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Einstein relation for a driven disordered quantum chain in subdiffusive regime

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A quantum particle propagates subdiffusively on a strongly disordered chain when it is coupled to itinerant hard-core bosons. We establish a generalized Einstein relation (GER) that relates such subdiffusive spread to an unusual time-dependent drift velocity, which appears as a consequence of a constant electric field. We show that GER remains valid much beyond the regime of the linear response. Qualitatively, it holds true up to strongest drivings when the nonlinear field–effects lead to the Stark-like localization. Numerical calculations based on full quantum evolution are substantiated by much simpler rate equations for the boson-assisted transitions between localized Anderson states.

Introduction- Over two decades after the outstanding discovery of the Anderson localization (AL) phenomena [1], the effect of the interplay between the disorder and many-body interactions on transport properties of metals started to be recognized as one of the fundamental unsolved problems in solid state physics [2, 3]. The importance of interactions on AL systems is now identified as a concept of the many-body localization (MBL) [4, 5]. The presence of MBL has been theoretically confirmed predominantly in systems that posses only spin or charge degrees of freedom [6–22]. Moreover, the existence of MBL has been found in a few experimental studies [23–28]. Among several characteristic features of strongly disordered systems is unusually slow time evolution of characteristic physical properties [27, 29–48] that typically emerges as subdiffusive dynamics as a precursor to MBL transition [18, 39, 49–54].

In this Letter we consider the effect of driving (via the constant electric field) on a quantum particle in a random chain coupled to itinerant hard-core bosons (HCB). We note that such a system simulates the propagation of a (single) charge coupled to spin degrees in strongly correlated systems, as e.g., the disordered Hubbard typemodels [44, 55, 56], being realized in cold-atom experiments [23–28]. It has long been assumed that the AL phenomenon is destroyed by the electron-phonon coupling via the mechanism of phonon-assisted hopping [57, 58]. Recently the absence of localization and the onset of normal diffusion of a particle coupled to standard itinerant bosons has been confirmed via a direct quantum evolution [59]. Still, the itinerant HCB appear to be a separate case with a transient or even persistent subdiffusive dynamics [54, 60]. While the subdiffusive dynamics has been found in various disordered interacting systems, the behavior of such system under constant driving remains predominantly unexplored [61] whereby in driven MBL systems the focus has been mostly on periodic drivings [9, 62-65].

Transport properties of disordered quantum interacting many-body systems depend on the disorder strength. Weakly disordered systems typically display generic transport properties. In particular, a one-dimensional (1D) chain reveals normal diffusion [39], i.e., a nonuniform particle density spreads as $\langle x^2(t) \rangle_0 = 2Dt$, where D is the diffusion constant. A weak external field, F, induces a drift, $\langle x(t) \rangle_F = \mu F t$, where μ is the mobility. According to the Einstein relation [66], $\mu = \beta D$, where $\beta = 1/k_B T$ with temperature T, the relation being valid also for quantum particles at high-enough T.

Strongly disordered chains of spinless fermions show MBL when the d.c. transport is completely suppressed. Here, we are interested in the intermediate case when the particles spread subdiffusively, i.e., with the d.c. value $D_0 = 0$ but $\langle x^2(t) \rangle_0 \propto t^{\gamma}$ with $0 < \gamma < 1$. There is a vast theoretical evidence for such subdiffusive evolution without external driving in disordered 1D systems, whereby the anomalous spread has been explained via the "weak–link" scenario [27, 37, 67, 68]. Despite $D_0 = 0$, one expects the relevance of generalized Einstein relation (GER) [69, 70]

$$\langle x(t) \rangle_F = F \frac{\beta}{2} \langle x^2(t) \rangle_0, \tag{1}$$

as long as the system remains in the linear response (LR) regime. However, subdiffusive systems display very slow relaxation, hence even a weak field can drive the system far from equilibrium. Then, β in Eq. (1) might be ill defined, hence the limits of the LR regime and the applicability of Eq. (1) should be methodically explored.

In the following we show that the GER holds true even for large fields within the quasiequilibrium LR when the temperature increases in time due to heating. For even stronger fields the particle dynamics gradually slows down (approaching the effective exponent $\gamma = 0$), related in this regime to the phenomenon of Stark localization. We also show that results obtained via full quantum evolution can be well explained with much simpler rate equations, where the transition rates between Anderson states are evaluated via the Fermi golden rule (FGR).

Model and method– We study a model of quantum particle moving in a disordered chain (Anderson model) and coupled to bosons,

$$H = -t_h \sum_{j} (c_{j+1}^{\dagger} c_j + \text{h.c.}) + \sum_{j} h_j n_j + g \sum_{j} n_j (a_j^{\dagger} + a_j) + \omega_0 \sum_{j} a_j^{\dagger} a_j - t_b \sum_{j} (a_{j+1}^{\dagger} a_j + \text{H.c.}).$$
(2)

where $n_j = c_j^{\dagger}c_j$ is local particle density and the random potential h_j is assumed to be uniformly distributed in [-W, W]. Bosons in Eq. (2) are itinerant due to finite hopping $0 < t_b < \omega_0/2$. We consider (predominantly) bosons being HCB with only two states per site. However, we briefly discuss also the coupling to standard bosons which leads to a normal diffusive transport [54].

In order to study the particle driven with a constant electric field F one considers either a system with periodic boundary conditions (p.b.c.) and time-dependent Peierls phase $t_h \rightarrow t_h \exp(-iFt)$ or a chain with open boundary conditions and additional electrostatic potential $H \rightarrow H - \sum_j jFn_j$. While both approaches are equivalent [71], the former one is more convenient for full quantum dynamics and the latter one with timeindependent H facilitates calculations of the transition rates between the Anderson states. Finally, we take $|t_h| = 1$ as the energy unit.

Numerical results – First, we numerically study the Hamiltonian, Eq. (2), with a Peierls driving $t_h(t) =$ $\exp(-iFt), F = \text{const.}$ We consider only relatively strong disorder, $W \geq 3$. It has been shown in Ref. [54] that in this regime (at F = 0) the particle coupled to HCB spreads subdiffusively, i.e., $\langle x^2(t) \rangle_0 \propto t^{\gamma}$ with $\gamma < 1$. The key question is whether the GER, Eq. (1), holds true and the transport anomaly shows up in the current that is induced by $F \neq 0$. In principle, Eq. (1) can be directly tested only for $F \to 0$, when $\beta(t) = \beta(0)$. otherwise the system's energy increases due to driving, $\Delta E(t) = F \langle x(t) \rangle_F$. Still, recalling that in the hightemperature regime $T \gg t_h$ the kinetic energy is proportional to the inverse temperature $E_k(t) \propto -\beta(t)$, where $E_k = \langle \sum_j e^{-iFt} c_{j+1}^{\dagger} c_j \rangle + \text{c.c.}$, the instantaneous $\beta(t)$ can be also directly monitored. Utilizing the latter proportionality, we rewrite Eq. (1) in a form that may be directly tested also for driven closed systems

$$R(t) = -\frac{\Delta E(t)}{F^2 E_k(t)} \propto \langle x^2(t) \rangle_0 \propto t^{\gamma}.$$
 (3)

Numerical calculations were performed on 1D systems with up to L = 14 sites with p.b.c. The size of the Hilbert space is given by $N_{\rm st} = L 2^L$, whereas the finite–size effects are discussed in the Supplemental Material [72]. Both energies in Eq. (3) were obtained by sampling over $N_{\rm s} = 10^3$ realizations of disorder. Full quantum time evolutions were performed while taking the advantage of the Lanczos technique [73] starting from the corresponding ground state of H. To achieve sufficient accuracy of time propagation, we used time step $\Delta t = 0.02$ and reached

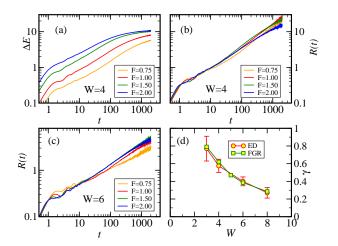


Figure 1. Results of full time propagation on systems with L = 14 for energy increase $\Delta E(t)$ in (a), and R(t) in (b) and (c). In (d) γ vs. W is shown, as obtained from fitting $R(t) \propto t^{\gamma}$ for $t \gtrsim 1$ in case of ED (circles) and using FGR (squares). In the latter case γ was extracted from $\langle x^2(t) \rangle_0 \propto t^{\gamma}$, see Ref. [54]. Note that unless otherwise specified, we have used: $\omega_0 = g = 1$, and $t_g = 0.5$.

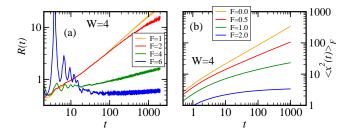


Figure 2. In (a) we show R(t) for W = 4 for different F > 0, up to maximal F = 6 using ED on L = 14 sites, and in (b) the spread $\langle x^2(t) \rangle_F$, using FGR for L = 400.

times $t \sim 10^3$. In Fig. 1(a) we show the sample-averaged energy increase $\Delta E(t) = (1/N_{\rm s}) \sum_i (E_i(t) - E_i(0))$, where $E_i(0)$ is the ground-state energy of H, Eq. (2), corresponding to *i*-th particular random-potential configuration $\{h_j\}$. Figs. 1(b) and (c) show the ratio R(t) for two values of disorder W = 4, 6. The main observation is that results are consistent with $R(t) \propto t^{\gamma}$, based on the assumption of the GER. In Fig. 1 (d) we show extracted exponents γ for different values of W along with those obtained from the spread of $\langle x^2(t) \rangle_0$ using analytical approach based on FGR, as discussed below.

Fig. 2a shows numerical results for R(t) for a fixed disorder strength W but various drivings F. It is evident that for stronger driving F > 2, exponent γ (as well as particle dynamics) is significantly reduced and eventually, for very strong $F \sim 6$ the particle becomes almost localized, here due to the Stark phenomenon.

Dynamics via rate equations.- In the following we de-

scribe the system's dynamics using the rate equations for the transitions between the localized Anderson states. The method has been shown to reproduce for F = 0 the subdiffusive particle dynamics as well as (at least qualitatively) values for the exponent γ , [54]. Direct comparison of numerical results obtained from ED and the rate equations is shown in the Supplemental Metarial [72]. We stress that it is essential to study the distribution of the transition rates and not just their average values, since the averaging erases the essential information on their large and singular fluctuations. In particular, averaging of localized and delocalized samples would (mistakenly) indicate that the particle is always delocalized.

Here, we recall only main steps of Ref. [54] for derivation of the transition rates, now taking into account $F \neq 0$. First we solve the single-particle eigenproblem for open boundary conditions

$$\sum_{j} \left[-t_h (c_{j+1}^{\dagger} c_j + \text{h.c.}) + (h_j - jF) n_j \right] = \sum_l \epsilon_l \varphi_l^{\dagger} \varphi_l,$$
(4)

where $\varphi_l^{\dagger} = \sum_j \phi_{lj} c_j^{\dagger}$ creates a particle in the localized Anderson–Stark state $|l\rangle$. Using the FGR one obtains transition rates between states l, l' which originate from the coupling to HCB,

$$\Gamma_{l,l'} = \int_{-\infty}^{\infty} \mathrm{d}t \; e^{-it\Delta_{l,l'}} \frac{1}{L} \sum_{q} |\eta_{l,l',q}|^2 \\ \times \left[f(\omega_q) e^{-i\omega_q t} + f(-\omega_q) e^{i\omega_q t} \right], \tag{5}$$

$$\eta_{l,l',q} = g \sum_{i} e^{-iqj} \phi_{l'j} \phi_{lj}, \qquad (6)$$

where $\omega_q = \omega_0 - 2t_B \cos(q)$, $f(\omega_q)$ is the Fermi-Dirac distribution function and $\Delta_{l,l'} = \epsilon_l - \epsilon_{l'}$. Within the FGR, the particle dynamics can be described via the rate equations for occupations $n_l(t) = \langle \varphi_l^{\dagger} \varphi_l \rangle(t)$,

$$\frac{\mathrm{d}n_l}{\mathrm{d}t} = \sum_{l'} (\Gamma_{l'l} n_{l'} - \Gamma_{ll'} n_l). \tag{7}$$

Fig. 2b shows the evolution of the averaged spread, $\langle x^2(t) \rangle_F = \sum_l (x_l - x_{l_0})^2 n_l(t)$, where $x_l = \sum_j j |\phi_{lj}|^2$, as obtained via rate equations at $\beta \to 0$ for L = 400 and open boundary conditions. Particle is initially put in the middle of the system, well away from the boundaries, i.e., $n_l(0) = \delta_{l,l_0}$. Due to strong disorder, W = 4, the particle spread is subdiffusive already for F = 0. For larger F > 1, the diffusion further slows down and eventually for $F \geq 2$ the particle tends to localize due to the Stark effect, i.e., $\langle x^2(t \to \infty) \rangle_F$ saturates. We stress a clear qualitative similarity between the spread and the rescaled drift, R(t), shown in Fig. 2a. This similarity persists even when both quantities are determined for strong F, well beyond the the LR regime relevant for Eq. (1).

Eqs. (5)-(7) can be studied numerically even for large systems. However, in order to derive the GER within

rate-equation approach, we rewrite Eq. (5) in a more symmetric form, representing it as $\Gamma_{l,l'} = \Gamma^0_{l,l'}[1 + \tanh(\beta \Delta_{l,l'}/2)]$, where $\Gamma^0_{l,l'}$ refer to rates for $\beta \to 0$,

$$\Gamma_{l,l'}^{0} = \frac{\pi}{L} \sum_{q} |\eta_{l,l',q}|^2 \left[\delta(\omega_q + \Delta_{l,l'}) + \delta(\omega_q - \Delta_{l,l'}) \right].$$
(8)

In general, $F \neq 0$ enters via the (symmetric) overlaps, $\eta_{l,l',q} = \eta_{l',l,q}$, and the (antisymmetric) energy differences, $\Delta_{l,l'} = -\Delta_{l',l}$. The antisymmetry of $\Gamma_{l,l'}$ originates solely from $\tanh(\beta \Delta_{l,l'}/2)$. The time-evolution of the particle drift due to $F \neq 0$ can be evaluated as the current, $I(t) = d\langle x(t) \rangle / dt = \sum_l x_l dn_l / dt$. Using Eq. (7) one then obtains

$$I(t) = -\sum_{l,l'} \frac{(x_l - x_{l'})^2}{2} \Gamma_{l,l'}^0 \times \left[\frac{n_l - n_{l'}}{x_l - x_{l'}} + (n_l + n_{l'}) \frac{\tanh[\frac{\beta(\epsilon_l - \epsilon_{l'})}{2}]}{x_l - x_{l'}} \right].$$
(9)

For high T, the second term may be expanded in β . Then, Eq. (9) becomes the Einstein relation which states that the current is induced by the gradient of the particle density (first term) and the gradient of the potential (second term), where the latter is weighted by β and the local density, $(n_l + n_{l'})/2$.

For strong disorder and weak F one may assume that $\epsilon_l \simeq \epsilon_l^0 - x_l F$, where ϵ_l^0 refers the Anderson state at F = 0. Since on average $\epsilon_l^0 - \epsilon_{l'}^0$ vanishes, the term $(\epsilon_l^0 - \epsilon_{l'}^0)/(x_l - x_{l'})$ does not contribute to the uniform current. Then, the meaning of Eq. (9) becomes even more evident,

$$I(t) \simeq \sum_{l,l'} \frac{(x_l - x_{l'})^2}{2} \Gamma^0_{l,l'} \left[-\frac{n_l - n_{l'}}{x_l - x_{l'}} + \frac{n_l + n_{l'}}{2} \beta F \right].$$
(10)

We may further simplify the analysis by neglecting the explicit momentum dependence of $|\eta_{l,l',q}|^2$,

$$|\eta_{l,l',q}|^2 \simeq |\eta_{l,l'}|^2 = \frac{1}{L} \sum_q |\eta_{l,l',q}|^2 = g^2 \sum_i (\phi_{l'i} \phi_{li})^2.$$
(11)

and assume an uniform bosonic density of states $1/L \sum_{q} \delta(\omega - \omega_q) \simeq \frac{1}{\Omega} \theta(\Omega - \omega)$ where $\Omega = \omega_0 + 2t_B$. Then the transition rates at $\beta \to 0$ read

$$\Gamma^{0}_{l,l'} \simeq \pi |\eta_{l,l'}|^2 \frac{1}{\Omega} \theta(\Omega - |\Delta_{l,l'}|).$$
(12)

In order to explain the interplay between strong disorder and strong driving we calculate $\Gamma_l = \sum_{l'\neq l} \Gamma_{l,l'}^0$ representing the inverse lifetime of a particle occupying the Anderson state $|l\rangle$, $\tau_l = 1/\Gamma_l$. As stressed before, it is essential to avoid averaging of Γ_l over disorder. Instead one may consider it as a random variable and discuss the probability density $f_{\Gamma}(\Gamma_l)$ or equivalently $f_{\tau}(\tau_l)$. Without driving [51, 54], the qualitative transport properties can be read out from the latter distribution using the random-trap model [70]. Namely, for $f_{\tau}(\tau_l) \propto 1/\tau_l^{\alpha+1}$ the normal diffusive transport exists for $\alpha \geq 1$, whereas for $0 < \alpha < 1$ the particle spreads subdiffusively with $\langle x^2(t) \rangle \propto t^{\gamma}$ and $\gamma = 2\alpha/(1+\alpha)$. By comparing the cumulative distribution functions one finds that the distribution $f_{\tau}(\tau_l) \propto 1/(\tau_l)^{\alpha+1}$ corresponds to $I(\Gamma) = \int_0^{\Gamma} f_{\Gamma}(\Gamma_l) d\Gamma_l \propto \Gamma^{\alpha}$, so the type of dynamics (i.e., the value of α) can be recognized directly from $I(\Gamma)$.

Fig. 3 shows the FGR results for $I(\Gamma)$. Results in panels a) and b) are obtained from Eqs. (5)-(6), whereas panel c) shows results for the simplified transition rates, Eq. (12), labeled as *Toy-model*. The dashed lines show $I(\Gamma) \propto \Gamma$ hence they mark the threshold for the normal diffusive transport. Comparing panels b) and c) it becomes quite evident that simplification via Eq. (11) is very accurate. One may also see that upon increasing F, the exponent α decreases and eventually becomes vanishingly small for $F \geq 2$. The latter result means that $f_{\Gamma}(\Gamma_l)$ acquires a $\delta(\Gamma_l)$ contribution or, in other words, that some states remain localized despite being coupled to HCB. Since this effect originates from strong electric field, it is legitimate to attribute it as the Stark localization.

Finally, we argue that the Stark localization doesn't occur if the particle is coupled to standard bosons, e.g., phonons. Then, the multi-boson processes significantly contribute to the transition rates, whereas previously, such contributions were strongly suppressed by the hard core–effects. As argued for the standard bosons [54], the rigid cut-off in Eq. (12) should be replaced by a smooth exponential cut-off, $\theta(\Omega - |\Delta_{l,l'}|) \rightarrow \exp(-|\Delta_{l,l'}|/\Omega)$. This seemingly harmless modification, changes the distribution of the transition rates, as shown in Fig. 3d. Even for very strong drivings and for very strong disorder the transitions rates are bounded from below $\Gamma_l \geq \Gamma_{\min}$. Therefore, the diffusion constant might be very small but nevertheless nonzero. Although the subdiffusive transport may show up for a quite long time-window, it is a transient phenomenon that will eventually be replaced by a normal diffusion, irrespectively of W or F.

The GER is expected to hold true within the LR theory [69, 70], whereas we have demonstrated that it remains applicable (at least qualitatively) for stronger drivings when assumptions of LR are not fulfilled in an obvious way. We note that in deriving Eq. (9) from the master equation (7) we have not assumed that driving is weak or that the transport is normal diffusive, since the anomalous transport and nonlinear (in F) effects are encoded in $\Gamma^0_{l,l'}$, see Eq. (12). The essential step in our derivation consist in expanding $tanh[\frac{\beta(\epsilon_l - \epsilon_{l'})}{2}]$ linearly in F. Here, β is the temperature of the bosonic bath so the bosonic bath must be in equilibrium (or close to equilibrium) and the expansion is justified when β is small.

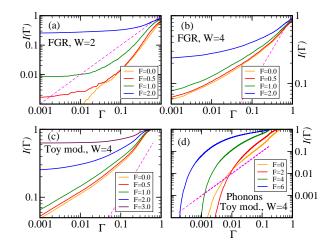


Figure 3. Cumulative distributions $I(\Gamma)$ in panels a) and b) for different F were obtained from Eqs. (5)-(6), based on FGR. In panel (c) we show results for the simplified (toy model) rates as given by, Eq. (12). The dashed lines in all panels represent the threshold for normal diffusion, $I(\Gamma) \propto \Gamma$.

One may also expect that the present model is oversimplified in that it describes only single quantum particle coupled to mutually noninteracting HCB. A more realistic description should account for nonzero density of fermions which, in turn, may induce effective interactions among the HCB. In order to check how the latter phenomena affects results presented in this manuscript, we have studied a similar system but with a boson-boson interactions. Results shown in the Supplemental Material [72] demonstrate that our qualitative conclusions hold true also for mutually interacting HCB [60].

Conclusions. – We have studied the transport properties of a quantum particle that propagates along a disordered chain and is coupled to hard-core bosons, whereby such a case can be considered as the simulation of the charge motion in the spin background in strongly correlated disordered systems. Without external driving, the particle exhibits anomalous subdiffusive propagation with vanishing diffusion constant. The main goal was to establish whether a generalized Einstein relation holds true in such a system. Namely, we have studied the relation between the drift originating from the electric field (F) and the spread of the particle density which grows in time mainly due to its inhomogeneous spatial distribution. Both quantities were determined in the presence of F. The GER was shown to hold true in the LR regime (as expected) but also within the quasiequilibrium evolution, when the energy (temperature) increases in time due to driving. In particular, we have demonstrated that a single exponent γ characterizes the anomalous dynamics of the spread $\langle x^2(t) \rangle_F$ and the drift $\langle x(t) \rangle_F \propto \langle x^2(t) \rangle_0 \propto t^{\gamma}$. Quite unexpectedly, the latter similarity between $\langle x^2(t) \rangle_F$ and $\langle x(t) \rangle_F$ holds true also

for much stronger fields beyond the regime of quasiequilibrium evolution. However for strong fields, γ decreases with increasing F and eventually, for very strong F, it vanishes marking the field-induced Stark localization. Qualitatively, all these properties were demonstrated to follow from the distribution of the transition rates between the Anderson states. We have also argued that the subdiffusive transport and localization should not occur when the particle is coupled to regular itinerant bosons with unbounded energy spectrum. In the latter case, strong driving may lead to a transient slowing down of the particle dynamics, nevertheless the asymptotic transport is expected to be normal diffusive. We cannot exclude that within a more accurate treatment of the multi-boson processes the normal diffusion eventually shows up also in the HCB model, however, for much longer times than for regular bosons.

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