Dissipative transport in dc-ac–driven tight-binding lattices

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Abstract. – We investigate the incoherent dissipative quantum transport of a particle in a periodic lattice being driven nonlinearly by dc-ac fields. The particle always diffuses slower, as compared to the force-free case, and the minimal diffusion is found for zero dc-bias and ac-field parameters that lead to dynamical localization (DL) in the nondissipative case. A current inversion occurs at weak dissipation. The amplitude of the negative current is *maximal* for a characteristic value of the dissipative strength, resembling a "stochastic resonance" like effect. For intermediate dissipation the current is positive and widely independent of both the ac-frequency and the dissipation. The negative current, as well as the stability of DL against dissipation are *universal* effects, in the sense that they are largely independent of the dissipative mechanism.

The model of a quantum particle moving in a periodic tight-binding (TB) lattice while coupled to a thermal bath is of great relevance in solid-state physics. It can serve as an idealized model for the diffusion of a quantum particle among intersitials inside a crystal [1], especially that of a charged particle in a metal [2]. It can also be invoked to investigate quantum effects in the current-voltage characteristic of a small Josephson junction [3] or of semiconductor superlattices driven by strong dc and ac fields [4], [5]. Finally, this multistate system can be related to the Luttinger liquid model [6] for the conductance between two one-dimensional quantum wires connected by a weak link.

The dissipative multistate system in the *absence* of time-dependent driving has been the object of intense research during the past years [7]-[10]. In contrast, others investigated localization effects in dc-ac–driven TB lattices in the absence of thermal noise and dissipation [11]. The effect of scattering on the driven TB particle has been included phenomenologically by employing an *ad hoc* stochastic Liouville equation [12] or a classical Boltzman equation [4]. The real-time path integral method has been recently used in [13], to evaluate the ac-conductance of a Luttinger liquid. Here, generalizing [10] to the case of ac-dc driving, and in the spirit of [13], we investigate the driven dissipative tunneling dynamics within a microscopic rigorous approach to dissipation.

As a starting model we consider the one-dimensional infinite, single-band tight-binding lattice described by the Hamiltonian $H(t) = H_{\rm TB} + H_{\rm ext}(t) + H_{\rm B}$. The first term $H_{\rm TB}$ is the Hamiltonian of the bare multistate system

$$H_{\rm TB} = -(\hbar\Delta/2)\sum_n (|n\rangle\langle n+1| + |n+1\rangle\langle n|) \ , \tag{1}$$

where $|n\rangle$ denotes a (Wannier) state localized at the n-th site, while $\hbar\Delta$ is the overlap integral between two neighboring sites. The driving influence is described by

$$H_{\rm ext}(t) = -q\hbar(\epsilon_0 + \hat{\epsilon}\cos\Omega t)/d, \quad q = d\sum_n n|n\rangle\langle n| \; , \tag{2}$$

where the operator q measures the particle's position on the lattice, and $\hbar\varepsilon(t)/d = \hbar(\epsilon_0 + \hat{\epsilon}\cos\Omega t)/d$ is the potential drop per lattice period d due to externally applied dc-ac fields. Finally, the term $H_{\rm B}$ describes the heath bath environment as an ensemble of harmonic oscillators bilinearly coupled to the particle's coordinate, *i.e.* [14]

$$H_{\rm B} = \frac{1}{2}\sum_{i=1}^{N}\left[\frac{p_i^2}{m_i} + m_i\omega_i^2\left(x_i - \frac{c_i}{m_i\omega_i^2}q\right)^2\right] \; . \tag{3}$$

The environmental influences are then completely captured in the spectral density $J(\omega) = \frac{\pi}{2}\sum_i (c_i^2/m_i\omega_i)\delta(\omega - \omega_i)$, which will be assumed to be continuous henceforth.

Suppose now that the particle has been prepared at time $t_0 = 0$ at the origin with the bath having a thermal distribution at temperature T. Then, the dynamical quantity of interest is the probability $P_n(t)$ for finding the particle at site n at time $t > 0$. In turn, the knowledge of $P_n(t)$ enables the evaluation of all the statistical quantitites of interest in the problem, as, for example, the position's expectation value $P(t)$, as well as the variance $S(t)$, *i.e.*

$$P(t) := \langle q\rangle_t = d\sum_{n=-\infty}^{n=\infty} nP_n(t) \; , \tag{4}$$

$$S(t) := \langle q^2\rangle_t - \langle q\rangle_t^2 = d^2\sum_{n=-\infty}^{n=\infty} n^2P_n(t) - P^2(t) \; . \tag{5}$$

A calculation of the quantities (4), (5) is indeed very complicated. In ref. [13] the ac-conductance of a Luttinger liquid was evaluated by path-integral methods to the lowest perturbative order Δ^2. As demonstrated in ref. [10] for the case of a dc-field, this approximation is equivalent to assume that the particle tunnels *incoherently* from site to site. This turns out to be a good approximation for high temperatures and/or strong enough dissipation [8]-[10]. In this case, the resulting dynamics is identical to that of a nearest-neighbor hopping model in which the occupation probabilities obey rate equations. Generalizing the reasoning of [10], and previous results on the driven, dissipative two-state system [15], in the regime where incoherent tunneling dominates (in addition to the conditions of the dc-field case, it is assumed that the bath correlations between tunneling transitions decay on a faster time scale as compared to the time scale $2\pi/\Omega$ of the driving-induced correlations) we find that

$$\dot{P}_n(t) = \gamma_{\rm f}(t)P_{n-1}(t) + \gamma_{\rm b}(t)P_{n+1}(t) - \gamma(t)P_n(t) \; . \tag{6}$$

Here, $\gamma_{\rm b}(t)$ and $\gamma_{\rm f}(t)$, are the time-dependent backward and forward rates, respectively, and $\gamma(t) = \gamma_{\rm f}(t) + \gamma_{\rm b}(t)$ is the incoherent tunneling rate in a dc-ac–driven two-state system [15]. The rates $\gamma_{\rm f}(t)$, $\gamma_{\rm b}(t)$ are conveniently expressed in terms of

$$\gamma(t) = \Delta^2\int_0^\infty {\rm d}\tau\, \exp[-Q'(\tau)]\cos Q''(\tau)\cos\eta(t+\tau, t) \; ,$$

$$\rho(t) = \Delta^2\int_0^\infty {\rm d}\tau\, \exp[-Q'(\tau)]\sin Q''(\tau)\sin\eta(t+\tau, t) \; ,$$

where $\rho(t)=\gamma_{\rm f}(t)-\gamma_{\rm b}(t)$ and $\eta(t,t')=\int_{t'}^{t}{\rm d}t''\varepsilon(t'')$. Here $Q'(t)$ and $Q''(t)$ represent the real and the imaginary part, respectively, of the bath correlation function ($\beta=1/k_{\rm B}T$)

$$Q(t)=\frac{d^2}{\pi}\int_0^\infty {\rm d}\omega\frac{J(\omega)}{\omega^2}\frac{\cosh[\hbar\omega\beta/2]-\cosh[\hbar\omega(\beta/2-it)]}{\sinh[\hbar\omega\beta/2]}\ . \tag{7}$$

The general solution of eq. (6) can now be obtained in the form

$$P_n(t)=\exp[-[F(t)+B(t)]]\Big(F(t)/B(t)\Big)^{-n/2}I_n\Big(2\sqrt{F(t)B(t)}\Big)\ ,$$

with $I_n(z)$ the modified Bessel function of order n, and

$$B(t)=\int_0^t {\rm d}t'\gamma_{\rm b}(t'),\quad F(t)=\int_0^t {\rm d}t'\gamma_{\rm f}(t')\ . \tag{8}$$

This in turns leads to the results

$$P(t)=d\,[F(t)-B(t)]\ ,\quad S(t)=d^2[F(t)+B(t)]\ . \tag{9}$$

In the dc-limit $\hat\epsilon\equiv 0$ one recovers the known relations $P(t)=d\rho_0\ t$ and $S(t)=d^2\gamma_0\ t$, where we set $\rho_0=\rho(\hat\epsilon=0)$ and $\gamma_0=\gamma(\hat\epsilon=0)$. Hence the particle diffuses linearly in time with nonlinear dc-mobility $\mu_0(\epsilon_0)=d^2\rho_0(\epsilon_0)/\hbar\epsilon_0$ and dc-diffusion coefficient $D_0(\epsilon_0)=d^2\gamma_0(\epsilon_0)/2$. In the following we investigate the mean square deviation $S(t)$ in the presence of dc-ac fields, as well as the time-averaged nonlinear mobility

$$\mu(\epsilon_0,\hat\epsilon)=\lim_{t\to\infty}\frac{d}{\hbar\epsilon_0}\frac{\Omega}{2\pi}\int_t^{t+2\pi/\Omega}{\rm d}t'\ \dot P(t')\ , \tag{10}$$

and the nonlinear diffusion coefficient

$$D(\epsilon_0,\hat\epsilon)=\lim_{t\to\infty}\frac{\Omega}{4\pi}\int_t^{t+2\pi/\Omega}{\rm d}t'\ \dot S(t')\ . \tag{11}$$

Incidently, the time-averaged nonlinear current $I(\epsilon_0,\hat\epsilon)$ of an ensemble of charged particles immediately follows from $I=e(\hbar\epsilon_0/d)\mu$, where e is the elementary electronic charge. From (9) we obtain

$$\mu(\epsilon_0,\hat\epsilon)=\frac{d^2\Delta^2}{\hbar\epsilon_0}\int_0^\infty {\rm d}\tau J_0\Big(\frac{\hat\epsilon}{\Omega}\sin\frac{\Omega\tau}{2}\Big)e^{-Q'(\tau)}\sin Q''(\tau)\sin\epsilon_0\tau\ , \tag{12}$$

$$D(\epsilon_0,\hat\epsilon)=\frac{d^2}{2}\Delta^2\int_0^\infty {\rm d}\tau J_0\Big(\frac{\hat\epsilon}{\Omega}\sin\frac{\Omega\tau}{2}\Big)e^{-Q'(\tau)}\cos Q''(\tau)\cos\epsilon_0\tau\ , \tag{13}$$

where J_0 is the zeroth-order Bessel function.

Up to now our results have been general. To make quantitative calculations we restrict ourselves to the specific case of Ohmic dissipation with an exponential cut-off $\omega_{\rm c}$ [14]

$$J(\omega)=(2\pi\hbar/d^2)\ \alpha\omega e^{-\omega/\omega_{\rm c}}\ , \tag{14}$$

where α is the Ohmic phenomenological dimensionless damping strength. Then, the real and the imaginary part $Q'(\tau)$ and $Q''(\tau)$ of $Q(\tau)$ in (7) assume the form

$$\begin{aligned}Q'(t)&=\alpha\ln(1+\omega_{\rm c}^2t^2)+4\alpha\ln\left|\frac{\Gamma(1+1/\hbar\beta\omega_{\rm c})}{\Gamma(1+1/\hbar\beta\omega_{\rm c}+it/\hbar\beta)}\right|\ ,\\ Q''(t)&=2\alpha\arctan(\omega_{\rm c}t)\ ,\end{aligned} \tag{15}$$

where $\Gamma(z)$ denotes the gamma function. For our simulations we choose $\omega_{\rm c}=20\Delta$.

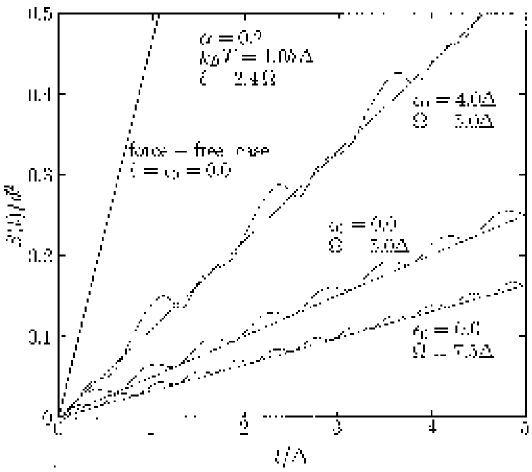

Fig. 1. – Dimensionless variance $S(t)/d^2 = (\langle q^2\rangle_t - \langle q\rangle_t^2\ )/d^2$ *vs.* time (full straight line and dot-dashed curves). S/d^2 is reduced as compared to the force-free case. It assumes its minimal values for zero dc-bias, high ac-frequencies Ω and when $\hat\epsilon \simeq 2.4\ \Omega$, corresponding closely to the conditions for dynamical localization in the nondissipative case. The dashed straight lines depict the curve $2D(\epsilon_0, \hat\epsilon)t$, where D is the diffusion constant in eq. (13).

The mean square deviation $S(t)$ *vs.* time is shown in fig. 1. For generic ϵ_0, $\hat\epsilon$ and Ω values, the diffusion is reduced as compared to the force-free case. For values of $\hat\epsilon$ and Ω such that $J_0(\hat\epsilon/\Omega) \simeq 0$, *i.e.* $\hat\epsilon/\Omega \simeq 2.4$, see the dot-dashed curves in fig. 1, the diffusion becomes very slow, especially for zero dc-bias and high driving frequencies Ω. This choice for $\hat\epsilon/\Omega$ corresponds to the condition for dynamical localization (DL) found for nondissipative TB systems [11]. Finally, the average slope of the curves in fig. 1 is well approximated by twice the diffusion coefficient (13).

In fig. 2 *a*) the dimensionless current $I(\epsilon_0, \hat\epsilon; \alpha)/ed\Delta$, is plotted *vs.* the dissipative strength α for different driving frequencies Ω. Two striking effects occur for weak damping and strong damping, respectively. *i*) A *negative current* at weak dissipation is observed. Moreover, for fixed $\hat\epsilon$ and Ω the amplitude of the negative current is *maximal* for a characteristic value $\alpha = \alpha^*$ of the Ohmic strength. *ii*) For stronger dissipation the current becomes independent of the ac-frequency and on dissipation on a wide range. As the frequency is increased further, the linear response regime $\hat\epsilon/\Omega \ll 1$ is approached and the current moves towards its dc-limit (full-line in fig. 2 *a*)). In fig. 2 *b*) $I(\epsilon_0, \hat\epsilon; \alpha)/ed\Delta$ is plotted *vs.* the applied dc-voltage ϵ_0 for different values of the applied ac-voltage $\hat\epsilon$. Again, a current reversal is observed.

To explain the results of figs. 1 and 2 it is convenient to expand $J_0\Big(\frac{\hat\epsilon}{\Omega}\sin\frac{\Omega\tau}{2}\Big)$ in Fourier series to obtain

$$\mathcal{R}(\epsilon_0, \hat\epsilon; \alpha) = J_0^2\Big(\frac{\hat\epsilon}{\Omega}\Big)\mathcal{R}_0(\epsilon_0; \alpha) + \sum_{n=-\infty, n\neq 0}^{\infty} J_n^2\Big(\frac{\hat\epsilon}{\Omega}\Big)\mathcal{R}_0(\epsilon_0 + n\Omega; \alpha)\ , \tag{16}$$

where $\mathcal{R}_0(\epsilon_0; \alpha) := \mathcal{R}(\epsilon_0, \hat\epsilon = 0; \alpha)$, and $\mathcal{R} = I$ or D. Thus, the ac-voltage produces new channels for dc-current flow or dc-diffusion due to photon emission ($n > 0$) and absorption ($n < 0$), each weighted by the factor $J_n^2(\hat\epsilon/\Omega)$.

Let us focus on the time-averaged current. The current inversion is due to the competition between the channels with $n = 0$, $n > 0$, each of which always gives a positive contribution to

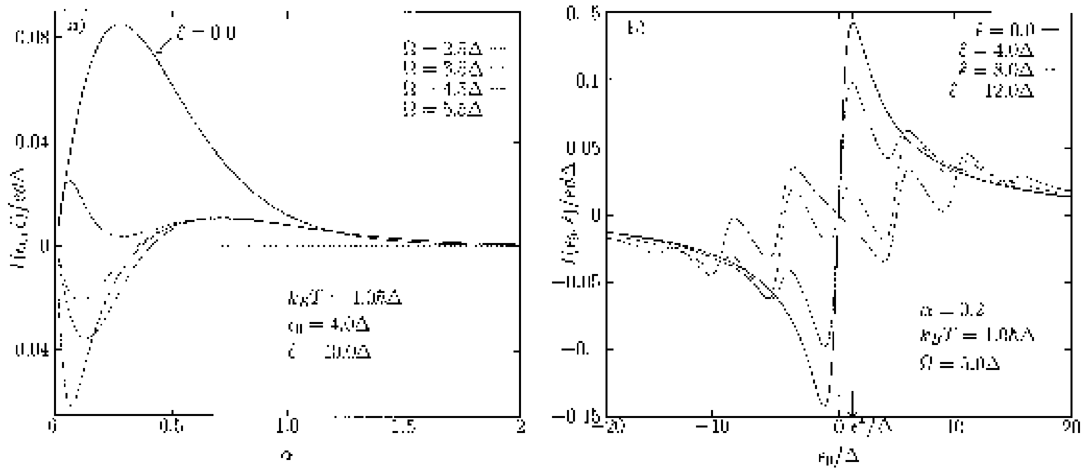

Fig. 2. – Dimensionless time-averaged current $I/ed\Delta$ plotted *vs.* the dissipative Ohmic strength α (fig. 2 *a*)) and *vs.* the dc-bias ϵ_0 (fig. 2 *b*)). For weak dissipation a negative current, which is *maximal* for an optimal value of α is found. For stronger dissipation the current becomes independent of the ac-frequency and on dissipation on a wide range.

the total current, and higher-order channels with $n < 0$ which may give a negative contribution. In fact, with the help of the blocking effect (*i.e.* $J_0(\hat{\epsilon}/\Omega) \simeq 0$) of the $n = 0$ channel it can be more favorable in current-gain (in absolute value) to absorb n photons than to emit n of them, even if the weight of the sidebands is the *same* and given by $J_n^2(\hat{\epsilon}/\Omega)$. For example, for the dot-dashed curves of fig. 2 *a*), 2 *b*) ($\Omega = 4.5\Delta$) the main contribution to the current is found to come from the first negative channel ($n = -1$) (not shown). Correspondingly, the maximal negative inversion occurs for $\alpha = \alpha^* \neq 0$ such that $|I_0(\epsilon_0 - \Omega; \alpha)|$ is maximal as a function of α (cf. fig. 2 *a*)). For fixed $\hat{\epsilon}$, $I(\epsilon_0, \hat{\epsilon}; \alpha)$ *vs.* ϵ_0 may have several minima $\epsilon_{\rm min}^{(n)}$ determined by the condition $\epsilon_{\rm min}^{(n)} + \epsilon^* = n\Omega$, where ϵ^* is the maximum of the dc-current I_0 *vs.* the dc-bias (see fig. 2 *b*)). Note that the position of these minima does not depend on the strength $\hat{\epsilon}$ of the ac-field. The ac-field strength determines instead the weight of the different channels. For the parameters chosen in fig. 2 *b*), the maximal negative current occurs when $\hat{\epsilon}$ is chosen such that the first channel dominates ($J_n^2(\hat{\epsilon}/\Omega) \simeq 0,\ n \neq 1$). The same line of reasoning can be used to explain the behaviour of the variance in fig. 1.

Finally, we observe that the structure (16) is *universal*, *i.e.* it does not depend on the specifics of the thermal bath. Dissipation determines instead the shape of the dc-current I_0, and of the dc-diffusion D_0. Hence, as long as the dc-current *vs.* the dc-bias presents the (physical) characteristics of being antisymmetric, positive for $\epsilon_0 > 0$ with a maximum at $\epsilon_0 = \epsilon^*$, a current reversal is possible even for a dissipative mechanism which is different from the Ohmic one we choose. In the same way the nonlinear diffusion will always be strongly reduced in the parameter regime of dynamical localization.

Indeed, a similar behaviour for the current *vs.* the dc-bias in semiconductor superlattices at room temperature has been predicted in [4] within a phenomenological approach based on a classical Boltzman equation with a single collision time ansatz. On the contrary, our results were obtained starting from a full *microscopic* analysis, with the only restriction being that of an incoherent tunneling dynamics. Recently, such a time-averaged negative current, (*i.e.* an absolute negative conductance) *vs.* the dc-bias has been very recently predicted theoretically and observed experimentally in semiconductor superlattices [4], [5], and in double quantum wells [16].

In conclusion, starting from a pure microscopic model, we investigated the quantum current as well as the diffusion of dissipative particles in TB lattices under the combined effects of dc-ac electric fields. For generic dc-ac fields, the particle diffuses slower, as compared to the force-free case, and it can be almost localized for appropriate values of the dc and ac driving strengths and driving frequencies. In addition, a negative current may occur, whose amplitude is maximal for an optimal value of the dissipative strength. Finally, for moderate-to-strong damping the current is positive and widely independent of the applied ac-frequency and dissipation.

Thus, our work provides a great potential for applications: It can be used to build quantum Brownian rectifiers moving particles "up-hill" in a tilted washboard potential, or to obtain a "down-hill" current, which is largely independent of the noise of the experimental device without the need of much fine tuning for the external ac-frequency.

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