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Fourier's law and many-body quantum systems

La loi de Fourier et les systèmes quantiques à n *corps*

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ABSTRACT

The topic of this article are transport properties of many-body quantum chains accompanying DMRG-type simulations of the Bose–Hubbard model. To set the stage, we first provide a very brief introduction to many-body quantum theory and tensor network approximations. Transport properties are studied via dynamical density correlation functions, in line with linear response theory. We observe diffusive behavior at "infinite temperature" $T \to \infty$. Finally, we mention other approaches to study transport, e.g., explicitly imposing a temperature gradient via thermal reservoirs at the boundary.

RÉSUMÉ

Cet article porte sur les propriétés de transport de chaînes quantiques à *n* corps en s'accompagnant de simulations de type « groupe de renormalisation de matrice de densité » du modèle de Bose–Hubbard. Pour dresser une vue d'ensemble, nous présentons d'abord une très brève introduction à la théorie quantique à *n* corps et aux approximations des réseaux de tenseurs. Les propriétés de transport sont étudiées à l'aide de fonctions dynamiques de corrélation de densité, en suivant la théorie de la réponse linéaire. Nous observons un comportement diffusif à « température infinie » $T \to \infty$. Enfin, nous mentionnons d'autres approches permettant d'étudier le transport, par exemple en imposant explicitement un gradient de température via des réservoirs thermiques aux bords.

1. Introduction

This article is concerned with Fourier's law and transport properties in general for many-body quantum systems. To start, one first has to relate the concept of thermal conduction to quantum mechanics. The approach presented here invokes linear response theory, i.e. the effect (to lowest order) of a small perturbation on the system initially in thermal equilibrium. Concerning transport, the idea is to quantify how a localized perturbation (effected by heating for example) spreads in

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time. After a brief introduction to many-body quantum theory, we will outline and present DMRG-type simulations of the quantum Bose–Hubbard model. Alternative approaches to study thermal conduction are reviewed in the final section.

2. Primer of many-body quantum theory

While a comprehensive introduction to quantum mechanics is beyond the scope of the present article (see, for example, the textbooks [1–3] for an introduction), we briefly outline the essential ingredients required in the next sections. The quantum system at the current time point is described by the so-called quantum wavefunction ψ, which is an element of the quantum Hilbert space $\mathcal{H}$ [4] corresponding to the physical system of interest. We take this Hilbert space to be finite-dimensional here, and imagine that the physical system consists of a finite lattice with L sites formed by, e.g., the atoms in an optical lattice or in a solid. Each site j is modeled by a complex d-dimensional vector space $\mathcal{V}_j$; for "qubits" $d = 2$, for example. Then the Hilbert space is the tensor product

$$\mathcal{H} = \bigotimes_{j=1}^{L} \mathcal{V}_j \tag{1}$$

The inner product on $\mathcal{H}$ is the usual ℓ^2 inner product, denoted $\langle\cdot|\cdot\rangle$, with the convention that it is linear in its *second* argument.

In particular, to represent a general wavefunction $\psi \in \mathcal{H}$, one requires d^L complex coefficients. Denoting by e_i the i-th unit vector, $i = 1, \dots, d$, the canonical orthonormal basis of $\mathcal{H}$ may be enumerated as $\{|i_1, \dots, i_L\rangle\}_{i_1,\dots,i_L=1}^{d}$ with

$$|i_1, \dots, i_L\rangle = e_{i_1} \otimes \cdots \otimes e_{i_L} \tag{2}$$

The wavefunction can thus be represented as

$$\psi = \sum_{i_1=1}^{d} \cdots \sum_{i_L=1}^{d} \alpha_{i_1,\dots,i_L} |i_1, \dots, i_L\rangle \tag{3}$$

using complex parameters $\alpha_{i_1,\dots,i_L} \in \mathbb{C}$.

Quantum mechanics associates an average energy with the wavefunction ψ and describes its time evolution via the so-called Hamiltonian operator H, i.e. a Hermitian matrix acting on $\mathcal{H}$. Specifically, the average energy is equal to $\langle\psi|H\psi\rangle$. The time evolution is governed by the famous Schrödinger equation

$$\mathrm{i}\hbar\partial_t \psi(t) = H\psi(t) \tag{4}$$

where i is the imaginary unit and $\hbar$ the reduced Planck constant, leading to the time dependence $\psi(t) = \mathrm{e}^{-\mathrm{i}Ht/\hbar}\psi(0)$. The *time evolution operator* $\mathrm{e}^{-\mathrm{i}Ht/\hbar}$ is unitary since H is Hermitian. For notational simplicity, we choose units such that $\hbar = 1$. Note that a time-dependent expression like $\langle\chi(t)|A\psi(t)\rangle$ (with ψ and χ quantum wavefunctions, and A an arbitrary matrix acting on $\mathcal{H}$) can be rewritten as

$$\langle\chi(t)|A\psi(t)\rangle = \left\langle \mathrm{e}^{-\mathrm{i}Ht}\chi \middle| A\mathrm{e}^{-\mathrm{i}Ht}\psi \right\rangle = \left\langle \chi \middle| \mathrm{e}^{\mathrm{i}Ht}A\mathrm{e}^{-\mathrm{i}Ht}\psi \right\rangle = \langle\chi|A(t)\psi\rangle \tag{5}$$

when using the so-called Heisenberg representation

$$A(t) = \mathrm{e}^{\mathrm{i}Ht}A\mathrm{e}^{-\mathrm{i}Ht} \tag{6}$$

By convention, ψ, χ, and A (without explicit time argument) are understood as initial ($t = 0$) or stationary states.

We assume that the Hamiltonian H is prescribed and well known. To provide a concrete example, the Hamiltonian of the Heisenberg model on a one-dimensional lattice reads

$$H = \frac{1}{2}\sum_{j=1}^{L}\left(\sum_{\alpha=x,y,z} J_\alpha \sigma_j^\alpha \sigma_{j+1}^\alpha + h\sigma_j^z\right) \tag{7}$$

where J_α and h are real parameters and σ_j^α is the α-th 2×2 Pauli matrix acting on lattice site j. The Pauli matrices are

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{8}$$

The expression $\sigma_j^\alpha\sigma_{j+1}^\alpha$ is a compact notation for the outer product of 2×2 identity operators and the Pauli matrices:

$$\sigma_j^\alpha\sigma_{j+1}^\alpha = \underbrace{I\otimes\cdots\otimes I}_{j-1} \otimes \sigma^\alpha \otimes \sigma^\alpha \otimes \underbrace{I\otimes\cdots\otimes I}_{L-j-1} \tag{9}$$

An important concept required for the following is the *thermal Gibbs ensemble* average: one imagines that the quantum system is in one of a number of states ψ_n with probability p_n. It will be convenient to define a corresponding *density matrix* as

$$\rho = \sum_n p_n \, |\psi_n\rangle\langle\psi_n| \tag{10}$$

where $|\psi_n\rangle\langle\psi_n|$ is the physicists' notation of the outer product of ψ_n with itself, i.e. applied to any $\chi \in \mathcal{H}$: $(|\psi_n\rangle\langle\psi_n|)\chi = \psi_n\langle\psi_n|\chi\rangle$. The density matrix of the thermal Gibbs ensemble at temperature T may be defined by letting the ψ_n's be the complete basis of eigenstates of H, i.e. $H\psi_n = \epsilon_n\psi_n$ for all $n = 1, \ldots, \dim(\mathcal{H})$ with energy $\epsilon_n \in \mathbb{R}$. The corresponding probabilities are chosen as $p_n = \frac{1}{Z}\mathrm{e}^{-\beta\epsilon_n}$ with inverse temperature $\beta = \frac{1}{k_\mathrm{B}T}$, k_B the Boltzmann constant and the "partition function" Z acting as normalization factor. Thus

$$\rho = \sum_n \frac{1}{Z}\mathrm{e}^{-\beta\epsilon_n} \, |\psi_n\rangle\langle\psi_n| = \frac{1}{Z}\mathrm{e}^{-\beta H}, \quad Z = \mathrm{tr}\left[\mathrm{e}^{-\beta H}\right] \tag{11}$$

The expression $\mathrm{e}^{-\beta H}$ is the matrix exponential of the Hamiltonian H multiplied by $-\beta$. Accordingly, the thermal Gibbs ensemble average of an operator A is defined as

$$\langle A\rangle_\mathrm{eq} = \sum_n \frac{1}{Z}\mathrm{e}^{-\beta\epsilon_n}\langle\psi_n|A\psi_n\rangle = \frac{1}{Z}\,\mathrm{tr}\left[\mathrm{e}^{-\beta H}A\right] \tag{12}$$

For later use, we denote the "connected correlation" (covariance) of two operators A and B as

$$\langle A; B\rangle_\mathrm{eq} = \langle AB\rangle_\mathrm{eq} - \langle A\rangle_\mathrm{eq}\langle B\rangle_\mathrm{eq} \tag{13}$$

Fourier's law of heat conduction can be regarded as a special case of (energy) transport properties in general. Here we focus on *linear response theory* for quantum systems [3] to investigate the question of how a small (local) perturbation of a system in thermal equilibrium influences (to lowest order) a measurable operator A at some later time (and potentially at some different location), i.e. the spatiotemporal dynamics of the perturbation. Starting from some time t_0, a small perturbation $\epsilon V(t)$ with $\epsilon \ll 1$ is assumed to act on the system. The perturbation is taken into account as an additional term in the Hamiltonian:

$$\tilde{H}(t) = H + \epsilon V(t)\,\theta(t - t_0) \tag{14}$$

with the Heaviside step function θ expressing the onset at t_0. Note that the time dependence in (14) is the explicit time dependence of the perturbation (e.g., a time-varying external field), not the Heisenberg representation in (6). The ensemble average of A under the dynamics induced by $\tilde{H}$ now likewise depends on time: starting from Eq. (12) at t_0, one obtains

$$\langle A\rangle_t = \sum_n \frac{1}{Z}\mathrm{e}^{-\beta\epsilon_n}\langle\psi_n(t)|A\psi_n(t)\rangle \tag{15}$$

where the $\psi_n(t)$, $t \le t_0$, are the eigenstates of H as before, but are subject to time evolution according to the perturbed Hamiltonian for $t \ge t_0$:

$$i\partial_t\psi_n(t) = \tilde{H}(t)\psi_n(t) \tag{16}$$

We keep the definition of $\langle\cdot\rangle_\mathrm{eq}$ in (12) independent of the perturbation. Linear response theory and the Kubo formalism [3] express the deviation of $\langle A\rangle_t$ from $\langle A\rangle_\mathrm{eq}$ as

$$\delta A(t) := \langle A\rangle_t - \langle A\rangle_\mathrm{eq} = -i\int_{t_0}^{t}\left\langle\left[\mathrm{e}^{\mathrm{i}H(t-\tau)}A\mathrm{e}^{-\mathrm{i}H(t-\tau)}, \epsilon V(\tau)\right]\right\rangle_\mathrm{eq}\mathrm{d}\tau + \mathcal{O}(\epsilon^2) \tag{17}$$

with $[A, B] = AB - BA$ the commutator of two operators A and B. Thus, we have expressed $\delta A(t)$ as a time integral over the equilibrium correlation between A and the perturbation $\epsilon V(\tau)$.

The Kubo formula (17) forms the starting point for the Green–Kubo relations [5,6], which express the conductivity as equilibrium-averaged autocorrelation of the current operator.

3. Tensor network methods

Simulating many-body quantum systems on (classical) computers poses a challenging task due to the inherent "curse of dimensionality". As detailed in the previous section, even storing all d^L complex coefficients of the wavefunction is not feasible if L exceeds on the order of 30 lattice sites (for $d = 2$). Thus physically inspired ansatzes and approximations are required, and the challenge has spurred the development of several computational approaches [7,8]. For quasi-one-dimensional lattice systems, the density matrix renormalization group (DMRG) framework [9–11] has emerged as one of the most successful methods. Modern formulations are based on tensor networks [12–18], and further developments and improvements of associated algorithms remain an active field of research.

While a detailed introduction to tensor network methods is beyond the scope of the present article, the following paragraphs try to convey the main principles: the central idea is to approximate the quantum wavefunction ψ as a tensor network, as illustrated in Fig. 1. On a one-dimensional lattice, this is known as "matrix product state" in the physics community. More formally, the wavefunction coefficients $\alpha_{i_1,\dots,i_L}$ (see Eq. (3) above) are interpreted as tensors of rank L, which are approximated as

$$\alpha_{i_1,\dots,i_L} \approx A^{(1)}_{i_1} \cdot A^{(2)}_{i_2} \cdots A^{(L)}_{i_L} \tag{18}$$

Here $A^{(j)}_i \in \mathbb{C}^{D_{j-1}\times D_j}$ is a complex matrix for each $i = 1,\dots,d$ and $j = 1,\dots,L$, the D_j are the so-called virtual bond dimensions (with dummy boundary dimensions $D_0 = D_L = 1$), and $\cdot$ is the usual matrix–matrix product. Alternatively, one may interpret $A^{(j)}$ as a rank-3 tensor in $\mathbb{C}^{d\times D_{j-1}\times D_j}$. We denote the largest occurring bond dimension by $D_{\max}$, i.e. $D_{\max} = \max\{D_0,\dots,D_L\}$. Thus the number of parameters on the right-hand side of Eq. (18) scales linearly with system size L, if $D_{\max}$ is bounded independent of L.

How is the approximation (18) justified? This question has been addressed by a large body of research in the physics community and is intimately related to physical "entanglement" [19]. In one sentence, the so-called "area law of entanglement" states that, at least for ground-state wavefunctions (lowest energy eigenstates) of Hamiltonians with local interactions (and away from a critical point), $D_{\max}$ can indeed be bounded independent of L. Thus, the tensor network ansatz (18) achieves a remarkable reduction from $\mathcal{O}(d^L)$ to $\mathcal{O}(d\,D^2_{\max}\,L)$ coefficients.

Moreover, typical quantum Hamiltonian operators on one-dimensional lattices can be *exactly* represented in tensor network form [12,20]. This works by the same principle as the MPS ansatz, but using two physical "legs" per lattice site (to represent a matrix instead of a vector), see Fig. 2, and is denoted "matrix product operator" (MPO).

Tensor networks with quasi-one-dimensional topology are well suited for efficient numerical manipulation; in particular, they can be efficiently contracted. For example, $\langle\psi|H\psi\rangle$ can be evaluated numerically exactly via a successive contraction

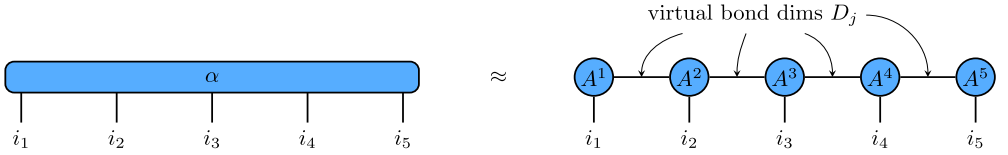

Fig. 1. The matrix product state (MPS) tensor network ansatz, shown for $L = 5$ lattice sites.

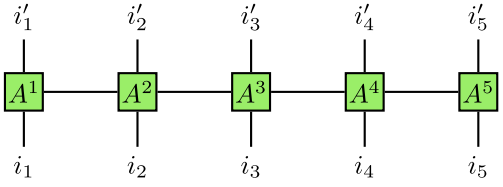

Fig. 2. A matrix product operator (MPO), shown for $L = 5$ lattice sites.

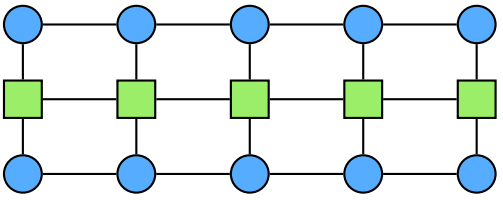

Fig. 3. Graphical representation of the tensor network for computing expectation values like $\langle\psi|H\psi\rangle$, with ψ the quantum wavefunction (blue) on a one-dimensional lattice and H the Hamiltonian (green). The network can be efficiently contracted from left to right (or right to left), with computational effort scaling linearly with system size L.

from left to right (or right to left), see Fig. 3. In a nutshell, this property explains the numerical efficiency of tensor network methods in one dimension. Efficient time evolution methods include Trotter splitting, the "time-evolving block decimation" (TEBD), and tangent space methods [12,15,18,21].

4. Diffusive scaling of dynamical correlation functions

As exemplification of transport in quantum systems, we numerically compute dynamical correlation functions using the tensor network methods discussed in the previous section. Here we consider the quantum Bose–Hubbard model with interaction strength $U = 5$ on a lattice with $L = 100$ sites. One expects qualitatively similar results for other (non-integrable) models, like the above Heisenberg model. In our case, the local Hilbert space dimension is $d = 3$ (restricted to a maximal occupancy of two particles per site), spanned by basis states corresponding to 0, 1, or 2 particles: $\{|0\rangle, |1\rangle, |2\rangle\}$. Instead of the Pauli matrices (8), we employ the local "density" (or "number") operator

$$n = \begin{pmatrix} 0 & & \\ & 1 & \\ & & 2 \end{pmatrix} \tag{19}$$

which is simply a diagonal matrix with respect to the basis $\{|0\rangle, |1\rangle, |2\rangle\}$.

In line with linear response theory, we investigate dynamical density correlation functions

$$\langle n_j(t); n_\ell(0)\rangle_{\mathrm{eq}} \tag{20}$$

with n_j denoting the density operator acting on lattice site j and the usual Heisenberg time dependence (6). For large system size L, one expects that finite-size (boundary) effects become negligible, such that the correlation function only depends on $j - \ell$ (and time t) in the thermodynamic limit $L \to \infty$ due to spatial translation invariance. Accordingly, we will label the reference site as $\ell = 0$. Diffusive behavior of the system is indicated by the correlation function matching the kernel of the heat equation, i.e.

$$\langle n_j(t); n_0(0)\rangle_{\mathrm{eq}} \simeq \frac{1}{\sqrt{4\pi \mathcal{D} t}} \exp\left(-\frac{j^2}{4\mathcal{D} t}\right) \tag{21}$$

with $\mathcal{D}$ the diffusion coefficient or conductivity.

The simulation results shown in Fig. 4 have been obtained in the "infinite temperature" limit $T \to \infty$, i.e. setting $\beta = 0$. Numerical simulation details can be found in [22]. The simulations are repeated for three values of the maximally allowed bond dimension $D_{\max}$, to ensure that the results are not sensitive to the $D_{\max}$ cut-off, i.e. to exclude artifacts of the tensor network approximation. Indeed, one observes a centered "heat peak" in Fig. 4, which spreads over time. The red dashed curve shows a Gaussian heat kernel of the form (21), with fitted diffusion coefficient $\mathcal{D} = 0.96$, and matches the correlation function quite well.

As a remark, the dynamical density correlation deviates strongly from a diffusive heat peak at finite temperatures $\beta \geq 1$ (data not shown).

5. Complementary approaches of studying transport

The approach presented here is one of many complementary ways of studying transport in quantum systems. In the absence of strong correlation, one typically invokes semiclassical kinetic theory and quantum Boltzmann equations [23–25], i.e. describing the collective carrier dynamics via a distribution function depending on single-particle position, momentum, and time.

Explicitly imposing temperature gradients can be achieved by introducing thermal reservoirs ("baths") at the left and right boundary of an (one-dimensional) quantum system. This leads to the following Lindblad equation [26] for the density matrix, which reads in general form

$$\partial_t \rho = -\frac{i}{\hbar}[H, \rho] + \sum_{n,m=1}^{N^2-1} h_{nm}\left(A_n \rho A_m^\dagger - \frac{1}{2}\left\{A_m^\dagger A_n, \rho\right\}\right) \tag{22}$$

Remarkably, explicit expressions for the nonequilibrium steady state (i.e. stationary solutions to the Lindblad equation) have been obtained for certain physical systems [27–29].

Especially for quantum systems out of equilibrium, where linear response theory is no longer applicable, insights into transport properties have also been gained by invoking the so-called holographic duality [30].

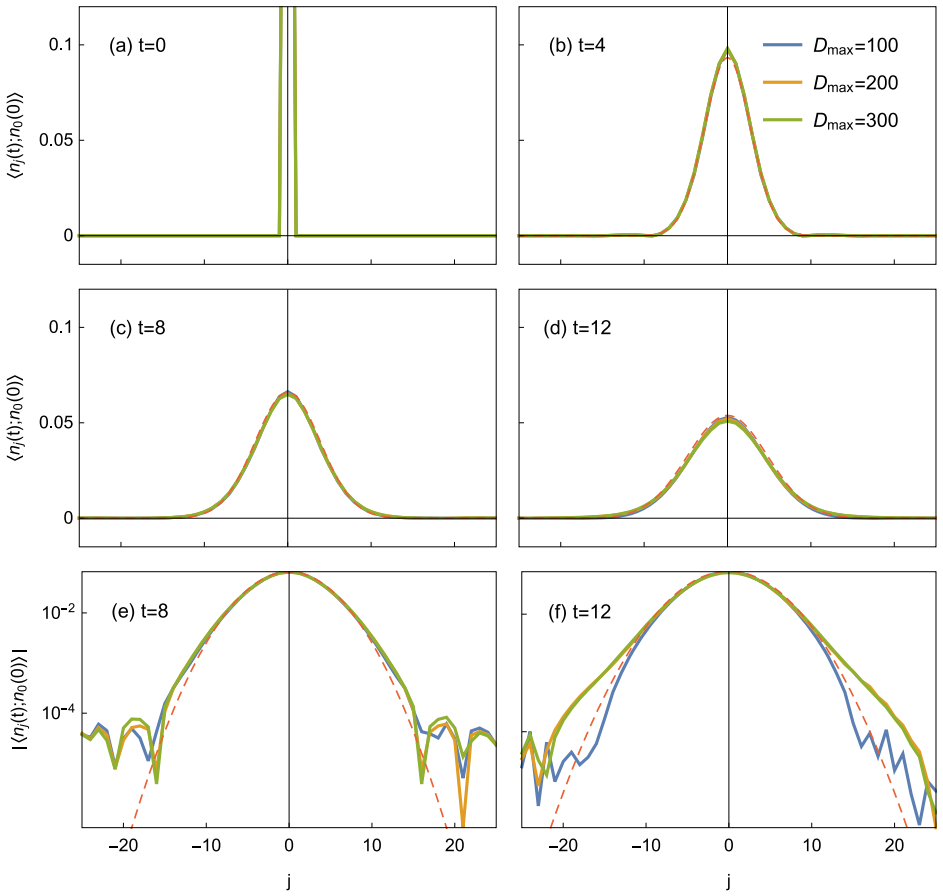

Fig. 4. Dynamical density correlation functions $\langle n_j(t); n_0(0)\rangle_{\mathrm{eq}}$ at four time points, for the quantum Bose–Hubbard model with $U = 5$ and at "infinite temperature" ($\beta = 0$). The curves for different maximal virtual bond dimensions $D_{\max}$ overlap (except for (f) and $|j| \geq 10$), indicating that the results are not significantly altered due to the $D_{\max}$ cut-off. The tip of the initial correlation peak in (a) is not visible due to the capped plot range. The dashed red curve is a Gaussian heat kernel of the form (21) with fitted diffusion coefficient $\mathcal{D} = 0.96$. The two bottom plots show the same data as the middle row, but on a logarithmic scale.

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