Unconventional Landau-Zener type transitions in many-body systems

Jonas Larson\textsuperscript{1,2,*}

\textsuperscript{1}Department of Physics, Stockholm University, AlbaNova University Center, Se-106 91 Stockholm, Sweden
\textsuperscript{2}Institut für Theoretische Physik, Universität zu Köln, De-50937 Köln, Germany
(Dated: October 30, 2013)

Landau-Zener transitions in a Lipkin-Meshkov-Glick model are considered, both as a single system and in a lattice where each individual site hosts a realization of the corresponding many-body problem. The single site mean-field problem is conceptually different from many other non-linear Landau-Zener models - it does not support any hysteresis and a new phenomenon appears where adiabaticity totally breaks down. More precisely, this breakdown occurs for isolated classical solutions propagating on a separatrix in phase space and during the Landau-Zener sweep they get locked to a fixed point which prohibits adiabatic following. Quantum fluctuations tend to destabilize these solutions such that for moderate particle numbers the phenomenon is lost. At the quantum level it is also shown that the non-adiabatic corrections \(P\) of the single site problem obey a power-law dependence on the Landau-Zener sweep velocity \(\lambda\) in the adiabatic regime, \(i.e.\ P \sim \lambda^2\). Furthermore, fluctuations in the populations of final diabatic states are found to grow linear with the particle number. In the full lattice problem, single-site Landau-Zener transitions interplay with inter-site particle dynamics which leads to a Franck-Condon effect. In general, even for relatively small lattices, remaining adiabatic becomes challenging.

PACS numbers: 03.75.-b, 03.65.Xp, 37.10.Jk

\[ P \sim \lambda^2 \]

I. INTRODUCTION

The Landau-Zener (LZ) formula gives an analytic expression for the transition probability when a system is swept through an avoided crossing \([1]\). More precisely, take a two-level system described, in the diabatic representation, by some state vector \(\psi(t) = [\psi_x(t)\,\psi_y(t)]^T\) which is a solution of the Schrödinger equation for a linear sweep in time, \(i.e.\ (\hbar = 1)\)

\[
\frac{\partial}{\partial t} \begin{bmatrix} \psi_x(t) \\ \psi_y(t) \end{bmatrix} = \begin{bmatrix} \lambda t & U \\ -U & -\lambda t \end{bmatrix} \begin{bmatrix} \psi_x(t) \\ \psi_y(t) \end{bmatrix},
\]

where \(\lambda\) is the sweep velocity and \(U\) the the coupling strength of the two diabatic energies. For an initial state \(\psi_x(-\infty) = 1, \psi_y(-\infty) = 0\), the probability for transfer from the \(x\)-adiabatic state to the \(y\)-adiabatic state at \(t = +\infty\) is \(P_y = \exp(-\Lambda)\) with the \textit{adiabaticity parameter} \(\Lambda = 2\pi U^2\). For fast sweeps, \(i.e.\ \lambda\) is large compared to \(U\), most of the population is swapped between the two adiabatic states. Thus, the process is highly non-adiabatic (\textit{adiabatic regime}). Furthermore, as the energy gap between the two diabatic energies goes as \(U\) it also follows that a large \(U\) favours adiabaticity.

Since adiabatic breakdown (\textit{i.e.} population transfer between adiabatic states) occurs predominantly in the vicinity of the crossing where the diabatic energies are approximately linear, the LZ model has seen numerous applications in all possible fields of physics; in molecular/chemical physics it demonstrates breakdown of the \textit{Born-Oppenheimer approximation} \([2]\), in cold atom physics it can be used to explain \textit{Bloch oscillations} \([3]\) or describe the formation of molecules when the gas is driven through a \textit{Feshbach resonance} \([4]\), for solid state Josephson junctions LZ physics can be used to analyze transport properties \([5]\) or interference effects \([6]\), it may also be used to understand \textit{critical slowing down} and the \textit{Kibble-Zurek mechanism} appearing when a system is driven through a critical point \([7]\), and it can be employed for \textit{state preparation} and \textit{coherent control} \([8]\).

Characteristic for the LZ problem is its exponential dependence on the coupling strength \(U\) and the sweep velocity \(\lambda\) – the transition probability is a smooth and monotonous function of both \(U\) and \(\lambda\). Furthermore, from the form of \(P_y\) it follows that the result for small \(\lambda\) (\textit{i.e.\ for adiabatic evolution}) is non-perturbative. Extensions to multi-level problems \([9, 11]\), many-body situations \([12, 16]\), and non-linear LZ transitions \([17, 20]\) have been considered. When the LZ model becomes non-linear both the exponential dependence and the smoothness of \(P_y\) may be lost \([17, 18]\). Such non-linear LZ problems typically arise in mean-field theories of quantum many-body problems. They especially find applications in cold atom research where the non-linearity stems from atom-atom interaction \([17, 20]\). It is particularly found that for strong enough non-linearity, adiabaticity cannot be achieved regardless of how slow LZ sweep \([21]\). This phenomenon has been identified as formation of \textit{swallowtail loops} describing a hysteresis effect. Recently this breakdown of adiabaticity was also experimentally verified in a cold atom setup \([23]\). In the absence of loops the transition probability is smooth and monotonous, but in the adiabatic regime it obeys a power-law dependence, \(i.e.\ P_y \sim \lambda^\nu\) for some power \(\nu\) \([18]\). Power-law dependences have also been predicted in many-body Landau-Zener (MBLZ) problems beyond the mean-field regime \([12, 13]\).

*Electronic address: jolarson@physto.su.se
The paper is structured in the following way. The full many-body problem is introduced in the following section, both at a second quantized and at a mean-field level. Its derivation in terms of cold atoms in optical lattices is presented in the Appendix. Some general remarks on the lattice problem are also given in Sec. II. In Sec. III, we consider the single site problem and focus on how already at this level the model displays some unexpected results. The many-site problem is considered in Sec. IV. To better understand the interplay between intra- and inter-site dynamics we start by analyzing the ground state properties and then turn the attention to the time-dependent MBLZ problem. We conclude with a summary in Sec. V.

II. MODEL SYSTEM

In this section we will introduce the full lattice model and derive the corresponding mean-field equations of motion. The derivation of the Hamiltonian in terms of cold atoms in optical lattices is presented in the Appendix.

A. Many-body Landau-Zener Hamiltonian

We will restrict the model to 2D \((xy, plane)\), to nearest neighbour tunneling and onsite interaction (tight-binding approximation), and to two orbital states, \(p_x\) and \(p_y\), on every site (single-band approximation). Note that these two approximations are generally met in optical lattice experiments. Furthermore, tunneling cannot accompany a change of orbital states (i.e. Dzyaloshinskii-Moriya terms are not present), orbital states are only interchanged via scattering of two \(p_x\)-orbitals into two \(p_y\)-orbitals or vice versa. A local shift in energy on every site is included which in a physical realization would correspond to a harmonic trap with frequency \(\omega\). For the full many-site problem it will turn out that the trap is indeed crucial. To sum up, the Hamiltonian is given by (in dimensionless variables, see the Appendix)

\[
H = H_0 + H_{\text{dd}} + H_{\text{ac}},
\]

with the ‘bare’ part

\[
H_0 = -\sum_{\alpha, \beta} \sum_{\langle ij \rangle} \alpha \beta \delta_{\alpha \beta} \hat{a}_{\alpha i}^\dagger \hat{a}_{\beta j} + \sum_{\alpha} \sum_{j} \left[ E_\alpha(t) + \frac{\omega^2}{2} (x_j^2 + y_j^2) \right] \hat{n}_{\alpha j},
\]

where \(\delta_{\alpha \beta} = 1\) is the number of \(\alpha\)-orbital particles in

These many-body results were, however, derived using adiabatic arguments from classical physics.

In this paper we consider the MBLZ problem for a Lipkin-Meshkov-Glick (LMG) model \([24]\) at a mean-field level, at a many-body level, and for a lattice extensions of the former. The MBLZ problem for a certain class of LMG models has been considered in the past \([19]\). The LMG model of Ref. \([19]\) appears for example in systems describing the bosonic Josephson effect. Importantly, the LMG model of Ref. \([19]\) has been considered in the past \([19]\). The LMG model of Ref. \([19]\) appears for example in systems involving coupling of the order parameter to its complex symmetry. Another LMG model is considered in the present paper. It arises for example in cold atom gases in optical lattices, and specifically the parity is preserved throughout the LZ sweep. As a result of the discrete \(Z_2\) parity symmetry is that in the thermodynamic limit this model possesses a quantum phase transition (QPT) of the Ising type which separates a polarized phase from a symmetry-broken phase. Hence, it does not come as a surprise that the physics of the parity LMG and the parity-broken LMG models are conceptually different. In fact, the parity LMG studied in this work shows novel features not encountered earlier in MBLZ problems. At the mean-field level, the emerging non-linear LZ problem involves coupling of the order parameter to its complex conjugate and not only to its absolute value which is typically the case for other non-linear LZ problems like the parity-broken LMG model \([17, 18]\). Furthermore, regardless of the strength of the non-linearity no swallowtail loops are formed. However, there are resonances when adiabaticity totally breaks down even for large \(U\) and small \(\lambda\) which expectedly should generate an adiabatic evolution. These resonances occur for solutions following a separatrix in classical phase space. The presence of ‘mobile’ fixed points located on the separatrix causes the adiabatic breakdown. While this breakdown of adiabaticity seems to be a new phenomenon in non-linear LZ problems, it is shown that the stability of these semiclassical solutions is severely sensitive for quantum fluctuations. As for other models, in the adiabatic regime the full MBLZ beyond the mean-field approximation obeys a power-law dependence \(P_{ex} \propto \lambda^2\) for the fraction of excitations \(P_{ex}\). It is noticeable, however, that the power \(\nu = 2\) of the parity LMG studied here is different from that found in the Tavis-Cummings model \([12]\).

In the lattice version of the problem, intra- and inter-site dynamics are coupled in a complex manner which results in a complicated evolution during the LZ sweep. More precisely, there is an intra-site time-scale (related to the adiabaticity parameter) which determines the probability for transitions between the two diabatic states, and there is an inter-site time-scale related to the mobility of particles within the lattice. For physically relevant parameters (considering atoms in optical lattices) intra-site adiabaticity is easier to fulfill than inter-site adiabaticity which describe a macroscopic flow of particles in the lattice. This is reminiscent of Franck-Condon physics, and similar situations can be found in pump-probe experiments in molecular and chemical physics \([25]\).
site \( j \); the ‘density-density’ interaction part

\[
\hat{H}_{dd} = \frac{U}{2} \sum_{\alpha} \sum_{j} \hat{n}_{\alpha j} (\hat{n}_{\alpha j} - 1) + \frac{U}{3} \sum_{\alpha\beta,\alpha\neq\beta} \sum_{j} \hat{n}_{\alpha j} \hat{n}_{\beta j}.
\]

(4)

and finally the ‘orbital changing’ term

\[
\hat{H}_{oc} = \frac{U}{6} \sum_{\alpha\beta,\alpha\neq\beta} \sum_{j} (\hat{a}_{\alpha j}^\dagger \hat{a}_{\alpha j} \hat{a}_{\beta j}^\dagger \hat{a}_{\beta j} + \hat{a}_{\beta j}^\dagger \hat{a}_{\beta j} \hat{a}_{\alpha j}^\dagger \hat{a}_{\alpha j}).
\]

The onsite energies \( E_{\alpha}(t) \) are given by \( E_{\alpha}(t) = -\lambda t \) and \( E_{y}(t) = \lambda t \) with \( \lambda (> 0) \) the velocity of the LZ sweep. Since these onsite terms induce a detuning between the two orbital states it is often seen as an ‘external field’, something that will be more clear in the next Section when we map the interaction part of the Hamiltonian onto a LMG model \[24\]. The particular relations between the strengths of the interaction terms derive from imposing the harmonic approximation in which the orbital states are taken to have the shapes of harmonic eigenstates. We note that for optical lattices, the harmonic approximation is usually valid when the tunneling and single-band approximations are justified \[26\] (For 

\[
i \frac{\partial \psi_{ij}}{\partial t} = -t_{ij} (\psi_{i,j+1} + \psi_{i,j-1}) - t_{ij} (\psi_{i,j+1} + \psi_{i,j-1})
\]

(5)

Thus, \( \hat{\psi}_{ij} \) couples to its own complex conjugate \( \psi_{ij}^* \). This peculiar coupling of the order parameter to its complex conjugate stems from the orbital changing term \( \hat{H}_{oc} \). Normally for Gross-Pitaevskii realizations appearing in atomic physics, the order parameter couples only to its density \( |\psi|^2 \) and not to \( \psi^* \). In the following we will see several more important consequences of the term \( \hat{H}_{oc} \).

Let us conclude this Subsection by some general remarks about the symmetries of the system. First of all, particle conservation, \( \left[ \hat{N}, \hat{H} \right] = 0 \) with \( \hat{N} = \sum_{\alpha j} \hat{n}_{\alpha j} \), implies a global \( U(1) \) symmetry. Non-zero tunneling breaks local onsite particle conservation, however if \( t_{xx} = t_{yy} = 0 \) we have a additional set of \( U(1) \) symmetries.

Since orbital changes come in pairs, there is a \( Z_2 \) parity symmetry corresponding to \( \hat{a}_{ij} \rightarrow \hat{a}_{ij} \). In the isotropic case \( E_{\alpha}(t) = E_{\beta}(t) \) we have as well the \( Z_2 \) symmetry of changing orbitals \( \hat{a}_{ij} \leftrightarrow \hat{a}_{ij} \).

B. Multiple time-scale many-body Landau-Zener

It was mentioned in the previous Subsection that the presence of the trap will influence the LZ physics of the present model. At first, this can be seen as strange since the trap shifts the energies of the two orbitals equally within every single site. In another language, it seems to be a local change of an effective chemical potential. But as we will explain next, this is indeed \textbf{not} a local density approximation and it derives from the properties of the tunneling.

The tunneling part of the Hamiltonian describes the
Figure 1: The classical energy surface $H_{cl}$ (the surfaces have been shifted upwards by 2/3 in order to separate them from the contour lines) for different ‘tilts’, $\lambda t/U = -0.5$ (a), $\lambda t/U = 0$ (b), and $\lambda t/U = 0.5$ (c). The contour lines give the constant energy curves, i.e. the instantaneous classical phase space trajectories (the geometry of the phase space is cylindrical). Thus, for an adiabatic sweep the classical trajectories follow the constant energy curves as the tilt is changed. Solid black circles mark the elliptic fixed points, while open circles display the limit fixed points.

kinetics of particles within the lattice. Hence, the tunneling coefficients $t_1$ and $t_2$ can be seen as inverse effective masses for the particles. Since $|t_1| > |t_2|$, a $p_x$-orbital particle is ‘heavier’ in the $y$-direction than in the $x$-direction, and oppositely for a $p_y$-orbital particle. Thus, an initially localized single $p_x$-orbital particle will diffuse more in the $x$-direction than in the $y$-direction. Furthermore, the effective mass is negative in the $x$-direction so the particle has both particle and hole properties. Now, if such a single $p_x$-orbital particle is confined in a harmonic potential, its ground state wave function is Gaussian in both directions, but its width in the $x$-direction is larger than in its $y$-direction. Naturally, the opposite holds true for a $p_y$-orbital particle. Interaction will couple the two orbital state, but as long as the interaction is not too strong (that is, we are not in the Thomas-Fermi regime [29]) the ground state of $N_{tot}$ particles will not be polar symmetric even if the harmonic potential is isotropic. That means that at sites at the boundary of the particle distribution, either $p_x$- or $p_y$-orbital particles will dominate. This demonstrates that the model goes beyond the local density approximation.

How does this intrinsic anisotropy affect the LZ driving? Starting with say $E_x \ll E_y$, all particles will reside in the $p_x$-orbitals and the particle distribution will be elongated in the $x$-direction. For $E_y \ll E_x$, on the other hand, the distribution will be elongated in the $y$-direction instead and all particles will populate $p_y$-orbitals. When we drive the LZ transition adiabatically it means that at every single site particles swap from $p_x$- to $p_y$-orbitals. Simultaneously, if we are to remain in the global ground state the external shape of the particle distribution must also change (otherwise we pay a price in potential energy); it should be rotated 90 degrees. At every populated site a non-linear LZ transition is realized, but in addition, the sites are coupled and particles can hop between them. The onsite LZ transition occurs on some characteristic time $\tau_{\text{intra}}$ that will depend on the interaction strength $U$ and onsite particle number $N$. The extrinsic dynamics during the LZ transition is characterized by some time $\tau_{\text{inter}}$ which depends on the tunneling amplitudes. Of course, this is a very simplified picture of the full coupled system, but it gives an idea of the complex dynamics. It follows that performing an adiabatic sweep would mean that $\lambda^{-1} \gg \tau_{\text{intra}}, \tau_{\text{inter}}$. Physically, if we have a macroscopic number of particles in our lattice the above scenario implies that we need to achieve a macroscopic current of particles within the lattice. For physically relevant parameters one would therefore expect that $\tau_{\text{inter}} > \tau_{\text{intra}}$. Then, if $\tau_{\text{inter}} > \lambda^{-1} > \tau_{\text{intra}}$ the onsite LZ transitions can be adiabatic while the overall particle distribution becomes excited.

III. SINGLE-SITE PROBLEM

The corresponding single-site problem of Eq. (2), i.e. when the tunneling terms vanish, is identical to $N$ equally interacting spin-1/2 particles in an external field. Such system is usually described by the LMG model which could also be seen as an infinite range Ising model. Thus, the single-site problem in itself is of general interest and could be realized for example with condensates loaded into the first excited states of a harmonic trapping potential or with spinor condensates with tunable scattering lengths between the different Zeeman levels. Already this problem is non-trivial and displays interesting new features that have not been encountered in other more
regular non-linear LZ. As a remark, from now on whenever we talk about ‘regular’ or ‘common’ non-linear LZ problem we mean a model where the order parameter couples to its density and not to the its phase (or its complex conjugate) as in the present work.

A. Mean-field analysis

To put the problem on a more familiar form, we can write the mean-field onsite equations of motion in the following way

\[
\frac{\partial}{\partial t} \begin{bmatrix} \psi_x \\ \psi_y \end{bmatrix} = \begin{bmatrix} \lambda t - \frac{U}{3} Z & \frac{2U}{3} \psi_y^* \psi_x \\ \frac{2U}{3} \psi_y \psi_x^* & -\lambda t + \frac{U}{3} Z \end{bmatrix} \begin{bmatrix} \psi_x \\ \psi_y \end{bmatrix},
\]

(9)

where we have introduced the orbital imbalance Z = |ψ_x|^2 − |ψ_y|^2 and normalized the order parameter to unity, i.e. |ψ_x|^2 + |ψ_y|^2 = 1. For positive sweep velocity λ and large negative times, the ‘ground state’ populates solely the p_x-orbital state, while only p_y-orbital states are populated for large positive times. From Eq. (9) we see how the two orbitals are only coupled once both of them are occupied. That implies that the mean-field dynamics is trivial whenever we initially only populate a single orbital state. This is, of course, a result from neglecting quantum fluctuations.

Instead of working with the complex order parameters ψ_x and ψ_y it is practical to introduce two new variables [31]: the imbalance Z defined above and the phase difference δ = θ_x − θ_y where θ_x is the phase of ψ_x. In terms of these new variables, the equations of motion become

\[
\begin{align*}
\dot{\delta} &= \lambda t + \frac{2U}{3} Z [1 - \cos(2\delta)], \\
\dot{Z} &= \frac{2U}{3} (1 - Z^2) \sin(2\delta).
\end{align*}
\]

(10)

These can be derived from the classical Hamiltonian

\[
H_{cl} = \lambda t Z + \frac{U}{3} Z^2 + \frac{1}{3} (1 - Z^2) \cos(2\delta).
\]

(11)

As we saw in the Introduction, for LZ problems it is common to work with the population transfer P_α telling how much state α is asymptotically populated (i.e. when t → +∞). Since the state is normalized we can equally well work with the imbalance Z instead. Directly from Eq. (10) we can say something about the evolution. If initially \(Z(-\infty) = ±1\) we see that the two equations decouple and only the phase δ(t) dynamically evolves. If |Z(−∞)| ≤ 1, at large negative times the phase grows rapidly meaning that sin(2δ) of the second equation is fast oscillating and that Z(t) follows adiabatically the evolution (adiabatic regime). In the vicinity of the crossing (λt ≈ 0) there is normally no clear separation of time-scales and this is where adiabaticity breaks down (sudden or critical regime).

We see that \(δ = δ_{ss} = π/2 + nπ (n ∈ N)\) minimizes the classical energy (since \(Z^2 ≤ 1\)). Naturally, treating t as a parameter these \(δ_{ss}\)'s are also elliptic fixed points for (10). The corresponding fixed point for the imbalance is \(Z_{ss} = -3\lambda t/4U\) (it should be remembered that for large |t| the imbalance is bounded by −1 ≤ Z ≤ 1). The classical energy for this ‘steady-state’ solution is \(E_{ss} = -3\lambda^2 t^2/8U - U/2\), i.e. an inverted parabola in terms of t. At λt = 0 we have that for the ‘ground state’ the two orbitals are equally populated and they differ in phase by π/2. Taking the shapes of the orbitals into account, this solution corresponds to a vortex with a unit winding number. \((Z_{ss}, δ_{ss}) = (±1, ±\arccos(3\lambda t/2U ± 1)/2)\) are two other ‘limit’ fixed points. These limit fixed points are somehow trivial in the sense that they do not describe dynamical transfer of population between the two orbitals. We will, however, see that they are of great importance for the dynamical properties of the model.

Finally, we note that the corresponding energy and steady-states could equally well be obtained from the non-linear eigenvalue problem

\[
\begin{bmatrix} -\lambda t - \frac{U}{3} Z & \frac{2U}{3} \psi_y^* \psi_x \\ \frac{2U}{3} \psi_y \psi_x^* & -\lambda t + \frac{U}{3} Z \end{bmatrix} \begin{bmatrix} \psi_x \\ \psi_y \end{bmatrix} = E_{ad} \begin{bmatrix} \psi_x \\ \psi_y \end{bmatrix}.
\]

(12)

Thus, \(E_{ad}\) is the corresponding non-linear adiabatic energy.

Comparing to the commonly studied non-linear LZ problem which supports either two or four classical energies [17], our system in contrast only allows for a single (non-trivial) energy \(E_{ss}\). Typically, the non-linear nature of these types of problems results in hysteresis and the forming of ‘swallowtail’ loops [17, 21]. This phenomenon of loop formation, i.e. appearance of additional solutions, is rather general and occurs in numerous different non-linear systems [32] and has also been experimentally verified in a cold atom realization of the LZ problem [23]. Indeed, the presence of loops for strong enough non-linearities seems to be a very common feature, and the fact that such hysteresis effect is lacking in the present model turns out to be more of an exception.

It is equally surprising that there exist only a single (physically non-trivial) solution to the eigenvalue problem (12) and not two as in its linear counterpart [23]. The meaning of this solution \((δ_{ss}, Z_{ss}) = (π/2, -3\lambda t/4U)\) should be clear: at large negative times \(t < -4U/3\lambda\) we assume λ > 0) all particles populate the p_x-orbital, for intermediate times \(-4U/3\lambda < t < 4U/3\lambda\) both orbitals are populated, and finally for \(t > 4U/3\lambda\) only the p_y-orbital is populated. This corresponds to the LZ transition between the two orbitals. The roles of the two orbitals are changed when we consider instead negative sweeps λ < 0, i.e. population is swapped from the p_y- to the p_x-orbital during the LZ sweep. For later purposes, we call these schemes ‘case-(a)’.

The fact that Eq. (12) only supports a single solution implies that it is not clear how the system will evolve for λ > 0 and when mainly the p_y-orbital is initially
the classical energy surface is symmetric with respect to
Fig. 1) with new characteristic frequencies $\Omega$
container the elliptic fixed point (shown as filled circles in
expectation, which warrants adiabatic evolution,
we give three examples of the full 3D surfaces in Fig. 1;
λt/U
by exploring the classical energy surface
level one can, however, get a deeper understanding of this
Subsection this difference between the two cases will be
for the case-($b$) and thereby corresponding to case-($b$). The initial phase
948]. Instantaneously we can esti-
the solutions wraps around the cylinder with some char-
characteristic frequency $\Omega >$. Instantaneously we can esti-
mate this frequency $\Omega > \approx \lambda /2$. In the transition regime
$-4U/3\lambda < t < 4U/3\lambda$, the solutions may start to en-
circle the elliptic fixed point (shown as filled circles in
Fig. 1) with new characteristic frequencies $\Omega_a$ and $\Omega_b$ for
the two respective cases.

For large enough $|t|$ we always have that $\Omega > \gg \lambda$
which warrants adiabatic evolution, i.e. the classical ac-
ction $I = \oint Z d\delta$, with the integration curve along the
classical phase space trajectory, stays constant (equiva-
ently, during one classical orbit the Hamiltonian change is minimal) [34]. In the vicinity of the LZ transition when
the classical energy surface of Fig. 1 ‘tips over’ there is no
clear separation in time scales and as mentioned earlier it is
in this sudden regime where adiabaticity breaks down.
Interestingly, especially in case-($b$) the characteristic fre-
cquency is considerably decreased in the critical regime
t $\sim 0$, i.e. $\Omega_a < \Omega_b \ll \Omega >$. This critical slowing down is
most pronounced in case-($b$) clarifying why also this case is
more sensitive to non-adiabatic contributions.

Numerical results from solving the set of equations (11)
are shown in Fig. 2 both for case-($a$) and case-($b$). The figure confirms that case-($b$) is indeed much more sen-
tive to non-adiabatic contributions than case-($a$). Such
an asymmetry does not exist in the linear LZ problem.
More precisely, the adiabatic energy surfaces of the linear
LZ problem (and also the regular non-linear LZ problem
for weak non-linearity) possesses two elliptic fixed points,
one global minimum at $\delta = \pi$ and one global maximum
at $\delta = 0$ (or equivalently for $\delta = 2\pi$ since the phase space
for the linear LZ model is given for $0 \leq \delta \leq 2\pi$). The
anomalous shape of the classical energy surface in our
model is also evident in the large amplitude oscillations
of $Z$ in the vicinity of $t \sim 0$ for the case-($b$) (see Fig. 1
(b)).

It was pointed out above that the non-linear LZ prob-
lem of Eq. (10) differs from other non-linear LZ models in
the sense that the order parameters $\psi_a$ couple to their
complex conjugates and not only to their densities $|\psi_a|$. It
turns out that this has a profound influence on the
dynamics. Figure 3 gives the asymptotic value $Z_\infty (\lambda)$
of the imbalance for large times as a function of the sweep
velocity $\lambda$ (in order to omit small fluctuations, the actual
value of $Z_\infty (\lambda)$ is obtained by averaging over a time in-
terval that is long compared to intrinsic oscillations but
short compare to the integration time). The initial and final
times, $t_i$ and $t_f$, are taken such that the two bare
orbital energies are well separated in energy. Over the
entire range of $\lambda$’s we find ‘resonances’ where adiabatic-
ity totally breaks down. Counterintuitively, these reso-
nances survive down to extremely slow sweep velocities

\begin{align*}
\lambda t/U &= -0.5 \ (a), \ \lambda t/U = 0 \ (b), \ \text{and} \ \lambda t/U = 0.5 \ (c).
\end{align*}

Note that the actual phase space has a cylindrical ge-
ometry due to the periodicity of the angle variable $\delta$.
If the process is adiabatic [34] it means that the classi-
ical solutions will evolve along the (instantaneous) con-
stant energy curves shown as contour lines in the figure.
Thus, provided the evolution is adiabatic and for large $|t|
the solutions wraps around the cylinder with some char-
acteristic frequency $\Omega >$. Instantaneously we can esti-
mate this frequency $\Omega > \approx \lambda /2$. In the transition regime
$-4U/3\lambda < t < 4U/3\lambda$, the solutions may start to en-
circle the elliptic fixed point (shown as filled circles in
Fig. 1) with new characteristic frequencies $\Omega_a$ and $\Omega_b$ for
the two respective cases.

For large enough $|t|$ we always have that $\Omega > \gg \lambda$
which warrants adiabatic evolution, i.e. the classical ac-
ction $I = \oint Z d\delta$, with the integration curve along the
classical phase space trajectory, stays constant (equiva-
ently, during one classical orbit the Hamiltonian change is minimal) [34]. In the vicinity of the LZ transition when
the classical energy surface of Fig. 1 ‘tips over’ there is no
clear separation in time scales and as mentioned earlier it is
in this sudden regime where adiabaticity breaks down.
Interestingly, especially in case-($b$) the characteristic fre-
cquency is considerably decreased in the critical regime
t $\sim 0$, i.e. $\Omega_a < \Omega_b \ll \Omega >$. This critical slowing down is
most pronounced in case-($b$) clarifying why also this case is
more sensitive to non-adiabatic contributions.

Numerical results from solving the set of equations (11)
are shown in Fig. 2 both for case-($a$) and case-($b$). The figure confirms that case-($b$) is indeed much more sen-
tive to non-adiabatic contributions than case-($a$). Such
an asymmetry does not exist in the linear LZ problem.
More precisely, the adiabatic energy surfaces of the linear
LZ problem (and also the regular non-linear LZ problem
for weak non-linearity) possesses two elliptic fixed points,
one global minimum at $\delta = \pi$ and one global maximum
at $\delta = 0$ (or equivalently for $\delta = 2\pi$ since the phase space
for the linear LZ model is given for $0 \leq \delta \leq 2\pi$). The
anomalous shape of the classical energy surface in our
model is also evident in the large amplitude oscillations
of $Z$ in the vicinity of $t \sim 0$ for the case-($b$) (see Fig. 1
(b)).

It was pointed out above that the non-linear LZ prob-
lem of Eq. (10) differs from other non-linear LZ models in
the sense that the order parameters $\psi_a$ couple to their
complex conjugates and not only to their densities $|\psi_a|$. It
turns out that this has a profound influence on the
dynamics. Figure 3 gives the asymptotic value $Z_\infty (\lambda)$
of the imbalance for large times as a function of the sweep
velocity $\lambda$ (in order to omit small fluctuations, the actual
value of $Z_\infty (\lambda)$ is obtained by averaging over a time in-
terval that is long compared to intrinsic oscillations but
short compare to the integration time). The initial and final
times, $t_i$ and $t_f$, are taken such that the two bare
orbital energies are well separated in energy. Over the
entire range of $\lambda$’s we find ‘resonances’ where adiabatic-
ity totally breaks down. Counterintuitively, these reso-
nances survive down to extremely slow sweep velocities

\begin{align*}
\lambda t/U &= -0.5 \ (a), \ \lambda t/U = 0 \ (b), \ \text{and} \ \lambda t/U = 0.5 \ (c).
\end{align*}

Note that the actual phase space has a cylindrical ge-
ometry due to the periodicity of the angle variable $\delta$.
\( \lambda \). In addition to the distinct resonance features, we also see an overall envelope shape showing a \( \lambda^{1/2} \) dependence for larger values on \( \lambda \).

\[
\text{Figure 4: Two examples of the classical phase space trajectories in the vicinity of } \lambda t \sim 0. \text{ The initial condition is as earlier, } Z(-500) = 0.95 \text{ and } \delta(-500) = \pi/2. \text{ The arrows mark the direction of time. In (a) the solution is on a 'resonance' (here } \lambda/U = 0.14 \text{ where little of the population is transferred between the diabatic states during the sweep. Specifically, during the interval marked by the dashed red lines the solution follows closely the limit fixed point. The length of this interval is } \pi/2 \text{ which exactly equals the distance that the limit fixed point } \delta_{ss} \text{ traverses during the LZ sweep. In (b), on the other hand, the transfer is large even if the sweep velocity is only slightly shifted } (\lambda/U = 0.143). \text{ Note that we plot the phase } \delta(t) \text{ and not the phase modulo } \pi.}
\]

The breakdown of adiabaticity in the regular non-linear LZ problem for small sweep velocities originates from the hysteresis effect which is present above some critical strength of non-linearity \[18\]. Dynamically, the breakdown occurs when two fixed points 'collide' in phase space and the solution is not able to precess around a single fixed point any longer. Clearly, the lack of adiabatic evolution in the present model cannot derive from the same mechanism. We can, however, understand this novel behaviour by exploring the classical trajectories in the critical regime. Figure 4 gives two examples of the classical solution \( (Z(t), \delta(t)) \) for times \( t \sim 0 \). We see that in both cases, away from the transition region the solution wraps around the phase space cylinder, either anti-clockwise \( d\delta(t)/dt < 0 \) or clockwise \( d\delta(t)/dt > 0 \) (seen from positive \( Z \)). In the upper plot, right before the reversal of \( \delta(t) \) the solution gets ‘locked’ to the vicinity of the limit fixed point \( (Z_{ss}, \delta_{ss}) = (1, \arccos(3\lambda t/2U + 1)/2) \). During the period when \( Z(t) \approx 1 \), the classical energy surface ‘tips over’ and the solution is no longer able to encircle the elliptic fixed point which means that adiabaticity necessarily is broken. To better understand the process, the two types of fixed points, elliptical and limit, are shown in Fig. 1. The limit fixed points, displayed as open circles, are located at the separatrix between orbitals encircling the elliptic fixed point and those wrapping around the cylinder. The example of Fig. 4(b) does not show the same locking to the limit fixed point (i.e. the trajectory lies within the separatrix), and during the LZ transfer the trajectory keeps encircling the elliptic fixed point \( Z_{ss} = -3\lambda t/U \).

Returning to the linear LZ problem we can understand why the same phenomena does not appear in that situation. The limit fixed points on the separatrix are settled to \( Z_{ss} = \pm 1 \) and \( \delta_{ss} = \pi/2, 3\pi/2 \) and thereby are immobile throughout the transfer. As a consequence of this stateness, the same slowing down does not occur in the linear LZ problem. Having understood the mechanism behind this new type of breakdown of adiabaticity we realize that the same phenomenon may not survive in the quantum system since quantum fluctuations will ‘delocalize’ the classical phase space trajectories. However, it is not clear whether these classical solutions will leave any remnants in the quantum evolution, similar to quantum scars in chaotic systems \[25\].

\[ \begin{align*}
\hat{H}_{\text{mb}} &= \lambda t (\hat{n}_x - \hat{n}_y) \\
&\quad + \frac{U}{2} \left[ \hat{n}_z^2 + \hat{n}_\gamma^2 + \frac{4}{3} \hat{n}_z \hat{n}_\gamma + \frac{1}{3} (\hat{a}_1^\dagger \hat{a}_2^\dagger \hat{a}_3 \hat{a}_4 + \hat{a}_3^\dagger \hat{a}_4^\dagger \hat{a}_1 \hat{a}_2) \right].
\end{align*} \tag{13} \]

In the Fock basis \( |n_x, n_y \rangle \) (\( \hat{n}_x |n_x, n_y \rangle = n_x |n_x, n_y \rangle \) and \( \hat{n}_y |n_x, n_y \rangle = n_y |n_x, n_y \rangle \)), \( \hat{H}_{\text{mb}} \) couples states along ladders of given parity, i.e. \( |n_x, n_y \rangle \leftrightarrow |n_x \pm 2, n_y \pm 2 \rangle \leftrightarrow |n_x \pm 4, n_y \pm 4 \rangle \leftrightarrow \ldots \). Thus, the onsite Hamiltonian is block-diagonal with block-sizes \( n \times n \) (\( n \in \mathbb{N} \)). Every individual block realizes an \( n \)-level LZ problem.

The block form of the Hamiltonian is also apparent by utilizing the Schwinger’s spin-boson mapping \[30\]: \( \hat{S}_z = \hat{a}_1^\dagger \hat{a}_2 - \hat{a}_2^\dagger \hat{a}_1, \hat{S}_x = \hat{a}_3^\dagger \hat{a}_4 + \hat{a}_4^\dagger \hat{a}_3 \) and \( \hat{S}_y = i (\hat{a}_2^\dagger \hat{a}_3 - \hat{a}_1^\dagger \hat{a}_4) \) where the spin operators obey the regular angular momentum commutation relations. The onsite Hamiltonian \( \hat{H}_{\text{mb}} \) takes the form

\[ \hat{H}_{\text{mb}} = \lambda t \hat{S}_z + \frac{U}{2} \left[ \hat{n} - \frac{2}{3} \right] - \frac{1}{3} \hat{S}_z^2. \tag{14} \]
Thereby, the Hamiltonian to be considered reads

\[ \hat{H}_{\text{LMG}} = \lambda \hat{S}_z - \frac{U}{6} \hat{S}_z^2. \]  

(15)

It is important to appreciate that we have scaled the second term by \( S^{-1} (S = N/2) \) in order for the model to be quantum critical [37] in the thermodynamic limit \( N \to \infty \). More precisely, as it now stands the two terms are both \( O(N) \) and the ferromagnetic (\( U > 0 \)) LMG model processes an Ising critical point at \( \lambda \hat{t}/U = \pm 1/3 \). For \( |\lambda| < U/3 \) the \( Z_2 \) parity symmetry (here corresponding to \( \hat{S}_x \to -\hat{S}_x, \hat{S}_y \to -\hat{S}_y, \) and \( \hat{S}_z \to \hat{S}_z \)) is spontaneously broken. When increasing \( \lambda t \), the ground state goes from highly polarized in the positive \( z \)-direction, where \( 1 \), and external field \( \lambda t \sigma_i^z \) in the \( z \)-direction, where \( \sigma_i \) are the Pauli matrices for spin \( i \). From now on, the second term, which only contributes a constant energy shift, will be dropped. Thereby, the Hamiltonian to be considered reads

\[ \hat{H}_{\text{LMG}} = \lambda \hat{S}_z - \frac{U}{6} \hat{S}_z^2. \]  

(15)

An important difference between the above references is that they consider an additional term \( \hat{S}_z \) in the Hamiltonian (in the original setting this corresponds to particle tunneling between the two orbitals). Including such a term leads to a breakdown of the \( Z_2 \) parity symmetry. As a consequence, the two versions of the LMG model, with or without the parity-breaking term, show very different properties [40]. In the following we therefore call our version of the model the parity LMG.

Driving the ferromagnetic LMG model through its critical point was analyzed in Refs. [13], and it was found that the non-adiabatic corrections obey a power-law dependence of the sweep velocity \( \lambda \). A similar behaviour was also demonstrated in the Tavis-Cummings model describing \( N \) spin-1/2 particles collectively interacting with a single boson mode [12]. The Tavis-Cummings model derives from the Dicke model [41] by imposing the rotating wave approximation which eliminates virtual processes. Due to the rotating wave approximation, the Tavis-Cummings and the Dicke models belong to different universality classes [12], and of the two it is the Dicke model which share the same universality class as \( H_{\text{LMG}} \) of Eq. (15). Also the LZ problem of the LMG model has been considered [19]. These studies were limited to the parity-broken version of the LMG model, and thereby the model was not critical and very different from ours. Another striking difference between the parity-broken LMG model and \( \hat{H}_{\text{LMG}} \) is that the former shows hysteresis on the mean-field level meaning that swallowtail loops may form. These loops inevitably lead to qualitative different dynamics compared to that of the model considered in this work.

The eigenenergies \( \varepsilon_n \) of \( \hat{H}_{\text{LMG}} \) are displayed in Fig. 6 for \( N = 20 \) particles. To clarify the role of the two parity solutions we have plotted them with different colours. In the thermodynamic limit, the critical points are at \( \lambda \hat{t}/U = \pm 1/3 \) for which the two parity states become degenerate. We note that going up in the spectrum, the degeneracy between the corresponding parity states occurs for smaller intervals \( \lambda \hat{t}/U \). Finally, for the most excited states the degeneracy only exists for \( \lambda \hat{t}/U = 0 \). Also for the finite size example of Fig. 6 the thermodynamic limit properties are clearly visible (the gap closing in the vicinity of \( \lambda \hat{t}/U = \pm 1/3 \)). Since the spectrum is symmetric with respect to \( \lambda \hat{t}/U = 0 \) it follows that the spectrum of the anti-ferromagnetic LMG is simply \(-\varepsilon_n \). This demonstrates the fact that the anti-ferromagnetic LMG hosts a first order QPT for vanishing external field (\( i.e. \) for \( \lambda = 0 \)). From this we can understand the big difference between case-(a) and case-(b). For the given Hamiltonian of Eq. (15), the case-(a) corresponds to studying the ferromagnetic LMG model while the case-(b) instead corresponds to the anti-ferromagnetic LMG model. This also tells us why the adiabaticity constrains are so different between the two cases, the rate of change \( d\varepsilon_n/dt \) relative to the energy gap is much smaller for case-(b) than case-(a) (remember that the two parity sectors are

![Figure 5: The spectrum of the LMD Hamiltonian \( \hat{H}_{\text{LMG}} \) for various \( \lambda \hat{t}/U \). The number of particles \( N = 20 \). The dotted black and solid red curves correspond to the two different parity solutions. The critical points of the LMG model occur at \( \lambda \hat{t}/U = \pm 1/3 \). This criticality can even be perceived in this finite size example by the appearance of a quasi degeneracy between the two lowest energy eigenvalues.](image-url)
the excitation fraction as is the introducing the operators $\hat{P}_n(t) = |\psi_n\rangle\langle \psi_n|$, where $|\psi_n\rangle$ is the $n$'th instantaneous eigenstate of $\hat{H}_{\text{LMG}}$, we define the excitation fraction as

$$P_{\text{ex}} = \lim_{t \to \infty} \frac{1}{N} \sum_{n=0}^{N} n \langle \psi(t) | \hat{P}_{n+1}(t) | \psi \rangle.$$  \hspace{1cm} (16)

Here, $|\psi(t)\rangle$ is the solution of the full time-dependent problem. Thus, $P_{\text{ex}}$ measures the amount of non-adiabatic excitations; $P_{\text{ex}} = 0$ corresponds to the case when only the ground state is populated (fully adiabatic) while $P_{\text{ex}} = 1$ is the opposite limit of a maximally excited system (fully diabatic if $t > 0$). Of course, $P_{\text{ex}}$ is nothing but the mean (scaled with the particle number) of the final distribution $P(n)$ of population of the various eigenstates $|\psi_n\rangle$. Note, since the diabatic and adiabatic states coincide in the large time limit, i.e. $\lim_{t \to \infty} \frac{\hat{S}_z}{\hat{H}_{\text{LMG}}} = 0$, we can connect the excitation fraction to the ‘magnetization’ according to $\langle \hat{S}_z \rangle = NP_{\text{ex}} - S$. To fully characterize the final distribution one would need all moments $\Delta^{(k)} n = \sum_n n^k P(n)$. Of particular interest is the Mandel $Q$-parameter [44]

$$Q = \frac{\Delta^{(2)} n - (\Delta^{(1)} n)^2}{\Delta^{(1)} n} - 1$$  \hspace{1cm} (17)

which says whether the distribution $P(n)$ is sub- ($Q < 0$) or super-Poissonian ($Q > 0$).

The full time-dependent problem has been integrated from $t = -200$ to $t = 200$ for various particle numbers $N$ and sweep velocities $\lambda$. The results for $P_{\text{ex}}$ are displayed in Fig. 6. For smaller systems we see some oscillations of $P_{\text{ex}}$ in the quasi-adiabatic regime which derive from the Landau-Zener-Stückelberg interferences. For larger system sizes these oscillations are washed out due to the presence of multiple paths which leads to an overall destructive interference effect. Thus, for these particle numbers the resonances of adiabatic breakdown found in the previous Subsection are destroyed by quantum fluctuations. To go to larger particle numbers in order to try and re-encounter any semi-classical behaviour becomes computationally very demanding. For $N$ on the order of few hundreds ($\sim 500$) we have not been able to recover any signatures of these classical effects. We see in the figure that for growing particle number $N$ the system becomes more sensitive to non-adiabatic excitations because of the increased density of states. More precisely, in the adiabatic and intermediate regime between adiabatic and diabatic we find that $P_{\text{ex}} \sim \sqrt{N}$.

It remains to establish whether the excitations depend exponentially or as a power-law on the sweep velocity $\lambda$ and how strong fluctuations are in the present many-body problem. By now it is clear that the LZ physics of the parity LMG model is qualitatively different from the parity-broken LMG [12] and the Tavis-Cummings model [12]. In the adiabatic regime different power-law dependences $P_{\text{ex}} \sim \lambda^\nu$ have been established in various types of LZ models; $\nu = 3/4$ for parity-broken LMG model [13], $\nu = 1$ for the Tavis-Cummings model [12], and $\nu = 1/3$ (quantum regime) or $\nu = 1$ (semi-classical regime) for a many-body fermionic model related to the Tavis-Cummings one [13]. For a sweep through the critical point of the parity LMG it was found that $\nu = 2$ deep in the adiabatic regime while $\nu = 3/2$ in the intermediate regime [13]. Such a dynamical situation is different from a full LZ sweep from $t = -\infty$ to $t = +\infty$ where Landau-Zener-Stückelberg interference can alter the excitations. Nevertheless, we expect similar power-law dependences and this is indeed also the case as has been verified numerically. Thus, for small sweep velocities $\lambda P_{\text{ex}} \sim \lambda^2$ (i.e. $\nu = 2$) and for for the regime where breakdown of adiabaticity considerably sets in $P_{\text{ex}} \sim \lambda^{3/2}$ (i.e. $\nu = 3/2$) and finally in the diabatic regime we re-
cover an exponential dependence $P_{\text{ex}} \sim [1 - \exp(-\kappa/\lambda)]$ for some $\lambda$-independent constant $\kappa$ (which is however $N$-dependent).

One of the main results of Ref. [12] was that the amount of fluctuations is greatly enhanced in interacting many-body LZ problems. While this is expected in the intermediate regime between adiabatic and diabatic, it was claimed in Ref. [12] that this phenomenon holds even in the quasi-adiabatic regime. Large number fluctuations of $P(n)$ imply a large $Q$-value of (17). In the quasi-adiabatic and intermediate regimes we have numerically found that $Q \sim \sqrt{N}$, while from Fig. 6 we can extract that in the corresponding regime $P_{\text{ex}} \sim \sqrt{N}$. Thus, the fluctuations grow as $\sqrt{N}$ relative to the non-adiabatic excitations in the system $(Q/P_{\text{ex}} \sim \sqrt{N})$ which agrees with the findings of [12].

IV. MANY-SITE PROBLEM

In the previous Section [11] we saw that at the mean-field level the single site problem became one of a non-linear two-level LZ system and at the many-body level we obtained a LMG LZ problem. Even at the single site level, the problem was highly non-trivial and led to several novel aspects. When we now turn to the full lattice problem it is not surprising that the complexity is drastically increased. The full problem can be seen as a lattice of coupled many-body LZ problems. However, the coupling between neighboring sites implies that the onsite particle number is no longer preserved, and as a consequence we cannot write the full many-body problem as a set of coupled LMG models with conserved onsite spin. Furthermore, we showed in Section II that the presence of a trap not only break the translational symmetry but also the symmetry between the density distributions of the two orbitals; the $p_x$-orbital density is elongated in the $x$-direction while the $p_y$-orbital density is stretched out along the $y$-direction. This extrinsic particle density will couple to the intra-well densities, i.e. there is an additional energy scale set by the trap. Thus, to adiabatically follow the system ground state the density of the particle cloud must be altered. One could imagine that the intra-well LZ transitions are adiabatic, but non-adiabatic excitations become manifest in the extrinsic degree of freedom describing the shape of the extrinsic distributions.

To numerically treat the many-site problem with a fair amount of populated sites we have to stick to a mean-field analysis. To consider the complete many-body problem on the lattice would require computer power beyond what we are capable of. The many-site mean-field problem of Eq. (5) is solved using the split-operator method [15]. For the many-site problem we can, in principle, consider both inter- ($Z_{\text{tot}}$) and intra-well ($Z_j$) imbalances, but we will only analyze the former. Previously, the onsite order parameter was normalized to unity. Now we normalize the full lattice order parameter to unity, which means that the onsite density is lower here. As we will see, one consequence of this is that the time-scales are much longer in the lattice problem (i.e. $\lambda$ in the intermediate regime is much smaller than in the previous section).

Figure 7: Ground state distributions (a)-(f) of the two $p_x$- (left) and $p_y$-orbitals (right) for different ratios $\lambda t$ ($\lambda t = -0.001$ (a) and (b), $\lambda t = 0$ (b) and (c), and $\lambda t = 0.001$ (e) and (f)), and the imbalance $Z_{\text{tot}}(\lambda t)$ (g). Apart from the regime $\lambda t \lesssim 10^{-4}$, the system ground state populations approximately only a single onsite orbital state (full polarization). The dimensionless parameters used are $\omega = 0.003$, $t_1 = -0.09$, $t_3 = 0.0045$, and $U = 0.38$. The latter three numerical values correspond to an optical lattice with an amplitude of 17 recoil energies which is chosen to be an experimentally relevant parameter [17]. The trap frequency is such that approximately a few hundred lattice sites are populated.

A. Ground state properties

Before entering into the full time-dependent problem, let us look at the ground state properties of the time-independent system, i.e. $\lambda t$ is taken as an external parameter that fixes the detuning between the two orbitals. At the mean-field level, every site hosts a qubit (spin-1/2 particle) characterized by a state $|\psi_{jz}\rangle = |\psi_{xj}\rangle$ which can be represented by a Bloch vector $R_j = (J_{xj}, J_{yj}, J_{zj}) = (2R_{\psi_{xj}^*\psi_{yj}}, 2\lambda(\psi_{xj}^*\psi_{yj}) + \psi_{xj}^*|\psi_{xj}|^2)$. The length of the Bloch vector gives the (scaled) onsite particle number (which is not preserved), and the $z$-component is nothing but the onsite particle imbalance. The LZ parameter $\lambda t$ acts as an external field which tries to align the onsite spins in the $z$-direction. Thus, for large $|\lambda t|$ we have $|R_j|/|R_j| = (0, 0, \pm 1)$, i.e. all the spins point either towards the north or the south.
pole on the Bloch sphere. For zero field, $\lambda t = 0$, we found in the previous Section that in the absence of a trap $R_j/|R_j| = (0, \pm 1, 0)$. Due to the non-zero tunneling terms $t_1$ and $t_2$, the full system organizes in an anti-ferromagnetic state with the spins alternating between pointing in the positive/negative $y$-direction between neighbouring sites [46].

Without a trap, the thermodynamic limit is often taken as letting the lattice size go to infinity while the particle density is kept fixed, i.e. $|R_j|$ is constant. With the knowledge of the previous section, upon driving the full system through a LZ transition we encounter a first order QPT at $\lambda t = 0$ where the full system jumps from positive to negative polarization in the $z$-direction. Only at the transition point $\lambda t = 0$ is the anti-ferromagnetic order restored. From the previous Subsection we also saw that there is an alternative thermodynamic limit which can be taken in a finite lattice, namely to increase the number of particles per site but simultaneously lower the interaction strength $U$ such that the system energy grows linear with the particle number. Both the mean-field as well as the LMG many-body analysis showed that a symmetry broken phase emerges between the two polarized phases. However, in a finite system we expect no true QPT’s but only signatures of them.

The above arguments are demonstrated in Fig. 7 where a confining harmonic trap has been included (hence the system is finite). In the upper plots (a)-(f) we give examples of of the ground state $p_x$-distributions (left plots) and $p_y$-distributions (right plots) for various $\lambda t$. Far from resonance, $\lambda t = 0$, we see that only $p_x$- or $p_y$-orbitals are populated (note the colourbars), and consequently the system is polarized in the $z$-direction. Furthermore, due to the different effective masses in the two directions the shape of the distributions are squeezed as earlier discussed. For zero field, $\lambda t = 0$ (c) and (d), the two distributions are identical but rotated 90 degrees. The full particle distribution is still not polar symmetric for $\lambda t = 0$. In the lower plot we show the total imbalance $Z_{\text{tot}}$ for the whole lattice. We find a regime around $\lambda t = 0$ where a mixing of the two orbitals exist. This corresponds to the broken symmetry phase of the LMG model. Thus, by properly taking the thermodynamic limits we find three phases of the system: large negative or positive $\lambda t$’s polarizes the system, and for small but finite $|\lambda t|$’s the system is in the broken symmetry phase that is characterized by anti-ferromagnetic inter-site ordering in the spin $y$-direction and large intra-site multi-particle entanglement. The QPT is of the Ising type [37]. In the literature of cold atoms on the $p$-bands of optical lattices [18] we may note that this Ising type transition in the superfluid regime has been overlooked.

B. Landau-Zener problem in the lattice

The argued interplay between inter- and intra-site dynamics while driving the system through the LZ transition should be understood from Fig. 7 In an adiabatic transition, the full particle distribution should go from Fig. 7(a) to Fig. 7(f), at the same time as the particles within each site are transfered from $p_x$-orbitals to $p_y$-orbitals (as in Fig. 7(g)). In the previous Section, the imbalance $Z$ (or correspondingly for the many-body situation $P_{\text{ex}}$) told us how adiabatic the transition was. From $Z_{\text{tot}}$ we have the amount of intrinsic excitations $P_{\text{ex}} = (1 - Z_{\text{tot}})/2$. This quantity is not capable of characterizing non-adiabaticity in the lattice since both inter- and intra-site excitations can exist. One direct measurement of how adiabatic the driving is would be to measure the instantaneous energy of the system and compare it to the corresponding ground state energy. However, as in Subsection III A if the system initially populates the ground state no population transfer will occur since the $p_y$-orbitals are not populated and quantum fluctuations are neglected at the mean-field level. In other words, we need to initially populate the $p_y$-orbitals and the system is thereby automatically in an excited state to begin with. Instead we will consider the widths of the $p_y$-distribution

$$\Delta y \alpha^2 = \frac{\langle \psi_y | \hat{a}^2 | \psi_y \rangle}{\langle \psi_y | \psi_y \rangle} - \frac{\langle \langle \psi_y | \hat{a} | \psi_y \rangle \rangle^2}{\langle \psi_y | \psi_y \rangle^2}$$  \hspace{1cm} (18)$$

where $\hat{a}$ $(\alpha = x, y)$ is the discrete position operator. From the above widths we define the squeezing measure

$$F_y(t) = \frac{\Delta y y^2}{\Delta y x^2}$$  \hspace{1cm} (19)$$

which tells how elongated the $p_y$-distribution is; $F_y(t) = 1$ no squeezing, $F_y(t) < 1$ squeezing in the $y$-direction, and $F_y(t) > 1$ squeezing in the $x$-direction. If the LZ sweep is adiabatic we have that at the final time $t_f$ $F_y(t_f) > 1$ and moreover $F_y(t)$ should be time-independent. Variations in $F_y(t)$ can only derive from non-adiabatic excitations, and we thereby introduce $\delta F_y(t)$ as the time-variance of the squeezing parameter at time $t$. In the following, $P_{\text{ex}}$ and $\delta F_y(t)$ will be our rough measures of intra- and inter-well non-adiabatic corrections respectively. But it should be kept in mind that there is not a one-to-one relation between these quantities and the LZ induced excitations.

In Fig. 8 we present numerical results from integrating Eq. (8) for various sweep velocities $\lambda$. The integration interval $[t_i, t_f]$ is taken long enough such that the diabatic states $|\psi_x\rangle$ and $|\psi_y\rangle$ are approximately decoupled at $t_i$ and $t_f$. The initial state is obtained from first finding the ground state (which will almost entirely populate the $p_x$-orbitals) for the given $\lambda$ and then by hand populate the $p_y$-orbitals with one percent and with the same distribution as the one for the $p_x$-orbitals. By increasing the initial population in the $p_y$-orbitals the evolution would in general be more adiabatic since the gap scales with $|\psi_y|^2$. However, this would also imply that the system would initially be more excited. In the figure we vary $\lambda$ while the remaining parameters are calculated from Wannier function overlap integrals (see the Appendix).
corresponding to an optical lattice with an amplitude of 17 recoil energies. This particular choice is meant to represent an experimentally relevant situation. The upper plot of Fig. 8 shows the intrinsic excitations $P_{\text{ex}}(\lambda)$ (a) and variance of the squeezing parameter $\delta F_y(\lambda)$ (b). The open circles mark calculated values, while the solid line is a 5th order polynomial least square fit. The parameters are the same as for Fig. 7, i.e. they correspond to a lattice amplitude of 17 recoil energies.

Figure 8: Intrinsic excitations $P_{\text{ex}}(\lambda)$ (a) and variance of the squeezing parameter $\delta F_y(\lambda)$ (b). The open circles mark calculated values, while the solid line is a 5th order polynomial least square fit. The parameters are the same as for Fig. 7, i.e. they correspond to a lattice amplitude of 17 recoil energies.

V. CONCLUSION

Some unusual features in MBLZ problems were studied. Starting with a LMG model we showed how the corresponding mean-field system is qualitatively different from other non-linear LZ systems studied in the past. The system does not support hysteresis, but breakdown of adiabaticity can instead occur due to a peculiarity of the classical phase space structure. One fixed point lives on a separatrix and moreover it is ‘mobile’ in the sense that when the explicit time-dependence of the Hamiltonian is considered as a parameter the fixed point position depends on this (parametrized) time. A classical solu-
tion that evolves along the separatrix will, during the LZ transition period, get locked to this fixed point and during this period the classical energy surface ‘tips over’ which prevents adiabatic evolution.

For particle numbers of a few hundred it was found that these classical solutions which break adiabaticity were not stable towards quantum fluctuations. Thus, in the fully quantum model and for moderate particle numbers the non-adiabatic corrections displayed a more smooth behaviour. However, these corrections did not obey an exponential behaviour as is the case for the linear two-level LZ problem, but they showed a power-law dependence on the sweep velocity. The quantum LMG model also displayed that large fluctuations are generated during the LZ sweep. In particular, the fluctuations grew linear with the particle number $N$. Simultaneously, the non-adiabatic corrections grew as $\sqrt{N}$ which suggests that even deep in the supposedly adiabatic regime fluctuations (enhanced by the large particle number) will dominate the evolution.

Finally a mean-field lattice version of the above system was considered. The novel feature here derived from an interplay between intra-site LZ transitions and inter-site particle dynamics. The ability of particles to tunnel between lattice sites resulted in a much stricter constrain for adiabaticity. An adiabatic evolution implied a macroscopic particle flow within the lattice. For physically relevant parameters it was found that the intra-site time-scale was much shorter than the inter-site time-scale which resulted in a Franck-Condon scenario. We also discussed how the present models could be experimentally realized in terms of cold bosonic atoms loaded into the $p$-bands of optical lattices. In such systems, time-of-flight measurements would provide direct insight into both internal and external excitations created during the LZ sweep.

All results of this work assume a relatively large particle number per site (typically $>10$) where mean-field approximations start to give a qualitative accurate description of the physics (the resonances found in Subsection III A is a clear exception) or when the many-body character of the LZ problem become particularly evident (Subsection III B). An interesting continuation would be to consider the opposite regime of a low filling and strong correlations, i.e., in the insulating phase. As recently pointed out [51], the physics of this system in the Mott insulator with unit filling is extremely rich and in particular realizes a XYZ Heisenberg model where the LZ sweep would represent a gradual change in the external field.

**Acknowledgments**

The author acknowledges Fernanda Pinheiro for stimulating discussions and help with the numerical codes, and VR (Vetenskapsrådet) for financial help.

**Appendix: Physical realization**

Effective models describing the MBLZ problems discussed in this paper could arise in various physical systems like trapped spinor condensates in optical lattices [52], ion traps [53], or atomic condensates occupying higher energy bands of optical lattices [48]. The following derivation considers the last option, more precisely an ultracold gas of bosonic atoms loaded into the $p$-bands (first excited) of a square optical lattice.

For the isotropic lattice, every lattice site hosts two degenerate atomic orbital states, the $p_x$- and $p_y$-orbitals. By tuning the lattice parameters this degeneracy can be lifted. In respect, an onsite LZ transition can be realized. Contrary to the single-body LZ problem, due to atom-atom interaction the present LZ transitions become non-linear. In analogy with atomic physics, the $p_x$-orbital state processes a node in the $x$-direction and thereby is also more extended in this direction. The same holds true for the $p_y$-orbital but instead in the $y$-direction. The lack of polar symmetry of the orbitals implies that an atom in a $p_x$-orbital state favours tunneling in the $x$-direction rather than in the $y$-direction. This results in an anisotropic tunneling behaviour of $p$-band atoms [46]. As discussed in the main text, the manifestation of this anisotropy becomes apparent when the atoms are confined in an external isotropic harmonic trapping potential [28].

From the single-particle Hamiltonian

$$\hat{H}_{sp} = -\frac{\hbar^2 \nabla^2}{2m} + V(r'),$$

(A.1)

where $m$ is the atomic bare mass and the potential $V(r') = V_{\text{lat}}(r') + V_{\text{trap}}(r')$ with

$$V_{\text{lat}}(r') = \tilde{V}_x \sin(kx') + \tilde{V}_y \sin(ky'),$$

$$V_{\text{trap}}(r') = \frac{m \omega^2}{2} (x'^2 + y'^2)$$

(A.2)

the optical lattice and the external trapping potentials respectively ($k$ being the lattice wave number and $\omega$ the trap frequency), the general form of the many-body Hamiltonian is

$$\hat{H}_{mb} = \int \frac{dr'}{r'} \hat{\Psi}^\dagger(r') \left[ \hat{H}_{sp} + \frac{\tilde{U}_0}{2} \hat{\Psi}^\dagger(r')\hat{\Psi}(r') \right] \hat{\Psi}(r').$$

(A.3)

Here, $\tilde{U}_0$ is the effective atom-atom interaction strength and $\hat{\Psi}(r')$ and $\hat{\Psi}^\dagger(r')$ are the atomic annihilation and creation operators respectively which obey the regular bosonic commutation statistics $[\hat{\Psi}(r''),\hat{\Psi}^\dagger(r')] = \delta(r'' - r')$. Throughout this article we worked with dimensionless variables where the recoil energy $E_R = \hbar^2 k^2 / 2m$ sets the energy scale giving a characteristic length $l = k^{-1}$ and time $\tau = \hbar / E_R$. The scaled dimensionless variables/parameters become $x = kx'$, $y = ky'$, $V_x = \tilde{V}_x / E_R$, $V_y = \tilde{V}_y / E_R$, $\omega = \sqrt{2m\omega/\hbar k^2}$. 


The Hamiltonian \([A3]\) is exact within the framework of two-body contact interactions. In order to derive the effective second quantized model \([2]\) we impose the single-band and tight-binding approximations, i.e. we will restrict the atoms to reside only on the two \(p\)-bands and only consider tunneling between nearest neighbours as well as only onsite interactions. To this end we expand the atom operators in the \(p\)-band Wannier functions

\[
\Psi(r) = \sum_{\alpha j} \psi_{\alpha j}(r) \hat{a}_{\alpha j},
\]

where \(\psi_{\alpha j}(r)\) is the \(p\)-orbital Wannier function at site \(R_j = (x_j, y_j) = (\pi J_x, \pi J_y)\), and \(\hat{a}_{\alpha j}\) annihilates an atom at site \(j\) in orbital \(\alpha\). Inserting \([A3]\) and its hermitian conjugate, in the expression \([A3]\) for the many-body Hamiltonian one derives Eq. \([2]\) in the single-band and tight-binding approximations and where the parameters are given by the overlap integrals; tunneling amplitude

\[
t_{\alpha \beta} = -\int dr \psi_{\alpha j}(r) \hat{H}_{sp} \psi_{\alpha j+1, \beta}(r),
\]

Without the LZ sweep, the onsite energies are assumed the same between the two orbitals and are thereby left out. In the isotropic case and in the harmonic approximation, i.e. \(w_{\alpha j}(r) \propto (x - \pi J_x)/2\sigma - (y - \pi J_y)^2/2\sigma\) with \(\sigma\) the width and similarly for \(w_{\beta j}(r)\), the interaction strengths obey \(U_{xx} = U_{yy} = 3U_{xy} = 3U_{yx}\). In the main text we define \(U = U_{xx}\) to parametrize all interaction terms.

[1] L. D. Landau, Phys. Z. Sowjetunion 2, 46 (1932); G. Zener, Proc. R. Soc. London Ser. A 137, 696 (1932).
[2] C. Y. Zhu, Y. Teranishi, H. Nakamura, Adv. Chem. Phys. 117, 127 (2001); A. W. Jasper, C. Y. Zhu, S. Nangia, D. G. Truhlar, Faraday Disc. 127, 1 (2004).
[3] O. Morsch, J. H. Müller, M. Cristiani, D. Ciampini, and E. Arimondo, Phys. Rev. Lett. 87, 140402 (2001).
[4] T. Köhler, K. Goral, and P. S. Julienne, Rev. Mod. Phys. 78, 1311 (2006).
[5] D. Averin and A. Bardas, Phys. Rev. Lett. 75, 1831 (1995).
[6] W. D. Oliver, Y. Yu, J. C. Lee, K. K. Berggren, L. S. Levitov, and T. P. Orlando, Science 310, 1653 (2005); M. Sillanpää, T. Lektinen, A. Paila, Y. Makhlin, and P. Hakonen, Phys. Rev. Lett. 96, 187002 (2006).
[7] B. Damski, Phys. Rev. Lett. 95, 035701 (2005); W. H. Zurek, U. Dorner, and P. Zoller, Phys. Rev. Lett. 95, 105701 (2005); J. Dziarmaga, Adv. Phys. 59, 1063 (2010).
[8] A. V. Shytov, D. A. Ivanov, and M. V. Feigelman, Eur. Phys. J. B 36, 263 (2003); J. Larson and S. Stenholm, J. Mod. Opt. 50, 1663 (2003); K. Saito, M. Wubs, S. Kohler, P. Hänggi, and Y. Kayaunma, Eur. Phys. Lett. 76, 22 (2006); C. Hicke, L. F. Santos, and M. I. Dykman, Phys. Rev. A 73, 012342 (2006); G. Z. Sun, X. D. Wen, B. Mao, J. A. Chen, Y. Yu, P. H. Wu, and S. Y. Han, Nature Commun. 1, 1050 (2010).
[9] O. Aatabek, R. Lefebvre, and M. Jacot, J. Chem. Phys. 81, 3874 (1984); C. E. Carroll and F. T. Hioe, J. Phys. A: Math. Gen. 19, 2061 (1986); V. L. Pokrovsky and N. A. Sinitsyn, Phys. Rev. B 65, 153105 (2002); J. Larson, Phys. Rev. A 73, 013823 (2006); N. A. Sinitsyn, Phys. Rev. A 87, 032701 (2013).
[10] Y. N. Demekov and V. N. Ostrovsky, J. Phys. B: At. Mol. Opt. Phys. 34, 2419 (2001).
[11] V. A. Yurovsky, A. Ben-Reuven, and P. S. Julienne, Phys. Rev. A 65, 043607 (2002).
[12] A. Altland, V. Gurarie, T. Kriecherbauer, and A. Polkovnikov, Phys. Rev. A 79, 042703 (2009).
[13] I. Tikhonenkov, E. Paz, Y. B. Band, M. Fleischhauer, and A. Vardi, Phys. Rev. A 73, 043605 (2006).
[14] P. Solinas, P. Ribeiro, and R. Mosseri, Phys. Rev. A 78, 052329 (2008); T. Caneva, R. Fazio, and G. E. Santoro, Phys. Rev. B 78, 104426 (2008); A. P. Itin and P. Törnä, arXiv:0901.4778.
[15] C. Kaszeta, S. Trotzky, Y.-A. Chen, I. Bloch, I. P. McCulloch, U. Schollwöck, and G. Orso, Phys. Rev. Lett. 106, 155302 (2011).
[16] Y. Qian, M. Gong, and C. Zhang, Phys. Rev. A 87, 013636 (2013).
[17] B. Wu and Q. Niu, Phys. Rev. A 61, 023402 (2000); O. Zobay and B. M. Garraway, Phys. Rev. A 61, 033603 (2000).
[18] J. Liu, L. Fu, B.-Y. Ou, S.-G. Chen, D.-I. Choi, B. Wu, and Q. Niu, Phys. Rev. A 66, 023404 (2002).
[19] C. Lee, Phys. Rev. Lett. 97, 150402 (2006); D. Witthaut, E. M. Graefe, and H. J. Korsch, Phys. Rev. A 73, 063609 (2006); K. Smith-Mannschott, M. Chuchem, M. Hiller, T. Kottos, and D. Cohen, Phys. Rev. Lett. 102, 230401 (2009).
[20] R. G. Unanyan and M. Fleischhauer, Phys. Rev. Lett. 90, 136001 (2003).
[21] M. Machholm, C. J. Pethick, and H. Smith, Phys. Rev. A 67, 053613 (2003); M. Machholm, A. Nicolin, C. J. Pethick, and H. Smith, Phys. Rev. A 69, 043604 (2004).
[22] To achieve this type of terms in spinor condensates one would need a significant large amplitude for scattering processes which convert atomic Zeeman levels. These are, however, often only on the order a few percent compared to other amplitudes.
[23] Y.-A. Chen, S. D. Huber, S. Trotzky, I. Bloch, and E. Altman, Nat. Phys. 7, 61 (2011).
[24] H. J. Lipkin, N. Meshkov, and A. J. Glick, Nucl. Phys. 62, 188 (1965).
[25] P. W. Atkins and R. S. Friedman, Molecular Quantum Mechanics (Oxford University Press, Oxford, 1999).
[26] J. Larson, S. Fernandez-Vidal, G. Morigi, and M. Lewenstein, New J. Phys. 10, 045002 (2008).
[27] A. Collin, J. Larson, and J.-P. Martikainen, Phys. Rev. A 81, 023605 (2010); T. Sowinski, M. Lacki, O. Dutta, J. Peterszewicz, P. Sierant, M. Gajda, J. Zakrzewski, and M. Lewenstein, arXiv:1304.6299.
[28] F. Pinheiro, J.-P. Martikainen, and J. Larson, Phys. Rev. A 85, 033638 (2012).
[29] C. J. Pethick and H. Smith, Bose-Einstein Condensation in Dilute Gases (Cambridge University Press, Cambridge, 2008).
[30] Since normalization and an overall phase constitute one constrain each, out of the four real variables only two are actually needed to fully characterize the physical state.
[31] E. M. Graefe, H. J. Korsch, and D. Witthaut, Phys. Rev. A 73, 013617 (2006); G.-F. Wang, D.-F. Ye, L.-B. Fu, X.-Z. Chen, and Z. Lie, Phys. Rev. A 74, 033414 (2006); D.-F. Ye, L.-B. Fu, and J. Liu, Phys. Rev. A 77, 013402 (2008); Z. Chen and B. Wu, Phys. Rev. Lett. 107, 065301 (2011); B. P. Venkatesh, J. Larson, D. H. J. O’Dell, Phys. Rev. A 83, 063606 (2011); S. Baharian and G. Baym, Phys. Rev. A 87, 013619 (2013); L. Dong, L. Zhou, B. Wu, B. Ramachandhran, and H. Pu, arXiv:1309.4369; J. Mumford, J. Larson, and D. H. J. O’Dell, arXiv:1309.7755.
[32] The adiabatic energies for the linear LZ problem are $E_{ad}^{\pm} = \pm \sqrt{\lambda t^2 + U^2}$.
[33] L. D. Landau and E. M. Lifschitz, Mechanics (Pergamon, Oxford, 1977).
[34] E. J. Heller, Phys. Rev. Lett. 53, 1515 (1984).
[35] J. J. Sakurai, Modern Quantum Mechanics (Addison Wesley, 1993).
[36] S. Sachdev, Quantum Phase Transitions, (Cambridge University Press, Cambridge, 2011).
[37] A. Michel, D. Jakob, T. I. Cirac, and P. Zoller, Phys. Rev. A 67, 013607 (2003).
[38] S. Morrison and A. S. Parkins, Phys. Rev. Lett. 100, 040403 (2008); D. I. Tsomokos, S. Ashhab, and F. Nori, New J. Phys. 10, 113020 (2008); G. Chen, L. Gang, J.-Q. Liang, and S. Jia, Opt. Express 17, 19682 (2009); J. Larson, Eur. Phys. Lett. 90, 54001 (2010).
[39] S. Dusuel and J. Vidal, Phys. Rev. B 71, 224420 (2005).
[40] R. H. Dicke, Phys. Rev. 93, 99 (1954).
[41] J. Larson, Phys. Rev. Lett. 108, 033601 (2012); M. Schiavo, M. Bordyuh, B. Oztqi, and H. E. Türeci, Phys. Rev. Lett. 109, 053601 (2012).
[42] S. N. Shevchenko, S. Ashhab, and F. Nori, Phys. Rep. 492, 1 (2010).
[43] L. Mandel and E. Wolf, Optical Coherence and Quantum Optics, (Cambridge University Press, Cambridge, 1995).
[44] M. D. Fleit, J. A. Fleck, and A. Steiger, J. Comput. Phys. 47, 412 (1982).
[45] A. Isacsson and S. M. Girvin, Phys. Rev. A 72, 053604 (2005).
[46] T. Müller, S. Fölling, A. Widera, and I. Bloch, Phys. Rev. Lett. 99, 200405 (2007).
[47] V. W. Scarola and S. Das Sarma, Phys. Rev. Lett. 95, 033003 (2005); C. J. Wu, W. V. Liu, J. Moore, and S. Das Sarma, Phys. Rev. Lett. 97, 190406 (2006); W. V. Liu and C. J. Wu, Phys. Rev. A 74, 013607 (2006); J. Larson, A. Collin, and J.-P. Martikainen, Phys. Rev. A 79, 033603 (2009).
[48] G. Wirth, M. Olschlager, and A. Hemmerich, Nature Phys. 7, 142 (2011).
[49] J. Ruostekoski and Z. Dutton, Phys. Rev. A 76, 063607 (2007).
[50] C. Schneider, D. Porras, and T. Schaetz, Rep. Prog. Phys. 75, 02401 (2012).