Transition from diffusive to ballistic dynamics for a class of finite quantum models

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The transport of excitation probabilities amongst weakly coupled subunits is investigated for a class of finite quantum systems. It is demonstrated that the dynamical behavior of the transported quantity depends on the considered length scale, e. g., the introduced distinction between diffusive and ballistic transport appears to be a scale-dependent concept, especially since a transition from diffusive to ballistic behavior is found in the limit of small as well as in the limit of large length scales. All these results are derived by an application of the time-convolutionless projection operator technique and are verified by the numerical solution of the full time-dependent Schrödinger equation which is obtained by exact diagonalization for a range of model parameters.

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There are certainly many ways in order to analyze the transport behavior of quantum systems: Linear response theory such as implemented in the Kubo-formula,1 2 3 4 5 6 (possibly represented by Green’s functions7 8 9 10 11), methods which concern reservoirs of the transported quantity, either explicitly12 13 14 or effectively15 or effectively16 17 18, and probably many more. However, except for those involving reservoirs, none of these methods allows to investigate the dependence of transport behavior on the length scale of a finite system. Unfortunately, the remaining methods which do involve baths are conceptually more subtle and computationally rather challenging16 17 18.

In this letter we will discuss a class of finite models which indeed exhibits scale-dependent transport of, e. g., excitation probabilities, energy or particles, according to the respective interpretations of the model. In particular, we will develop a method which allows for the complete characterization of the available types of transport and their dependence on the considered length scale. It will be especially demonstrated that the numerically exact solution of the full time-dependent Schrödinger equation perfectly agrees with the theoretical predictions which are obtained from this method: For intermediate length scales diffusive behavior is found, that is, the dynamics of the transported quantity is well described by a respective diffusion equation and the spatial variance of an initial excitation profile increases linearly in time. Contrary, in the limit of small as well as large length scales diffusive behavior breaks down. This non-diffusive transport type turns out to be “ballistic” which is to be understood in terms of a quadratic increase of the spatial variance. (See the last page of this letter for a classification of these findings in the framework of standard solid state theory.)

According to Fig. 1 our model consists of _N_ identical, weakly coupled, subunits featuring a non-degenerate ground state with energy \( \varepsilon_0 = 0 \) as well as _n_ excited states with equidistant energies \( \varepsilon_i, i = 1, 2, \ldots, n \). We will focus on the (invariant) “one-excitation subspace” which is spanned by the set \( \{\mu, i\} \), where \( \{\mu, i\} \) corresponds to the excitation “sitting” in the \( i \)th exited state of the \( \mu \)th subunit. Using this notation, the total Hamiltonian \( H = H_0 + \lambda V \), the sum of a local part \( H_0 \) and an interaction part \( V \), is given by

\[
H_0 = \sum_{\mu} \sum_i \varepsilon_i \left| \mu, i \right\rangle \left\langle \mu, i \right| ,
\]

\[
V = \sum_{\mu} \sum_{i,j} c_{ij} \left| \mu, i \right\rangle \left\langle \mu + 1, i \right| + \text{H.c.}
\]

We use periodic boundary conditions, i. e., we identify \( \mu = N \) with \( \mu = 0 \). The \( c_{ij} \) form a normalized Gaussian random matrix with zero mean, \( \lambda \) is an overall coupling constant. Obviously, \( V \) corresponds to nearest-neighbor hopping.

This system may be viewed as a simplified model for, e. g., a chain of coupled molecules or quantum dots, etc. In this case the hopping of an excitation from one subunit to another corresponds to transport of energy, especially if \( \Delta E \gg \delta \varepsilon \). The model may also be viewed as a tight-binding model for particles on a lattice. In this case the hopping corresponds to transport of particles. There are \( n \) “orbitals” per lattice site but no particle-particle interaction in the sense of a Hubbard model [cf. Eq. (2)].

FIG. 1: A model of \( N \) identical, weakly coupled, subunits featuring a non-degenerate ground state, an energy gap \( \Delta E \) and an energy band \( \delta \varepsilon \) with \( n \) equidistant states. The dots indicate excitation probabilities and are supposed to visualize a state from the investigated “single-excitation space”.

\[\text{FIG. 1: A model of } N \text{ identical, weakly coupled, subunits featuring a non-degenerate ground state, an energy gap } \Delta E \text{ and an energy band } \delta \varepsilon \text{ with } n \text{ equidistant states. The dots indicate excitation probabilities and are supposed to visualize a state from the investigated “single-excitation space”.
\]
Due to the independence of \( c_{ij} \) from \( \mu \), these are systems without disorder in the sense of, say, Anderson [19], in spite of the fact that the \( c_{ij} \) are random. For some literature on this model class, see [20, 21, 22, 23].

The total state of the system is naturally represented by a time-dependent density matrix \( \rho(t) \). We denote by \( \Pi_{\mu} \equiv \sum_i |\mu, i\rangle \langle \mu, i| \) the operator which projects onto the exited states |\( \mu, i\rangle \) of the \( \mu \)th subunit’s band. Thus, the quantity \( P_{\mu}(t) = \text{Tr}[\Pi_{\mu} \rho(t)] \) represents the probability for finding an excitation of the \( \mu \)th subunit, while all other subunits are in their ground state.

Our aim is to describe the dynamical behavior of these local probabilities and to develop explicit criteria that enable a clear distinction between diffusive and ballistic transport. We will call the behavior diffusive, if the \( P_{\mu}(t) \) fulfill a discrete diffusion equation

\[
P_{\mu} = \kappa (P_{\mu+1} + P_{\mu-1} - 2 P_{\mu})
\]

with some diffusion constant \( \kappa \). As well known from the work of Fourier, such a diffusion equation decouples with respect to, e. g., cosine-shaped spatial density profiles, i. e., the above equation yields

\[
\hat{F}_q = -2(1 - \cos q) \kappa F_q , \quad F_q \equiv C_q \sum_\mu \cos(q \mu) P_\mu
\]

with \( q = 2\pi k/ N, k = 0, \ldots, N/2 \) and an appropriate normalization constant \( C_q \). Hence, if the model indeed shows diffusive behavior, then all modes \( F_q \) have to relax exponentially. But if the modes \( F_q \) are found to relax exponentially only for some regime of \( q \), the model is said to behave diffusively on the corresponding length scale \( l = 2\pi/ q \). The dynamics of the \( F_q \), as resulting from the quantum system, is most conveniently expressed in terms of expectation values of “mode operators” \( \Phi_q \),

\[
F_q(t) = \text{Tr}[\Phi_q \rho(t)] , \quad \Phi_q \equiv C_q \sum_\mu \cos(q \mu) \Pi_\mu
\]

where we now choose \( C_q = \sqrt{2/\pi N} \) for \( q \neq 0, \pi \) as well as \( C_0 = C_\pi = \sqrt{1/\pi N} \) such that \( \text{Tr}[\Phi_q \Phi_q^\dagger] = \delta_{qq'} \), the mode operators are orthonormal.

A strategy for the analysis of the dynamical behavior of the \( F_q \) is provided by the projection operator techniques [1, 24, 25, 26]. In order to apply these techniques one first defines an appropriate projection superoperator \( \mathcal{P} \). Formally, this is a linear map which projects any density matrix \( \rho(t) \) to a matrix \( \mathcal{P} \rho(t) \) that is determined by a certain set of relevant variables. Moreover, the map has to be a projection in the sense of \( \mathcal{P}^2 = \mathcal{P} \). In the present case a suitable projection superoperator is defined by

\[
\mathcal{P} \rho(t) \equiv \sum_q \text{Tr}[\Phi_q \rho(t)] \Phi_q = \sum_q F_q(t) \Phi_q
\]

Due to the orthonormality of the mode operators this map is indeed a projection operator. The great advantage of this approach is given by the fact that it directly yields an equation of motion for the relevant variables, in our case the Fourier amplitudes \( F_q \). We concentrate here on a special variant of these techniques which is known as time-convolutionless (TCL) projection operator method [20, 24]. Considering initial states with \( \mathcal{P} \rho(0) = \rho(0) \), this method leads to a time-local differential equation of the form \( \dot{F}_q(t) = -\gamma \dot{q} F_q(t) \). So far, this formulation is exact. Modes with different \( q \) do not couple due to the translational invariance of the model.

Nevertheless, the exact \( F_q(t) \) is hard to determine but the TCL method also yields a systematic perturbation expansion for the rate \( \Gamma_q(t) \) in powers of the coupling constant \( \lambda \), namely, \( \Gamma_q(t) = \lambda^2 \Gamma_{q,2}(t) + \lambda^4 \Gamma_{4,q}(t) + \ldots \) (all odd order contributions vanish). Note that a truncation of the above TCL expansion may yield reasonable results even and especially in the regime where the elements of the perturbation matrix are larger than the level spacing of \( H_0 \), i. e., the regime where standard time-independent perturbation theory breaks down.

In leading order a straightforward calculation yields

\[
\hat{F}_q(t) = -2(1 - \cos q) \gamma_2(t) F_q(t)
\]

where the rate \( \gamma_2(t) \) is defined by \( \gamma_2(t) = \int_0^t d\tau f(\tau) \) and the two-point correlation function \( f(\tau) \) is given by (time arguments refer to the interaction picture)

\[
f(\tau) = \frac{1}{n} \text{Tr}[V(t)V(t_1) \Pi_\mu] , \quad \tau = t - t_1.
\]

This function is completely independent from \( \mu \) because of the translational invariance of the model. Of course, \( f(\tau) \) depends on the concrete realization of the random interaction \( V \). But due to the law of large numbers, the crucial features of \( V \) are nevertheless the same for the overwhelming majority of all realizations of \( V \), as long as \( \sqrt{n} \gg 1 \). And in fact, \( f(\tau) \) typically assumes the form in Fig. 2. It decays like a standard correlation function on a time scale of the order \( \tau_e = 1/\delta \varepsilon \). The area under this first peak is approximately given by \( \gamma = 2\pi n \lambda^2/\delta \varepsilon \). However, unlike standard correlation functions, due to the equidistant level spacing of the local bands, \( f(\tau) \) is a strictly periodic function with the period \( T = 2\pi n/\delta \varepsilon \). Consequently, its time-integral \( \gamma_2(t) \) nearly represents a step function, see Fig. 2.

Thus, for \( \tau_e < t < T \) we find from Eq. (7)

\[
\dot{F}_q(t) = -2(1 - \cos q) \gamma F_q(t).
\]

The comparison with Eq. (4) clearly indicates diffusive behavior with a diffusion constant \( \kappa = \gamma \). And indeed, for modes which decay on a time scale \( t \) with \( \tau_e < t < T \) we find an excellent agreement between Eq. (8) and the numerical solution of the full time-dependent Schrödinger equation, obtained by incorporating Bloch’s theorem and exactly diagonalizing the Hamiltonian within decoupled subspaces. A “typical” example for a single realization of
The random matrix $V$ is shown in Fig. 3. Note that the size of the system is chosen adequately large such that there are only small fluctuations of the order of $1/n$ which arise due to the discrete spectrum, see, e. g., 20, 21.

However, until now the above picture is not complete for two reasons. The first reason is that $F_q(t)$ may decay on a time scale that is long compared to $T$. According to Eq. (7), this will happen, if $2(1-\cos q)\gamma T \gg 1$ is violated. If we approximate $2(1-\cos q) \approx q^2 = 4\pi^2/l^2$ for rather small $q$ (large $l$), this leads to the condition

$$
\left( \frac{4\pi^2 n \lambda}{l \delta \epsilon} \right)^2 \gg 1. \tag{9}
$$

If this condition is satisfied for the largest possible $l$, i. e., for $l = N$, the system exhibits diffusive behavior for all modes. If, however, the system is large enough to allow for some $l$ that violates condition (9), diffusive behavior breaks down in the long-wavelength limit. This result is again backed up by numerics, see Fig. 4.

Towards what transport type does the system deviate from diffusive, if condition (9) is violated? In this regime we have to consider time scales with $t \gg T$, as already mentioned above. We may thus approximate $\gamma_2(t) \approx 2\gamma t/T$, see Fig. 2. Plugging $\kappa = 2\gamma t/T$ into Eq. (3) yields a spatial variance $\sigma^2 \equiv \langle \mu^2 \rangle - \langle \mu \rangle^2 = 2\gamma^2 t^2/T$, contrary to $\sigma^2 = 2\gamma t$ which results for $\kappa = \gamma$. ($\kappa = \gamma$ applies in the regime where condition (9) is satisfied.) This change of the time-scaling of $\sigma^2$ clearly indicates the transition from diffusive to ballistic transport. The validity of the TCL approach in the ballistic regime is again backed up by numerics: Here, the TCL theory obviously predicts a Gaussian decay of $F_q(t)$ which is in agreement with the numerical results, see Fig. 5.

In a second case transport may be non-diffusive, if the corresponding $F_q(t)$ decay on a time scale that is short compared to $\tau_c$. This will happen, if $2(1-\cos q) \gamma \tau_c \ll 1$ is violated. We may approximate $2(1-\cos q) \approx 4\pi^2/l^2$ for the largest possible $q$ (smallest possible $l$). Hence, the above inequality may be written as

$$
\frac{8\pi n \lambda^2}{\delta \epsilon^2} \ll 1. \tag{10}
$$

If this inequality is violated, diffusive behavior breaks
down in the limit of short-wavelength modes. Moreover, if the second order still yields reasonable results for not too large λ, we expect a linearly increasing rate γ2(t) and thus a Gaussian decay, that is, according to the above reasoning, ballistic transport. For increasing wavelength, however, the corresponding inequality will eventually be satisfied, thus allowing for diffusive behavior. Also these conclusions are in accord with numerics, see Fig. 4.

Standard solid state theory always predicts ballistic transport for a translational invariant model without particle-particle interactions. Nevertheless, in the limit of many bands (many orbitals per site) and few sites (few k-values) two features may occur: i) The band structure in k-space becomes a disconnected set of points rather than the usual set of distinct smooth lines. It is hence impossible to extract velocities by taking the derivatives of the dispersion relations. ii) The eigenstates of the current operator no longer coincide with the Bloch eigenstates of the Hamiltonian and the current becomes a non-conserved quantity, even without impurity scattering. It is straightforward to check that both features occur in the regime where condition \(\Gamma\) is fulfilled. This is the regime where standard solid state theory breaks down due to the fact that the system is to "small".

On the other hand, our numerical simulations clearly reveal that the TCL projection operator technique is applicable both in the diffusive and in the ballistic regime and that it correctly describes the transition between these regimes. Recall that all analytical results have been obtained from the second order contribution \([\text{Eq. (17)}]\) of the TCL expansion. And in fact, it is possible to demonstrate that higher-order contributions are confidently negligible. We omit the details of the determination of the higher orders of the TCL expansion (several examples are discussed in \([24]\)), since this is beyond the scope of this letter and since the excellent agreement with the numerical simulations is surely evident.

However, the fact that already the second-order TCL equation \([\text{Eq. (17)}]\) yields an excellent quantitative agreement with the numerics, by contrast to standard perturbation theory, can be understood from the following argument. We first note that for \(\lambda = 0\) the energy eigenvalues of the Hamiltonian are N-fold degenerate, corresponding to the resonant transitions \(|\mu, i\rangle \rightarrow |\mu \pm 1, i\rangle\) between neighboring subunits induced by the interaction. While standard perturbation theory is spoiled by the presence of these resonant transitions, the TCL expansion works perfectly well even in the case of exact degeneracies. In fact, an analysis of the structure of the higher-order correlation functions reveals that for an interaction Hamiltonian \(V_d\) which includes only the resonant transitions, the second-order TCL equation \([\text{Eq. (17)}]\) is \textit{exact} on average (for arbitrary \(\lambda\)) with small fluctuations of order \(\lambda/n\). This is due to the fact that the TCL method is based on an expansion in terms of the ordered cumulants of \(V_d\) \([20]\), the higher-orders of which vanish by virtue of the Gaussian character of the coupling matrix elements. This implies that the second order TCL equation already reproduces exactly the effect of all resonant transitions, which is the crucial reason for the success of the TCL projection operator approach.

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