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Fourier's law of heat conduction: Quantum mechanical master equation analysis

Lian-Ao Wu and Dvira Segal
Chemical Physics Theory Group, Department of Chemistry, and Center for Quantum Information and Quantum Control, University of Toronto, 80 St. George Street, Toronto, Ontario M5S 3H6, Canada

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We derive the macroscopic Fourier's Law of heat conduction from the exact gain-loss time convolutionless quantum master equation under three assumptions for the interaction kernel. To second order in the interaction, we show that the first two assumptions are natural results of the long time limit. The third assumption can be satisfied by a family of interactions consisting of an exchange effect. The pure exchange model directly leads to energy diffusion in a weakly coupled spin-1/2 chain.

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Introduction. Fourier's law, connecting the rate of heat flow within a body to the temperature profile along the flow path, is an empirical law based on observation. Despite its fundamental nature, a derivation of this law from first principles does not yet exist [1].

In classical systems, extensive numerical simulations [2] and rigorous derivations [1,3,4] manifested the applicability of Fourier's law for specifically designed nonlinear systems. It is still a great challenge to derive this macroscopic law from microscopic *quantum* principles. Quantum simulations of heat flow in spin chains pointed out the validity of Fourier's law, in connection with the onset of quantum chaos [5,6]. More recent studies have focused on the derivation of this law from Schrödinger dynamics [7–9]. By using the Hilbert space average method, Michel *et al.* demonstrated the emergence of heat diffusion within a quasi degenerate level local Hamiltonian using the truncated Dyson series for the short-time displacement operator [7]. Using this approach, the transition from diffusive to ballistic dynamics at different length scales was further explored [9]. These works successfully manifested the onset of Fourier's law for a specific class of quantum models. The rigorous derivation of this law from quantum dynamics for general Hamiltonians is still a great challenge.

In this paper we employ the most general nonperturbative microscopic master equation of the gain-loss form to derive the Fourier's law quantum mechanically. Unlike the derivation in Ref. [7], applicable for a class of modular designed models, we use the most general local Hamiltonian. The diffusive behavior is obtained by making three assumptions on the interacting kernel in the microscopic master equation. These assumptions can be traced down to the structure of coupling between local sites. At weak coupling, approaching the long time limit, we furthermore demonstrate that the first and second assumptions are independent of the specific form of the interaction, and the exchange interaction plays the decisive role in order for the third assumption to hold.

Master equation. Consider a system with N local units (particles), each has the same M (could be infinite) dimensional eigenspace spanned by bases $\{|n\rangle\}$, possibly coupled to their own baths. The eigenspace of all N particles is spanned by bases $\{|\mathbf{n}\rangle = |n_1\rangle_1 |n_2\rangle_2 |n_i\rangle_i \ldots |n_N\rangle_N\}$. The most general Hamiltonian of the system and its bath is

$$H = H_0 + \lambda H_I, \tag{1}$$

where $H_0 = H_S + H_B$ and $H_S = \Sigma_{i=1}^{N} \Sigma_{n_i} \epsilon_{n_i}(i) |n_i\rangle_i \langle n_i|$ is the system Hamiltonian. We assume that the energy spectra of the sites are identical, $\epsilon_n(i) = \epsilon_n(j) \geq 0$, and the ground state energy is set as zero. H_B is the bath Hamiltonian, consisting degrees of freedom other than included in the system. The bath may act locally on each site, $H_B = \Sigma_{i=1}^{N} H_B(i)$, where $H_B(i)$ couples to the ith local site. The second term H_I includes interactions between system particles, where λ characterizes the strength of these interactions. It can be generally written as $H_I = \Sigma |\mathbf{n}\rangle\langle\mathbf{m}| B_{\mathbf{nm}}$, where $B_{\mathbf{nm}}$'s are the matrix elements of either system or bath operators. Practically, our derivation of the Fourier law does not require the existence of local thermal reservoirs, thus we focus later on a closed system, as done in Ref. [7] for a specific model [see text after Eq. (5)]. The dynamics obeys the Liouville equation $\frac{\partial}{\partial t} \rho_{tot}(t) = -i\lambda [H_I(t), \rho_{tot}(t)] \equiv \lambda \mathcal{L}(t) \rho_{tot}(t)$, where ρ_{tot} is the density matrix of the total system, and we work in the interaction representation $H_I(t) = e^{iH_0 t} H_I e^{-iH_0 t}$. The Liouville superoperator $\mathcal{L}(t)$ is defined by this equation. The super projection operation of interest, $\rho(t) = \mathcal{P} \rho_{tot}(t)$, defines the *relevant* part of the total density matrix for the open system. This part exactly satisfies the time-local master equation [10]

$$\frac{\partial}{\partial t} \rho(t) = \mathcal{K}(t) \rho(t), \tag{2}$$

given that the initial state is in the relevant subspace, $\mathcal{P} \rho_{tot}(0) = \rho_{tot}(0)$. The time-convolutionless generator $\mathcal{K}(t)$ is in general an extremely complicated object, calculated using perturbative expansions [10]. Though the time-local master equation (2) is less well known than the Nakajima-Zwanzig equation [11,12], it is easy to show that these forms are equivalent for non-diverging superoperators [13]. In order to project the diagonal part of the total density $\rho_{tot}(t)$ we use the following projection [13,12]:

$$\mathcal{P} \rho_{tot} = \sum |\mathbf{n}\rangle\langle\mathbf{n}| \mathrm{tr}\{|\mathbf{n}\rangle\langle\mathbf{n}| \rho_{tot}\} \otimes \rho_B, \tag{3}$$

where ρ_B is the bath thermal equilibrium density matrix, and the trace is taken over both system and bath states. Note that $\mathrm{tr}\{|\mathbf{n}\rangle\langle\mathbf{n}| \rho_{tot}\} = P_{\mathbf{n}}$ defines the probability to find the system in state $|\mathbf{n}\rangle$. The time-local master equation can be exactly written as [14]

$$\frac{dP_{\mathbf{n}}}{dt} = \sum_{\mathbf{m}} W_{\mathbf{nm}}(t)P_{\mathbf{m}} - \sum_{\mathbf{m}} W_{\mathbf{mn}}(t)P_{\mathbf{n}}, \tag{4}$$

where the rates, or interacting kernels $W_{\mathbf{nm}}(t)$, are complicated functionals of the interaction $H_I(t)$. Assuming that $\mathcal{P}L(t)\mathcal{P}=0$, which is true for closed systems [12] and for many open systems [10], to second order in H_I the expansion $\mathcal{K}(t)=\int_0^t ds\mathcal{P}L(t)\mathcal{L}(s)\mathcal{P}$ holds. One then obtains

$$W_{\mathbf{mn}}(t) = 2\lambda^2 \,\mathrm{Re}\int_0^t d\tau D_{\mathbf{nm}}(\tau)e^{i(E_{\mathbf{n}}-E_{\mathbf{m}})\tau}, \tag{5}$$

where $B_{\mathbf{nm}}(\tau)=e^{iH_B\tau}B_{\mathbf{nm}}e^{-iH_B\tau}$, and $D_{\mathbf{nm}}(\tau)=\mathrm{tr}_B\{B_{\mathbf{nm}}(\tau)B_{\mathbf{mn}}\rho_B\}$. The total energy $E_{\mathbf{n}}=\sum_{i=1}^N\epsilon_{n_i}(i)$ is an eigenvalue of H_S. For a closed system $D_{\mathbf{nm}}(\tau)=|B_{\mathbf{mn}}|^2$, where $B_{\mathbf{nm}}$'s are c numbers.

The gain-loss master equation (2) was introduced for a *closed* system, and proved vigorously in Ref. [12]. In the long time limit, or Markovian limit, the time-dependent interacting kernel $W(t)$ becomes a constant matrix for both open or closed systems [15]. In what follows we focus on a *closed* system (no local reservoirs), and study energy diffusion between system units due to the (system induced) H_I coupling. The starting point of our derivation is the exact equation (2) with a *nonperturbative* kernel W.

Assumptions and derivation. First consider a one-dimensional system. We employ the nearest neighbor interaction form $H_I=\sum_{i=1}^{N-1}V(i,i+1)$, where the symmetry $V(i,i+1)=V(i+1,i)$ holds. Our *first assumption* is that the interacting kernel matrix W takes the same symmetry as the interaction, i.e., $W=\sum_{i=1}^{N-1}W(i,i+1)$ and $W(i,i+1)=W(i+1,i)$. This "localization" assumption implies that the many-site correlation (kernel W) is given by the sum of two-site correlations $W(i,i+1)$. This assumption is not trivial as the interacting kernels are not lineally related to the interaction H_I. The matrix elements of W are therefore given by

$$W_{\mathbf{nm}}(t) = \sum_{i=1}^{N-1} W_{n_in_{i+1},m_im_{i+1}}(i,i+1;t)\prod_{j\neq i,i+1}\delta_{n_jm_j}. \tag{6}$$

As diagonal elements ($\mathbf{n}=\mathbf{m}$) do not contribute to Eq. (4), they are allowed to be exceptions of the assumption. Our *second assumption* describes energy conservation between initial and final system states,

$$W_{n_in_{i+1},m_im_{i+1}}(i,i+1;t) = \begin{cases} w_{n_in_{i+1}}(i,i+1;t); & n_i=m_{i+1} \text{ and } n_{i+1}=m_i \\ 0; & \text{otherwise.}\end{cases} \tag{7}$$

Besides energy conservation, this condition also implies that the local spectra are *anharmonic*, see discussion after Eq. (17). In the *third assumption*, we assume that $w_{n_in_{i+1}}(i,i+1;t)=w(i,t)$, independent of the n_i and n_{i+1} quantum numbers. The probability of finding the ith particle in state $|n_i\rangle_i$ is

$$P_{n_i}(i) = \mathrm{tr}\{|n_i\rangle_i\langle n_i|\rho_{tot}\} = \sum_{n_j\neq n_i} P_{\mathbf{n}}. \tag{8}$$

Incorporating Eqs. (6)–(8) into (4) we obtain

$$\frac{dP_n(i)}{dt} = w(i,t)[P_n(i+1)-P_n(i)] - w(i-1,t)[P_n(i)-P_n(i-1)], \tag{9}$$

where for convenience we use the short notation $P_n(i)$. In deriving (9) we have also utilized the symmetry $W(i,i+1)=W(i+1,i)$ which holds exactly for a closed system at second order [see text after Eq. (5)]. Next we write an equation of motion for the internal energy at each site, $u(i)=\sum\epsilon_nP_n(i)$,

$$\frac{du(i)}{dt} = w(i,t)[u(i+1)-u(i)] - w(i-1,t)[u(i)-u(i-1)]. \tag{10}$$

The continuous version of this equation is

$$\frac{\partial u(x,t)}{\partial t} = a^2\frac{\partial}{\partial x}\left(w(x,t)\frac{\partial u(x,t)}{\partial x}\right), \tag{11}$$

where a is the distance between neighboring sites. Generalization of this derivation to a three-dimensional simple cubic lattice is straightforward, leading to Eq. (11) with $\mathbf{r}$ and $\boldsymbol{\nabla}$ replacing $\frac{\partial}{\partial x}$ and x. Applying the continuity equation for the energy density, $\frac{\partial u(\mathbf{r},t)}{\partial t}=-\boldsymbol{\nabla}\cdot\mathbf{J}(\mathbf{r},t)$, $\mathbf{J}$ is the heat current, we exactly obtain the Fourier law

$$\mathbf{J}(\mathbf{r},t) = -w(\mathbf{r},t)a^2\boldsymbol{\nabla}u(\mathbf{r},t) = -\kappa(\mathbf{r},t)\boldsymbol{\nabla}T(\mathbf{r},t). \tag{12}$$

Here $T(\mathbf{r},t)$ denotes the temperature profile and $\kappa(\mathbf{r},t)=w(\mathbf{r},t)a^2C_V$ with $C_V=\partial u/\partial T$ as the specific heat. The heat conductivity κ is essentially time dependent due to the explicit time dependence of the microscopic rates $w(\mathbf{r},t)$. In the long time, or Markovian limit, the microscopic rates and the temperature profile become constants, leading to a time-independent relation. Equation (12) is the main result of our paper. It characterizes the intrinsic properties of a closed system. We emphasize that it was derived from the exact master equation (2) for a generic local Hamiltonian. While most studies in this context analyze the onset of the Fourier's law in nonequilibrium steady-state situations [2], here we have shown that an isolated system prepared with an arbitrary nonuniform temperature may relax obeying Fourier's dynamics [1].

An exact model in the second order. We present next a model Hamiltonian that exactly satisfies the three assumptions leading to Fourier's law in the Markovian limit. We assume a closed system, and employ a pure exchange interaction form

$$H_I = \sum_{i=1}^{N-1} J_{i,i+1}\mathcal{E}^{(i,i+1)}. \tag{13}$$

Here $\mathcal{E}^{(i,i+1)}$ is the permutation operator and $J_{i,i+1}$ are nearest-neighbor coupling constants (superexchange for spin system), taken as constants $J_{i,i+1}=J$ and set to one in the following discussion. In the two-level case ($M=2$), since $\mathcal{E}^{(i,i+1)}=\frac{1}{2}(1+\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_{i+1})$, Eq. (13) is simply the Heisenberg spin-1/2 exchange interaction model. The correlation function in (5) is given by

$$D_{\mathbf{nm}}(\tau) = \sum_{i=1}^{N-1} \delta_{n_i m_{i+1}} \delta_{n_{i+1} m_i} \prod_{j \neq i,i+1} \delta_{n_j m_j}, \tag{14}$$

when $\mathbf{n} \neq \mathbf{m}$, satisfying the first assumption. Furthermore, the second assumption is fulfilled here exactly as the matrix W has the exact form of Eq. (7) with $w(i,t)=2\lambda^2 t$. In order to check the validity of the second-order approximation, we compare this result with the exact solution for a three unit system, $N=3$ and $M=2$. Let the initial state be $|1\rangle_1|0\rangle_2|0\rangle_3$. We can get an exact solution for the dynamics for the interaction (13), $dP_1(2)/dt=w(t)[P_1(1)+P_1(3)-2P_1(2)]$, where $w(t)=\frac{\sqrt{2}\lambda \sin(2\sqrt{2}\lambda t)}{2\cos^2(\sqrt{2}\lambda t)-1}$. For weak coupling (small λ), $w(t)=2\lambda^2 t$, which is the same as the second order result. While this model satisfies all three assumptions, in the long time limit it does not lead to the standard Fourier's law with a constant conductivity.

However, the energy difference between spin states of site i may slightly differ from that of site $i+1$, $\Delta_{n_i,n_{i+1}}(i) = [\epsilon_{n_i}(i)-\epsilon_{n_{i+1}}(i)]-[\epsilon_{n_i}(i+1)-\epsilon_{n_{i+1}}(i+1)] \neq 0$. This effect may originate from thermal fluctuations. In this case, $w_{n_i n_{i+1}}(i,t) = 2\lambda^2 \frac{\sin(\Delta_{n_i,n_{i+1}}(i))t)}{\Delta_{n_i,n_{i+1}}(i)}$. At short times, if the difference $\Delta_{n_i,n_{i+1}}(i)$ is small, one again finds $w(t) \propto t$. In contrast, at long times $w_{n_i n_{i+1}}(i) \rightarrow 2\pi\lambda^2 \delta(\Delta_{n_i,n_{i+1}}(i))$. When the energy spectrum of each spin state forms a band that is dense enough [16], the Fermi's Golden rule is obtained, $w_{n_i n_{i+1}}(i)=2\pi\lambda^2\Gamma(0)$, where $\Gamma(0)$ is the density of states at zero detuning.

Thus, this simple exchange model exactly reproduces the long time Fourier law (12) with $\kappa=2\pi\lambda^2 a^2 C_V \Gamma(0)$. This result manifests that the local sites do not need to acquire exactly identical spectra. It also provides a microscopic explanation of the validity of Fourier's law in spin chains with Heisenberg-type interactions [17].

Long time (Markovian) limit. Next we show that at second order in the interacting kernel the first two assumptions [Eqs. (6) and (7)] are model independent in the long time limit, and the third assumption is valid for family of interactions with exchange effect. We consider the most general interaction $V(i,i+1)$ for a one-dimensional system. It is easy to show that

$$B_{\mathbf{nm}} = \sum_{i=1}^{N-1} V_{n_i n_{i+1}, m_i m_{i+1}}(i,i+1) \prod_{l \neq i,i+1} \delta_{n_l m_l}. \tag{15}$$

In the long time (Markovian) limit Eq. (5) reduces to

$$W_{\mathbf{mn}}(t \rightarrow \infty) = 2\pi\lambda^2 |B_{\mathbf{mn}}|^2 \delta(E_{\mathbf{n}} - E_{\mathbf{m}}), \tag{16}$$

using $\frac{\sin[(E_{\mathbf{n}}-E_{\mathbf{m}})t]}{(E_{\mathbf{n}}-E_{\mathbf{m}})} \rightarrow \pi\delta(E_{\mathbf{n}}-E_{\mathbf{m}})$ when $t \rightarrow \infty$. Assuming the bound states are nondegenerate, a somewhat tedious calculation shows that the first assumption is satisfied, and the off-diagonal matrix elements are given by

$$W_{n_i n_{i+1}, m_i m_{i+1}}(i,i+1;t) = 2\pi\lambda^2 |V_{n_i n_{i+1}, m_i m_{i+1}}(i,i+1)|^2 \times \delta(\Delta_{n_i n_{i+1}, m_i m_{i+1}}), \tag{17}$$

where $\Delta_{n_i n_{i+1}, m_i m_{i+1}} = \epsilon_{n_i} + \epsilon_{n_{i+1}} - \epsilon_{m_i} - \epsilon_{m_{i+1}}$. Since $\epsilon_n \geq 0$, the delta function in Eq. (17) implies that $\epsilon_{n_i} = \epsilon_{m_{i+1}}$ and $\epsilon_{n_{i+1}} = \epsilon_{m_i}$, provided that the energy spectra are *anharmonic*. Therefore, in the nondegenerate case, only transitions between the quantum states $n_i = m_{i+1}$ and $n_{i+1} = m_i$ exist, in accordance with the second assumption. In contrast, when the energy spectra are *strictly harmonic*, the delta function can be satisfied for a large number of combinations, $\epsilon_{n_i} - \epsilon_{m_i} = \epsilon_{m_{i+1}} - \epsilon_{n_{i+1}} = j\omega_0$. Here ω_0 is the energy difference between subunit states (equal for all N) and j is an integer. In this case the second assumption does not hold, and we cannot derive Eq. (9) and the subsequent result (12). Thus, interestingly, in order to derive Fourier's law, the system spectrum should be anharmonic, in accordance with classical results [1,2].

At second order, the first two assumptions are therefore the results of the Markovian limit. As discussed above, we can expect that there is a dense band structure around each level ϵ_n, originating from bath fluctuations or quantum tunneling between sites. Defining the density of states at the energy difference around Δ as $\Gamma(\Delta)$, we obtain [16]

$$w_{n_i n_{i+1}}(i) = 2\pi\lambda^2\Gamma(0)|V_{n_i n_{i+1}, n_{i+1} n_i}(i,i+1)|^2, \tag{18}$$

which manifests that the third assumption is valid, depending on the form of specific Hamiltonians. We calculate next the microscopic rates for different types of interactions. Assuming translational symmetry in the system, we need only discuss a pair of sites, for instance between site 1 and 2, $V_{n_1 n_2, n_2 n_1}(1,2) = \langle n_1 n_2 | V(1,2) | n_2 n_1 \rangle$.

In general, particles at each site may be electrons or atoms. To simplify, we consider the case with one particle at each site. Our first example is the short-range delta interaction, $V(1,2)=g\delta(r_{12})$, where $r_{12}=|x_2-x_1|$, and $x_1(x_2)$ is the coordinate of the first (second) particle. Physically, this interaction describes particles that move almost independently in the site interior, while collisions, leading to energy exchange between particles, occur at the edge points $x_1=x_2$. This picture is appropriate for describing phonon collisions in solids [18]. For this type of interaction the matrix elements become

$$V_{n_1 n_2, n_2 n_1}(1,2) = g \int dx |\phi_{n_1}(x)|^2 |\phi_{n_2}(x)|^2. \tag{19}$$

This integral is almost independent of quantum numbers n_1 and n_2 for many systems [19]. Therefore, the third assumption is generally valid for short-range interactions. For example, in one-dimensional infinite square well (width d) with the wave function $\phi_n(x)=\sqrt{\frac{2}{d}} \sin \frac{n\pi x}{d}$, the matrix element $V_{n_1 n_2, n_2 n_1}(1,2)=1/d$ is completely independent of quantum numbers, assuming $d > a$ so that two particles could collide.

Our second example is the long-range interaction. We choose the general form $V(1,2)=V(r_{12})(\lambda_1+\lambda_2\mathcal{E}^{(1,2)})$, where the λ's are constants and $\mathcal{E}^{(1,2)}$ is the spacious exchange operator [20]. Considering the first-order contribution to this potential, $V(1,2)=|x_2-x_1|(\lambda_1+\lambda_2\mathcal{E}^{(1,2)})$, the matrix elements $V_{n_1 n_2, n_2 n_1}(1,2)$ become the sum of the direct (D) and exchange (E) terms,

$$V^D_{n_1 n_2, n_2 n_1}(1,2) = \lambda_1 \int dx_1 dx_2 \phi^*_{n_1}(x_1)\phi^*_{n_2}(x_2)|x_2 - x_1| \times \phi_{n_1}(x_2)\phi_{n_2}(x_1),$$

$$V^E_{n_1n_2,n_2n_1}(1,2) = \lambda_2 \int dx_1 dx_2 |\phi_{n_1}(x_1)|^2 \times |\phi_{n_2}(x_2)|^2 |x_2 - x_1|.$$

In what follows we take $\lambda_1 = \lambda_2 = 1$. If the overlap between the wave functions of two particles is zero, the direct integral diminishes because of the orthogonality of two states, and the exchange integral $(x_2 > x_1)$ is $V^E_{n_1n_2,n_2n_1}(1,2) = a + \langle n_2 | x_2' | n_2 \rangle - \langle n_1 | x_1 | n_1 \rangle$, where $x_2' = x_2 - a$ is the relative coordinate of particle 2. If the wave function, $\phi_n(x)$ has a well-defined parity, $\langle n | x | n \rangle = 0$ for the relative coordinate of each particle, implying that $V_{n_1n_2,n_2n_1}(1,2) = a$ is a constant. This satisfies the third assumption. Note that the result is independent of the details of the local Hamiltonian.

If the overlap is not zero, yet small, the direct integral is expected to be small. Considering again the one-dimensional infinite square well, when $a/d < 1$, two particles will overlap. Numerical calculations show that for quantum numbers n_1, n_2 ranging from 1 to 20 the direct integrals are less than one-tenth of the exchange integrals and $V_{n_1n_2,n_2n_1}(1,2)$ is almost a constant, very close to a (derivation around 3% when $0.4 < a/d < 1$). The larger the values of a/d, the smaller the ratio between the direct and the exchange integrals.

We also calculate the interaction $V(1,2)$ for the harmonic potential $V(r_{1,2}) = r_{12}^2$. We find that when a/d varies from 0.7 to 0.95 the exchange integral is almost a constant with deviations from 14% to 4%, and the ratio between the direct and exchange integrals is 0.14–0.1.

The temperature dependence of the heat conductivity κ results from the interplay between the specific heat and the interaction kernel. The specific heat, defined per unit, can be easily calculated for different models, e.g., for a spin chain of ω_0 spacing, $C_V = \frac{\omega_0^2}{T^2} e^{\omega_0/T} (e^{\omega_0/T} + 1)^{-2}$. In contrast, our approach does not directly bring in the temperature dependence of the kernel $W_{\mathbf{mn}}$. Physically, since $V_{n_1n_2,n_2n_1}(1,2)$ is a function of the intersite separation, the lattice vibrations can modify it, thus introduce temperature dependent transition rates. This effect can be successfully included by phenomenologically introducing a temperature dependent interaction [21,22]. Here we adopt the simple form $V_T(r_{12}) = V(r_{12}) \gamma(r_{12}, T)$, where T may be the average temperature of site 1 and 2, and $\gamma(r_{12}, T) = \exp[-\alpha f(T) r_{12}]$. In the case of interacting ions [21], α is inversely proportional to the Fermi velocity and $f(T) = T$. When $f(T) \to \infty$, $V_T(r_{12}) \to \frac{2}{\alpha f(T)} V(0) \delta(r_{12})$. Therefore, for high temperatures $\kappa \propto 1/f(T)^2$, as the lattice specific heat typically saturates. For the ionic solid of Ref. [21] one obtains $\kappa \propto 1/T^2$, in agreement with standard expectations [18].

Summary. We have presented a microscopic quantum derivation of Fourier's law of heat conduction that is not limited to specifically designed models. The derivation relies on three assumptions that are satisfied in weak coupling and at long times for a family of exchange interaction potentials. Our analysis naturally implies that energy diffusion cannot emerge in closed harmonic models, in agreement with the behavior of classical systems.

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