Local temperature of an interacting quantum system far from equilibrium

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A theory of local temperature measurement of an interacting quantum electron system far from equilibrium via a floating thermoelectric probe is developed. It is shown that the local temperature so defined is consistent with the zeroth, first, second, and third laws of thermodynamics, provided the probe-system coupling is weak and broadband. For non-broadband probes, the local temperature obeys the Clausius form of the second law and the third law exactly, but there are corrections to the zeroth and first laws that are higher order in the Sommerfeld expansion. The corrections to the zeroth and first laws are related, and can be interpreted in terms of the error of a nonideal temperature measurement. These results also hold for systems at negative absolute temperature.

I. INTRODUCTION

Nonequilibrium Green's functions (NEGFs) [1] provide a systematic method to study the local properties of interacting quantum systems far from equilibrium; however, a corresponding thermodynamic description has generally been lacking, outside the limit where a local equilibrium exists [2]. The concept of a local temperature has been extended to nonequilibrium systems under the assumption of local equilibrium [2], but it has proven far more challenging to generalize to systems where the local equilibrium hypothesis does not hold [3,4]. Without local equilibrium, different temperatures may be obtained by different measurement protocols [4]. Furthermore, 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 [5,6], the lattice temperature [7,8], the nuclear temperature [9], etc. This distinction is particularly acute in the extreme limit of elastic quantum transport [10–12], where electron and phonon temperatures are completely decoupled. The consensus has thus been that the various schemes for measuring the temperature of a system far from equilibrium can at best deliver an operational definition of the local temperature.

In this article, we systematically reexamine this fundamental issue, building upon the findings of Meair *et al.* [11], who argued that the temperature $\bar{T}_p$ measured by a floating thermoelectric probe can be interpreted as the local temperature of a nonequilibrium electron system, consistent with the laws of thermodynamics. While $\bar{T}_p$ does not have the same fundamental basis in statistical mechanics as the temperature of an equilibrium system, nonetheless it was shown that (i) $\bar{T}_p$ is largely independent of the details of the probe-sample coupling, (ii) the temperature inferred from an independent electrical noise measurement coincides with that measured by a floating probe, and (iii) the temperature so defined is consistent with both the zeroth and second laws of thermodynamics. These results were obtained within linear response and to leading order in the Sommerfeld expansion.

In the present article, a theory of local temperature measurement is developed that extends the analysis of Ref. [11] to interacting quantum systems under steady-state conditions arbitrarily far from equilibrium, using the method of NEGFs. In addition to the zeroth and second laws, the conditions under which $\bar{T}_p$ is consistent with the first and third laws of thermodynamics are investigated. It is shown that the local temperature defined by a floating thermoelectric probe is consistent with the zeroth, first, second, and third laws of thermodynamics, provided the probe-system coupling is weak and broadband. For non-broadband probes, the local temperature obeys the Clausius form of the second law and the third law exactly, but there are corrections to the zeroth and first laws that are higher order in the Sommerfeld expansion. The exact agreement with Clausius' statement of the second law and with the third law implies that the local temperature metric $\bar{T}_p$ defines an ordering of temperatures and an absolute zero, but not necessarily an absolute temperature scale. The corrections to the zeroth and first laws are shown to be related, and can be interpreted in terms of the error of a nonideal temperature measurement. This analysis also applies to systems with negative absolute temperature [13–16] (population inversion).

It is also shown that for a probe with broadband coupling, $\bar{T}_p$ is directly related to the mean local excitation energy of the system, in the same way as it is in an equilibrium system. Our findings make a compelling case to interpret the temperature measured by a noninvasive, broadband thermoelectric probe as the local temperature of a nonequilibrium electron system. This definition goes far beyond a mere operational notion, although it does not have the same fundamental status as the temperature of a system in equilibrium.

This article is organized as follows: In Sec. II, the probe equilibration conditions are defined and expressed using the NEGF formalism. Prior results [10,12] obtained within linear-response theory are also summarized here, introducing the Onsager coefficients that are useful in the sequel. In Sec. III, the local spectrum and distribution function sampled by the probe are defined, and the charge and heat currents flowing into the probe are related to these local properties of the nonequilibrium quantum system. It is shown that the probe equilibration problem is determined entirely by the local occupancy and energy of the system for a noninvasive, broadband probe. Sections IV–VII examine the extent to which the temperature $\bar{T}_p$ measured by a noninvasive local probe is consistent with the zeroth, first, second, and third laws of thermodynamics, respectively, even when the system probed is arbitrarily far from equilibrium. Section VIII draws together the various threads presented throughout the paper, and concludes that $\bar{T}_p$ provides far more than a mere operational definition of

temperature out of equilibrium. Appendix A derives some important properties of the local spectrum and distribution function of a nonequilibrium steady state, while Appendix B examines an alternative to the zeroth-law scenario investigated in Sec. IV.

II. CURRENT FORMULA AND PROBE TEMPERATURE

Our approach is motivated by the experimental technique of scanning thermal microscopy [17], whose resolution has recently been brought down to the nanometer range [18–21]. The system's local temperature is defined via an external local probe weakly coupled to the system via a tunnel barrier [10]. At its other end, the probe is connected to a macroscopic electron reservoir whose chemical potential and temperature "float" until neither electric current nor heat current flow between the probe and the system [10,11]:

$$I_p^{(\nu)} = 0, \quad \nu = 0,1, \tag{1}$$

where $-eI_p^{(0)}$ and $I_p^{(1)}$ are the electric current and heat current, respectively, flowing into the probe. The probe is then in local equilibrium with a system that is itself arbitrarily far from equilibrium. Several investigators have proposed related definitions of a floating thermal probe [5,6,22–30]. It should be noted that a number of other schemes for measuring the temperature of electron systems also exist [31], but these generally lack the high spatial resolution available in a scanning probe.

The starting point of our analysis is the NEGF formula for the steady-state electric and heat currents flowing into a probe coupled locally to a nonequilibrium quantum system with arbitrary interactions [32,33]:

$$I_p^{(\nu)} = -\frac{i}{h} \int_{-\infty}^{\infty} d\omega (\omega - \mu_p)^\nu \operatorname{Tr}\{\Gamma^p(\omega)(G^<(\omega) + f_p(\omega)[G^r(\omega) - G^a(\omega)])\}, \tag{2}$$

where $\nu = 1$ gives the electronic contribution to the heat current and $\nu = 0$ the electron number current. The probe is assumed to consist of a noninteracting electron reservoir with Fermi-Dirac distribution

$$f_p(\omega) = \{1 + \exp[(\omega - \mu_p)/k_B T_p]\}^{-1} \tag{3}$$

and tunneling-width matrix

$$[\Gamma^p(\omega)]_{n\sigma,m\sigma'} = 2\pi \delta_{\sigma\sigma'} \sum_{k \in p} V_{nk} V_{mk}^* \delta(\omega - \epsilon_{k\sigma}). \tag{4}$$

Here $|n\rangle$, $|m\rangle$ are single-particle basis orbitals (e.g., atomic orbitals) in the system, while the states in the probe are labeled $|k\rangle$. The coupling matrix elements V_{nk} can be calculated in the tunneling regime using standard methods for scanning probes [10,34]. In Eq. (2), $G^r(\omega)$, $G^a(\omega)$, and $G^<(\omega)$ are Fourier transforms of the retarded, advanced, and Keldysh "lesser" Green's functions describing electron propagation/occupancy within the system [1]:

$$G_{n\sigma,m\sigma'}^r(t) = -i\theta(t)\langle\{d_{n\sigma}(t), d_{m\sigma'}^\dagger(0)\}\rangle, \tag{5}$$

$$G_{n\sigma,m\sigma'}^a(t) = i\theta(-t)\langle\{d_{n\sigma}(t), d_{m\sigma'}^\dagger(0)\}\rangle, \tag{6}$$

and

$$G_{n\sigma,m\sigma'}^<(t) = i\langle d_{m\sigma'}^\dagger(0)\, d_{n\sigma}(t)\rangle, \tag{7}$$

respectively. Equation (2) is an exact formal result, valid for arbitrary interactions and for arbitrary steady-state thermal and/or electric bias.

The probe temperature of an interacting electron system with arbitrary bias is determined by solving the conditions (1) with $I_p^{(\nu)}$ given by Eq. (2). Equations (1) and (2) represent two coupled nonlinear equations for the two unknowns, T_p and μ_p. *A priori*, a solution to the probe equilibration problem might not exist at all, or might not be unique if it did exist. However, it was shown in Ref. [16] that for any weak probe-system coupling $\Gamma^p(\omega)$, the solution to Eqs. (1) and (2) exists and is unique. T_p was shown to be positive provided the system does not have local population inversion, and negative if it does.

Given that the probe equilibration conditions (1) constitute a well-posed problem [16], the present article addresses the related question of how the measured value of T_p depends on the actual probe-system coupling $\Gamma^p(\omega)$ for a system far from equilibrium. That is, to what extent do various thermometers measure different temperatures of the same nonequilibrium quantum system? The thermodynamic interpretation of such a local nonequilibrium temperature is also explored.

A. Linear response results

We summarize here the formalism for linear thermoelectric response of an open quantum system, because several of the key concepts and formulas will be useful by analogy in treating the far-from-equilibrium system. Consider a general system with M electrical contacts. Each contact α is connected to a reservoir at temperature T_α and electrochemical potential μ_α. In linear response, the electric current $-eI_\alpha^{(0)}$ and heat current $I_\alpha^{(1)}$ flowing into reservoir α may be expressed as

$$I_\alpha^{(\nu)} = \sum_{\beta=1}^M \left[\mathcal{L}_{\alpha\beta}^{(\nu)}(\mu_\beta - \mu_\alpha) + \mathcal{L}_{\alpha\beta}^{(\nu+1)}\left(\frac{T_\beta - T_\alpha}{T_0}\right) \right], \tag{8}$$

where $\mathcal{L}_{\alpha\beta}^{(\nu)}$ ($\nu = 0,1,2$) is an Onsager linear-response coefficient [35].

In a thermal transport experiment, the system is driven out of equilibrium by a thermal bias applied between the hot and cold electrodes, but the system forms an open electric circuit. Under these conditions, the chemical potentials μ_α may be eliminated from Eq. (8), yielding the following expression for the total heat current flowing into the probe, which forms the third terminal of the thermoelectric circuit:

$$I_p^Q \equiv I_p^{(1)} = \sum_{\beta=1}^2 \tilde{\kappa}_{p\beta}(T_\beta - T_p) + \kappa_{p0}(T_0 - T_p). \tag{9}$$

Here $\tilde{\kappa}_{\alpha\beta}$ is the thermal conductance between electrodes α and β, and κ_{p0} is the thermal coupling of the probe to the ambient environment at temperature T_0. The environment could be, for example, the blackbody radiation or gaseous atmosphere surrounding the circuit, or the cantilever/driver on which the temperature probe is mounted.

Equations (1) and (9) can be solved for the temperature of a probe in thermal and electrical equilibrium with, and coupled

locally to, the system [10]

$$\bar{T}_p = \frac{\tilde{\kappa}_{p1}T_1 + \tilde{\kappa}_{p2}T_2 + \kappa_{p0}T_0}{\tilde{\kappa}_{p1} + \tilde{\kappa}_{p2} + \kappa_{p0}}. \tag{10}$$

The effect of κ_{p0} on local temperature measurement, an important issue in nanoscale thermometry [18–21], was discussed in Refs. [10,12]. In the present paper, we are concerned with establishing the fundamental theoretical basis for defining a local temperature of a nonequilibrium quantum system, not with the nonidealities inherent in experimental thermometry. Therefore, unless otherwise specified, we will take $\kappa_{p0} = 0$ in the remainder of the present paper.

In the absence of an external magnetic field $\mathcal{L}_{\alpha\beta}^{(\nu)} = \mathcal{L}_{\beta\alpha}^{(\nu)}$ and the thermal conductances are given by [10]

$$\tilde{\kappa}_{\alpha\beta} = \frac{1}{T}\left[\mathcal{L}_{\alpha\beta}^{(2)} - \frac{[\mathcal{L}_{\alpha\beta}^{(1)}]^2}{\tilde{\mathcal{L}}_{\alpha\beta}^{(0)}} \right. $$
$$\left. - \mathcal{L}^{(0)}\left(\frac{\mathcal{L}_{\alpha\gamma}^{(1)}\mathcal{L}_{\alpha\beta}^{(1)}}{\mathcal{L}_{\alpha\gamma}^{(0)}\mathcal{L}_{\alpha\beta}^{(0)}} + \frac{\mathcal{L}_{\gamma\beta}^{(1)}\mathcal{L}_{\alpha\beta}^{(1)}}{\mathcal{L}_{\gamma\beta}^{(0)}\mathcal{L}_{\alpha\beta}^{(0)}} - \frac{\mathcal{L}_{\alpha\gamma}^{(1)}\mathcal{L}_{\gamma\beta}^{(1)}}{\mathcal{L}_{\alpha\gamma}^{(0)}\mathcal{L}_{\gamma\beta}^{(0)}} \right) \right], \tag{11}$$

with

$$\tilde{\mathcal{L}}_{\alpha\beta}^{(0)} = \mathcal{L}_{\alpha\beta}^{(0)} + \frac{\mathcal{L}_{\alpha\gamma}^{(0)}\mathcal{L}_{\gamma\beta}^{(0)}}{\mathcal{L}_{\alpha\gamma}^{(0)} + \mathcal{L}_{\gamma\beta}^{(0)}} \tag{12}$$

and

$$\frac{1}{\mathcal{L}^{(0)}} = \frac{1}{\mathcal{L}_{12}^{(0)}} + \frac{1}{\mathcal{L}_{13}^{(0)}} + \frac{1}{\mathcal{L}_{23}^{(0)}}. \tag{13}$$

B. Elastic transport

Within elastic electron transport theory, the linear response coefficients needed to evaluate Eq. (10) are given by [33,36,37]

$$\mathcal{L}_{\alpha\beta}^{(\nu)} = \frac{1}{h}\int d\omega \, (\omega - \mu_0)^\nu \, T_{\alpha\beta}(\omega)\left(-\frac{\partial f_0}{\partial \omega} \right), \tag{14}$$

where f_0 is the equilibrium Fermi-Dirac distribution of the electrodes at chemical potential μ_0 and temperature T_0. The elastic transmission function may be expressed as [38,39]

$$T_{\alpha\beta}(\omega) = \text{Tr}\{\Gamma^\alpha(\omega)G^r(\omega)\Gamma^\beta(\omega)G^a(\omega)\}, \tag{15}$$

where $\Gamma^\alpha(\omega)$ is the tunneling-width matrix for lead α.

III. RELATION OF PROBE CURRENTS TO LOCAL PROPERTIES OF THE SYSTEM

A. Local properties of the nonequilibrium system

One can define the *mean local spectrum* sampled by the probe as

$$\bar{A}(\omega) \equiv \text{Tr}\{\Gamma^p(\omega)A(\omega)\}/\text{Tr}\{\Gamma^p(\omega)\}, \tag{16}$$

where the spectral function of the (nonequilibrium) system is

$$A(\omega) = \frac{i}{2\pi}[G^r(\omega) - G^a(\omega)]. \tag{17}$$

Equation (16) defines a density of states averaged over the orbitals coupled to the probe. In the tunneling regime, the probe-sample coupling decreases exponentially with distance, so $\bar{A}(\omega)$ is a measure of the local density of states.

In equilibrium, $G^<$ may be expressed as

$$G_{\text{eq}}^<(\omega) = 2\pi i \, A(\omega) f_{\text{eq}}(\omega). \tag{18}$$

This relation motivates the following definition of the *local nonequilibrium distribution function*, as sampled by the probe

$$f_s(\omega) \equiv \frac{\text{Tr}\{\Gamma^p(\omega)G^<(\omega)\}}{2\pi i \, \text{Tr}\{\Gamma^p(\omega)A(\omega)\}}. \tag{19}$$

$\bar{A}(\omega)$ and $f_s(\omega)$ satisfy the necessary conditions for a spectrum and a distribution function, respectively. In particular, $\bar{A}(\omega) \geqslant 0$ and $0 \leqslant f_s(\omega) \leqslant 1$ (see Appendix A and Ref. [16] for proofs and further discussion).

The mean occupancy and energy of the electronic orbitals sampled by the probe are

$$\langle N \rangle \equiv \int \frac{d\omega}{2\pi i} \frac{\text{Tr}\{\Gamma^p(\omega)G^<(\omega)\}}{\text{Tr}\{\Gamma^p(\omega)\}} = \int_{-\infty}^{\infty} d\omega \, \bar{A}(\omega) f_s(\omega), \tag{20}$$

$$\langle E \rangle \equiv \int \frac{d\omega}{2\pi i} \frac{\omega \, \text{Tr}\{\Gamma^p(\omega)G^<(\omega)\}}{\text{Tr}\{\Gamma^p(\omega)\}} = \int_{-\infty}^{\infty} d\omega \, \omega \bar{A}(\omega) f_s(\omega), \tag{21}$$

respectively.

For the case of maximally local coupling of the probe to the system,

$$[\Gamma^p(\omega)]_{ij} = \bar{\Gamma}^p(\omega)\delta_{in}\delta_{jn}, \tag{22}$$

where n is a single localized orbital in the sample, $\bar{A}(\omega) = A_{nn}(\omega) \equiv \rho(\omega)$ is just the local density of states, and

$$f_s(\omega) = f_n(\omega) = \frac{G_{nn}^<(\omega)}{G_{nn}^<(\omega) - G_{nn}^>(\omega)}. \tag{23}$$

1. Elastic transport regime

In the regime of elastic quantum transport, one can express

$$f_s(\omega) = \sum_{\alpha=1}^{M} \lambda_\alpha(\omega) f_\alpha(\omega), \tag{24}$$

where $f_\alpha(\omega)$ is the equilibrium Fermi-Dirac distribution of reservoir α and $\lambda_\alpha(\omega) = \rho_\alpha(\omega)/\rho(\omega)$, where

$$\rho_\alpha(\omega) = \frac{1}{2\pi}[G^r(\omega)\Gamma^\alpha(\omega)G^a(\omega)]_{nn} \tag{25}$$

is the *injectivity* [40,41] of reservoir α, i.e., the local density of states associated with electrons injected by α. The coefficients $\lambda_\alpha(\omega)$ satisfy the condition

$$1 = \sum_\alpha \lambda_\alpha(\omega). \tag{26}$$

In the elastic transport regime, the local nonequilibrium distribution function $f_s(\omega)$ is thus a linear combination of the various Fermi functions of the reservoirs, with energy-dependent coefficients. For a quantum system connected to source and drain electrodes under electrical bias, this leads to an energy distribution with two characteristic steps at the source and drain Fermi energies (see Fig. 1), as observed experimentally in mesoscopic metal wires [42,43]. For a
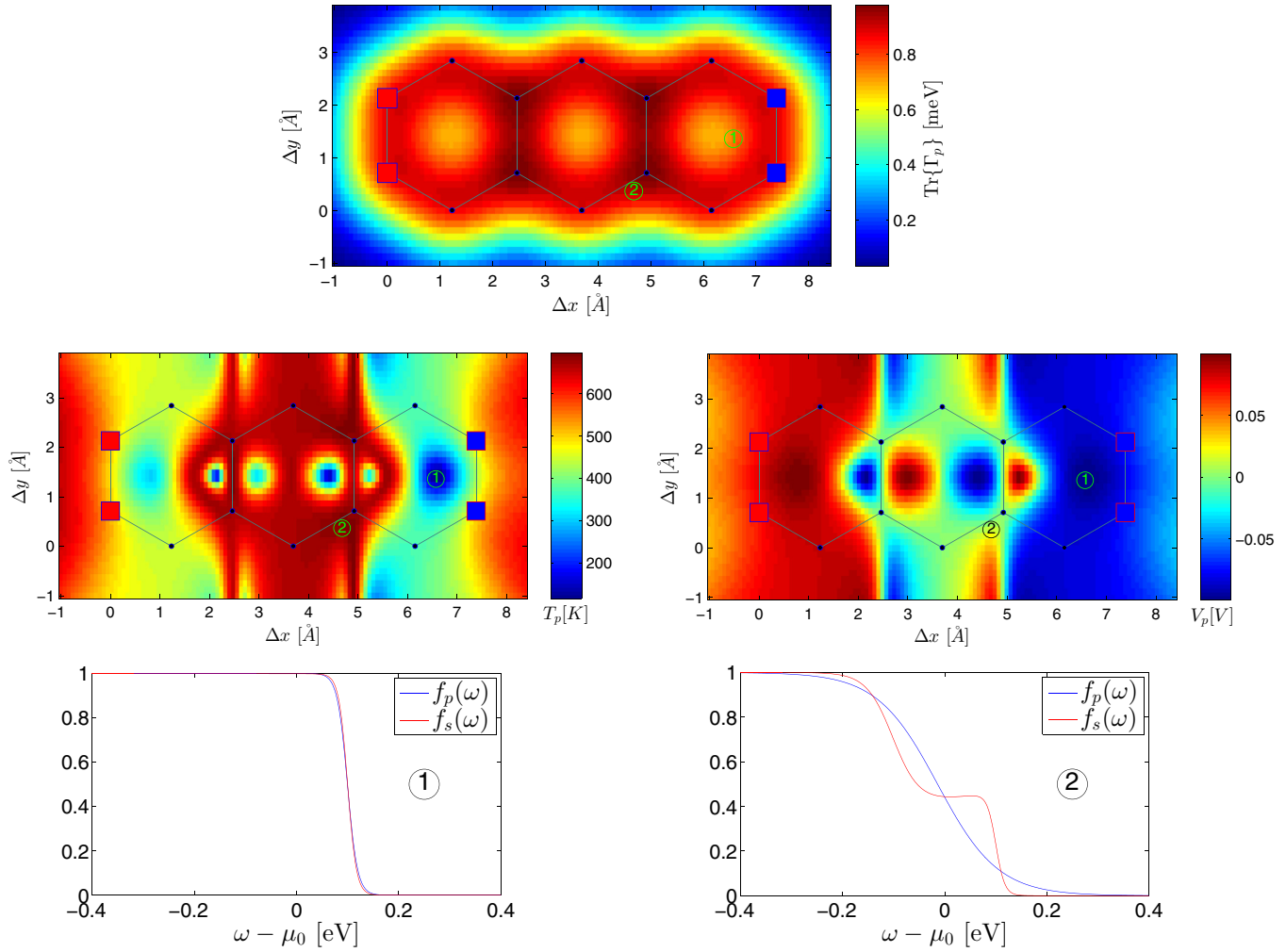
FIG. 1. Measurements of a floating thermoelectric probe scanned 3.5 Å above the plane of carbon nuclei in a single-molecule junction containing an anthracene molecule. The electronic structure of the molecule is illustrated in the topmost panel, which shows $\text{Tr}\{\Gamma^p(\mu_0)\}$ as a function of the probe's horizontal position. The local temperature $\bar{T}_p$ and voltage $\bar{V}_p \equiv -\bar{\mu}_p/e$ are shown in the left and right panels of the middle row, respectively. The probe is modeled as an atomically sharp Au tip and $\Gamma^p(\omega)$ was taken as a constant evaluated at the Au Fermi energy (broadband limit). The thermoelectric bias of the junction is applied by two electrodes covalently bonded to the molecule at the points labeled by the blue squares (electrode 1) and red squares (electrode 2), with $T_1 = 100$ K, $T_2 = 300$ K, and $\mu_2 - \mu_1 = 0.2$ eV. The local energy distribution of the system $f_s(\omega)$ and the Fermi-Dirac distribution of the probe $\bar{f}_p(\omega)$ are shown in the lower two panels for two different probe positions, corresponding to a cold spot and a hot spot, respectively (indicated by circles in the top panels). The zeroth and first moments of the probe's and system's local energy distributions are equal, as described by Eqs. (20)–(21) and (35)–(36).

Fermi system, the coefficients $\lambda_\alpha(\mu_0)$ exhibit characteristic $2k_F$ oscillations as a function of position [40,41], leading to oscillations of the local energy density and temperature [6,10–12] in the linear-response regime.

B. Effective two-terminal current formulas

It is useful to rewrite Eq. (2) in terms of the local distribution $f_s(\omega)$ within the system, as sampled by the probe. Using Eqs. (17) and (19), Eq. (2) can be rewritten as

$$I_p^{(\nu)} = \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega (\omega - \mu_p)^\nu \text{Tr}\{\Gamma^p(\omega)A(\omega)\}[f_s(\omega) - f_p(\omega)].$$

(27)

This has the structure of a two-terminal current formula with sample-probe "transmission function"

$$T_{ps}(\omega) = 2\pi \, \text{Tr}\{\Gamma^p(\omega)A(\omega)\}.$$

(28)

Note, however, that there is no assumption of elastic transport, and that f_s is not in general an equilibrium distribution. Equation (27) is an exact result which merely represents rewriting Eq. (2).

For a given bias of the system, let us denote the Fermi-Dirac distribution of the probe once it has reached local equilibrium with the system [as defined by Eq. (1)] by $\bar{f}_p(\omega)$. Let us now derive a formula for the currents into the probe when the probe is biased away from this local equilibrium point. We will assume that the local nonequilibrium distribution $f_s(\omega)$ is independent of the probe bias (noninvasive probe;

see Ref. [16]). We note that $f_s(\omega)$ is independent of probe bias provided $\Gamma^p \ll \sum_{\alpha \neq p} \Gamma^\alpha$ (weak probe-sample coupling). Writing $f_s - f_p = f_s - \bar{f}_p + \bar{f}_p - f_p$, it is evident that $I_p^{(0)}$ is given by Eq. (27) with the local nonequilibrium distribution f_s replaced by the equilibrium distribution $\bar{f}_p$. To see that the same holds for $I_p^{(1)}$, one can also write $\omega - \mu_p$ in the integrand of Eq. (27) as $\omega - \bar{\mu}_p + \bar{\mu}_p - \mu_p$, and note that all the integrals involving $f_s - \bar{f}_p$ vanish due to the conditions of Eq. (1). The currents flowing into the probe are then given by the effective two-terminal formula

$$I_p^{(\nu)} = \frac{1}{h} \int_{-\infty}^{\infty} d\omega (\omega - \mu_p)^\nu\, T_{ps}(\omega)[\bar{f}_p(\omega) - f_p(\omega)], \quad (29)$$

where both f_p and $\bar{f}_p$ are equilibrium Fermi-Dirac distributions. Although this formula has the same form as the two-terminal current formula of elastic transport theory [33,36,44,45], note that it holds for arbitrary interactions within the system and that no assumption of elastic transport has been made. These effects are encoded in the spectral function $A(\omega)$ of the interacting nonequilibrium system appearing in Eq. (28). Equation (29) is no longer exact, because the dependence of f_s on probe bias has been neglected (assumption of noninvasive probe).

Because Eq. (29) has the same form as the two-terminal current formula of elastic transport theory, one can define Onsager coefficients for the probe-sample junction analogous to Eq. (14):

$$\mathcal{L}_{ps}^{(\nu)} = \frac{1}{h} \int d\omega\, (\omega - \bar{\mu}_p)^\nu\, T_{ps}(\omega) \left(-\frac{\partial \bar{f}_p}{\partial \omega} \right). \quad (30)$$

In terms of these coefficients, one may express the thermopower and thermal conductance of the probe-sample junction as

$$S_{ps} = -\frac{1}{eT_p} \frac{\mathcal{L}_{ps}^{(1)}}{\mathcal{L}_{ps}^{(0)}}, \quad (31)$$

$$\kappa_{ps} = \frac{1}{T_p} \left(\mathcal{L}_{ps}^{(2)} - \frac{[\mathcal{L}_{ps}^{(1)}]^2}{\mathcal{L}_{ps}^{(0)}} \right) \geqslant 0, \quad (32)$$

respectively. $\kappa_{ps} \geqslant 0$ was proven in Ref. [16].

C. Broadband limit

If the probe-sample coupling is broadband, we may approximate $\Gamma^p(\omega) \approx \Gamma^p(\mu_0)$, where μ_0 is the electrochemical potential of the source, drain, and probe electrodes when the whole system is in equilibrium. Writing

$$\mathrm{Tr}\{\Gamma^p(\mu_0)\} = \bar{\Gamma}^p \quad (33)$$

and using Eq. (16), with $\Gamma^p(\omega)$ replaced by $\Gamma^p(\mu_0)$, Eq. (27) may be expressed as

$$I_p^{(\nu)} = \frac{\bar{\Gamma}^p}{\hbar} \int_{-\infty}^{\infty} d\omega (\omega - \mu_p)^\nu\, \bar{A}(\omega)[f_s(\omega) - f_p(\omega)]. \quad (34)$$

When the probe is in local equilibrium with the sample, as defined by Eq. (1), Eqs. (20), (21), and (34) imply

$$\langle N \rangle|_{f_s} = \langle N \rangle|_{\bar{f}_p}, \quad (35)$$

$$\langle E \rangle|_{f_s} = \langle E \rangle|_{\bar{f}_p}. \quad (36)$$

That is to say, the mean local occupancy and energy of the nonequilibrium system are the same as if its local (nonequilibrium) spectrum $\bar{A}(\omega)$ were populated by the equilibrium Fermi-Dirac distribution of the probe. A noninvasive measurement of $\bar{\mu}_p$, $\bar{T}_p$ thus constitutes a measurement of the local occupancy and energy of the system, in the broadband limit. The quantity $\langle E \rangle - \bar{\mu}_p \langle N \rangle$ is a monotonically increasing function of $\bar{T}_p$ at fixed $\bar{\mu}_p$, and is a measure of the mean excitation energy of the system (see Sec. V). Thus $\bar{T}_p$ is directly related to the degree of local energy excitation, in the same way that it is in an equilibrium system. Certainly, then, a floating thermoelectric probe provides more than a mere operational definition of local temperature.

The principle underlying Eqs. (35)–(36), that a floating thermoelectric probe whose coupling to the system is broadband measures the zeroth and first moments of the system's local energy distribution, is illustrated in Fig. 1. For this example, the electronic transport was considered elastic, as described in Sec. III A 1. The electronic structure of the system (an anthracene molecule covalently bonded to two metal electrodes) was modeled via Hückel theory, and the floating thermoelectric probe was modeled as an atomically sharp Au tip scanned at a constant height of 3.5 Å above the plane of carbon nuclei in the junction. The probe-system coupling was calculated by the method of Refs. [10,12]. The probe temperature $\bar{T}_p$ and chemical potential $\bar{\mu}_p$ were obtained by finding the roots of Eq. (2) numerically at finite bias [46]. At both the cold spot and hot spot indicated, the probe's Fermi-Dirac distribution matches the zeroth and first moments of the local energy distribution. It should be emphasized that this particular nanostructure is merely an example, chosen to illustrate the general principles involved in a scanning thermoelectric measurement, and the methods and approximations used to treat it in no way limit the applicability of the arguments given in the remainder of the paper.

IV. ZEROTH LAW

In a previous article [11], it was shown that the local temperature measured by a scanning thermoelectric probe is consistent with the *zeroth-law of thermodynamics*, also known as the *transitive property of equilibrium*: if the local temperatures and chemical potentials of two nonequilibrium quantum systems, as measured by the probe, are equal, then the two systems will be in thermal and electrical equilibrium with each other when connected by a transmission line coupled locally to the same two points. This result was proven within linear response and to leading order in the Sommerfeld expansion.

This scenario can be extended to the nonlinear response regime, as discussed in Appendix B. However, here we focus on another zeroth-law scenario, namely, under what conditions will two different thermometers measure the same local temperature of a single nonequilibrium quantum system?

A. Ideal probe: Local, noninvasive, broadband

It is well known in the field of scanning probe microscopy [34] that the image of any physical property depends on the spatial resolution of the probe. This dependence drops

out in the limit of maximally local coupling given by Eq. (22), for which $\bar{A}(\omega)$ reduces to the local density of states $\rho(\omega)$. For the sake of clarity, we focus on this limit of a locally coupled probe throughout the remainder of the paper. It is straightforward to extend these results to probes with arbitrary spatial resolution.

The local density of states $\rho(\omega)$ is independent of Γ^p provided the coupling of the probe to the sample is not so strong that it perturbs the local spectrum (noninvasive probe). This may be seen explicitly as follows. Using Dyson's equations for G^r and G^a,

$$G^{r/a}(\omega) = [\mathbf{1}\omega - H^{(1)} - \Sigma^{r/a}(\omega)]^{-1}, \qquad (37)$$

where $H^{(1)}$ is the one-body Hamiltonian of the system and $\Sigma^{r/a}(\omega)$ is the retarded/advanced self-energy describing 2-body interactions and coupling of the system to the external reservoirs, it can be shown that

$$A(\omega) = \frac{1}{2\pi} G^r(\omega)\Gamma(\omega)G^a(\omega), \qquad (38)$$

where

$$\Gamma(\omega) \equiv -i(\Sigma^a - \Sigma^r) = \sum_\alpha \Gamma^\alpha - i\left(\Sigma_{\text{int}}^a - \Sigma_{\text{int}}^r\right). \qquad (39)$$

Here $\Gamma^\alpha(\omega)$ is the tunneling-width matrix describing coupling of reservoir α to the system, where α can represent source, drain, probe, etc., and $\Sigma_{\text{int}}(\omega)$ is the self-energy due to two-body interactions. Let $G_0^{r/a} = \lim_{\Gamma^p \to 0} G^{r/a}$ and $\Gamma_0 = \lim_{\Gamma^p \to 0} \Gamma$. Then $A_0(\omega) = G_0^r \Gamma_0 G_0^a / 2\pi$ is the spectral function of the system in the absence of probe-system coupling, and one can show that

$$\frac{\rho(\omega)}{\rho_0(\omega)} = 1 - \pi\rho_0(\omega)\Gamma^p(\omega) + \frac{(G_0^r \Gamma^p G_0^a)_{nn}}{(G_0^r \Gamma_0 G_0^a)_{nn}} + \mathcal{O}(\rho_0\Gamma^p)^2. \qquad (40)$$

Any perturbation of the local spectrum by the probe can thus be safely neglected [47] provided $\rho_0(\omega)\Gamma^p \ll 1$. Similarly, the nonequilibrium distribution $f_s(\omega)$ is unaffected by the probe [16] provided $\Gamma^p \ll \sum_{\alpha \neq p} \Gamma^\alpha$, where $\alpha = 1, 2, \ldots$ denote the reservoirs of charge and energy used to drive the system out of equilibrium.

For any probe with such a maximally local, weak, broadband coupling to the system, the measured value of the local temperature depends only on the nonequilibrium state of the system, and is independent of the properties of the probe. The probe temperature and chemical potential are directly related to the mean energy and occupancy of the localized orbital to which it is coupled. Any two such thermometers will measure exactly the same local temperature of the system, and thus satisfy the transitive property of equilibrium. The local temperature so defined is thus consistent with the zeroth law of thermodynamics.

The two conditions on the probe-system coupling needed to ensure consistency with the zeroth law, that it should be both weak and broadband, are eminently reasonable, since they are needed to ensure that the measurement does not strongly perturb the system, and that the measurement depends on the spectrum of the system rather than that of the thermometer, respectively. We define such a measurement, where in addition the thermal coupling of the probe to the ambient environment

is negligible ($\kappa_{p0} = 0$), as an *ideal temperature measurement*, and denote the value by $\hat{T}_p$.

B. Beyond the broadband limit

To investigate deviations from the zeroth law far from equilibrium beyond the broadband limit, one can solve Eqs. (1) and (2) for $\bar{T}_p$, treating $\Gamma^{p\prime}(\mu_0)$, $\Gamma^{p\prime\prime}(\mu_0)$, etc., as perturbations. Let us define

$$\Gamma^p(\omega) \equiv \bar{\Gamma}^p[1 + \lambda g(\omega)], \qquad (41)$$

where λ is a dimensionless parameter that is taken to be small and $g(\mu_0) = 0$. The temperature measured by the probe is

$$\bar{T}_p = \hat{T}_p + \delta T_p, \qquad (42)$$

where $\hat{T}_p$ is the result for $\lambda = 0$, and it can be shown that the temperature error δT_p of a nonideal thermometer with $\Gamma^p(\omega) \neq$ constant is

$$\delta T_p = \lambda \frac{\delta I_p^{(1)} + e\hat{T}_p S_{ps} \delta I_p^{(0)}}{\kappa_{ps}} + \mathcal{O}(\lambda^2), \qquad (43)$$

where S_{ps} and κ_{ps} are given by Eqs. (31) and (32), respectively, with Eq. (30) evaluated for $T_{ps}(\omega) \to 2\pi\bar{\Gamma}^p\rho(\omega)$ and $\bar{f}_p(\omega) \to \hat{f}_p(\omega) = f_p(\hat{\mu}_p, \hat{T}_p; \omega)$, where $\hat{\mu}_p \equiv \lim_{\lambda \to 0} \bar{\mu}_p$ is the result of an *ideal voltage measurement*. Here

$$\delta I_p^{(\nu)} = \frac{\bar{\Gamma}^p}{\hbar} \int_{-\infty}^{\infty} d\omega(\omega - \hat{\mu}_p)^\nu g(\omega)\rho(\omega)[f_s(\omega) - \hat{f}_p(\omega)]. \qquad (44)$$

If one assumes that $g(\omega)$ is a slowly varying function with

$$g(\omega) = g_1(\omega - \hat{\mu}_p) + g_2(\omega - \hat{\mu}_p)^2 + \cdots, \qquad (45)$$

then one can show that

$$\delta T_p = \frac{\lambda\bar{\Gamma}^p}{\hbar} \left(\frac{g_1 + e\hat{T}_p S_{ps} g_2}{\kappa_{ps}} \right)$$
$$\times \int_{-\infty}^{\infty} d\omega(\omega - \hat{\mu}_p)^2 \rho(\omega)[f_s(\omega) - \hat{f}_p(\omega)] \qquad (46)$$

plus corrections involving higher powers of $(\omega - \hat{\mu}_p)$ in the integrand.

In order to make further progress analytically, it is necessary to consider the limit of linear response. For small thermoelectric bias, transport in nanostructures is largely elastic at room temperature and below, so one can use Eq. (24) in Eq. (46), and expand $f_\alpha(\omega)$ and $\hat{f}_p(\omega)$ about the equilibrium distribution $f_0(\omega)$. We consider separately the cases of thermal and electrical bias.

1. Thermal bias

Evaluating Eq. (46) for a thermal bias, and keeping only the leading term of the Sommerfeld expansion, one obtains

$$\delta T_p = \lambda g_1 \frac{7\pi^2}{5} \frac{(k_B T_0)^2}{\bar{T}_{ps}(\mu_0)} \sum_\alpha \bar{T}_{p\alpha}'(\mu_0)(T_\alpha - T_p), \qquad (47)$$

where

$$\bar{T}_{p\alpha}(\omega) = 2\pi\bar{\Gamma}^p\rho_\alpha(\omega) \qquad (48)$$

is the transmission probability from reservoir α into the probe, evaluated in the broadband limit for the probe-sample coupling. One thus finds

$$\frac{\delta T_p}{\Delta T} \sim (k_B T_0)^2 \left.\frac{d \ln \Gamma^p}{d\omega}\right|_{\omega=\mu_0} \left.\frac{d \ln \bar{T}_{p\alpha}}{d\omega}\right|_{\omega=\mu_0} \quad (49)$$

for the temperature error as a fraction of the thermal bias. The temperature error between any two thermometers is thus higher order in the Sommerfeld expansion for the case of a linear thermal bias, and hence is expected to be numerically negligible for nanosystems at room temperature and below. Note that the maximum temperature error between any two thermometers is bounded by ΔT for a pure thermal bias [10], because the equilibration of a thermometer at a value of T_p outside the range $[T_2, T_1]$ would violate the second law of thermodynamics.

2. Electrical bias

Let us next consider a pure electrical bias, with both source and drain electrodes held at ambient temperature. Evaluating Eq. (46), one obtains

$$\frac{\delta T_p}{T_0} \simeq \lambda g_1 \frac{7\pi^2}{10} \frac{(k_B T_0)^2}{\bar{T}_{ps}(\mu_0)} \sum_\alpha \bar{T}''_{p\alpha}(\mu_0)(\mu_\alpha - \hat{\mu}_p), \quad (50)$$

where the leading-order term of the Sommerfeld expansion vanishes due to condition (1). This temperature error should be compared to the temperature shift of an ideal probe due to the Peltier effect in the system [48],

$$\frac{T_p - T_0}{T_0} \simeq \frac{\bar{T}_{p1} \bar{T}'_{p2} - \bar{T}_{p2} \bar{T}'_{p1}}{\bar{T}^2_{ps}} \Delta\mu. \quad (51)$$

The relative temperature error of a nonideal thermometer thus scales as

$$\frac{\delta T_p}{T_p - T_0} \sim (k_B T_0)^2 \left.\frac{d \ln \Gamma^p}{d\omega}\right|_{\omega=\mu_0} \frac{\bar{T}''_{p\alpha}(\mu_0)}{\bar{T}'_{p\alpha}(\mu_0)}. \quad (52)$$

As in the case of a thermal bias, the error is higher order in the Sommerfeld expansion, and hence expected to be numerically negligible for nanosystems at room temperature and below.

V. FIRST LAW

In this section, we investigate whether the temperature measured by a floating thermoelectric probe is consistent with the first law of thermodynamics. We first consider a noninteracting system driven arbitrarily far from equilibrium, and show that the local temperature inferred from an ideal temperature measurement is consistent with the first law. We then consider an interacting system, where not only the local distribution $f_s(\omega)$ but also the local density of states $\rho(\omega)$ depends on the nonequilibrium state of the system, and hence on the local temperature. For this case, we show that deviations from the first law are higher order in the Sommerfeld expansion.

A. Noninteracting system

As in Sec. IV A–IV B, we focus here on the case of maximally local coupling given by Eq. (22), for which the

quantities discussed in this section have an obvious meaning. It is straightforward to generalize the arguments herein to arbitrary probe-sample coupling.

For a given nonequilibrium steady state of the system, the temperature of the probe is determined by

$$0 = I_p^{(1)} = \frac{\bar{\Gamma}^p}{\hbar} \int_{-\infty}^{\infty} d\omega\, (\omega - \bar{\mu}_p)[1 + \lambda g(\omega)]\rho(\omega)$$
$$\times [f_s(\omega) - \bar{f}_p(\omega)], \quad (53)$$

where we have used Eqs. (27) and (41). From Eqs. (53) and (44), it follows immediately that

$$\langle E \rangle|_{f_s} - \bar{\mu}_p \langle N \rangle|_{f_s} = \langle E \rangle|_{\bar{f}_p} - \bar{\mu}_p \langle N \rangle|_{\bar{f}_p} - \lambda \frac{\hbar}{\bar{\Gamma}^p} \delta I_p^{(1)}, \quad (54)$$

where $\langle E \rangle$ and $\langle N \rangle$ are the mean energy and occupancy, respectively, of the localized orbital of the system coupled to the probe, defined by Eqs. (20) and (21). To leading order in the Sommerfeld expansion, Eq. (43) gives

$$\lambda \frac{\hbar}{\bar{\Gamma}^p} \delta I_p^{(1)} = \frac{\hbar}{\bar{\Gamma}^p} \kappa_{ps} \delta T_p = C_s^{(1)}(\bar{\mu}_p, \bar{T}_p)\delta T_p, \quad (55)$$

where the one-body contribution to the local specific heat is

$$C_s^{(1)}(\mu_p, T_p) = \frac{1}{T_p} \int_{-\infty}^{\infty} d\omega\, (\omega - \mu_p)^2 \rho(\omega)\left(-\frac{\partial f_p}{\partial\omega}\right) \geqslant 0. \quad (56)$$

Consider now a small change in bias of the nonequilibrium system, leading to a new nonequilibrium steady state characterized by the same value of the local chemical potential $\bar{\mu}_p$, but by a different local temperature $\bar{T}'_p$. The heat ΔQ_s added locally to the system under this change of bias satisfies

$$\Delta Q_s \equiv \Delta \langle E - \bar{\mu}_p N \rangle = C_s^{(1)}(\bar{\mu}_p, \bar{T}_p)\, \Delta(\bar{T}_p - \delta T_p)$$
$$= C_s^{(1)}(\bar{\mu}_p, \bar{T}_p)\Delta\hat{T}_p, \quad (57)$$

where Eqs. (54)–(56) have been used. Here $\bar{T}_p - \delta T_p = \hat{T}_p$ is the result of an *ideal temperature measurement* by a broadband probe coupled weakly to the system, as discussed above in Sec. IV. Thus deviations from the zeroth and first laws under nonideal measurement conditions are not independent, and Eq. (57) implies that it is $\hat{T}_p$ that should be identified as the true local temperature of the system, directly related to the local energy excitation.

Note that Eq. (57) also holds for systems with $\bar{T}_p < 0$ (absolute negative temperature), although the interval $[\bar{T}_p, \bar{T}'_p]$ cannot contain 0 since $\langle E \rangle$ and $\bar{f}_p(\omega)$ are discontinuous at $\bar{T}_p = 0$ (they are continuous functions of $\bar{\beta}_p \equiv 1/k_B \bar{T}_p$). Absolute negative temperatures do not characterize any generic equilibrium state, but allow one to quantify population inversion in a nonequilibrium system with a bounded spectrum [13]. Negative temperature solutions to Eq. (1) exist for strongly driven systems [16].

B. Interacting system

In an interacting system, not only the local distribution $f_s(\omega)$ but also the local spectrum $\rho(\omega)$ depends on temperature,

so that $C_s = C_s^{(1)} + C_s^{(2)}$, where

$$C_s^{(2)}(\mu_p, T_p) = \int_{-\infty}^{\infty} d\omega \, (\omega - \mu_p) f_p(\omega) \left. \frac{\partial \rho(\omega)}{\partial T_p} \right|_{\mu_p} \quad (58)$$

is the two-body contribution to the local specific heat. Due to the limited phase space for two-body scattering in Fermi systems [49] at temperatures well below the Fermi temperature, $\partial \rho(\omega)/\partial T \propto T$ so that $C_s^{(2)}$ is two orders higher in the sense of a Sommerfeld expansion than $C_s^{(1)}$.

The arguments of Sec. V A can be extended straightforwardly to the case of an interacting nonequilibrium system, leading to the result

$$\Delta Q_s \equiv \Delta \langle E - \bar{\mu}_p N \rangle = C_s^{(1)}(\bar{\mu}_p, \bar{T}_p) \Delta \hat{T}_p$$
$$+ \int_{-\infty}^{\infty} d\omega \, (\omega - \bar{\mu}_p) \bar{f}_p(\omega) \Delta \rho(\omega), \quad (59)$$

where $\Delta \rho(\omega)$ is the change in the local spectrum due to the small change in bias of the nonequilibrium system. For the case of a system driven out of equilibrium by a thermal bias alone, it is clear from the above discussion that the two-body term in Eq. (59) is two orders higher in the Sommerfeld expansion than the one-body term, and hence comparable to the error arising from a nonideal temperature measurement. However, the size of the two-body term for general thermoelectric bias remains an open question.

Formally, one can write $\Delta \rho(\omega) \equiv \Delta \hat{T}_p \partial \rho(\omega)/\partial \hat{T}_p$, where $\partial \rho(\omega)/\partial \hat{T}_p$ is the temperature derivative of the spectrum of a fictitious equilibrium interacting system whose local spectrum coincides with that of the actual interacting nonequilibrium system. In that case, of course, the first law applies also to the two-body contribution to ΔQ_s, which characterizes the role of correlations in local heating of the nonequilibrium system.

VI. SECOND LAW

In a previous article [11], it was shown that if a nonequilibrium system is used as a heat bath to drive a thermoelectric process, the maximum electrical work generated satisfies Carnot's theorem, with $\bar{T}_p$ as the absolute temperature of the bath. That result was obtained within linear response for noninteracting systems. In this section, we demonstrate that the temperature measured by a floating thermoelectric probe satisfies Clausius' statement of the second law of thermodynamics, that no process is possible whose sole effect is to transfer heat from a system at some temperature T to a system at a higher temperature T'. The arguments of this section apply to steady-state systems arbitrarily far from equilibrium, and with arbitrary interactions. The relation between probe temperature and the direction of heat flow was discussed in a different context by Caso *et al.* [25,29].

Let us consider the junction between the probe and the system. If the probe is biased away from the local equilibrium temperature $\bar{T}_p$ to some other temperature T_p, then a heat current $I_p^{(1)}$ will flow across the junction in accordance with Eq. (29). It should be emphasized that $I_p^{(1)}$ is the *heat flowing into the probe*, which is well defined, since the (macroscopic) probe is arbitrarily close to equilibrium in the presence of this microscopic heat current; by contrast, the *heat flowing out of*

the system is not well defined, since the system is far from equilibrium.

Equation (29) expresses the heat current $I_p^{(1)}$ in terms of the difference between two equilibrium Fermi-Dirac distributions, $\bar{f}_p = f(\bar{\mu}_p, \bar{T}_p)$ and $f_p = f(\mu_p, T_p)$. $T_{ps}(\omega)$ in Eq. (29) is given by Eq. (28) and satisfies $T_{ps}(\omega) \geqslant 0$ since both $\Gamma^p(\omega)$ and $A(\omega)$ are positive-definite. Thus Eq. (29) gives the heat current across a fictitious two-terminal junction between two equilibrium reservoirs with transmission function $T_{ps}(\omega)$.

A. Thermal bias of probe

Let us first consider the case where the probe is thermally biased, but held at the equilibrium chemical potential $\bar{\mu}_p$. Then $f_p(\omega) = f(\bar{\mu}_p, T_p; \omega)$, and

$$(\omega - \bar{\mu}_p)[\bar{f}_p(\omega) - f_p(\omega)] \gtrless 0 \quad \text{if} \quad \beta_p \gtrless \bar{\beta}_p, \quad (60)$$

where $\beta_p \equiv 1/k_B T_p$. Thus the integrand for $I_p^{(1)}$ in Eq. (29) is everywhere positive for $\beta_p > \bar{\beta}_p$ and negative for $\beta_p < \bar{\beta}_p$, so that

$$\text{sgn}(I_p^{(1)}) = \text{sgn}(\beta_p - \bar{\beta}_p). \quad (61)$$

That is to say, heat flows into the probe if it is biased to a temperature below the local temperature $\bar{T}_p$, and out of the probe for a bias above the local temperature, consistent with the second law of thermodynamics. This statement holds provided T_p and $\bar{T}_p$ have the same sign; if $T_p > 0$ and $\bar{T}_p < 0$, then heat flows into the probe, in accordance with Eq. (61) (a system at absolute negative temperature is "hotter" than any positive temperature [13]), while the heat flow is reversed if the signs are reversed.

This analysis rules out the possibility of multiple-valued solutions of $I_p^{(1)} = 0$ at fixed $\mu_p = \bar{\mu}_p$. The uniqueness of the probe temperature in the absence of electrical bias in the system (which precludes local Peltier cooling/heating effects) was previously proven in Ref. [27].

B. Probe as open electric circuit

Under the thermal bias conditions discussed above, a small electric current $I_p^{(0)}$ may flow across the junction between the probe and the system due to thermoelectric effects. To rigorously check the applicability of the Clausius formulation of the second law, we must consider a probe forming an open electric circuit, so that only heat may be exchanged between the probe and the system in steady state. This leads to the condition $I_p^{(0)} = 0$, which can be solved for the chemical potential shift $\Delta \mu_p = \mu_p - \bar{\mu}_p$ of the probe as a function of the thermal bias $T_p - \bar{T}_p$.

For thermal biases achievable in the laboratory, the resulting thermoelectric voltage $\Delta \mu_p$ may be treated within linear response. Writing

$$\bar{f}_p \equiv f_p(\bar{\mu}_p, \bar{T}_p) = f_p(\mu_p, \bar{T}_p) + [\bar{f}_p - f_p(\mu_p, \bar{T}_p)]$$
$$\cong f_p(\mu_p, \bar{T}_p) - \Delta \mu_p \left(\frac{\partial \bar{f}_p}{\partial \omega} \right), \quad (62)$$

the open-circuit thermoelectric voltage may be obtained from Eq. (29) as

$$\mathcal{L}_{ps}^{(0)} \Delta\mu_p \cong -\frac{1}{h}\int_{-\infty}^{\infty} d\omega\, T_{ps}(\omega)[f_p(\mu_p,\bar{T}_p) - f_p(\mu_p,T_p)],$$

$$(63)$$

where $\mathcal{L}_{ps}^{(0)}$ is given by Eq. (30). The right-hand side of Eq. (63) is just the electric current $I_p^{(0)}$ flowing when $\Delta\mu_p = 0$. The heat current flowing into the probe when it forms an open electric circuit may then be expressed as

$$I_p^{(1)} \cong I_p^{(1)}\big|_{\Delta\mu_p=0} - \frac{\mathcal{L}_{ps}^{(1)}}{\mathcal{L}_{ps}^{(0)}} I_p^{(0)}\big|_{\Delta\mu_p=0}, \qquad (64)$$

where the first term is the heat current at $\Delta\mu_p = 0$ discussed above, and the second term is a small thermoelectric correction, which has the opposite sign of the first term. The thermoelectric correction is well known in the theory of electronic heat transport [35,50]. It represents negative feedback arising from the "interference" of charge and heat transport processes [35], and cannot exceed the magnitude of the first term without leading to a violation of the second law. Although the latter condition has not been established in general for transport between an equilibrium system and a system far from equilibrium, it must hold for the case at hand due to the mapping onto a fictitious junction between two equilibrium systems provided by Eq. (29).

Thus, we have shown that the temperature measured by a floating thermoelectric probe satisfies Clausius's statement of the second law for arbitrary steady-state thermoelectric bias conditions of the system, and for arbitrary thermal bias between the probe and the system. For a rigorous mathematical proof, see Ref. [16].

VII. THIRD LAW

In this section, we investigate whether the local temperature of a nonequilibrium quantum system is consistent with the third law of thermodynamics. From Eq. (59), it follows that

$$\lim_{\bar{T}_p\to 0^+}\Delta Q_s \equiv \lim_{\bar{T}_p\to 0^+}\Delta\langle E - \bar{\mu}_p N\rangle = C_s^{(1)}(\bar{\mu}_{p0},\bar{T}_p)\Delta\bar{T}_p,$$

$$(65)$$

where $C_s^{(1)}$ is given by Eq. (56) and $\bar{\mu}_{p0} = \lim_{\bar{T}_p\to 0^+}\bar{\mu}_p$. Provided $\rho(\bar{\mu}_{p0}) \neq 0$, the low-temperature limit of $C_s^{(1)}$ may be straightforwardly calculated as

$$\lim_{\bar{T}_p\to 0^+} C_s^{(1)}(\bar{\mu}_p,\bar{T}_p) = \frac{\pi^2}{3}\rho(\bar{\mu}_{p0})k_B^2\bar{T}_p. \qquad (66)$$

Similarly, it can be shown that the leading-order behavior of the probe-sample thermal conductance κ_{ps} defined in Eq. (32) is

$$\lim_{\bar{T}_p\to 0^+}\kappa_{ps} = \frac{\pi^2\bar{\Gamma}^p}{3\hbar}\rho(\bar{\mu}_{p0})k_B^2\bar{T}_p. \qquad (67)$$

Note that if $\rho(\bar{\mu}_{p0}) = 0$, both C_s and κ_{ps} vanish as higher powers of $\bar{T}_p$. The fact that both $C_s \to 0$ and $\kappa_{ps} \to 0$ as $\bar{T}_p \to 0^+$ indicates that the local temperature inferred from the measurement by a floating thermoelectric probe is completely consistent with the third law of thermodynamics. Furthermore,

it can be shown [46] that the local entropy of the system goes to zero whenever $\bar{T}_p \to 0$.

Equations (66) and (67) also hold in the limit $\bar{T}_p \to 0^-$, with $\bar{T}_p$ replaced by $|\bar{T}_p|$. These statements may be considered analogues of the third law [13] as it applies to the state of maximum energy in a system with a bounded spectrum.

VIII. CONCLUSIONS

In the present article, a theory of local temperature measurement of an interacting quantum electron system arbitrarily far from equilibrium via a floating thermoelectric probe was developed. For a probe-system coupling that is both weak and broadband, it was shown that the local temperature and chemical potential of the probe are completely determined by the zeroth and first moments of the local energy distribution in the system [cf. Eqs. (35)–(36) and Fig. 1]. The local temperature $\bar{T}_p$ so defined is thus directly related to the mean local excitation energy of the system (57), just as it is in an equilibrium system.

For a noninvasive broadband probe, it was shown that $\bar{T}_p$ is consistent with the zeroth, first, second, and third laws of thermodynamics. For non-broadband probes, the local temperature obeys the Clausius form of the second law and the third law exactly, but there are deviations from the zeroth and first laws that are higher order in the Sommerfeld expansion. It was shown that the corrections to the zeroth and first laws are related, and can be interpreted in terms of the error inherent in a nonideal temperature measurement. This analysis also applies to systems with negative absolute temperature [13–16] (population inversion).

The exact agreement with Clausius's statement of the second law and with the third law implies that the local temperature metric $\bar{T}_p$ defines an ordering of temperatures and an absolute zero, but not necessarily an absolute temperature scale. The first law defines absolute temperature differences, and it was shown that discrepancies with the first law in probes that are not broadband arise from deviations from ideal measurement (zeroth law). In this sense, a noninvasive broadband probe can be used to define an absolute temperature scale for nonequilibrium quantum electron systems. All such thermometers will measure the same temperature, and the temperature scale so defined is consistent with the laws of thermodynamics, as elucidated above. However, other types of thermometers [11,31] may not yield precisely the same temperature, and the values of $\bar{T}_p$, $\bar{\mu}_p$ determined by a floating thermoelectric probe may not be consistent with alternative formulations of the laws of thermodynamics, all of which are equivalent for equilibrium systems (see Appendix B for a discussion of an alternative formulation of the zeroth law).

The ability to consistently define local thermodynamic variables such as the temperature [11,46] or chemical potential [48,51,52] points to the possibility of constructing a thermodynamic description—if only a partial one—of far-from-equilibrium quantum systems.

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.,

$$\langle \hat{Q} \rangle = \text{Tr}\{\hat{\rho}\hat{Q}\} = \sum_{\mu,\nu} \rho_{\mu\nu} \langle \nu|\hat{Q}|\mu\rangle. \tag{A1}$$

The "lesser" and "greater" Green's functions [1] used in the paper are defined as

$$G^{<}_{\alpha\beta}(t) \equiv i\langle d^{\dagger}_{\beta}(0)d_{\alpha}(t)\rangle, \tag{A2}$$

while its Hermitian conjugate is

$$G^{>}_{\alpha\beta}(t) \equiv -i\langle d_{\alpha}(t)d^{\dagger}_{\beta}(0)\rangle, \tag{A3}$$

where

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

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

The spectral representation uses the eigenbasis of the Hamiltonian $\hat{H}|\nu\rangle = E_{\nu}|\nu\rangle$, where ν denotes a many-body energy eigenstate. One may write the "lesser" Green's function as

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

while the "greater" Green's function becomes

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

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

$$A(\omega) \equiv \frac{1}{2\pi i}(G^{<}(\omega) - G^{>}(\omega)), \tag{A7}$$

and can be expressed in the spectral representation as

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

1. Sum rule for the spectral function

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

$$\int_{-\infty}^{\infty} d\omega A_{\alpha\beta}(\omega) = \sum_{\mu,\nu} \rho_{\mu\nu}\langle\nu|d^{\dagger}_{\beta}d_{\alpha}|\mu\rangle$$
$$+ \sum_{\mu',\nu} \rho_{\nu\mu'}\langle\mu'|d_{\alpha}d^{\dagger}_{\beta}|\nu\rangle$$
$$= \sum_{\mu,\nu} \rho_{\mu\nu}\langle\nu|d^{\dagger}_{\beta}d_{\alpha} + d_{\alpha}d^{\dagger}_{\beta}|\mu\rangle$$
$$= \sum_{\mu,\nu} \rho_{\mu\nu}\delta_{\mu\nu}\delta_{\alpha\beta}$$
$$= \delta_{\alpha\beta}\,\text{Tr}\,\{\hat{\rho}\}$$
$$= \delta_{\alpha\beta}. \tag{A9}$$

In our theory of local thermodynamic measurements, the quantity of interest is the local spectrum of the system sampled by the probe $\bar{A}(\omega)$, defined in Eq. (16). This obeys a further sum rule in the broadband limit (*ideal probe*), discussed below.

Local spectrum in the broadband limit

The probe-system coupling is energy-independent in the broadband limit, $\Gamma^p(\omega) = $ constant, and we write $\text{Tr}\,\{\Gamma^p\} = \bar{\Gamma}^p$ for its trace. The local spectrum sampled by the probe $\bar{A}(\omega)$ defined in Eq. (16) can be written in the broadband limit as

$$\bar{A}(\omega) = \frac{1}{\bar{\Gamma}^p}\sum_{\alpha,\beta}\langle\beta|\Gamma^p|\alpha\rangle A_{\alpha\beta}(\omega). \tag{A10}$$

In this limit, it obeys a further sum rule:

$$\int_{-\infty}^{\infty} d\omega\bar{A}(\omega) = \frac{1}{\bar{\Gamma}^p}\sum_{\alpha,\beta}\langle\beta|\Gamma^p|\alpha\rangle\int_{-\infty}^{\infty} d\omega A_{\alpha\beta}(\omega)$$
$$= \frac{1}{\bar{\Gamma}^p}\sum_{\alpha,\beta}\langle\beta|\Gamma^p|\alpha\rangle\delta_{\alpha\beta} \tag{A11}$$
$$= 1.$$

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 $\bar{A}(\omega)$ 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 $\hat{Q}$,

$$\langle\hat{Q}(t)\rangle = \sum_{\mu,\nu} \rho_{\mu\nu}\langle\nu|\hat{Q}(t)|\mu\rangle$$
$$= \sum_{\mu,\nu} \rho_{\mu\nu}\langle\nu|e^{i\frac{\hat{H}}{\hbar}t}\hat{Q}e^{-i\frac{\hat{H}}{\hbar}t}|\mu\rangle \tag{A12}$$
$$= \sum_{\mu,\nu} \rho_{\mu\nu}e^{-i\frac{E_{\mu}-E_{\nu}}{\hbar}t}\langle\nu|\hat{Q}|\mu\rangle.$$

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,

$$-i\langle\alpha|G^<(\omega)|\alpha\rangle \equiv -iG^<_{\alpha\alpha}(\omega)$$
$$= 2\pi \sum_{\mu,\mu'} \rho_{\mu\mu}|\langle\mu|d^\dagger_\alpha|\mu'\rangle|^2$$
$$\times \delta\left(\omega - \frac{E_\mu - E_{\mu'}}{\hbar}\right) \geqslant 0. \quad \text{(A13)}$$

Similarly,

$$i\langle\alpha|G^>(\omega)|\alpha\rangle \equiv iG^>_{\alpha\alpha}(\omega)$$
$$= 2\pi \sum_{\mu,\mu'} \rho_{\mu\mu}|\langle\mu'|d^\dagger_\alpha|\mu\rangle|^2$$
$$\times \delta\left(\omega - \frac{E_{\mu'} - E_\mu}{\hbar}\right) \geqslant 0. \quad \text{(A14)}$$

It follows that

$$\langle\alpha|A(\omega)|\alpha\rangle = \frac{1}{2\pi}\langle\alpha|-iG^<(\omega) + iG^>(\omega)|\alpha\rangle \geqslant 0. \quad \text{(A15)}$$

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

4. $0 \leqslant f_s(\omega) \leqslant 1$ and $\bar{A}(\omega) \geqslant 0$

The nonequilibrium distribution function $f_s(\omega)$ was defined in Eq. (19) as

$$f_s(\omega) \equiv \frac{\mathrm{Tr}\{\Gamma^p(\omega)G^<(\omega)\}}{2\pi i\,\mathrm{Tr}\{\Gamma^p(\omega)A(\omega)\}}. \quad \text{(A16)}$$

We have $\Gamma^p(\omega) > 0$ by causality [1]:

$$\mathrm{Im}\,\Sigma^r_p(\omega) = -\frac{1}{2}\Gamma^p(\omega) < 0. \quad \text{(A17)}$$

Let $\Gamma^p|\gamma_p\rangle = \gamma_p|\gamma_p\rangle$, where $\gamma_p \geqslant 0$ and some γ_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 Γ^p, yielding

$$f_s(\omega) = \frac{\sum_{\gamma_p} \gamma_p \langle\gamma_p|G^<(\omega)|\gamma_p\rangle}{2\pi i \sum_{\gamma_p} \gamma_p \langle\gamma_p|A(\omega)|\gamma_p\rangle}$$
$$= \frac{\sum_{\gamma_p} \gamma_p \langle\gamma_p|-iG^<(\omega)|\gamma_p\rangle}{\sum_{\gamma_p} \gamma_p \langle\gamma_p|-iG^<(\omega) + iG^>(\omega)|\gamma_p\rangle}. \quad \text{(A18)}$$

Therefore

$$0 \leqslant f_s(\omega) \leqslant 1. \quad \text{(A19)}$$

Similarly,

$$\bar{A}(\omega) \equiv \frac{\mathrm{Tr}\{\Gamma^p(\omega)A(\omega)\}}{\mathrm{Tr}\{\Gamma^p(\omega)\}}$$
$$= \frac{\sum_{\gamma_p} \gamma_p \langle\gamma_p|-iG^<(\omega) + iG^>(\omega)|\gamma_p\rangle}{\sum_{\gamma_p} \gamma_p} \geqslant 0. \quad \text{(A20)}$$

APPENDIX B: ALTERNATIVE ZEROTH-LAW SCENARIO

In this appendix, we consider the question investigated previously in Ref. [11]: If the local temperatures and chemical potentials of two nonequilibrium quantum systems, as measured by a scanning thermoelectric probe, are equal, will the two systems be in thermal and electrical equilibrium with each other when connected by a transmission line coupled locally to the same two points? This question was answered in the affirmative [11] for a noninteracting system within linear response and to leading order in the Sommerfeld expansion. Here we extend the previous analysis to consider two systems under arbitrary steady-state nonequilibrium conditions.

In this section, we consider noninteracting electrons and neglect the spin-orbit interaction, so we omit the spin index. Let the fermion creation and annihilation operators of system A be denoted by $d^\dagger$, d and the corresponding Green's functions of system A by G^r, G^a, and $G^<$, as defined in Sec. II. Let the fermion creation and annihilation operators in system B be denoted by $f^\dagger$, f and denote the retarded, advanced, and Keldysh "lesser" Green's functions describing electron propagation/occupancy within system B by $g^r_{nm}(t) = -i\theta(t)\langle\{f_n(t), f^\dagger_m(0)\}\rangle$, $g^a_{nm}(t) = i\theta(-t)\langle\{f_n(t), f^\dagger_m(0)\}\rangle$, and $g^<_{nm}(t) = i\langle f^\dagger_m(0) f_n(t)\rangle$, respectively.

Suppose there is a point a in system A with local temperature $\bar{T}_p$ and chemical potential $\bar{\mu}_p$ as determined by a measurement specified by Eqs. (1) and (27), and that there is a corresponding point b in system B characterized by the same values of $\bar{T}_p$ and $\bar{\mu}_p$. The question is whether points a and b will be in equilibrium with each other when connected by a transmission line permitting the exchange of energy and charge.

Let the Hamiltonian coupling systems A and B be

$$H_{AB} = \sum_{\substack{n \in a \\ m \in b}} [V_{nm}d^\dagger_n f_m + \mathrm{H.c.}]. \quad \text{(B1)}$$

Then it can be shown using standard NEGF methods [32,33,39] that the electric current I_{AB} and energy current I^E_{AB} flowing from system B into system A are given by

$$I_{AB} = -\frac{e}{h}\int_{-\infty}^\infty d\omega\,\mathrm{Tr}\{[G^r(\omega) - G^a(\omega)]Vg^<(\omega)V^\dagger$$
$$+ G^<(\omega)V[g^a(\omega) - g^r(\omega)]V^\dagger\}, \quad \text{(B2)}$$

$$I^E_{AB} = \frac{1}{h}\int_{-\infty}^\infty d\omega\,\omega\,\mathrm{Tr}\{[G^r(\omega) - G^a(\omega)]Vg^<(\omega)V^\dagger$$
$$+ G^<(\omega)V[g^a(\omega) - g^r(\omega)]V^\dagger\}, \quad \text{(B3)}$$

respectively.

For the case where H_{AB} couples only a single localized orbital in system A to a single localized orbital in system B

with matrix element V, Eqs. (B2) and (B3) can be simplified to

$$I_{AB}^{(\nu)} = \frac{2\pi|V|^2}{\hbar} \int_{-\infty}^{\infty} d\omega\, \omega^\nu \rho_a(\omega)\rho_b(\omega)[f_b(\omega) - f_a(\omega)], \quad \text{(B4)}$$

where $\nu = 0$ gives the fermion number current and $\nu = 1$ gives the energy current. Here $f_a(\omega)$ and $f_b(\omega)$ are the local nonequilibrium distributions at points a and b, respectively, defined according to Eqs. (19) and (23), and $\rho_a(\omega)$ and $\rho_b(\omega)$ are the local densities of states at points a and b, respectively.

Notice that it is problematic in the present case to define a heat current, since neither system A nor system B possesses a local equilibrium. Nonetheless, the conditions

$$I_{AB}^{(\nu)} = 0, \quad \nu = 0, 1, \quad \text{(B5)}$$

suffice to define thermoelectric equilibrium between the two systems, and are equivalent to the conditions given by Eq. (1) for the case where the heat current can be defined.

Equations (1) and (27) imply

$$0 = \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega\, \omega^\nu \Gamma^p(\omega)\rho_a(\omega)[f_a(\omega) - f_p(\omega)], \quad \nu = 0, 1, \quad \text{(B6)}$$

$$0 = \frac{1}{\hbar} \int_{-\infty}^{\infty} d\omega\, \omega^\nu \Gamma^p(\omega)\rho_b(\omega)[f_b(\omega) - f_p(\omega)], \quad \nu = 0, 1. \quad \text{(B7)}$$

In linear response, it can be shown [11] that Eqs. (B6) and (B7) imply Eq. (B5) to leading order in the Sommerfeld expansion. Under general nonequilibrium conditions in systems A and B, Eqs. (B6) and (B7) imply Eq. (B5) provided $\Gamma^p(\omega)$, $\rho_a(\omega)$, and $\rho_b(\omega)$ can all be treated in the broadband limit. That is to say, they can be taken as constant in the region where $f_b(\omega) - f_a(\omega)$ and $f_a(\omega) - f_p(\omega)$ differ significantly from zero. Thus, the conditions for the validity of the zeroth law are somewhat more stringent for the scenario considered here than for the scenario considered in Sec. IV.

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