_p(\omega) \right],
\]

with \(\nu = \{0, 1\}\),

where one may think of

\[
T_{ps}(\omega) = 2\pi \text{Tr} \{\Gamma_p(\omega) A(\omega)\}
\]

as a local transmission function between the macroscopic probe terminal and the nonequilibrium quantum system. \(f_s(\omega)\) is the nonequilibrium distribution function of the system, as sampled by the probe, and is defined by [13]

\[
f_s(\omega) = \frac{\text{Tr} \{\Gamma_p(\omega) G^< (\omega)\}}{2\pi \text{Tr} \{\Gamma_p(\omega) A(\omega)\}}.
\]

In Eqs. (2–3), \(A(\omega) = (G^<(\omega) - G^>(\omega))/2\pi i\) is the spectral function. \(G^< (\omega)\) and \(G^> (\omega)\) are the Fourier transforms of the Keldysh “lesser” and “greater” Green’s functions [58], describing the nonequilibrium electron and hole distributions within the system, respectively (see Appendix A for details). \(\Gamma_p(\omega)\) is the tunneling width matrix describing the coupling of the probe to the system, and \(f_p(\omega; \mu_p, T_p) = 1/(1 + \exp(\omega - \mu_p - T_p)/T_p))\) is the Fermi-Dirac distribution of the probe. We note that the expression in Eq. (1) is completely general and allows for arbitrary interactions within the quantum system, and arbitrary bias conditions of the reservoirs.

Since the spectral function \(A(\omega)\) is positive-semidefinite and the probe-system coupling \(\Gamma_p(\omega)\) is positive-definite (see Appendix A), we note that

\[
\text{Tr} \{A(\omega) \Gamma(\omega)\} = \text{Tr} \left\{ A^{1/2}(\omega) A^{1/2}(\omega) \Gamma(\omega) \right\} = \text{Tr} \left\{ A^{1/2}(\omega) \Gamma(\omega) A^{1/2}(\omega) \right\} \geq 0,
\]

where \(A^{1/2}(\omega)\) is the positive-semidefinite square root of \(A(\omega)\). \(A^{1/2}(\omega) \Gamma(\omega) A^{1/2}(\omega)\) becomes positive-semidefinite when \(A^{1/2}(\omega)\) and \(\Gamma(\omega)\) are positive-semidefinite [59] and therefore we have

\[
T_{ps}(\omega) \geq 0, \ \forall \omega \in \mathbb{R}.
\]

We note that \(f_s(\omega)\) satisfies the property of a distribution function, namely,

\[
0 \leq f_s(\omega) \leq 1 \ \forall \omega \in \mathbb{R},
\]
as shown in appendix A. We start our analysis with the following postulate, and explain its physical significance.

**Postulate 1** The local probe-system transmission function \( T_{ps} : \mathbb{R} \rightarrow [0, \infty) \) and the nonequilibrium distribution function \( f_s : \mathbb{R} \rightarrow [0, 1] \) are measurable over any interval \([a, b] \subseteq \mathbb{R}\), and \( T_{ps}(\omega) \) satisfies

\[
0 < \int_{-\infty}^{\infty} d\omega T_{ps}(\omega) < \infty, \tag{7}
\]

and

\[
\left| \int_{-\infty}^{\infty} d\omega \omega T_{ps}(\omega) \right| < \infty. \tag{8}
\]

The measurability of \( T_{ps}(\omega) \) and \( f_s(\omega) \) is taken to lend meaning to the currents in Eq. (1). We point out that the finiteness of the two integrals given in Eqs. (7) and (8) is somewhat redundant since the limiting case must have \( \omega_{-} \rightarrow \pm \infty \) while \( \omega_{-} \rightarrow -\infty \) is ruled out based on the principle that any physical spectrum has a finite ground-state energy. We note that Eqs. (7), (8) also imply

\[
0 < \int_{-\infty}^{\infty} d\omega T_{ps}(\omega) f_s(\omega), \int_{-\infty}^{\infty} d\omega T_{ps}(\omega) f_p(\omega) < \infty \tag{9}
\]

and

\[
\int_{-\infty}^{\infty} d\omega \omega T_{ps}(\omega) f_s(\omega), \int_{-\infty}^{\infty} d\omega \omega T_{ps}(\omega) f_p(\omega) < \infty. \tag{10}
\]

### III. LOCAL MEASUREMENTS

The local voltage and temperature of a nonequilibrium quantum system, as measured by a scanning thermoelectric probe, is defined by the simultaneous conditions of vanishing net charge dissipation and vanishing net heat dissipation into the probe \(13, 15, 44, 45, 52, 60\):

\[
I_{p}^{(\nu)} = 0, \quad \nu \in \{0, 1\}, \tag{11}
\]

\[
\text{FIG. 1: Illustration of the measurement setup: The quantum conductor represented below is in a nonequilibrium steady state. A weakly-coupled scanning tunneling probe noninvasively measures the local voltage (\( \mu_p \)) and local temperature (\( T_p \)) simultaneously. By requiring both a vanishing net charge exchange (\( I_{p}^{(0)} = 0 \)) and a vanishing net heat exchange (\( I_{p}^{(1)} = 0 \)) with the system. The nonequilibrium steady state has been prepared, in this particular illustration, via the electrical and thermal bias of the strongly-coupled reservoirs (1 and 2). The measurement method itself is completely general and does not depend upon (a) how such a nonequilibrium steady-state is prepared, (b) how far from equilibrium the quantum electron system is driven, and (c) the nature of interactions within that system.}
\]

where \( \nu = 0, 1 \) correspond to the electron number current and the electronic contribution to the heat current, respectively. Eq. (11) gives the conditions under which the probe is in local equilibrium with the sample, which is itself arbitrarily far from equilibrium.

We define the system’s local temperature and voltage using a probe that is weakly coupled via a tunnel barrier. The other end of this scanning probe \(4, 5\) is the macroscopic electron reservoir whose temperature and voltage are both adjusted until Eq. (11) is satisfied. A weakly coupled probe is a useful theoretical construction for our analysis, and the extension of our results beyond the weak-coupling limit is an open question. We explain the physical basis of weak coupling below, and derive some useful formulae.

#### A. Noninvasive measurements

When the coupling of the probe to the system is weak, we may take \( T_{ps}(\omega) \) in Eq. (2) and the local nonequilibrium distribution function \( f_s(\omega) \) to be independent of the probe Fermi-Dirac distribution \( f_p(\omega) \). While both these
quantities depend upon the local probe-system coupling in an obvious manner, the weak-coupling condition essentially implies that the nonequilibrium steady state of the system is unperturbed by the introduction of the probe terminal. The voltage and temperature of the probe itself play no role in preparing the nonequilibrium steady state. In other words, the probe does not drive the system but merely exchanges energy and particles across a weakly-coupled tunnel barrier and constitutes a noninvasive measurement.

Given a system prepared in a certain nonequilibrium steady state (e.g., by a particular bias of the strongly coupled reservoirs), the currents given by Eq. (11) are functions of the probe Fermi-Dirac distribution specified by its temperature and chemical potential

\[ I_p^{(\nu)} \equiv I_p^{(\nu)}(\mu_p, T_p). \]  

(12)

It can be seen that the currents are continuous functions of \( \mu_p \in (-\infty, \infty) \) and \( T_p \in (0, \infty) \) with continuous gradient vector fields defined by

\[ \nabla I_p^{(\nu)} = \left( \frac{\partial I_p^{(\nu)}}{\partial \mu_p}, \frac{\partial I_p^{(\nu)}}{\partial T_p} \right). \]  

(13)

With \( k_B \) set to unity, we compute the gradients of the currents using Eq. (11). We find the gradient of the number current to be

\[ \nabla I_p^{(0)} = \left( -\mathcal{L}^{(0)}_{ps} \frac{\partial I_p^{(0)}}{\partial T_p}, \frac{\partial I_p^{(0)} - \mathcal{L}^{(1)}_{ps}}{T_p} \right). \]  

(14)

The gradient of the heat current reduces to

\[ \nabla I_p^{(1)} = \left( -\mathcal{L}^{(1)}_{ps} - I_p^{(0)}, -\frac{\partial \mathcal{L}^{(2)}_{ps}}{T_p} \right), \]  

(15)

where we define the response coefficients \( \mathcal{L}^{(\nu)}_{ps} \) as

\[ \mathcal{L}^{(\nu)}_{ps} \equiv \mathcal{L}^{(\nu)}_{ps}(\mu_p, T_p) \]

\[ = \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega (\omega - \mu_p) f_{ps}(\omega) \frac{\partial f_{ps}}{\partial \omega}, \]  

(16)

which are easily seen to be finite [61].

Although the coefficients \( \mathcal{L}^{(\nu)}_{ps} \) formally resemble the Onsager linear-response coefficients [62] of an elastic quantum conductor [63], it is very important to note that we do not make the assumptions of linear response, local equilibrium, or elastic transport in the above definition of \( \mathcal{L}^{(\nu)}_{ps} \). The system itself may be arbitrarily far from equilibrium with arbitrary inelastic scattering processes. The coefficients above appear naturally when we calculate the gradient fields defined by Eq. (11), and the gradient operator is of course given by the first derivatives. Our main results follow from an analysis of the properties of these gradient fields.

IV. UNIQUENESS AND THE SECOND LAW

We now turn to one of the central problems which we set out to address: \( I_p^{(\nu)}(\mu_p, T_p) = 0 \), with \( \nu = (0, 1) \), is a system of coupled nonlinear equations in two variables that defines our local voltage and temperature measurement. There is no a priori reason to expect a unique solution, if a solution exists at all. We begin the section with statements of the second law of thermodynamics, and conclude by showing that the uniqueness of the measurement emerges as a consequence.

A. Statements of the second law

We note that \( \forall \mu_p \in (-\infty, \infty) \) and \( T_p \in (0, \infty) \),

\[ \mathcal{L}^{(0)}_{ps}(\mu_p, T_p) > 0 \]

\[ \mathcal{L}^{(2)}_{ps}(\mu_p, T_p) > 0, \]  

(17)

since \( T_{ps}(\omega) \geq 0 \), and the measure of \( T_{ps}(\omega) \) and the Fermi-function derivative are both nonzero and strictly positive. This leads to two statements of the second law of thermodynamics, related to the Clausius statement, which are presented in the following two lemmas. The idea is to choose the correct contour for each case, and to evaluate the line integral over the current gradients in Eqs. (14) and (15). A cursory glance at the number current gradient in Eq. (11) suggests that the contour should be defined over a constant temperature, while the heat current gradient in Eq. (15) suggests a line integral over a constant voltage contour.

Lemma 1 The number current contour defined by \( I_p^{(0)}(\mu_p, T_p) = 0 \) exists for all \( T_p \in (0, \infty) \) and defines a function \( M : (0, \infty) \rightarrow \mathbb{R} \) where \( \mu_p = M(T_p) \), such that the second law of thermodynamics is obeyed:

\[ I_p^{(0)}(\mu_p', T_p) > 0, \text{ if } \mu_p' < M(T_p) \]

\[ I_p^{(0)}(\mu_p', T_p) < 0, \text{ if } \mu_p' > M(T_p). \]  

(18)

Proof. We first show that \( I^{(0)}(\mu_p, T_p) = 0 \) is satisfied for all \( T_p \in (0, \infty) \). For any \( T_p \in (0, \infty) \), we have

\[ \lim_{\mu_p \to -\infty} I_p^{(0)}(\mu_p, T_p) = \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega T_{ps}(\omega) f_s(\omega) \]

\[ - \lim_{\mu_p \to -\infty} f_p(\omega) \]

\[ = \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega T_{ps}(\omega) f_s(\omega) > 0, \]  

(19)
and
\[ \lim_{\mu_p \to \infty} I_p^{(0)}(\mu_p, T_p) = \frac{1}{h} \int_{-\infty}^{\infty} d\omega T_{ps}(\omega) [f_p(\omega) - f_p(0)] = 1 \int_{-\infty}^{\infty} T_{ps}(\omega) (f_s(\omega) - 1) < 0. \]

This ensures at least one solution due to the continuity of the currents, but does not ensure uniqueness.

We note that \( I_p^{(0)} \) is monotonically decreasing along \( dI = (d\mu_p, 0) \)

\[ \Delta I_p^{(0)} = \int_{\mu_p}^{\mu_p'} \nabla I_p^{(0)} \cdot dI = \int_{\mu_p}^{\mu_p'} - C_p^{(0)} d\mu_p \]

due to the fact that \( C_p^{(0)} \) is positive, and more explicitly:
\[ \Delta I_p^{(0)} = \frac{1}{h} \int_{-\infty}^{\infty} d\omega T_{ps}(\omega) [f_p(\mu_p, T_p; \omega) - f_p(\mu_p', T_p; \omega)] \]
\[ > 0, \text{ if } \mu_p' < \mu_p \]
\[ < 0, \text{ if } \mu_p' > \mu_p. \]

This implies the existence of a unique solution to \( I_p^{(0)}(\mu_p, T_p) = 0 \) for every \( T_p \in (0, \infty) \) which we denote by \( \mu_p = M(T_p) \), and Eq. (15) is implied by Eq. (22).  

We also note that the number current \( [\mu_p = M(T_p)] \) contour is vertical when the temperature approaches absolute zero, as shown in Fig. 2 since \( L_p^{(1)} / T_p \to 0 \) as \( T_p \to 0 \), and implies a vanishing Seebeck coefficient for the probe-system junction near absolute zero.

An “ideal potentiometer” was initially proposed \([37]\) by merely requiring \( I_p^{(0)} = 0 \). Subsequently, Büttiker \([64, 65]\) clarified that this definition holds only near absolute zero due to the absence of thermoelectric corrections. Such a voltage probe determines the voltage uniquely at zero temperature in the linear response regime, and is relevant for experiments in mesoscopic circuits \([10, 11]\) which are carried out at cryogenic temperatures. However, at higher temperatures and/or larger bias voltages, where the sample may be heated by both the Joule and Peltier effects, thermoelectric corrections to voltage measurements must be considered. Indeed, Bergfield and Stafford \([60]\) argue that an ideal voltage probe must be required to equilibrate thermally with the system \( (I_p^{(1)} = 0) \), without which “a voltage will develop across the system-probe junction due to the Seebeck effect.”

Voltage probes have been used extensively in the theoretical literature to mimic the effects of various scattering processes, such as inelastic scattering \([64, 66, 74]\) and dephasing \([71, 72]\) in mesoscopic systems. A modern variation of Büttiker’s voltage probe, additionally requiring that the probe exchange no heat current, has been used to model inelastic scattering in quantum transport problems at finite temperature \([32, 42, 74, 76]\). The probe technique, as a model for scattering, has also been extensively studied beyond the linear response regime \([77, 78]\).

Lemma 1 implies that a “voltage probe” (defined only by \( I_p^{(0)} = 0 \)) requires the simultaneous specification of a probe temperature \( T_p \) so that \( \mu_p = M(T_p) \) is uniquely determined. Fig. 2 illustrates that the measured voltage shows a large dependence on the probe temperature. Therefore, it is important to define a simultaneous temperature measurement by imposing \( I_p^{(1)}(\mu_p, T_p) = 0 \).

**Lemma 2** The heat current contour defined by \( I_p^{(1)}(\mu_p, T_p) = c \), where \( c \) is some constant, obeys the second law of thermodynamics, namely,
\[ I_p^{(1)}(\mu_p, T_p) > c, \text{ if } T_p' < T_p \]
\[ < c, \text{ if } T_p' > T_p. \]

**Proof.** We follow an analogous argument to lemma 1 and show the monotonicity of \( I_p^{(1)}(\mu_p, T_p) \) along a certain contour in the \( \mu_p-T_p \) plane. Naturally, the contour we choose is along a fixed \( \mu_p \) [cf. Eq. (15)] since we know that \( L_p^{(2)} \) is positive. Therefore we have \( \Delta I_p^{(1)} = I_p^{(1)}(\mu_p, T_p) - I_p^{(1)}(\mu_p, T_p) = \int_{\mu_p}^{T_p} \nabla I_p^{(1)} \cdot d\mu \), where \( d\mu = (0, dT_p) \) and explicitly,
\[ \Delta I_p^{(1)} = \frac{1}{h} \int_{-\infty}^{\infty} d\omega (\omega - \mu_p) T_{ps}(\omega) [f_p(\mu_p, T_p; \omega) - f_p(\mu_p, T_p; \omega)] \]
\[ > 0, \text{ if } T_p' < T_p \]
\[ < 0, \text{ if } T_p' > T_p. \]
This implies Eq. (24).

We stated lemma 2 with a constant $c$ [80], not necessarily $c = 0$, unlike lemma 1. This is because we do not a priori know whether the contour $I_p^{(1)} = 0$ exists, and we derive a necessary and sufficient condition for its existence in Sec. V.D.

Analogous to Lemma 1, Lemma 2 implies that a “temperature probe” [37] (defined only by $I_p^{(1)} = 0$) requires the simultaneous specification of a probe voltage $\mu_p$ so that the temperature $T_p = \tau_0(\mu_p)$ (cf. footnote 80) is uniquely determined. Fig. 3 illustrates that the measured temperature shows a large dependence on the probe voltage. Therefore, it becomes important to simultaneously measure the voltage by imposing $I_p^{(0)} = 0$. If the temperature probe is not allowed to equilibrate electrically with the system, then a temperature difference will build up across the probe-system junction due to the Peltier effect, leading to an error in the temperature measurement.

Clearly, depending upon the probe voltage, the “temperature probe” could measure any range of values, rendering the measurement somewhat meaningless (see Fig. 3). Analogously, the “voltage probe” could measure any range of values depending upon the probe temperature (see Fig. 2). Thermoelectric probes (also referred to as dual probes, and voltage-temperature probes) treat temperature and voltage measurements on an equal footing, and implicitly account for the thermoelectric corrections exactly. Only such a dual probe is in both thermal and electrical equilibrium with the system being measured, and therefore yields an unbiased measurement of both quantities. A mathematical proof of the uniqueness of a voltage and temperature measurement is therefore of fundamental importance.

We may also deduce that $T_p = 0$ cannot be obtained as a measurement outcome since

$$\lim_{T_p \to 0} I_p^{(1)}(\mu_p, T_p) = \int_{-\infty}^{\infty} d\omega (\omega - \mu_p) T_{ps}(\omega)[f_s(\omega) - \lim_{T_p \to 0} f_p(\mu_p, T_p)]$$

$$= \int_{-\infty}^{\mu_p} d\omega (\omega - \mu_p) T_{ps}(\omega)(f_s(\omega) - 1) + \int_{\mu_p}^{\infty} d\omega (\omega - \mu_p) T_{ps}(\omega)f_s(\omega)$$

$$> 0,$$ (25)

consistent with the third law of thermodynamics. However, temperatures arbitrarily close to absolute zero are, in principle, possible [13].

Lemmas 1 and 2 are equivalent to the Clausius statement of the second law [81]: “No process is possible whose sole effect is to transfer heat from a colder body to a warmer body.” Lemma 2 gives us the direction in which heat will flow [cf. Eq. (24)] when the probe is biased away from thermal equilibrium $I_p^{(1)}(\mu_p, T_p) = 0$: whenever the probe is hotter than the temperature corresponding to local thermal equilibrium, with the chemical potential held constant, heat flows out of the probe and vice versa. Similarly, Lemma 1 gives us the direction in which particle flow occurs when the probe is biased away from equilibrium $I_p^{(0)}(\mu_p, T_p) = 0$: whenever the probe is at a higher chemical potential than the one corresponding to local electrical equilibrium, with temperature held constant, particles flow out of the probe and vice versa.

The problem of a unique measurement of a “voltage probe” (defined only by $I_p^{(0)} = 0$), or a “temperature probe” (defined only by $I_p^{(1)} = 0$) has been attempted previously by Jacquet and Pillet [12] for transport beyond linear response, and to our knowledge is the only work in this direction. However, in Ref. [12], the bias conditions considered are quite restrictive and the result assumes noninteracting electrons. Lemma 1 and lemma 2 respectively, generalize the result to arbitrary bias conditions, and arbitrary interactions within a quantum electron system while also providing a useful insight via the Clausius statement of the second law of thermodynamics. However, the question we would like to answer in this article pertains to the uniqueness of a thermoelectric probe measurement, defined by both $I_p^{(0)} = 0$ and $I_p^{(1)} = 0$. A result for such dual probes has been obtained only in the linear response regime and for noninteracting electrons [59].

**Theorem 1** The coefficients $\mathcal{L}_{ps}^{(\nu)}$ satisfy the inequality

$$\mathcal{L}_{ps}^{(0)} \mathcal{L}_{ps}^{(2)} - (\mathcal{L}_{ps}^{(1)})^2 > 0.$$ (26)
Proof. We may define functions $g(\omega)$ and $h(\omega)$ as

$$g(\omega) = \sqrt{T_{ps}(\omega) \left( - \frac{\partial f_p}{\partial \omega} \right)}$$  \hspace{1cm} (27)$$

and

$$h(\omega) = (\omega - \mu_p) \sqrt{T_{ps}(\omega) \left( - \frac{\partial f_p}{\partial \omega} \right)}.$$  \hspace{1cm} (28)$$

We note that $g(\omega)$ and $h(\omega)$ belong to $L^2(\mathbb{R})$. Noting that $g$ and $h$ are real, we apply the Cauchy-Schwarz inequality

$$\left| \int_{-\infty}^{\infty} d\omega g(\omega) h(\omega) \right|^2 \leq \int_{-\infty}^{\infty} d\omega |g(\omega)|^2 \int_{-\infty}^{\infty} d\omega |h(\omega)|^2.$$  \hspace{1cm} (29)$$

The integral appearing on the lhs is $L_{ps}^{(1)}$, while on the rhs we have the product of $L_{ps}^{(0)}$ and $L_{ps}^{(2)}$, respectively. We drop the absolute value on the lhs by noting that $L_{ps}^{(1)}$ is real and write

$$(L_{ps}^{(1)})^2 \leq L_{ps}^{(0)} L_{ps}^{(2)}.$$  \hspace{1cm} (30)$$

We drop the equality case above by noting that $g$ and $h$ are linearly independent except for the trivial case when $T_{ps}(\omega) = 0 \forall \omega$, or when the probe coupling is narrowband $[T_{ps}(\omega) = \gamma \delta(\omega - \omega_0)]$ which we discuss in sec V C.

The proof above can be easily extended to show the positive-definiteness of the linear response matrices widely used for elastic transport calculations (e.g., in Refs. [62] and [82]). Theorem 1 implies a positive thermal conductance (see e.g., Ref. [82]), which is necessary for positive entropy production consistent with the second law of thermodynamics.

**B. Uniqueness**

**Theorem 2** The local temperature and voltage of a nonequilibrium quantum system, measured by a thermoelectric probe, is unique when it exists.

**Proof.** The tangent vectors $t^{(v)}$ for $I_p^{(v)}$ are along

$$t^{(0)} = \left( - \frac{L_{ps}^{(1)}}{I_p}, L_{ps}^{(0)} \right)$$  \hspace{1cm} (31)$$

and

$$t^{(1)} = \left( \frac{L_{ps}^{(2)}}{I_p} - L_{ps}^{(1)}, I_p - I_p^{(0)} \right) = \left( \frac{L_{ps}^{(2)}}{I_p} - L_{ps}^{(1)} \right), \text{ if } I_p^{(0)} = 0,$$  \hspace{1cm} (32)$$

respectively, such that we have

$$\int_{s_1}^{s_2} ds \frac{t^{(v)} \cdot \nabla I_p^{(v)}}{|t^{(v)}|} = 0,$$  \hspace{1cm} (33)$$

where $s$ is a scalar that labels points along the contour $I_p^{(v)} = \text{constant}$.

We now compute the change in $I_p^{(1)}$ along the contour $I_p^{(0)} = 0$. The points along $I_p^{(0)} = 0$ are labeled by the continuous parameter $\xi$ such that $\mu_p = \mu_p(\xi)$ and $T_p = T_p(\xi)$. $\xi$ is chosen to be increasing with increasing temperature. The change $\Delta I_p^{(1)}$ becomes

$$\Delta I_p^{(1)} = \int_{\xi_1}^{\xi_2} d\xi \frac{t^{(0)} \cdot \nabla I_p^{(1)}}{|t^{(0)}|} = \int_{\xi_1}^{\xi_2} d\xi \frac{1}{|t^{(0)}| T_p} \left( (L_{ps}^{(1)})^2 - L_{ps}^{(0)} L_{ps}^{(2)} \right)$$  \hspace{1cm} (34)$$

due to theorem 1. Therefore $I_p^{(1)} = 0$ (or for that matter $I_p^{(1)} = c$, for any $c$) is satisfied at most at a single point along $I_p^{(0)} = 0$.

**Theorem 2** is a form of the second law of thermodynamics that gives us the direction in which the heat current flows along the contour $I_p^{(0)} = 0$ (cf. Eq. (34)). The heat current $I_p^{(1)}$ decreases monotonically along the contour $I_p^{(0)} = 0$. Therefore we may find only one point along $I_p^{(0)} = 0$ that also satisfies $I_p^{(1)} = 0$, which implies a unique solution to Eq. (1) when it exists.

Indeed, Onsager points out in his 1931 paper [82] that for positive entropy production, the linear response matrix will have to be positive-definite (which translates to our condition in Theorem 1). However, that analysis rests upon the assumption of linear response near equilibrium. Our result in Theorem 2 does not require such a condition for the nonequilibrium state of the system, but instead emerges out of the analysis of the currents flowing into a weakly-coupled probe. In addition, we obtain a strict mathematical proof of theorem 1. We point out that theorem 2 holds even when the physically expected postulate fails, making the uniqueness result in theorem 2 very general.

**V. EXISTENCE**

A unique local measurement of temperature and voltage is only part of our main problem. An equally important part is to derive the conditions for the existence of a solution. The main idea behind this analysis is to follow the number current contour $I_p^{(0)} = 0$ and ask what happens to the heat current $I_p^{(1)}$ as we traverse towards
higher and higher temperatures, $T_p \to \infty$. We noted that near $T_p = 0$, the heat current into the probe must be positive, consistent with the third law of thermodynamics [cf. Eq. (11)]. Since we know that the heat current is monotonically decreasing along the number current contour (Theorem 2), we could guess whether or not a solution occurs depending upon the asymptotic value of the heat current along that contour as $T_p \to \infty$. In this way, we find a necessary and sufficient condition for the existence of a solution while analyzing the problem for positive temperatures (see Fig. 4 for an illustration of this case). On the other hand, when this condition is not met, one can immediately prove that a negative temperature must satisfy the measurement condition $I_p^{(\nu)} = 0$, $\nu = \{0, 1\}$. This latter condition corresponds to a system exhibiting local population inversion which leads to negative temperature solutions, as illustrated in Fig. 4.

Our results here are again completely general and are valid for electron systems with arbitrary interactions, arbitrary steady state bias conditions, and for any weakly-coupled probe. However, our analysis here leads us to demarcate between two extremes of the probe-system coupling. We conclude that an ideal probe is one which operates in the broadband limit. A measurement by such a probe depends only on the properties of the system that it couples to, and is independent of the spectral properties of the probe itself. The broadband limit lends itself to an easier physical interpretation of the population inversion condition as well, and we discuss this important limit in Sec. V.B.

The other extreme is that of a narrow-band probe which is capable of probing the system at just one value of energy, leading to a nonunique measurement (see also the proof of theorem 1), and is discussed in Sec. V.C. Only this pathological case leads to an exception to Theorem 2.

The simplest system which could, in principle, exhibit population inversion is a two-level system. Therefore, our results, including that of the previous section, have been illustrated by using a two-level system. The details of the nonequilibrium two-level system and its coupling to the thermoelectric probe are given in Sec. V.D.

Our analysis starts with a rearrangement of the currents given by Eq. (1) and a restatement of the measurement condition [cf. Eq. (11)] in terms of energy currents, and we also define some useful quantities along the way. We may rewrite the number current in Eq. (1) as

$$I_p^{(0)} = \langle \hat{N} \rangle |f_s - \langle \hat{N} \rangle |f_p,$$

where

$$\langle \hat{N} \rangle |f_s \equiv \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega T_p s(\omega) f_s(\omega),$$

and similarly

$$\langle \hat{N} \rangle |f_p \equiv \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega T_p s(\omega) f_p(\omega).$$

The quantity $\langle \hat{N} \rangle |f_s$ is the rate of particle flow into the probe from the system, while $\langle \hat{N} \rangle |f_p$ gives the rate of particle flow out of the probe and into the system.
Similarly, the rate of energy flow into the probe from the system is
\[
\langle \dot{E} \rangle_{f_s} = \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega \omega T_{ps}(\omega) f_s(\omega),
\]
while
\[
\langle \dot{E} \rangle_{f_p} = \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega \omega T_{ps}(\omega) f_p(\omega)
\]
gives the rate of energy outflux from the probe back into the system. The net energy current flowing into the probe is given by \( I_p^E = \langle \dot{E} \rangle_{f_s} - \langle \dot{E} \rangle_{f_p} \).

The local equilibration conditions in Eq. (11) now become
\[
\langle \dot{N} \rangle_{f_p} = \langle \dot{N} \rangle_{f_s} \quad (\text{and} \quad \langle \dot{E} \rangle_{f_p} = \langle \dot{E} \rangle_{f_s})
\]
(40)
The equation for the rate of energy flow above is equivalent to the condition \( I_p^{(1)} = 0 \) when \( I_p^{(0)} = 0 \) since
\[
I_p^E(\mu_p, T_p) \equiv \langle \dot{E} \rangle_{f_p} - \langle \dot{E} \rangle_{f_s} = I_p^{(1)} + \mu_p I_p^{(0)}.
\]
The equality of the local temperature and voltage while the local distribution function \( f_s(\omega) \). The probe measures the appropriate voltage and temperature when it exchanges no net charge and energy with the system.

We may introduce a characteristic rate of particle flow [cf. Eq. (7)] as
\[
\langle \dot{N} \rangle_{f_{e1}} = \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega T_{ps}(\omega)
\equiv \frac{\gamma_p}{\hbar}.
\]
This leads to the following inequalities:
\[
0 < \langle \dot{N} \rangle_{f_s} < \frac{\gamma_p}{\hbar},
\]
\[
0 < \langle \dot{N} \rangle_{f_p} < \frac{\gamma_p}{\hbar}.
\]
The equality of the local inequality for \( \langle \dot{N} \rangle_{f_s} \) above excludes \( f_s(\omega) \equiv 0 \) while the local inequality excludes \( f_s(\omega) = 1 \) \( \forall \omega \in \mathbb{R} \), and we retain the strict inequalities imposed by Eq. (43) (see also Eqs. (9) and (10) and the preceding discussion).

We similarly introduce a characteristic rate for the energy flow between the system and probe:
\[
\langle \dot{E} \rangle_{f_{e1}} = \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega \omega T_{ps}(\omega)
\equiv \frac{\gamma_p}{\hbar} \omega_c,
\]
where \( \omega_c < \infty \) (due to postulate 1) can interpreted as the centroid of the probe-sample transmission function. We find that \( \omega_c \to \infty \) necessarily implies a positive temperature solution. We remind the reader that \( \omega_c \to -\infty \) is physically impossible due to the principle that any physical system must have a lower bound for the energy \((\langle H \rangle \geq -c \text{ for some finite } c \in \mathbb{R})\).

The quantities \( \langle \dot{N} \rangle_{f_s}, \langle \dot{N} \rangle_{f_p}, \langle \dot{N} \rangle_{f_{e1}}, \langle \dot{E} \rangle_{f_s}, \langle \dot{E} \rangle_{f_p}, \langle \dot{E} \rangle_{f_{e1}} \) are all finite due to postulate [cf. Eqs. (7,10)].

A. Asymptotic Properties, and Conditions for the Existence of a Solution

Traversing along \( I_p^{(0)} = 0 \) results in a monotonically decreasing heat current \( I_p^{(1)} \) (Theorem 2). Here, we traverse the contour from low temperatures \((T_p \to 0)\) to higher temperatures \((T_p \to \infty)\) as discussed in Theorem 2. This implies a monotonically increasing \( \langle \dot{E} \rangle_{f_p} \) due to Eq. (41). We proceed to calculate the asymptotic value of \( \langle \dot{E} \rangle_{f_p} \) along the number current contour.

Let the asymptotic scaling of \( \mu_p = M(T_p) \) defined by the contour \( I_p^{(0)}(\mu_p, T_p) = 0 \) (lemma 1) be
\[
\lim_{T_p \to \infty} \frac{M(T_p)}{T_p} = \Lambda.
\]
(45)
We use the above limiting value to calculate \( \langle \dot{N} \rangle_{f_p} \) along the contour \( \mu_p = M(T_p) \):
\[
\lim_{T_p \to \infty} \langle \dot{N} \rangle_{f_p} = \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega T_{ps}(\omega)
\times \lim_{T_p \to \infty} \frac{1}{1 + \exp \left( \frac{\omega - M(T_p)}{T_p} \right)}
= \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega T_{ps}(\omega) \frac{1}{1 + \exp (-\Lambda)}
= \frac{1}{1 + \exp (-\Lambda)} \frac{\gamma_p}{\hbar}.
\]
(46)
The above limiting value satisfies the inequality in Eq. (43) for any \( \Lambda \in \mathbb{R} \). The points on the contour satisfy \( \langle \dot{N} \rangle_{f_p} = \langle \dot{N} \rangle_{f_s} \) by construction, therefore \( \Lambda \) is computed from the equation
\[
\frac{1}{1 + \exp (-\Lambda)} \frac{\gamma_p}{\hbar} = \langle \dot{N} \rangle_{f_s}.
\]
(47)
It is important to note that the asymptotic scaling defined by Eq. (45) does not mean that the scaling is linear. For example, a sublinear scaling \( M(T_p) = \alpha T_p^n \) with \( n < 1 \) merely corresponds to \( \Lambda = 0 \) which could satisfy Eq. (47) if the nonequilibrium system is prepared in that way. However, \( \Lambda \to \pm \infty \) do not obey the strict inequality in Eq. (43). \( \Lambda \to \infty \) corresponds to a trivial and unphysical nonequilibrium distribution \( f_s(\omega) \equiv 1 \), and likewise, \( \Lambda \to -\infty \) corresponds to \( f_s(\omega) \equiv 0 \) \( \forall \omega \).
The asymptotic value of \( \langle \hat{E} \rangle \big|_{f_p} \) along the \( I_p^{(0)} = 0 \) contour is simply
\[
\lim_{T_p \to -\infty} \langle \hat{E} \rangle \big|_{f_p} = \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega \, \omega T_{ps}(\omega)
\cdot \lim_{T_p \to -\infty} \frac{1}{1 + \exp\left(\frac{\omega - M(T_p)}{\hbar} \right)}
= \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega \, \omega T_{ps}(\omega) \frac{1}{1 + \exp(-\Lambda)}
= \frac{1}{1 + \exp(-\Lambda)} \frac{\gamma_p}{\hbar} \omega_c
= \omega_c \langle \hat{N} \rangle \big|_{f_s}.
\] (48)

**Theorem 3** A positive temperature solution exists if and only if there is no net population inversion, i.e., when
\[
\frac{\langle \hat{E} \rangle \big|_{f_s}}{\langle N \rangle \big|_{f_s}} < \omega_c.
\] (49)

**Proof.** \( \langle \hat{E} \rangle \big|_{f_s}/\langle \hat{N} \rangle \big|_{f_s} < \langle \hat{E} \rangle \big|_{f_s}/\langle \hat{N} \rangle \big|_{f_s} \) when \( T_p \to 0 \) along the contour \( I_p^{(0)} = 0 \) [cf. Eq. (25) and Eq. (41)]. The asymptotic limit of \( \langle \hat{E} \rangle \big|_{f_s}/\langle \hat{N} \rangle \big|_{f_s} \) is \( \omega_c \) [cf. Eq. (48)]. \( \langle \hat{E} \rangle \big|_{f_p} \) is continuous \( \forall \mu_p \in (-\infty, \infty) \), \( T_p \in (0, \infty) \) and is monotonically increasing along \( I_p^{(0)} = 0 \) (Theorem 2). We use the intermediate value theorem. \( \blacksquare \)

**Corollary 3.1** There exists a negative temperature solution for a nonequilibrium system with net population inversion, i.e., when
\[
\frac{\langle \hat{E} \rangle \big|_{f_s}}{\langle N \rangle \big|_{f_s}} > \omega_c.
\] (50)

**Proof.** Let \( f_p(\mu_p, T_p) \) be the Fermi-Dirac distribution with \( T_p > 0 \); we define the Fermi-Dirac distribution
\( f_p^{(-)} \equiv f_p(\mu_p, -T_p) = 1 - f_p \).

\[
f_p^{(\nu)}(\mu_p, -T_p) = \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega (\omega - \mu_p)^\nu T_{ps}(\omega) [f_s(\omega) - (1 - f_p(\omega))]
= \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega (\omega - \mu_p)^\nu T_{ps}(\omega) [f_p(\omega) - (1 - f_s(\omega))]
= \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega (\omega - \mu_p)^\nu T_{ps}(\omega) [f_p(\omega) - f_p^{-}(\omega)]
= -I_p^{(\nu)}.
\] (51)

\( I_p^{(\nu)} = 0 \) with \( \nu = \{0, 1\} \) is now understood to solve the complementary nonequilibrium system with \( f_p^{-}(\omega) \equiv 1 - f_s(\omega) \).

\[ f_p^{-}(\omega) \] is of course a completely valid nonequilibrium distribution function and satisfies Eq. (38). We apply Theorem 3 and find that
\[
\frac{\langle \hat{E} \rangle \big|_{f_p^{-}}}{\langle \hat{N} \rangle \big|_{f_p^{-}}}
= \frac{\gamma_p}{\hbar} \omega_c - \frac{\langle \hat{E} \rangle \big|_{f_s}}{\langle \hat{N} \rangle \big|_{f_s}}
\leq \frac{\langle \hat{E} \rangle \big|_{f_s}}{\langle \hat{N} \rangle \big|_{f_s}} - \omega_c \langle \hat{N} \rangle \big|_{f_s}
\geq \frac{\langle \hat{E} \rangle \big|_{f_s}}{\langle \hat{N} \rangle \big|_{f_s}} > \omega_c \langle \hat{N} \rangle \big|_{f_s}.
\] (52)

For the case that \( \langle \hat{E} \rangle \big|_{f_s} = \omega_c \langle \hat{N} \rangle \big|_{f_s} \), \( T_p = \pm \infty \), corresponding to \( f_p = 1/2 \), independent of energy. \( \blacksquare \)

**B. Ideal Probes: The Broadband Limit**

In the broadband limit, the probe-system coupling becomes energy independent, and we may write \( \Gamma(\omega) = \Gamma(\mu_0) \). The spectrum of the system, sampled locally by the probe, is given by
\[
\bar{A}(\omega) \equiv \frac{\text{Tr} \{ \Gamma(\omega) A(\omega) \}}{\text{Tr} \{ \Gamma(\omega) \}}
= \frac{\text{Tr} \{ \Gamma(\mu_0) A(\omega) \}}{\text{Tr} \{ \Gamma(\mu_0) \}}.
\] (53)

The occupancy and energy of the system, respectively, are given by
\[
\langle N \rangle \big|_{f_p} = \int_{-\infty}^{\infty} d\omega \, \bar{A}(\omega) f_s(\omega)
\langle E \rangle \big|_{f_p} = \int_{-\infty}^{\infty} d\omega \, \omega \, \bar{A}(\omega) f_s(\omega).
\] (54)

The measurement conditions in Eq. (11) become simply
\[
\frac{\langle N \rangle \big|_{f_p}}{\langle E \rangle \big|_{f_p}} = \frac{\langle N \rangle \big|_{f_s}}{\langle E \rangle \big|_{f_s}}.
\] (55)

The above equations imply that an ideal measurement of voltage and temperature constitutes a measurement of the zeroth and first moments of the local energy distribution of the system. That is to say, when the probe is in local equilibrium with the nonequilibrium system, the local occupancy and energy of the system are the same as they would be if the system’s local spectrum were populated by the equilibrium Fermi-Dirac distribution \( f_p \equiv f_p(\mu_p, T_p) \) of the probe.

We may now write the condition for the existence of a positive temperature solution (Theorem 3) simply as
\[
\frac{\langle E \rangle \big|_{f_p}}{\langle N \rangle \big|_{f_p}} < \omega_c,
\] (56)
where \( \omega_c \) is the centroid of the spectrum given by
\[
\omega_c = \int_{-\infty}^{\infty} d\omega \, \bar{A}(\omega).
\] (57)
The eigenstates of the closed two-level Hamiltonian (see Sec. V D) \( \epsilon \) corresponds to the unique solution (shown in the left panel). The resonances in the spectrum inhibiting population inversion: 

\[
\text{there exists a negative temperature solution for a system exhibiting population inversion:}
\]

\[
f_s(\omega) \geq \omega_c.
\]

The advantage of the broadband limit is that one may write the measurement conditions, as well as the condition for the existence of a solution, in terms of the local expectation values of the energy and occupancy directly, instead of using the rate of particle and energy flow into the probe. We also do not need to introduce a “characteristic tunneling rate.” We note that \( \omega_c \) in Eq. (57) is the centroid since the local spectrum \( A \) normalizes to unity within the broadband limit (see Appendix A.1).

A local measurement by a weakly-coupled broadband thermoelectric probe is ideal in the sense that the result is independent of the properties of the probe, and depends only on the nonequilibrium state of the system and the subsystem thereof sampled by the probe. Such a measurement provides more than just an operational definition of the local temperature and voltage of a nonequilibrium quantum system, since the thermodynamic variables are determined directly by the moments (54) of the local (nonequilibrium) energy distribution.

C. Nonunique Measurements: The Narrowband Limit

A narrowband probe is one that samples the system only within a very narrow window of energy. The extreme case of such a probe-system coupling would be a Dirac-delta function:

\[
\Gamma_p(\omega) = 2\pi V_p^\dagger V_p \delta(\omega - \omega_0),
\]

which gives \( T_{ps}(\omega) = 2\pi \text{Tr} \{ V_p A(\omega) V_p^\dagger \} \delta(\omega - \omega_0) \) which we write simply as

\[
T_{ps}(\omega) = \gamma(\omega) \delta(\omega - \omega_0),
\]

where \( \gamma(\omega) = 2\pi \text{Tr} \{ V_p A(\omega) V_p^\dagger \} \) has dimensions of energy.

We previously noted that Theorem 1 does not hold for \( T_{ps} \) given by Eq. (60). One can verify straightforwardly that, for a probe-sample transmission that is extremely narrow, we will have

\[
\mathcal{L}_{ps}^{(0)} \mathcal{L}_{ps}^{(2)} - (\mathcal{L}_{ps}^{(1)})^2 = 0.
\]

This results in a nonunique solution since following the proof of theorem 1 would give us [cf. Eq. (54)] \( \Delta I_p^{(1)} = 0 \). In fact, it would lead to a family of solutions.
We may solve for the solution explicitly. The number current reduces to
\[ I_p^{(0)} = \frac{2(\omega_0)}{\hbar} (f_p(\omega_0) - f_s(\omega_0)), \] (62)
while the heat current is given by
\[ I_p^{(1)} = (\omega_0 - \mu_p) \frac{2(\omega_0)}{\hbar} (f_p(\omega_0) - f_s(\omega_0)), \] (63)
which trivially vanishes for vanishing number current. Therefore, the family of solutions to the measurement is simply given by
\[ f_p(\omega_0; \mu_p, T_p) = f_s(\omega_0), \] (64)
which is linear in the \( \mu_p - T_p \) plane and is given by
\[ \mu_p = \omega_0 - T_p \log \left( \frac{1 - f_s(\omega_0)}{f_s(\omega_0)} \right). \] (65)
f\( s(\omega) \) has the following explicit form:
\[ f_s(\omega) = \frac{\text{Tr} \left\{ V_p G^< (\omega) V_p^\dagger \right\}}{2\pi i \text{Tr} \left\{ V_p A(\omega) V_p^\dagger \right\}}. \] (66)

A narrowband probe is therefore unsuitable for thermoelectric measurements. Even if a probe were to sample the system at just two distinct energies \( \omega_1 \) and \( \omega_2 \), theorem 1 would hold and the thermoelectric measurement would be unique. Indeed, the narrowband probe is a pathological case whose only function is to highlight a certain theoretical limitation for the measurement of the temperature and voltage.

D. Example: Two-level system

Net population inversion is essentially a quantum phenomenon, since classical Hamiltonians are generally unbounded above due to the kinetic energy term, i.e., there does not exist a finite \( c \in \mathbb{R} \) that satisfies \( \langle H \rangle < c \). In other words, \( \omega_c \to \infty \) generally holds for classical systems and negative temperatures are not possible. The simplest quantum system where a net population inversion can be achieved is a two-level system. We therefore illustrated our results for a two-level system in figs. 2 to 4.
The system Hamiltonian here was taken to be
\[ H = \begin{bmatrix} \epsilon_1 & V \\ V^* & \epsilon_2 \end{bmatrix}, \] (67)
whose values were set as \( V = \frac{2(1-i)}{3}, \epsilon_1 = 1/3 \) and \( \epsilon_2 = -1/3 \), such that the eigenvalues are \( \epsilon_{\pm} = \pm 1 \) and units are taken as eV. We introduce two reservoirs that are strongly coupled locally to each site with \( \Gamma_1 = \text{diag}(0.5, 0) \) and \( \Gamma_2 = \text{diag}(0, 0.5) \), while the probe coupling is taken as \( \Gamma_p = \text{diag}(0.01, 0.1) \), which is about five times weaker than the coupling to the reservoirs that bias the system.

We used two different bias conditions: (a) To illustrate the case without a net population inversion in figs. 2 to 4 the reservoirs had a symmetric \( \mu_1 - \mu_2 = 0 \) voltage bias \( \mu_1 - \mu_2 = 1eV; \) (b) to illustrate the case with a net population inversion in fig. 5 the reservoirs had a symmetric voltage bias of \( \mu_1 - \mu_2 = 4eV \). The two reservoirs are held at \( T = 300K \) for both cases.

It has been previously noted that the probe-system coupling strength does not strongly affect the measured temperature and voltage even when varied over several orders of magnitude, but we remind the reader that our theoretical results depend upon the assumption of a weakly-coupled probe (noninvasive measurements). How weak is weak enough is a different, and perhaps more subtle, theoretical question. Numerically, however, we do find that the probe measurements are not much altered even when the probe coupling strength is comparable to that of the strongly-coupled reservoirs.

VI. CONCLUSIONS

The local temperature and voltage of a nonequilibrium quantum system are defined in terms of the equilibration...
of a noninvasive thermoelectric probe, locally coupled to the system. The simultaneous temperature and voltage measurement is shown to be unique for any system of fermions in steady state, arbitrarily far from equilibrium, with arbitrary interactions within the system, and the conditions for the existence of a solution are derived. In particular, it is shown that a positive temperature solution exists provided the system does not have a net local population inversion; in the case of population inversion, a unique negative temperature solution is shown to exist. These results provide a firm mathematical foundation for temperature and voltage measurements in quantum systems far from equilibrium.

Our analysis reveals that a simultaneous temperature and voltage measurement is uniquely determined by the local spectrum and nonequilibrium distribution of the system [cf. Eq. (41)], and is independent of the properties of the probe for broadband coupling (ideal probe). Such a measurement therefore provides a fundamental definition of local temperature and voltage, which is not merely operational.

In contrast, prior theoretical work relied almost exclusively on operational definitions [12, 37–40], leading to a competing panoply of often contradictory predictions for the measurement of such basic observables as temperature and voltage. Measurements of temperature or voltage, taken separately (see, e.g., Refs. [12 and 37], are shown to be ill-posed: a thermometer out of electrical equilibrium with a system produces an error due to the Peltier effect across the probe-sample junction, while a potentiometer out of thermal equilibrium with a system produces an error due to the Seebeck effect.

Our results put the local thermodynamic variables temperature and voltage on a mathematically rigorous footing for fermion systems under very general nonequilibrium steady-state conditions, a necessary first step toward the construction of nonequilibrium thermodynamics [8–15]. Our analysis includes the effect of interactions with arbitrary interactions within the system, and the bosons themselves [53, 54] were not addressed in the present analysis. Moreover, we did not explicitly consider magnetic systems, which require separate consideration of the spin degree of freedom, and its polarization. Future investigation of probes that exchange bosonic or spin excitations may enable similarly rigorous analysis of local thermodynamic variables in bosonic and magnetic systems, respectively.

**Appendix A: The nonequilibrium steady state**

The nonequilibrium steady state is described by a density matrix $\hat{\rho}$ that is time-independent. The expectation values of observables are given by their usual prescription in statistical physics, e.g.,

$$\langle \hat{Q} \rangle = \text{Tr} \left\{ \hat{\rho} \hat{Q} \right\} = \sum_{\mu,\nu} \rho_{\mu\nu} \langle \nu | \hat{Q} | \mu \rangle. \quad (A1)$$

The “lesser” and “greater” Green’s functions used in the paper are defined as follows

$$G^\lesssim_{\alpha\beta}(t) \equiv i \langle d^\dagger_{\beta}(0) d_{\alpha}(t) \rangle, \quad (A2)$$

while its Hermitian conjugate is

$$G^\gtrsim_{\alpha\beta}(t) \equiv -i \langle d_{\alpha}(t) d^\dagger_{\beta}(0) \rangle, \quad (A3)$$

where

$$d_{\alpha}(t) = e^{i \frac{H}{\hbar} t} d_{\alpha}(0) e^{-i \frac{H}{\hbar} t} \quad (A4)$$

evolves according to the Heisenberg equation of motion for a system with Hamiltonian $H$. Here, $\alpha, \beta$ denote basis states in the 1-body Hilbert space of the system.

The spectral representation uses the eigenbasis of the Hamiltonian $H |\nu\rangle = E_\nu |\nu\rangle$, where $\nu$ denotes a many-body energy eigenstate. One may write the “lesser” Green’s function as

$$G^\lesssim_{\alpha\beta}(\omega) = 2\pi i \sum_{\mu,\mu',\nu} \rho_{\mu\nu} \langle \nu | d^\dagger_{\beta} | \mu' \rangle \langle \mu' | d_{\alpha} | \mu \rangle \times \delta \left( \omega - \frac{E_\mu - E_{\mu'}}{\hbar} \right), \quad (A5)$$

while the “greater” Green’s function becomes

$$G^\gtrsim_{\alpha\beta}(\omega) = -2\pi i \sum_{\mu,\mu',\nu} \rho_{\mu\nu} \langle \nu | d_{\alpha} | \mu' \rangle \langle \mu' | d^\dagger_{\beta} | \mu \rangle \times \delta \left( \omega - \frac{E_{\mu'} - E_{\nu}}{\hbar} \right). \quad (A6)$$

The spectral function $A(\omega)$ is given by

$$A(\omega) \equiv \frac{1}{2\pi i} \left( G^\lesssim(\omega) - G^\gtrsim(\omega) \right), \quad (A7)$$

and can be expressed in the spectral representation as

$$A_{\alpha\beta}(\omega) = \sum_{\mu,\mu',\nu} \left[ \rho_{\mu\nu} \langle \nu | d^\dagger_{\beta} | \mu' \rangle \langle \mu' | d_{\alpha} | \mu \rangle + \rho_{\nu\mu'} \langle \mu' | d_{\alpha} | \mu \rangle \langle \mu | d^\dagger_{\beta} | \nu \rangle \right] \times \delta \left( \omega - \frac{E_\mu - E_{\mu'}}{\hbar} \right). \quad (A8)$$

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1. Sum rule for the spectral function

Eq. (A8) leads to the following sum rule for the spectral function:

\[
\int_{-\infty}^{\infty} d\omega A_{\alpha\beta}(\omega) = \sum_{\mu,\nu} \rho_{\mu\nu} \langle \nu|d_{\beta}^{\dagger}d_{\alpha}|\mu\rangle + \sum_{\mu,\nu'} \rho_{\nu\nu'} \langle \mu'|d_{\alpha}d_{\beta}|\nu\rangle = \sum_{\mu,\nu} \rho_{\mu\nu} \langle \nu|\delta_{\alpha\beta}|\mu\rangle = \sum_{\mu,\nu} \rho_{\mu\nu} \delta_{\alpha\beta} \delta_{\nu\mu} = \delta_{\alpha\beta} \text{Tr} \{\hat{\rho}\} = \delta_{\alpha\beta}.
\]

(A9)

In our theory of local thermodynamic measurements, the quantity of interest is the local spectrum of the system sampled by the probe \(\hat{A}(\omega)\), defined in Eq. (53). This obeys a further sum rule in the broadband limit (ideal probe), discussed below.

\(\text{a. Local spectrum in the broadband limit}\)

The probe-system coupling is energy independent in the broadband limit, \(\Gamma^p(\omega) = \text{const}\), and we write \(\text{Tr} \{\Gamma^p\} = \Gamma^p\) for its trace. The local spectrum sampled by the probe \(\hat{A}(\omega)\) defined in Eq. (53) can be written in the broadband limit as

\[
\hat{A}(\omega) = \frac{1}{\Gamma^p} \sum_{\alpha,\beta} \langle \beta|\Gamma^p|\alpha\rangle A_{\alpha\beta}(\omega).
\]

(A10)

In this limit, it obeys a further sum rule:

\[
\int_{-\infty}^{\infty} d\omega \hat{A}(\omega) = \frac{1}{\Gamma^p} \sum_{\alpha,\beta} \langle \beta|\Gamma^p|\alpha\rangle \int_{-\infty}^{\infty} d\omega A_{\alpha\beta}(\omega) = \frac{1}{\Gamma^p} \sum_{\alpha,\beta} \langle \beta|\Gamma^p|\alpha\rangle \delta_{\alpha\beta} = 1.
\]

(A11)

The broadband limit is special in that the measurement is determined by the local properties of the system itself, and is not influenced by the spectrum of the probe. In this limit, the local spectrum \(\hat{A}(\omega)\) obeys the sum rule (A11) since the probe samples the same subsystem at all energies. One should not expect such a local sum rule to hold outside the broadband limit, since the probe samples different subsystems at different energies.

2. Diagonality of \(\hat{\rho}\)

We have, for any observable \(\hat{Q}\),

\[
\langle \hat{Q}(t) \rangle = \sum_{\mu,\nu} \rho_{\mu\nu} \langle \nu|\hat{Q}(t)|\mu\rangle = \sum_{\mu,\nu} \rho_{\mu\nu} \langle \nu|e^{-\frac{i\hat{H}t}{\hbar}}\hat{Q}e^{\frac{i\hat{H}t}{\hbar}}|\mu\rangle = \sum_{\mu,\nu} \rho_{\mu\nu} e^{-\frac{E_\nu-E_\mu}{\hbar}t} \langle \nu|\hat{Q}|\mu\rangle.
\]

(A12)

The system observables must be independent of time in steady state. Therefore \(\hat{\rho}\) must be diagonal in the energy basis, as seen from the above equation. The nondiagonal parts of \(\hat{\rho}\) in the energy basis, when they exist, must be in a degenerate subspace so that \(E_\mu = E_\nu\) in the above equation.

For states degenerate in energy, the boundary conditions determining the nonequilibrium steady state will determine the basis in which \(\hat{\rho}\) is diagonal. Henceforth, we work in that basis.

3. Positivity of \(-iG^< (\omega)\) and \(iG^> (\omega)\)

Working in the energy eigenbasis in which \(\hat{\rho}\) is diagonal,

\[
-i\langle \alpha|G^< (\omega)|\alpha\rangle = iG^<_{\alpha\alpha}(\omega) = 2\pi \sum_{\mu,\mu'} \rho_{\mu\mu'} \langle \mu|d_{\alpha}d_{\alpha}'|\mu'\rangle \frac{d}{\hbar} \left( \omega - \frac{E_\mu - E_{\mu'}}{\hbar} \right) \geq 0.
\]

(A13)

Similarly,

\[
i\langle \alpha|G^> (\omega)|\alpha\rangle = iG^>_{\alpha\alpha}(\omega) = 2\pi \sum_{\mu,\mu'} \rho_{\mu\mu'} \langle \mu|d_{\alpha}'d_{\alpha}|\mu'\rangle \frac{d}{\hbar} \left( \omega - \frac{E_{\mu'} - E_\mu}{\hbar} \right) \geq 0.
\]

(A14)

It follows that

\[
\langle \alpha|A(\omega)|\alpha\rangle = \frac{1}{2\pi} \langle \alpha| -iG^< (\omega) + iG^> (\omega)|\alpha\rangle \geq 0.
\]

(A15)

Therefore, all three operators \(-iG^< (\omega), iG^> (\omega),\) and \(A(\omega)\) are positive-semidefinite.

4. \(0 \leq f_s(\omega) \leq 1\)

The nonequilibrium distribution function \(f_s(\omega)\) was defined in Eq. (53) as

\[
f_s(\omega) = \frac{\text{Tr} \{\Gamma^p(\omega)G^< (\omega)\}}{2\pi i \text{Tr} \{\Gamma^p(\omega)A(\omega)\}}
\]

(A16)

We have \(\Gamma^p(\omega) > 0\) by causality (58):

\[
\text{Im} \sum_{\rho}^\rho(\omega) = -\frac{1}{2} \sum_{\rho}^\rho(\omega) < 0.
\]

(A17)
Let $\Gamma^p|\gamma_p\rangle = \gamma_p|\gamma_p\rangle$, where $\gamma_p \geq 0$ and some $\gamma_p$ satisfy $\gamma_p > 0$. The energy dependence is taken to be implicit. The traces in Eq. (A16) may be evaluated in the eigenbasis of $\Gamma^p$, yielding:

$$f_s(\omega) = \frac{\sum \gamma_p \gamma_p |G(\omega)|^2 |\gamma_p\rangle}{2\pi i \sum \gamma_p \gamma_p A(\omega) |\gamma_p\rangle} = \frac{\sum \gamma_p \gamma_p |G(\omega)|^2 |\gamma_p\rangle - iG(\omega) |\gamma_p\rangle}{\sum \gamma_p \gamma_p |\gamma_p\rangle - iG(\omega) + iG(\omega) |\gamma_p\rangle}.$$  

(A18)

Therefore

$$0 \leq f_s(\omega) \leq 1.$$  

(A19)

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