Occupation Statistics of a BEC for a Driven Landau-Zener Crossing

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We consider an atomic Bose-Einstein condensate (BEC) loaded in a biased double-well trap with tunneling rate K and inter-atomic interaction U. The BEC is prepared such that all N atoms are in the left well. We drive the system by sweeping the potential difference $\mathcal{E}$ between the two wells. Depending on the interaction $u = NU/K$, and the sweep rate $\dot{\mathcal{E}}$, we distinguish three dynamical regimes: *adiabatic*, *diabatic*, and *sudden* and consider the occupation statistics of the final state. The analysis goes beyond mean-field theory and is complemented by a semiclassical picture.

The theoretical and experimental study of driven atomic Bose-Einstein Condensates (BEC) in a few site system using optical lattice technology has sparked an intense research activity in recent years [1, 2, 3, 4]. Beyond their scientific challenge, these studies also aim to realize a new generation of nano-scale devices such as an atom transistor [5]. Consequently, a lot of effort has been invested in the study of the prototype two-site (dimer) system, either within the framework of a nonlinear mean-field approach [1], optionally using higher order cumulants [6], or adopting a conventional many-body perspective [7, 8, 9, 10]. Such investigations have revealed many interesting phenomena related to eigenvalue spectra, the structure of the eigenstates, wavepacket dynamics, e.g. of the Bloch-Josephson type, and leaking dynamics due to dissipative edges.

Driven dimers prove to be even more challenging [11, 12, 13, 14, 15]. The scenario investigated in these studies involves many-body Landau-Zener (LZ) transitions induced by sweeping the potential difference $\mathcal{E}$ between the two wells. Specifically, one assumes that initially $\mathcal{E}$ is very negative, and that all $n = N$ atoms are in the first well. Then $\mathcal{E}$ is increased at some constant rate $\dot{\mathcal{E}}$ to a very large positive value. The objective is to calculate how many atoms (n) remain in the first well. The analysis in the majority of published works is based on the study of the discrete nonlinear Schrödinger equation, which is a mean-field approach [11, 12]. There are only a few studies that have made further progress within the framework of a full quantum mechanical treatment of the system [13, 14, 15]. However, they all focus on calculating the average occupation $\langle n\rangle$, while a theory for the occupation statistics $P(n)$, and in particular for the variance $\mathrm{Var}(n)$ is still lacking.

Outline. – In this Letter, we consider a driven dimer with inter-site hopping amplitude K, and inter-atomic interaction U. The dimensionless parameter $u = NU/K$ can be either positive (repulsive) or negative (attractive) and its magnitude determines the interaction regime which is either Rabi ($|u| < 1$), Josephson ($1 < |u| < N^2$), or Fock ($|u| > N^2$). Depending on the sweep rate $\dot{\mathcal{E}}$ we distinguish *adiabatic*, *diabatic*, and *sudden* dynamical scenarios, consider the occupation statistics of the final state, and show that the latter depends on u. Our analysis goes beyond mean-field theory, and is complemented by a semiclassical picture.

Modeling. – The simplest model that describes interacting bosons on a lattice is the Bose-Hubbard Hamiltonian (BHH). For a two-site (dimer) system:

$$\mathcal{H} = \sum_{i=1}^{2}\left[\mathcal{E}_i\hat{n}_i + \frac{1}{2}U\hat{n}_i(\hat{n}_i-1)\right] - \frac{K}{2}\sum_{i\neq j}\hat{b}_i^\dagger\hat{b}_j, \qquad (1)$$

where $\hat{b}_i$ and $\hat{b}_i^\dagger$ are bosonic annihilation and creation operators, and $\hat{n}_i = \hat{b}_i^\dagger\hat{b}_i$ counts the number of particles at site $i = 1, 2$. We use units such that $\hbar = 1$. The BHH has two constants of motion: the energy E and the total number of particles $N = \hat{n}_1 + \hat{n}_2$. Given N, the Hilbert-space has dimension $\mathcal{N} = N+1$, and the Fock basis states are $|n\rangle \equiv |n_1{=}n, n_2{=}N{-}n\rangle$. Below we assume an even $N \gg 1$ and define $j = N/2$, hence $\mathcal{N} = 2j+1$. The BHH for a given N is formally equivalent to the Hamiltonian of a spin j particle. Defining $J_z \equiv (\hat{n}_1 - \hat{n}_2)/2$ and $J_+ \equiv \hat{b}_1^\dagger\hat{b}_2$ it can be re-written as:

$$\hat{H} = U\hat{J}_z^2 + \mathcal{E}\hat{J}_z - K\hat{J}_x, \qquad (2)$$

where $\mathcal{E} = \mathcal{E}_1 - \mathcal{E}_2$ is the bias. In the absence of interaction this Hamiltonian can be reinterpreted as describing a spin in a magnetic field with precession frequency $\Omega = (-K, 0, \mathcal{E})$.

The many-body Landau-Zener scenario that we consider assumes that initially the bias is very negative and that all particles are in the first site $|\Psi(t{=}0)\rangle = |N\rangle$. This is the ground state in the case of an attractive interaction ($U < 0$), and it is equivalent to a preparation in the most excited state if $U > 0$ [a]. The bias $\mathcal{E}$ is raised with some constant sweep rate $\dot{\mathcal{E}}$. Once the bias becomes large and positive the occupation statistics $P(n) \equiv |\langle n|\Psi(t)\rangle|^2$ reach a steady state. Below we use the following terminology: (i) if at the end of the sweep we observe the Fock state $|0\rangle$, then we call it an idealized adiabatic process; (ii) if we observe the Fock state $|N\rangle$, we call it an idealized sudden process; and (iii) if the system ends up in a

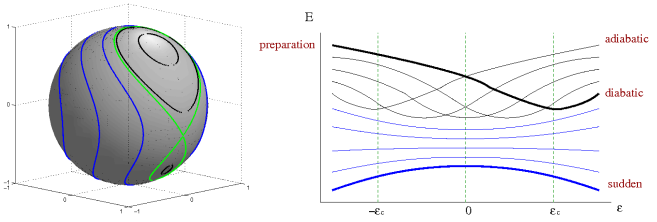

FIG. 1: (Color online) Phase space and corresponding energy levels (conceptual plot). The sea levels are in blue, the separatrix in green, and the islands are black.

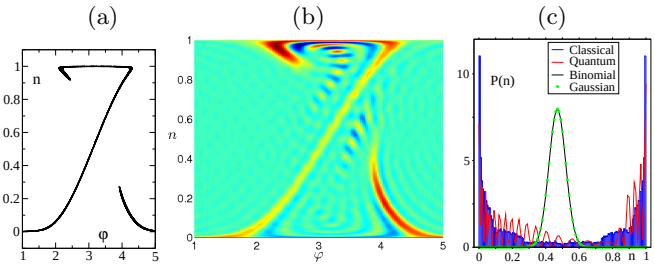

FIG. 2: (Color online) Dynamical evolution in a situation in which the mean-field (Gaussian) approximation does not hold: $N = 100$ particles are prepared in one site of a symmetric ($\mathcal{E}$=0) double well, and then evolved with a u=2 Hamiltonian. The initial wavepacket is stretched along the separatrix. (a) Classical probability distribution in phase space. (b) Wigner representation of the corresponding quantum state. (c) Quantum probability n distribution (red line) compared with the semiclassical (blue histogram) and with the mean-field (binomial/Gaussian) predictions. In all these plots n is scaled to the range $[0, 1]$. The average occupation $\langle n\rangle = 47$ is associated here with a huge super-binomial variance $\mathrm{Var}(n) = 1530$ instead of the binomial value $\mathrm{Var}(n) \sim 25$.

Fock state $|n_c\rangle$, where $n_c \neq 0, N$, we call it an idealized diabatic process.

Phase Space. – In order to analyze the dynamics for finite U it is convenient to rewrite the BHH using canonical variables. Formally we are dealing with two coupled oscillators and thus we can define action-angle variables as $\hat{b}_i \equiv \sqrt{\hat{n}_i}\exp(i\varphi_i)$. Note that the translation-like operator $\exp(i\varphi)$ is in fact non-unitary because it annihilates the ground state, but this is irrelevant for $N \gg 1$. With these coordinates the BHH takes a form that resembles the Josephson (pendulum) Hamiltonian:

$$\mathcal{H} \;\approx\; \frac{NK}{2}\left[\frac{1}{2}u(\cos\theta)^2 + \varepsilon\cos\theta - \sin\theta\cos\varphi\right], \qquad (3)$$

where θ is an alternative way to express the occupation difference $J_z \equiv (n_1 - n_2)/2 \equiv \mathsf{n} \equiv (N/2)\cos(\theta)$, and the scaled biased is $\varepsilon \equiv \mathcal{E}/K$. It is important to realize that φ and θ do not commute. The classical phase space is described either using the canonical coordinates (φ, n), with $\mathsf{n} \in [-N/2, N/2]$, or equivalently using the spherical coordinates (φ, θ). In the former case the total area of phase space is $2\pi N$ with a Planck cell $2\pi\hbar$ and $\hbar$=1, while in the latter case the phase space has total area 4π with a Planck cell $4\pi/N$. Within the semiclassical approximation, a quantum state is described as a distribution in phase space, and the eigenstates are associated with stripes that are stretched along contour lines $\mathcal{H}(\varphi, \theta) = E$. The energy levels E_n can be determined via WKB quantization of the enclosed phase space area.

Separatrix. – The phase space topology becomes non-trivial, i.e. has more than one component, if $|u| > 1$ and $|\varepsilon| < \varepsilon_c$ where $\varepsilon_c = (u^{2/3} - 1)^{3/2}$ (see Fig. 1a for an illustration). In this regime, a separatrix divides the phase space into three regions: two *islands* that contain the upper energy levels and a *sea* that contains the lower energy levels. In this description and in the numerics below we assume $U > 0$ and adopt the following enumeration convention: we define n=0 as the most excited level, while n=N corresponds to the lowest one. Note that the replacement $U \mapsto -U$ merely inverts the order of the levels and for $U < 0$ the n=0 level corresponds to the ground state [a].

Fig. 1b is an illustration of the energy levels as a function of the bias. Each level is associated via WKB quantization with one of the contours lines in Fig. 1a. For the sake of our later analysis we define n_c as the level which is closest to the separatrix for $|\varepsilon| = \varepsilon_c$. At this critical value of the bias one of the islands has a vanishing phase space area, while the area of the other is $A_c \approx 4\pi\varepsilon_c/u$. Using WKB quantization we get

$$n_c \;=\; \frac{A_c}{4\pi/N} \;\approx\; (1 - u^{-2/3})^{3/2}\, N, \qquad (4)$$

where the approximation for A_c has been tested against a numerical calculation. The analysis here parallels the one in Ref.[11].

Simulation. – As a preliminary step we have made a simulation of the undriven wavepacket dynamics with $\mathcal{E}$=0 and u=2. For this value of u the separatrix crosses the north pole of the phase space, and therefore the wavepacket stretches along it, as illustrated in Fig. 2a (classical) and in Fig. 2b (quantum mechanical). It should be appreciated that this type of dynamics cannot be properly addressed by the mean-field approximation. The mean-field equation merely describes the Hamiltonian evolution of a single *point* in phase space and therefore assumes that the wavepacket looks like a minimal Gaussian at any moment. Whenever the motion is in the vicinity of the separatrix the mean-field description becomes inapplicable and consequently the n distribution is likely *not* to be binomial (Fig. 2c).

Coming back to the bias-sweep scenario one wonders what the effect is of the separatrix motion on the occupation statistics. It should be clear that this separatrix motion in unavoidable here: For $\varepsilon < -\varepsilon_c$ the wavepacket is localized in the upper level. When $\varepsilon = -\varepsilon_c$ the separatrix emerges. As long as $-\varepsilon_c < \varepsilon < 0$ the wavepacket remains trapped in the top of the big island. This island

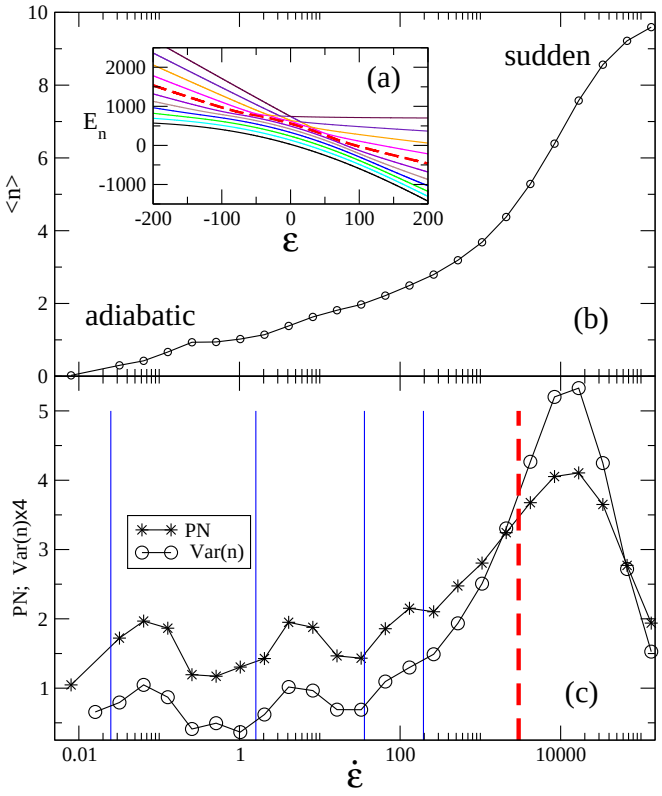

FIG. 3: (Color online) (a) Parametric evolution of the adiabatic energy levels versus the bias $\mathcal{E}$ [a] for a BEC with N=10 particles, U=15 and K=60. The dashed line corresponds to the level n_c=4. (b) Average occupation $\langle n\rangle$ versus the sweep rate $\dot{\mathcal{E}}$. (c) Participation number (PN) and Var(n) versus $\dot{\mathcal{E}}$. The vertical lines indicate the various adiabatic thresholds (blue) and the diabatic threshold (orange).

gradually shrinks. When ε becomes larger than zero, the wavepacket can partially tunnel out from the shrinking island to the levels of the expanding island. When $\varepsilon = +\varepsilon_c$ the shrinking island disappears and the remaining part of the wavepacket is squeezed out along the $n = n_c$ contour, resembling the dynamics of Fig. 2.

In Fig. 3 we plot the average occupation $\langle n\rangle$ and the participation number (PN) of the distribution $P(n)$ at the end of the sweep as a function of $\dot{\mathcal{E}}$. The plot of $\langle n\rangle$ does not provide much information regarding the nature of the crossing process. It is much more informative to look at PN. For very slow rates, the wavepacket follows a strict adiabatic process and ends at n=0. For a somewhat larger sweep rate the wavepacket exits in a superposition of n=0 and n=1 states, indicated by PN=2. We also resolve the possibility of ending entirely at n=1 or at n=2 or at n=3. In the case shown in Fig. 3 we have $n_c \approx 4$. For larger sweep rates we observe a qualitatively different behavior that can be described as a crossover from an adiabatic/diabatic behavior to a sudden behavior at the peak value PN=4. In order to appreciate the deviation of the numerical results from the mean-field theory prediction, we plot Var(n) versus $\langle n\rangle$ in Fig. 4 and compare with the binomial expectation. Below we further analyze the observed results.

Thresholds. – The various thresholds that are involved in the adiabatic-diabatic-sudden crossovers can be cast into an inequality of the form

$$\dot{\mathcal{E}} \;\ll\; \omega_{\rm osc}^2 \,/\, \kappa, \tag{5}$$

where $\omega_{\rm osc}$ is a characteristic frequency of the unperturbed dynamics and κ is the coupling parameter that determines the rate of the driven transitions. In the strict quantum adiabatic framework, $\omega_{\rm osc}$ is simply the level spacing and κ is determined by the slopes of the intersecting levels. In order to determine the adiabatic thresholds in Fig. 3 we observe that for the intersection of the n=0 level with the n=(N−n) level the difference in slope is $\kappa = (N-n)$, because asymptotically, $d(E_n - E_m)/d\mathcal{E} \sim (n-m)$. In the absence of interaction ($u \ll 1$), the level spacing is $\omega_{\rm osc} = K$ and only nearby levels are coupled, leading to the standard Landau-Zener adiabaticity condition $\dot{\mathcal{E}} \ll K^2$. With strong interaction there is an Nth order coupling between the n=0 level and the n=N level, which allows tunneling from the top of one island to the top of the other island (as illustrated in Fig. 1). An estimate for this coupling is $K_{\rm eff} = [NK]/[2^{N-1}(N-1)!](K/U)^{N-1}$ [7]. We note that in this regime similar considerations can be applied to the bottom sea level in order to determine if we have adiabatic, gradual, or sequential crossing [16]. The various quantum adiabatic thresholds are summarized in Fig. 5.

For large N it might be practically impossible to satisfy the strict adiabaticity condition which is associated with the possibility to tunnel from the top of one island to the top of the other. Then the relevant mechanism for transition, i.e. the emission to the level n_c as described in the previous section, becomes semiclassical. The frequency that governs this transition is $\omega_{\rm osc} \sim |NUK|^{1/2}$. It is the oscillation frequency at the bottom of the sea, which determines the level spacing there and, with some logarithmic correction [17], also the level spacing in the vicinity of the separatrix. It follows that the diabatic-sudden crossover involves the threshold condition $\dot{\mathcal{E}} \ll |NUK|$ as indicated in Fig. 5 and calculated for the simulations of Fig. 3.

Scaling. – The essence of the diabatic-sudden crossover involving *sea* levels can be captured by the toy Hamiltonian $\mathcal{H} = h(t)\cdot J$, where J is a spin entity with $j_{\rm eff} = (N-n_c)/2$, and $h(t)$ is a field with constant magnitude $|h(t)| = \omega_{\rm osc}$ corresponding to the mean level spacing. The sweep is like rotation of $h(t)$ in the plane with some angular rate ω. On the basis of this simple model, we suggest a sub-binomial scaling relation between the mean and the variance of the occupation statistics:

$$Y \;=\; (1-X)\frac{X-c}{1-c}; \quad \text{with} \quad c = \frac{n_c}{N}, \tag{6}$$

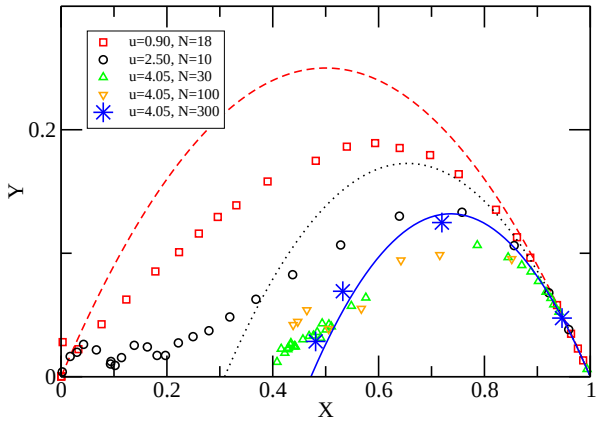

FIG. 4: (Color online) $Y = \mathrm{Var}(n)/N$ versus $X = \langle n\rangle/N$. Symbols correspond to numerical data, while lines indicate the sub-binomial scaling relation Eq.(6) with u=2.5 (dotted) and u=4.05 (solid). No fitting is involved. As a reference we also plot the standard binomial scaling (dashed line) which would strictly apply in the absence of interaction (u=0). There is a clear crossover from a binomial to the sub-binomial scaling, and the agreement becomes better for large N. Note that the super-binomial data point $(X, Y) = (0.47, 15.3)$ that corresponds to the distribution in Fig. 2 is out-of-scale.

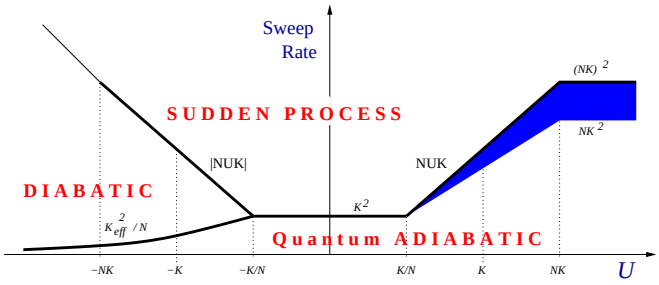

FIG. 5: (Color online) Diagram of the $(U, \dot{\mathcal{E}})$ dynamical regimes for a ground state preparation. In the Rabi regime $|U| < K/N$ we have a crossover from adiabatic to sudden behavior. For $K/N < U < NK$ (or $U > NK$) we have a broad crossover from adiabatic gradual (or sequential [16]) behavior to sudden behavior. For $U < -K/N$ we have two crossovers: the first from quantum adiabatic to diabatic behavior, and the second from diabatic to sudden behavior. The diabatic behavior can be regarded as a classical non-linear adiabatic behavior. For $U < -NK$ the distinction between the diabatic and the sudden regime is blurred because the final state is the same.

where $X = \langle n\rangle/N$, and $Y = \mathrm{Var}(N)/N$. Our numerical data is reported in Fig. 4 together with the binomial (c=0) and sub-binomial scaling relation Eq.(6). The numerics confirm the expected u-dependent crossover from binomial to sub-binomial statistics, where the latter, with no fitting parameters, sets a lower bound for the variance.

Summary. – In view of the strong research interest in counting statistics of electrons in mesoscopic devices, it is somewhat surprising that the issue of occupation statistics of BECs has been explored only for equilibrium phase transitions. Getting into this issue in the dynamical context is motivated by state-of-the-art experiments that are aimed in counting individual particles [2, 3, 4]. We have shown that in the case of a many-body Landau-Zener transition the mean-field binomial expectation is not realized, however a sub-binomial scaling relation still works quite well. By looking at the occupation statistics, in particular at the participation number of the final distribution, we were able to resolve all the details of the adiabatic-diabatic-sudden crossovers, and to verify theoretical estimates for the threshold of each crossover.

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[a] A ground state preparation of a $U < 0$ system with increasing $\mathcal{E}$, is equivalent to a most excited state preparation of a $|U| > 0$ system with decreasing $\mathcal{E}$. The latter convention has been adopted in our simulations.