Coupled transport in a linear-stochastic Schrödinger equation

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Abstract. I study heat and norm transport in a one-dimensional lattice of linear Schrödinger oscillators with conservative stochastic perturbations. Its equilibrium properties are the same of the discrete nonlinear Schrödinger equation in the limit of vanishing nonlinearity. When attached to external classical reservoirs that impose nonequilibrium conditions, the chain displays diffusive transport, with finite Onsager coefficients in the thermodynamic limit and a finite Seebeck coefficient.

Keywords: stochastic particle dynamics, transport processes/heat transfer
1. Introduction

Within the vast class of nonequilibrium classical and quantum phenomena, the physics of coupled transport (CT) is a growing field with potentially revolutionary technological innovations. The knowledge of systems where two or more species of irreversible flows may occur and influence one another dates back to the discoveries by Seebeck and Peltier of thermoelectricity in the first half of the XIX century. The basic principle of a thermoelectric material is the capacity of converting a temperature difference into a voltage and vice-versa. More generally, depending on the physical nature of the microscopic carriers, analogous CT effects may also involve different kind of unbalance, like chemical potential differences (thermodiffusion) or spin voltages (thermomagnetism).

From the point of view of applications, the possibility to control a heat flow by means of an auxiliary current within the same medium allows to build solid-state miniaturized versions of power generators or refrigerators with no mechanical parts. At present, however, the conversion efficiency of these materials is still too low compared to the one of common thermo-mechanical machines. As a result, the use of CT devices is limited to a quite restricted number of special applications.

In recent years, mounting evidence has been provided that the aim of a significant improvement of CT technologies necessarily requires a deeper understanding of the fundamental physical mechanisms that underlie CT processes [1–5]. In the absence of a complete theory, many approaches have been proposed to tackle the problem. In the context of statistical mechanics, the study of simple models of coupled oscillators represents undoubtedly a powerful strategy for unveiling the basic microscopic mechanisms of transport phenomena [6–8]. Among them, the discrete nonlinear Schrödinger (DNLS) equation [9] is a natural candidate to study CT of energy and mass (norm) in several setups, ranging from nonlinear optics [10, 11] to cold atoms [12–14] and micromagnetic systems [15, 16]. In one dimension, the DNLS equation reads

$$i\dot{z}_n = -\nu|z_n|^2z_n - z_{n+1} - z_{n-1}. \quad (1)$$
It describes the dynamics of a chain of $N$ coupled anharmonic oscillators (with $1 \leq n \leq N$) with complex amplitudes $z_n$ ($|z_n|^2$ is the local norm) and a real nonlinearity coefficient $\nu$. In the standard nonequilibrium setup, the DNLS chain interacts with two external reservoirs that exchange energy and norm and impose temperature and chemical potentials [17, 18]. While for sufficiently large temperatures, the DNLS model displays normal transport with a non-vanishing Seebeck coefficient [17, 19] and diffusive spreading of energy- and norm correlations [20], in the low-temperature regime, the quasi-conservation of the phase differences yields anomalous transport on long time scales [20]. More in general, it was shown that the nonlinearity of the system plays a relevant role for the determination of its nonequilibrium properties. Some examples are the strong dependence of the Onsager coefficients on the thermodynamical variables [17], the observation of interfacial regions and dynamical transitions for low temperatures and large chemical potential differences [21] and the spontaneous creation of nonequilibrium barriers and localized structures for very large (even negative) temperatures [22].

For vanishing nonlinearity, the DNLS equation reduces to a chain of complex harmonic oscillators, the discrete Schrödinger (DS) equation. In this limit transport is ballistic (i.e. currents do not depend on the system size) and stationary profiles are flat [17], in analogy with the well known behaviour of a chain of real harmonic oscillators connected to boundary reservoirs [23]. Since in the DS equation energy and norm are carried by $N$ noninteracting phonon modes, the related currents are independent on the system size $N$ and can be fully characterized in the framework of Landauer theory of electronic transport [24, 25].

A particularly effective strategy to bridge the gap between nonlinear models and harmonic systems is to replace nonlinear interactions by suitable stochastic perturbations of a linear dynamics [26]. This approach proved to be very effective in the context of anomalous heat conduction, allowing to obtain explicit representations of the nonequilibrium invariant measure [27] and analytical expressions of stationary temperature profiles associated to anomalous currents [28–30]. In a few words, the method consists in adding local stochastic collisions that conserve exactly momentum and energy of a chain of harmonic oscillators. Such collisions mimic the effect of nonlinearities and introduce some degree of ergodicity and irreversibility that would otherwise be completely missing in a purely harmonic system. It is important to notice that as long as one considers a chain of real harmonic oscillators, the nature of the interaction potential and the symmetries of the model prevent any coupling between momentum- and heat currents [19, 31]. As a result, no CT is expected in this context.

Analogous studies focused on CT are scarce [32]. For the DS chain, it was shown in [33] that the addition of phase noise to the deterministic dynamics allows to recover nonequilibrium stationary states that satisfy the Fourier law. This class of perturbations, however, conserves only the total norm, while the conservation of the total energy is lost. As a result, the exploration of the transport properties of the system is limited to the set of states at infinite temperature (and infinite chemical potential) [18, 33].

In this paper I present a discrete linear-stochastic Schrödinger equation that conserves exactly both the total energy and the total norm and naturally allows to study CT problems in the whole space of thermodynamic variables. This model has the same symmetries of the DNLS equation and recovers its typical transport properties, which
are characterized by diffusive currents and a nonzero Seebeck coefficient. The paper is organized as follows. In section 2, I introduce the model and discuss the relevant thermodynamic observables that are used to characterize nonequilibrium steady states. In section 3, I discuss the main features of the nonequilibrium steady states as obtained from numerical simulations. Finally, section 4 is devoted to the conclusions and to a discussion of open problems and future perspectives.

2. Model and observables

I begin this section by reviewing the equilibrium properties of the one dimensional DS equation

\[ i\hat{z}_n = -z_{n+1} - z_{n-1}. \]  \hspace{1cm} (2)

Upon identifying the set of canonical variables \( z_n \) and \( i\hat{z}_n^* \), equation (2) can be derived from the Hamilton equations \( \dot{\hat{z}}_n = -\partial H / \partial (i\hat{z}_n^*) \) for the Hamiltonian

\[ H = \sum_{n=1}^{N} (z_n^* z_{n+1} + z_n z_{n+1}^*). \]  \hspace{1cm} (3)

The model has two exactly conserved quantities, namely the total energy \( H \) and the total norm

\[ A = \sum_{n=1}^{N} |\hat{z}_n|^2. \]  \hspace{1cm} (4)

In terms of Fourier amplitudes \( \tilde{z}_k = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{-2\pi i kn} z_n \) (with \( k = 1, \ldots, N \)), the Hamiltonian can be rewritten in the diagonal form

\[ H = \sum_{k=1}^{N} |\tilde{z}_k|^2 \omega_k, \]  \hspace{1cm} (5)

where \( \omega_k = 2 \cos(2\pi k / N) \) is the energy spectrum of the system and \( |\tilde{z}_k|^2 \) represents the power of the \( k \)th mode, with the constraint \( \sum_{k=1}^{N} |\tilde{z}_k|^2 = A \).

The thermodynamical properties of the DS equation are determined by two parameters: the total norm density \( a = A/N \) and the total energy density \( h = H/N \), which can be mapped to a couple of values of temperature \( T \) and chemical potential \( \mu \) via a classical grand-canonical distribution. To derive this mapping, one can start from the partition function of the system

\[ Z = \int \prod_{k=1}^{N} d\tilde{z}_k d\tilde{z}_k^* e^{-(H - \mu A)/T}, \]  \hspace{1cm} (6)

which can be explicitly computed and rewrites in the standard equipartition form

\[ Z = \prod_{k=1}^{N} \frac{2\pi}{\beta(\omega_k - \mu)}, \]  \hspace{1cm} (7)

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where the Boltzmann constant was set to 1. Hence, from the knowledge of the free energy $F = -T \log(Z)$, one can derive [34] an equation of state for $a$ and $h$ in the form

$$a = -\frac{T \text{sign}(\mu)}{\sqrt{\mu^2 - 4}}$$
$$h = T + \mu a$$

(8)

with the condition $|\mu| > 2^{1}$. Equation (8) fully specifies the equilibrium phase diagram of the model, as shown in figure 1. Here, the lower dashed line represents the ground state $h = -2a$, while the horizontal dashed line $h = 0$ identifies the set of states at infinite temperature. The grey region $R_f$ is a forbidden region, while $R_p$ is the region of positive temperature states. In analogy to what was found for the DNLS equation [35], the DS equation displays a region $R_n$ of negative temperature states located above the infinite temperature line. The symmetric nature of $R_n$ and $R_p$ (which is found also in some spin systems [36]) derives from the fact that for every accessible state $(a, h)$ corresponding to some temperature $T$, there exists a symmetric state $(a, -h)$ characterized by the temperature $-T$. In view of this symmetry, in this paper I will focus to the nonequilibrium properties of the DS model within the region $R_p$. A discussion of more general situations involving both $R_p$ and $R_n$ will be given in a forthcoming paper.

2.1. Conservative noise

The stochastic version of the DS equation is obtained from the deterministic one, equation (2), by adding suitable conservative random ‘shakings’ of local phases, which occur at rate $\gamma_c$. To illustrate this stochastic dynamics, let me consider the local energy on a generic site $n$

$$e_n = 2\rho_n \rho_{n-1} \cos(\phi_n - \phi_{n-1}) + 2\rho_n \rho_{n+1} \cos(\phi_{n+1} - \phi_n)$$

(9)

where $\rho_n = |z_n|$ and $\phi_n = \text{arg}(z_n)$. The goal is to define a local transformation on the lattice site $n$ that conserves both the energy $e_n$ and the local norm $\rho_n^2$. If the transformation restricts to the phase $\phi_n$, the conservation of the norm holds straightforwardly, while from equation (9) it follows the condition

$$A \cos(\phi_n - \alpha) + B \cos(\phi_n - \beta) = E$$

(10)

where $A = \rho_{n-1}$, $B = \rho_{n+1}$, $\alpha = \phi_{n-1}$, $\beta = \phi_{n+1}$ and $E$ are now fixed parameters. This linear goniometric equation has two (possibly identical) solutions in the interval $[0, 2\pi)$: one solution corresponds to the state before the shaking operation, the other one to the shaken state. Shaking operations are performed on the whole DS chain at random times, whose separation $\tau$ are independent and identically distributed variables extracted from a Poissonian distribution $P(\tau) \sim \exp(-\gamma_c \tau)$. In between two successive realizations of the conservative noise, the evolution of the system follows the deterministic dynamics defined in equation (2), except for the two boundary sites, which are coupled to external stochastic reservoirs. Their dynamics is described in the following subsection, along with a presentation of the nonequilibrium observables that are considered in this paper.

1 This condition ensures the existence of a well defined partition function in (6) and (7).
2.2. The nonequilibrium setup

A typical setup adopted for the study of CT problems amounts to put the system in contact with two boundary reservoirs at temperature $T_L$ and $T_R$ and chemical potential $\mu_L$ and $\mu_R$, respectively. For the stochastic DS equation this task can be accomplished by introducing a suitable Langevin equation. Focusing on the last lattice site $n = N$, which is in contact with the right reservoir, the Langevin equation writes

$$i\dot{z}_N = -(1 + i\gamma)z_{N-1} + i\gamma\mu_R z_N + \sqrt{\gamma T_R} \eta(t),$$

where $\eta(t)$ is a complex Gaussian white noise with zero mean and unit variance, $\gamma$ is the bath coupling parameter and open boundary conditions are assumed. An analogous equation holds for the left reservoir, which is coupled to the first site $n = 1$ and imposes a temperature $T_L$ and a chemical potential $\mu_L$.

When the chain is steadily kept out of equilibrium by some thermodynamic force, the main observables are the two currents associated to the conserved quantities: the norm flux $j_a$ and the energy flux $j_h$. Their explicit expressions are

$$j_a = 2\langle \text{Im}(z_n^* z_{n+1}) \rangle$$

$$j_h = 2\langle \text{Re}(z_n^* z_{n+1}) \rangle$$

where the angular brackets denote a time average. Within the linear response regime, thermodynamic forces and currents are related by the celebrated Onsager relations. Upon introducing the heat flux $j_q = j_h - \mu j_a$, they write

$$j_a = -L_{aa} \frac{d\mu}{dx} + L_{aq} \frac{d\beta}{dx}$$

$$j_q = -L_{qa} \frac{d\mu}{dx} + L_{qq} \frac{d\beta}{dx}.$$
where the coefficients $L_{ij}$ are the entries of the symmetric and positive-definite Onsager matrix $L$ and the two gradient terms identify the thermodynamic forces, with $\beta = 1/T$ and $x = n/N$. Within this representation, CT is clearly related to non-vanishing off-diagonal elements $L_{aq} = L_{qa}$. Indeed, the Seebeck coefficient, that quantifies the strength of the coupling between the two currents, is defined as [19]

$$S = \beta \frac{L_{aq}}{L_{aa}}$$

and the thermodiffusive conversion efficiency is determined by the figure of merit [1]

$$ZT = \frac{L_{aq}^2}{\det L}.$$  

Steady states are additionally described in terms of the (averaged) profiles of local norm and local energy

$$a_n = \langle |z_n|^2 \rangle$$

$$h_n = \langle e_n \rangle$$

or, equivalently, by means of local measurements of temperature $T_n$ and chemical potential $\mu_n$. For these two last quantities, suitable explicit microcanonical definitions can be consistently derived from the thermodynamic relations $1/T = \partial s/\partial h$ and $\mu/T = -\partial s/\partial a$, where $s$ is the microcanonical entropy density of the system. I refer to [17, 38] and references therein for details.

Numerical simulations of the dynamics of the stochastic DS equation were performed by implementing a 4th-order Runge–Kutta scheme with minimum timestep $\delta t = 10^{-4}$ time units. Without any loss of generality, the Langevin coupling parameter $\gamma$ has been set to 1. In order to sample accurately the nonequilibrium steady states, the system was evolved for a time interval $t_s$ equal to $5 \times 10^6$ time units after a transient evolution of $10^6$ time units. It was verified that $t_s$ was long enough to observe stationary currents and profiles in the whole range of thermodynamic parameters and for the system sizes explored in this paper.

3. Steady states

In this section, I discuss the transport properties of the stochastic DS chain. As a preliminary test for the consistency of the nonequilibrium setup, it was verified that for $\gamma_c = 0$ the chain displays ballistic transport and flat profiles, as shown in figure 2 for a pure temperature unbalance. Similarly to the behaviour of the chain of real oscillators [23], the temperature of the chain settles to a constant value which is the average between $T_L$ and $T_R$. The same occurs for the chemical potential.

For finite $\gamma_c$, the response of the system is radically different, as shown in figure 3 for $\gamma_c = 1$. The linear-stochastic chain displays non-flat profiles of temperature and chemical potential that interpolate between the values imposed by the external reservoirs. Figures 3(a) and (b) show the stationary profiles obtained with the same choice of
boundary conditions used for the integrable limit of figure 2. Depending on the choice of the external thermal and chemical unbalances, also nonlinear profiles may emerge, as shown in figures 3(c) and (d) for a pure chemical unbalance, see in particular the profile of $\mu(x)$. More in general, if the system is locally in equilibrium, a consistent representation of the stationary profiles requires that the relations (8) are satisfied for every $x \in [0, 1]$. In figures 3(b) and (d) it is verified that this is indeed the case (up to numerical precision) by computing $a(x)$ and $h(x)$ in two independent ways: (i) from the direct computation through the definitions (17) and (18), respectively (solid lines); (ii) from the profiles of $T(x)$ and $\mu(x)$ and using the equations of state (8) (open symbols). These profiles are also reported parametrically in the phase diagram $(a, h)$, where they give rise to almost straight paths in the region $R_p$, see figure 1.

For fixed differences of the thermodynamic parameters $\Delta T = T_R - T_L$ and $\Delta \mu = \mu_R - \mu_L$, the two currents $j_a$ and $j_h$ of the stochastic DS chain are inversely proportional to the system size $N$, as shown in figure 4(a). These results confirm that transport is normal and that the Onsager coefficients are finite in the thermodynamic limit, in analogy to what was observed in the presence of nonlinearities [17]. In any case, although the diffusive scaling holds in principle for every finite $\gamma_c$, the magnitude of stationary currents is found to depend on $\gamma_c$, see figure 4(b). In particular, the observed trends indicate that in the limit of very frequent stochastic moves, transport is effectively suppressed as a consequence of the dynamic decoupling of Schrödinger oscillators. This effect is qualitatively similar to the behaviour of quantum systems subjected to strong dephasing noise, where the suppression of unitary evolution is often referred to as the quantum Zeno effect [39]. On a more quantitative level, the observed decay $j \sim \gamma_c^\alpha$ with $\alpha \simeq -0.8$ (dot-dashed line in figure 4(b)) appears quite different from

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**Figure 2.** Stationary nonequilibrium profiles in the integrable limit $\gamma_c = 0$ as a function of $x = n/N$ for a chain of $N = 400$ lattice sites and $\mu_L = \mu_R = -10$, $T_L = 1$, $T_R = 4$. (a) Temperature and chemical potential profiles computed with the appropriate microcanonical observables over small spatial subchains of 10 sites around $n$. (b) Local norm and energy densities corresponding to the profiles in (a). (c) Fluxes of norm (circles) and energy (squares) versus $N$ for the same thermodynamic parameters.
The result $\alpha = -1$ expected for pure-dephasing white noise [40]. A detailed analysis of this problem would demand a careful study of the statistical properties of the conservative noise, a task that goes beyond the aims of the present paper.

Finally, a numerical evaluation of the Seebeck coefficient of the system was performed on the isochemical line $\mu = -4$ for temperatures in the range $1 \leq T \leq 4$ (and local norms of order 1), see figure 5(a). The value of $S(\mu, T)$ was obtained from the Onsager matrix through equation (15), see [17, 19] for details. In short, given a reference state $(T, \mu)$, the Onsager matrix was computed by applying fixed thermal and
chemical unbalances to this state and by inverting equation (14). If these unbalances are small enough, the profiles of $T(x)$ and $\mu(x)$ are linear and the resulting Onsager matrix is independent on the system size $N$. It was verified for two chains lengths $N = 200$ and $N = 400$ that the choice $\Delta T = 0.4$ and $\Delta \mu = 0.4$ is compatible with linear response in the specified region of parameters (data not shown). Accordingly, figure 5 displays the results obtained with $N = 400$. It was also checked that, within statistical errors, the Onsager matrix is symmetric and positive-definite. Altogether, the finite and positive Seebeck coefficient confirms that the stochastic DS displays CT. Moreover, the decreasing character of $S(T)$ in figure 5(a) suggests that in the limit of very high temperatures, CT is suppressed by the incoherent nature of the oscillators’ dynamics. For the same thermodynamical parameters, the figure of merit $ZT$ obtained from equation (16) is shown in figure 5(b). It essentially follows the behaviour of $S(T)$, with a moderate decrease from the value $ZT \simeq 12$ attained for $T = 1$.

4. Conclusions

Introduced in this paper is a linear-stochastic model of coupled complex oscillators that displays CT in the sense of linear irreversible thermodynamics. The model consists in a one-dimensional DS chain endowed with stochastic moves that act on the local phases and conserve simultaneously the total energy and the total norm. Due to the linear nature of the deterministic dynamics, the equilibrium properties of the system are fully accessible through an equation of state that was derived within the grand-canonical formalism [34]. The resulting equilibrium phase diagram is two-dimensional and represents the limit of low norm densities of the analogous diagram obtained for the DNLS equation [35]. Nonequilibrium stationary states crucially depend on the stochastic dynamics: despite the intrinsically discrete character of the conservative moves, I
have shown that they are sufficient to introduce irreversibility in the system. Indeed, numerical simulations indicate that such a model displays diffusive transport and a finite Seebeck coefficient, similarly to what is found in the DNLS equation [17, 19].

An interesting open question that naturally arises in this context concerns the possibility of performing an analytical description of the nonequilibrium problem for the stochastic Schrödinger model, in analogy to what was done for the chain of real harmonic oscillators [29]. Practically, this task requires finding a solution for the Fokker–Planck equation, where a purely dynamical propagator is combined with the contribution of conservative collisions [29]. The importance of such an approach is clearly related to the opportunity of understanding and controlling the mechanisms of conversion efficiency in interacting systems.

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