Many-body interband tunneling as a witness for complex dynamics in the Bose-Hubbard model

Andrea Tomadin,1 Riccardo Mannella,1 and Sandro Wimberger1,2

1Dipartimento di Fisica, Università degli Studi di Pisa, Largo Pontecorvo 3, 56127 Pisa, Italy
2CNISM, Dipartimento di Fisica del Politecnico, C. Duca degli Abruzzi 24, 10129 Torino, Italy

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A perturbative model is studied for the tunneling of many-particle states from the ground band to the first excited energy band, mimicking Landau-Zener decay for ultracold, spinless atoms in quasi-one dimensional optical lattices subjected to a tunable tilting force. The distributions of the computed tunneling rates provide an independent and experimentally accessible signature of the regular-chaotic transition in the strongly correlated many-body dynamics of the ground band.

The experimental advances in atom and quantum optics allow the experimentalist to directly study a plethora of minimal models which have been developed to describe usually much more complex phenomena occurring in solid states [1,2,3]. Bose-Einstein condensates loaded into optical lattices, which perfectly realize spatially periodic potentials, are used, e.g., to implement the Wannier-Stark problem [4,5,6] as a paradigm of quantum transport where atoms move in a tilted lattice. Up to now all experiments on the Wannier-Stark system with ultracold atoms have been performed in a regime where atom-atom interactions are either negligible [1] or reduce to an effective mean-field description [3,7]. State-of-the-art setups are, however, capable to achieve small filling factors of the order of one atom per lattice site [2]. Moreover, the atom-atom interactions can be tuned by the transversal confinement and by Feshbach resonances [3,8], resulting in strong interaction-induced correlations.

The regime of strong correlations in the Wannier-Stark system was addressed in [9,10], revealing the sensitive dependence of the system’s dynamics on the Stark force \( F \). The single-band Bose-Hubbard model of [6,10] is defined by the following Hamiltonian with the creation \( \hat{a}^\dagger \), annihilation \( \hat{a} \), and number operators \( \hat{n}_{l,1} \) for the first band of a lattice \( l = 1 \ldots L \):

\[
\sum_l F l \hat{n}_{l,1} - \frac{J_1}{2} \left( \hat{a}_{l+1,1}^\dagger \hat{a}_{l,1} + \text{h.c.} \right) + \frac{U_1}{2} \hat{n}_{l,1} (\hat{n}_{l,1} - 1) .
\] (1)

A transition from a regular dynamical (dominated by \( F \)) to a quantum chaotic regime (with comparable values of \( J_1, U_1, F \)) was found [9,10]. The transition was quantitatively studied using the distribution of the spacings between next nearest eigenenergies of the Hamiltonian [9]. This analysis [3,10] verifies that the normalized level spacings \( s \equiv \Delta E / \Delta E \) obey a Poisson (\( P(s) = \exp(-s) \)) and a Wigner-Dyson (WD: \( P(s) = s \pi / 2 \exp(-\pi s^2 / 4) \)) distribution in the regular and chaotic case, respectively [11]. \( P(s) \) and the cumulative distribution functions (CDF: \( C(s) \equiv \int_0^s ds' P(s') \)) are shown for typical cases in Fig. 4 where we scanned \( F \) to emphasize the crossover between the regular and the chaotic regime. Statistical tests are also shown which confirm the analysis of [3,10] in a more systematical manner [12].

As shown in [3], the strong correlations in the quantum chaotic regime induce a fast and irreversible decay of the Bloch oscillations, which otherwise would persist in the ideal, non-interacting case. Therefore, the crossover between the two regimes discussed above could be measured in experiments by observing just the mean momentum as a function of time. Here we introduce a new, robust and hence also experimentally accessible prediction for this crossover. In the presence of strong interactions parameterized by \( U_1 \), the single-band model should be extended to allow for interband transitions [13], as recently realized.

FIG. 1: (a,b) CDF (stairs) and \( P(s) \) (stairs in insets) for \( N = 5 \) atoms, \( L = 8 \), lattice depth \( V = 10 \) recoil energies (fixing \( J_1 = 0.038 \), \( U_1 = 0.032 \), \( F \approx 0.063 \) (a) and 0.021 (b), with WD (solid) and Poisson distributions (dashed). (c) \( \chi^2 \) test with values close to zero for good WD statistics. The dashed line marks the transition to quantum chaos as \( F \) is tuned. (d) \( \chi^2 \) test with the number of levels in intervals of length \( \Delta E \) (with normalized mean spacing), for the cases of (a) (squares) and (b) (circles), with the random matrix predictions for Poisson (dashed) and WD (solid) [11].
at\ F = 0\ in\ experiments\ with\ fermionic\ interacting\ atoms\ 3.\ Instead\ of\ using\ a\ numerically\ hardly\ tractable\ complete\ many-bands\ model,\ we\ introduce\ a\ perturbative\ decay\ of\ the\ many-particles\ modes\ in\ the\ ground\ band\ to\ a\ second\ energy\ band.\ Our\ novel\ approach\ to\ study\ the\ Landau-Zener-like\ tunneling\ between\ the\ first\ and\ the\ second\ band\ 1,\ 3,\ 5,\ 12,\ 13\ leads\ to\ predictions\ for\ the\ expected\ decay\ rates\ and\ their\ statistical\ distributions.\ As\ we\ will\ show,\ the\ latter\ are\ drastically\ affected\ by\ the\ dynamics\ in\ the\ ground\ band,\ and\ they\ therefore\ provide\ a\ measurable\ witness\ for\ the\ regular-chaotic\ transition.

We\ first\ derive\ the\ individual\ decay\ rates\ of\ the\ dominating\ interband\ coupling\ channels.\ These\ decay\ rates\ will\ serve\ to\ effectively\ open\ the\ single-band\ model\ 11\ for\ mimicking\ losses\ arising\ from\ the\ interband\ coupling.\ Our\ analysis\ starts\ from\ the\ following\ “unperturbed”\ Hamiltonian\ for\ the\ first\ two\ bands:\

\[ H_0 = \sum_{l=1}^{L} \left[ \varepsilon_1 \hat{n}_{1,l} + \varepsilon_2 \hat{n}_{1,l} - \frac{J_1}{4} (\hat{a}_{1,l+1} \hat{a}_{1,l} + \text{h.c.}) + F(\hat{n}_{1,l} + \hat{n}_{1,l} + \frac{U_0}{2} \hat{n}_{1,l} (\hat{n}_{1,l} - 1)) \right]. \tag{2} \]

For\ a\ moment,\ we\ neglect\ the\ hopping\ in\ the\ lower\ band,\ where\ the\ single-particle\ Wannier\ functions\ 13\ are\ more\ localized\ than\ in\ the\ upper\ band.\ In\ the\ latter\ we\ neglect\ the\ interactions,\ since\ initially\ only\ a\ few\ particles\ populate\ the\ excited\ levels.\ A\ closer\ analysis\ of\ the\ full\ two-bands\ system\ 12\ shows\ that\ there\ are\ two\ dominating\ mechanisms\ that\ promote\ particles\ to\ the\ second\ band.\ The\ first\ one\ is\ a\ single-particle\ dipole\ coupling\ arising\ from\ the\ force\ term:\

\[ H_1 = F \cdot D \sum_j \left( \hat{a}_{l,2} \hat{a}_{l,1} + \hat{a}_{l,1} \hat{a}_{l,2} \right), \tag{3} \]

where\ \( D \)\ depends\ only\ on\ the\ lattice\ depth\ \( V \)\ (measured\ in\ recoil\ energies\ according\ to\ the\ definition\ in\ 12).\ The\ second\ one\ is\ a\ many-body\ effect,\ describing\ two\ particles\ of\ the\ first\ band\ entering\ the\ second\ band\ together:\

\[ H_2 = \frac{U_x}{2} \sum_{l=1}^{L} \left( \hat{a}_{l,1} \hat{a}_{l,1} \hat{a}_{l,1} \hat{a}_{l,1} + (1 \leftrightarrow 2) \right). \tag{4} \]

The\ cross-band\ interaction\ is\ characterized\ by\ the\ parameter\ \( U_x \equiv \hat{a}_s \int dx \chi_1^2 \chi_2^2 \approx 0.5 U_1 \)\ (for\ \( V = 3 \ldots 10 \)\ 12),\ for\ \( U_1 = \hat{a}_s \int dx \chi_1^2 \),\ with\ renormalized\ scattering\ length\ \( \hat{a}_s \)\ 8,\ 12\ and\ the\ Wannier\ functions\ \( \chi_1, \chi_2 \)\ localized\ in\ each\ well\ for\ the\ first\ or\ second\ band.\ To\ justify\ the\ following\ perturbative\ approach,\ it\ is\ crucial\ to\ realize\ that\ the\ terms\ 3 and\ 11\ must\ be\ small\ compared\ with\ the\ band\ gap\ \( \Delta \equiv \varepsilon_2 - \varepsilon_1 \)\ (not\ necessarily\ small\ with\ respect\ to\ the\ single\ band\ terms\ in\ 11),\ and\ indeed\ \( FD, U_x, U_1 \ll \Delta \)\ for\ the\ parameters\ considered\ here.

For\ the\ first\ perturbation,\ the\ decay\ channel\ of\ a\ given\ unperturbed\ Fock\ state\ labelled\ \( |b\rangle\)\ (with\ a\ total\ number\ of\ atoms\ \( N \)\ and\ \( n_h \)\ atoms\ in\ an\ arbitrary\ well\ \( h \))\ is:

\[ |b; N \rangle \otimes |\text{vac} \rangle \rightarrow |b'; N - 1 \rangle \otimes |w \rangle, \quad n_h = n_h - 1. \tag{5} \]

Here,\ \( |w \rangle = \sum_{m=-\infty}^{+\infty} J_{m-w}(J_2/F) \hat{a}_{m,2} \otimes |\text{vac} \rangle \)\ is\ the\ single-particle\ eigenstate\ for\ the\ Wannier-Stark\ problem,\ localized\ around\ the\ site\ \( w \)\ in\ the\ second\ band,\ with\ the\ Bessel\ function\ of\ the\ first\ kind\ \( J_m(x) \)\ 14.\ The\ expectation\ value\ of\ \( \langle 3 \rangle \)\ for\ \( |b; N \rangle\)\, equal\ to\ the\ first-order\ \( \delta E(b) \),\ is\ zero\ because\ the\ operator\ does\ not\ conserve\ the\ number\ of\ particles\ within\ the\ bands.\ The\ decay\ width\ at\ first-order\ is\ given\ by\ the\ matrix\ element\ of\ the\ perturbation\ between\ the\ initial\ and\ final\ state\ according\ to\ Fermi’s\ Golden\ Rule,\ and\ only\ the\ first\ term\ in\ \( \langle 3 \rangle \)\ gives\ a\ nonzero\ contribution\ 12:

\[ \langle k | b' \rangle \sum_{l=1}^{L} \hat{a}_{l,2} \hat{a}_{l,1} | b \rangle \otimes |\text{vac} \rangle = \sum_{l=1}^{L} J_{l-w}(J_2/F) \delta(n_l', n_l - 1) \sqrt{n_l} \prod_{m \neq l} \delta(n_m', n_m) \tag{6} \]

The\ \( \delta(\cdot, \cdot) \)\ acts\ as\ a\ selection\ rule\ for\ the\ Fock\ states\ that\ are\ coupled\ by\ the\ perturbation.\ The\ tunneling\ mechanism\ does\ not\ include\ any\ income\ of\ energy\ from\ an\ external\ source,\ so\ the\ initial\ and\ final\ energies\ \( E_0(b) = \langle \text{vac} | b |\text{H}_0 | b \rangle \langle b | \text{vac} \rangle \)\ and\ \( E_0(b', w) = \langle w | b |\text{H}_0 | b \rangle \langle b | \text{vac} \rangle \),\ respectively,\ must\ be\ equal\ as\ required\ by\ the\ Golden\ Rule.\ The\ condition\ on\ the\ energy\ conservation\ is,\ however,\ relaxed\ to\ account\ for\ the\ uncertainty\ \( \Delta E(b) \)\ of\ the\ unperturbed\ energy\ levels\ of\ the\ initial\ and\ final\ states\ in\ the\ lower\ band\ arising\ from\ the\ hopping\ in\ this\ band\ initially\ neglected\ in\ \( \langle 2 \rangle \).\ A\ detailed\ derivation\ is\ given\ in\ \( \langle 12 \rangle \),\ and\ here\ we\ only\ state\ the\ result:

\[ \Delta E(b) = 2\pi (J_1/2)^2 \sum_{b'} \delta(E(b) - b') = 2\pi (J_1/2)^2 \sum_l \sum_{\Delta l = \pm 1} n_l^2 \delta(n_l + \Delta l + 1, n_l). \tag{7} \]

The\ level\ density\ \( \rho(E, b) \)\ around\ the\ unperturbed\ energy\ \( E_0(b) \)\ of\ a\ Fock\ state\ \( b \)\ is\ then\ approximated\ by\ a\ rectangular\ profile,\ of\ width\ \( \Delta E(b) \)\ and\ unit\ area:\

\[ \rho(E, b) = \chi \left( |E - E_0(b)| / \Delta E(b) \right) \tag{8} \]

Hence\ the\ energy\ \( \Delta \)\ required\ to\ promote\ a\ particle\ to\ the\ second\ band\ is\ supplied\ by\ the\ decrease\ of\ the\ interaction\ \( \chi U_1 \)\ and\ by\ the\ work\ of\ the\ force\ \( \chi F \)\ exerted\ on\ the\ promoted\ particle.

The\ total\ width\ \( \Gamma_1(b) \)\ for\ the\ decay\ via\ the\ allowed\ channels\ \( K \),\ is\ proportional\ to\ the\ square\ of\ the\ matrix\ element\ and\ to\ the\ level\ density\ \( \rho(E, b) \):

\[ \Gamma_1(b) = 2\pi (F D)^2 \sum_{(h, w) \in K} \left| J_{h-w}(J_2/F) \cdot \sqrt{n_h} \right|^2 \frac{1}{\Delta E(b) \Delta E(b')} \tag{9} \]
\[ J_n(x) \] significantly contributes only for \(|n| \ll |x|\). If \( U_1, \Delta E(b) \ll \Delta \), the energy conservation is roughly given by \(|\Delta| \approx F(h - w)\). Requiring that the Bessel function in (9) is substantially larger than zero, we obtain the inequality \(|\Delta| \leq |J_2|\). The last condition does not depend on \( F \), since a twofold effect is at work: a stronger force produces a larger energy gain when a particle moves along the lattice, but the extension \(|J_2/F|\) of the single-particle state shrinks. Therefore, increasing \( F \) results in an increased energy matching and a strongly reduced “geometrical” matching condition – we apply the truncation \(|\Delta| \leq |J_2|\), such that the energy matching cannot be realized by just tuning the lattice depth. The decay can, however, be activated by an increase of the interactions, which can be experimentally achieved by acting on the transversal confining potential of a quasi-one dimensional lattice, or by a Feshbach resonance [8]. In the calculations presented below, we augmented the dimensional lattice, or by a Feshbach resonance [8]. In the regular regime (f), a log-normal distribution (dotted) well fits the data, with a scaling \( P(\Gamma) \propto \Gamma^{-\varepsilon} \) for the largest \( \Gamma \) (dashed line in the inset of (f) with \( x = 1 \)). In the chaotic case, a global power-law behavior with \( x \approx 2 \) is found (dashed line in the inset of (b)).
Fokk state can act as a privileged decay channel for many eigenstates. Many states then share similar rates, leading to thinner distributions. Therefore, the thinner distribution of Fig. 2(b) is a direct signature of the chaotic dynamics evidenced in (a), as compared with the regular case in (c,f). In Fig. 2(f), we found a good agreement with the expected log-normal distribution of decay rates \( \Gamma \approx 2 \) (dashed lines in (b,d)).

In summary, our perturbative opening of the single-band Wannier-Stark system allows one to study Landau-Zener-like interband tunneling within a many-body description of the dynamics of ultracold atoms. The statistical characterization of the tunneling rates (mean values and form of the distributions) provides clear and robust signatures of the regular-to-chaotic transition for future experiments. A more detailed analysis of the interband coupling in a full-blown model, in which at least two bands are completely included, calls for huge computational resources to access the complete quantum spectra. Nonetheless, our results are a first step in the direction of studies for which “horizontal” and “vertical” quantum transport along the lattice are simultaneously present and influence each other in a complex manner.

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