Spin polarization through floquet resonances in a driven central spin model

Claeys, P.W.; De Baerdemacker, S.; El Araby, O.; Caux, J.-S.

DOI
10.1103/PhysRevLett.121.080401

Publication date
2018

Document Version
Final published version

Published in
Physical Review Letters

Citation for published version (APA):

General rights
It is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), other than for strictly personal, individual use, unless the work is under an open content license (like Creative Commons).

Disclaimer/Complaints regulations
If you believe that digital publication of certain material infringes any of your rights or (privacy) interests, please let the Library know, stating your reasons. In case of a legitimate complaint, the Library will make the material inaccessible and/or remove it from the website. Please Ask the Library: https://uba.uva.nl/en/contact, or a letter to: Library of the University of Amsterdam, Secretariat, Singel 425, 1012 WP Amsterdam, The Netherlands. You will be contacted as soon as possible.
Spin Polarization through Floquet Resonances in a Driven Central Spin Model

Pieter W. Claeys, Stijn De Baerdemacker, Omar El Araby, and Jean-Sébastien Caux

1Department of Physics and Astronomy, Ghent University, Krijgslaan 281 S9, B-9000 Gent, Belgium
2Center for Molecular Modeling, Ghent University, Technologiepark 903, 9052 Gent, Belgium

(Received 7 January 2018; published 21 August 2018)

Adiabatically varying the driving frequency of a periodically driven many-body quantum system can induce controlled transitions between resonant eigenstates of the time-averaged Hamiltonian, corresponding to adiabatic transitions in the Floquet spectrum and presenting a general tool in quantum many-body control. Using the central spin model as an application, we show how such controlled driving processes can lead to a polarization-based decoupling of the central spin from its decoherence-inducing environment at resonance. While it is generally impossible to obtain the exact Floquet Hamiltonian in driven interacting systems, we exploit the integrability of the central spin model to show how techniques from quantum quenches can be used to explicitly construct the Floquet Hamiltonian in a restricted many-body basis and model Floquet resonances.

Introduction.—Periodically driven systems have a rich history ranging from the simple kicked rotor to recent experimental progress on cold atoms in optical fields [1,2]. The dynamics in driven systems has remarkable features, such as the absence of a well-defined adiabatic limit [3,4] and the heating to an infinite temperature which is expected to occur [5–9]. The same physical mechanism underlies these phenomena—in the presence of periodic driving, it is possible for states to interact resonantly. States whose energies are separated by an integer multiple of the driving frequency will interact strongly, leading to Floquet or many-body resonances [10–12].

While this is generally seen as a disadvantage because of the experimental problems posed by heating, there is hope that in large but finite systems such many-body resonances can be well understood and even controlled. This opens up ways of engineering specific many-body resonant quantum states by adiabatically tuning the driving frequency to resonance. Such “driven driving” protocols, if smartly conceived, could even lead to states with properties beyond these associated with the (physical) driving Hamiltonians [13–18]. This is illustrated on the central spin model, which is adiabatically driven such that the central spin becomes completely decoupled from its environment, incompatible with the physics of the instantaneous Hamiltonians. This model describes the (inhomogeneous) interaction of a central spin on which a magnetic field is applied with an environment of surrounding spins, being important in the study of quantum dots, solid-state nuclear magnetic resonance, and the nitrogen-vacancy defect in diamond, a promising qubit system [19]. A major experimental challenge remains the decoherence due to the presence of an environment, motivating numerous studies [20–30]. Surprisingly, Floquet resonances can here be used to construct pure spin states, seemingly at odds with the inevitable interaction with the environment and resulting decoherence effects.

All such resonances are encoded in the spectrum of the Floquet Hamiltonian, governing periodic dynamics. However, due to the exponential scaling of the Hilbert space and the inherently nondiagonal nature of time evolution operators, it is generally impossible to obtain this Hamiltonian in realistically sized interacting systems. In the present Letter, we exploit that the system is driven by periodically switching between integrable Hamiltonians [31,32], and we show how techniques from quantum quenches in integrability can be adapted to accurately model such transitions by constructing a (numerically) exact Floquet Hamiltonian in a restricted Hilbert space spanned by the resonant (Bethe ansatz) eigenstates of the integrable time-averaged Hamiltonian. This also presents a first step toward applying the toolbox from integrability to driven systems, where integrability is generally expected to lose its usefulness because of the general nonintegrability of the Floquet Hamiltonian [33–35].

Floquet theory.—The key result in the study of periodically driven systems is the Floquet theorem [36], recasting the unitary evolution operator as

\[ U(t) = \mathcal{P}(t)e^{-iH_F t}, \]

with \( \mathcal{P}(t) \) a periodic unitary operator with the same period \( T \) as the driving, satisfying \( \mathcal{P}(T) = 1 \), and \( H_F \) the Floquet Hamiltonian (with \( \hbar = 1 \)). Considering time evolution over...
one full cycle leads to the Floquet operator, from which $H_F$ can be extracted as

$$U_F \equiv U(T) = e^{-iH_F T}. \tag{2}$$

Simultaneously diagonalizing these operators leads to

$$H_F = \sum_n \epsilon_n |\phi_n\rangle \langle \phi_n|, \quad U_F = \sum_n e^{-i\epsilon_n T} |\phi_n\rangle \langle \phi_n|, \tag{3}$$

with quasienergies $\epsilon_n = \theta_n / T$. These provide the Floquet equivalent of quasimomenta in Bloch theory, similarly defined only up to shifts $k \times 2\pi / T, k \in \mathbb{N}$, and quasienergies separated by shifts $k \times 2\pi / T, k \in \mathbb{N}$, are said to be quasigeometric. Crucially, the Floquet Hamiltonian itself defined only up to shifts $k \times 2\pi / T, k \in \mathbb{N}$, is crucial to consider finite systems with a bounded spectrum, since the unbounded spectrum in infinitely large systems immediately leads to a proliferation of many-body resonances, and lead to so-called “infinite-temperature states.” Here, it is crucial to consider finite systems with a bounded spectrum, since the unbounded spectrum in infinitely large systems immediately leads to a proliferation of many-body resonances, and “infinite-temperature” Floquet eigenstates at all possible driving frequencies. However, by tuning the driving frequency in finite systems, it remains possible to target specific resonances of nontrivial states, as will be illustrated.

### The central spin model

The model Hamiltonian is

$$H = B_z S_z^0 + \sum_{j=1}^L A_j \vec{S}_0 \cdot \vec{S}_j, \tag{6}$$

with $S^+_0$ and $S^-_0$ the spin operators of the central spin and the environment, respectively. These are taken to be spin-1/2 particles, and the coupling constants are commonly chosen as $A_j = \exp[-(j-1)/L]$, corresponding to a quantum dot in a 2D Gaussian envelope [50]. However, the integrability of the central spin model is versatile enough that our proposed method holds for arbitrary spins and parameterizations. For consistency with the literature on integrability, we set $\epsilon_j = -A_j^{-1}$ and $\epsilon_0 = 0$. The exact Bethe ansatz eigenstates

$$|B_z; v_1, \ldots, v_N\rangle = \prod_{a=1}^N \left( \sum_{j=0}^{L} \frac{S^+_a}{\epsilon_j - v_a} \right) |\downarrow \cdots \downarrow\rangle \tag{7}$$

depend on variables $\{v_1, \ldots, v_N\}$ satisfying Bethe equations

$$B_z^{-1} + \frac{1}{2} \sum_{j=0}^{L} \frac{1}{\epsilon_j - v_a} = \sum_{b \neq a}^{N} \frac{1}{v_b - v_a} \quad \forall \ a = 1, \ldots, N, \tag{8}$$

leading to energies

$$E(B_z; \{v_1, \ldots, v_N\}) = \frac{1}{2} \sum_{a=1}^{N} v_a^{-1} - \frac{1}{4} \sum_{j=1}^{L} A_j - \frac{1}{2} B_z. \tag{9}$$

Integrability now has two major advantages. First, these equations can be efficiently solved in a time scaling polynomially with the system size. This should be contrasted with the conventional diagonalization of the Hamiltonian matrix in an exponentially large Hilbert space, allowing for exact results for large system sizes. Second, it allows for the systematic targeting of eigenstates through the Bethe equations. The key to our proposed approach is that overlaps $\langle B_z; v_1, \ldots, v_N|B_z; w_1, \ldots, w_N\rangle$ between eigenstates of central spin Hamiltonians with different magnetic fields $B_{\perp 1} \neq B_{\perp 2}$ can also be efficiently calculated numerically [51].

Returning to Floquet dynamics, a protocol is considered where $B_z$ is periodically switched between values $B_{\perp 1}$ and $B_{\perp 2}$. To fix ideas, the eigenphases of the Floquet operator have been given in Fig. 1 for different driving periods $T$, with total spin projection 0, $\eta = 0.5$, and $B_z$ switched between 1.2 and 0.8. These calculations have been performed using exact diagonalization on a small system with $L = 5$ in order to avoid a visual clutter of eigenstates but are representative for larger system sizes. Next to the spectrum of the Floquet operator, two energy measures of a Floquet state $|\phi_n\rangle$ are
FIG. 1. Phase spectrum of the Floquet operator, quasienergies, and dynamical energies for a periodically driven central spin Hamiltonian at different driving periods $T$. The dotted (blue) lines mark the edges of the Brillouin zone $\pm \pi(\theta_n)$ and $\pm \pi/T (\theta_n/T)$, while the vertical dotted line denotes $T_c = 2\pi/W$. The ground state and highest excited state are highlighted red using the approximative results from integrability (see below).

$$\theta_n = \langle \phi_n | H_F | \phi_n \rangle, \quad \frac{\partial \theta_n}{\partial T} = \langle \phi_n | H_{av} | \phi_n \rangle,$$  

(10)

with $\theta_n/T$ the quasienergies and $\partial_T \theta_n$ the dynamical contribution to the quasienergies [34,63]. This second quantity is convenient for the visualization of avoided crossings in the spectrum of the Floquet Hamiltonian.

At small driving periods, the spectrum of $H_F$ reduces to that of $H_{av}$ and both energies coincide. The onset of many-body resonances can be observed at $T_c = 2\pi/W$, with $W = E_{\text{max}} - E_{\text{min}}$ the bandwidth of $H_{av}$. At this critical frequency, the energy difference between the ground state and the highest excited state exactly matches the driving frequency. These states are then quasidegenerate and interact resonantly, which can be clearly observed in the avoided crossing between their respective quasienergies in $\langle H_F \rangle$ [64] and the crossing between their respective energies in $\langle H_{av} \rangle$. Further increasing the driving period, more and more resonances are introduced. Remarkably, the off-resonant parts of the spectrum can often be accurately approximated using $H_{av}$ [12,65].

Resonant transitions.—Resonances have a major influence on the concept of adiabaticity, with distinct effects on the eigenstates of the Floquet Hamiltonian and the time-averaged Hamiltonian [65–70]. Starting from an eigenstate of the Floquet Hamiltonian and adiabatically changing the driving frequency [71], the initial state will adiabatically follow the eigenstate of the Floquet Hamiltonian. Across resonance, this would result in a transition from, e.g., the ground state to a highly excited state of the time-averaged Hamiltonian, since the eigenstates of the Floquet Hamiltonian adiabatically connect these states.

Focusing on the ground and highest excited state and adiabatically increasing the driving period across resonance, starting from the ground state of $H_{av}$ leads to

$$U(T_n) \ldots U(T_2) U(T_1) |\phi_0(\bar{B}_z)\rangle,$$

(11)

with $T$ slowly increased from $T_1$ to $T_n$ and $\bar{B}_z = \eta B_{z,1} + (1 - \eta) B_{z,2}$. We will refer to this state as the “adiabatic ground state,” which is expected to adiabatically follow the corresponding eigenstate of the Floquet Hamiltonian through the frequency sweep, leading to transitions between resonant states. For the small system with $L = 5$, such transitions are shown in Fig. 2 for the first- ($T \approx T_c$) and second-order ($T \approx 2T_c$) resonance. Slowly increasing the driving period, the system ends up in the highest excited state of $H_{av}$ in the second resonance, while it undergoes another resonance in the first transition before the highest excited state can be reached. Since the initial state is not an exact eigenstate of $H_F$, but only a (good) approximation, oscillations are introduced in all expectation values corresponding to contributions from excited eigenstates of $H_F$ to $|\phi_0(\bar{B}_z)\rangle$ (see the inset in Fig. 2). These arise from higher-order contributions to the Magnus expansion and are as such controllable (e.g., by decreasing $|B_{z,2} - B_{z,1}|$). Still, it is clear that the ground state adiabatically follows the eigenstates of the Floquet Hamiltonian if
the driving period is varied adiabatically. In order to have a clear transition between two states, it is important that the resonance is isolated, where only a single state is quasidegenerate with the ground state. For the ground and highest excited state, the first and second resonances are guaranteed to be isolated because of the two-band nature and the low density of states at the edge of the spectrum (see Fig. 1). Note how \(\langle S^0_0 \rangle\), as shown in the lower panel in Fig. 2, vanishes at the first resonance and nears its maximal value of 1/2 in the second resonance.

**Modeling the resonant transition.**—In general, such calculations require constructing the evolution operators for both driving Hamiltonians at each value of the driving period and constructing and subsequently diagonalizing the Floquet operator. Each step involves the full Hilbert space, making such calculations unfeasible for realistic system sizes. However, knowledge acquired from quantum quenches (see, e.g., [72] and references therein) can be transferred to the present situation under the following key assumption. Namely, we assume that each many-body resonance can be modeled as a two-level system including only the corresponding quasidegenerate eigenstates of \(H_{av}\). This assumes that quasidegenerate states do not interact strongly with off-resonant states or other quasidegenerate states with a different quasienergy, similar in spirit to strong quasidegenerate perturbation theory. This approximation can be validated through the Floquet-Magnus expansion and is expected to hold if the deviations of the driving Hamiltonians are small with respect to the time-averaged Hamiltonian \(H_{av}\). This approximation can be modeled as a two-level system including only the corresponding quasidegenerate eigenstates of \(H_{av}\). This assumes that quasidegenerate states do not interact strongly with off-resonant states or other quasidegenerate states with a different quasienergy, similar in spirit to strong quasidegenerate perturbation theory. This approximation can be validated through the Floquet-Magnus expansion and is expected to hold if the deviations of the driving Hamiltonians are small with respect to the time-averaged Hamiltonian \(H_{av}\). The Floquet operator can then be constructed in the two-dimensional basis \(\{\phi_0(\vec{B}_z), \phi_f(\vec{B}_z)\}\) spanned by the relevant quasidegenerate eigenstates of the time-averaged Hamiltonian

\[
U_F = \begin{bmatrix}
\langle \phi_0(\vec{B}_z) | U_F | \phi_0(\vec{B}_z) \rangle & \langle \phi_0(\vec{B}_z) | U_F | \phi_f(\vec{B}_z) \rangle \\
\langle \phi_f(\vec{B}_z) | U_F | \phi_0(\vec{B}_z) \rangle & \langle \phi_f(\vec{B}_z) | U_F | \phi_f(\vec{B}_z) \rangle
\end{bmatrix}.
\] (12)

Explicitly writing out the Floquet operator (12) and expanding in the eigenstates of the driving Hamiltonians, each matrix element is given by

\[
\langle \phi_f(\vec{B}_z) | U_F | \phi_f(\vec{B}_z) \rangle = \sum_{m,n} e^{-i(1-\eta)E_m(\vec{B}_z)T} e^{-i\eta E_n(\vec{B}_z)T} \times \langle \phi_f(\vec{B}_z) | \phi_m(\vec{B}_z) \rangle \times \langle \phi_m(\vec{B}_z) | \phi_n(\vec{B}_z) \rangle \times \langle \phi_n(\vec{B}_z) | \phi_f(\vec{B}_z) \rangle.
\] (13)

The calculation of each matrix element generally involves a double summation over the Hilbert space of energies and overlaps, which in turn involve summations over the Hilbert space. Integrability already provides numerically efficient expressions for the energies and the overlaps. As noticed in quantum quenches, another important feature of Bethe states is that they offer a basis in which only a very small minority of eigenstates carry a substantial correlation weight, allowing summations over the full Hilbert space to be drastically truncated [52,53]. Such a truncation scheme is presented in Supplemental Material [51], and the induced error can be checked from sum rules. In practice, this allows for a numerically exact construction of the matrix elements (13) for relatively large systems. The resulting \(2 \times 2\) operator can be easily diagonalized, and integrability allows for an efficient calculation of expectation values from its eigenstates [54–59]. So the main approximation in this scheme is the restriction of the Hilbert space to a two-dimensional space, but within this space the Floquet operator is numerically exact. While we focus on the interaction between the ground and the highest excited state only, this makes it possible to systematically reconstruct part of the Floquet spectrum by including an increasing number of states in this basis. The accuracy can already be appreciated from Figs. 1 and 2, where the avoided crossings near the resonances are well approximated but do not take into account the resonances involving other states. The results are extended in Figs. 3 and 4 to...
different system sizes and average magnetic fields. The period beyond which the two-level approximation fails because another state needs to be included can also be estimated [51] and is marked in both figures. Note that this period lies outside the figure for the second-order resonance.

Discussion.—While the expectation value of $H_{\text{av}}$ varies smoothly from the initial to the final value, the behavior of the central spin is highly dependent on the order of the resonance. The magnetization $\langle S^z_0 \rangle$ vanishes at the first resonance, while it nears the maximal value 1/2 at the second resonance. Such a protocol could then be used to realize a state with magnetization exceeding that of both states, incompatible with any stationary central spin Hamiltonian, since a maximal value of 1/2 implies a pure state decoupled from its environment.

A simple way to understand this behavior follows from the structure of the ground and the highest excited state, where the environment spins tend to align either antiparallel or parallel to the central spin. These can be approximated by treating the environment as a single collective spin, and in this space the Hamiltonian simplifies to

$$ H \approx \bar{B}_z S_0^z + A_p \vec{S}_b \cdot \vec{S}_0. \quad (14) $$

Although not a necessary assumption [51], some intuition can be gained by taking $|B_z| \ll |A_p S_b|$, where the relevant eigenstates can be approximated as

$$ |\phi_{\pm} \rangle \approx \frac{1}{\sqrt{2}} \left( |1/2, -1/2 \rangle_b \pm |1/2, 1/2 \rangle_b \right). $$

At resonance, the Floquet states are approximately given by $|\phi \rangle = (1/\sqrt{2})(|\phi_+ \rangle \pm e^{i\theta} |\phi_- \rangle)$, where the relative phase $\theta$ is a priori unknown. However, the magnetization of the central spin depends on this relative phase as $\langle \phi | S_0^z | \phi \rangle = 1/2 \cos(\theta)$. The different magnetizations hence correspond to different relative phases acquired by these states. This relative phase can be deduced from second-order perturbation theory, expanding the matrix elements of the Floquet operator (13) at resonance for small deviations from the average magnetic field $(B_z - \bar{B}_z)$ [51]. Evolving either state over a full driving cycle will lead to a global phase and introduce off-diagonal corrections on the initial state, which are shown to interfere either constructively or destructively, depending on the order of the resonance. This is reflected in the dependence of the off-diagonal elements on the order of the resonance $k$ through terms $e^{i\pi nk\Delta\theta}$, and perturbation theory leads to relative phases $\pi/2$ and $3\pi/2$ in the first resonance, while it leads to relative phases 0 and $\pi$ in the second resonance. These explain the observed magnetization $\langle S^z_0 \rangle = 0$ or $\pm 1/2$ and the decoupling of the central spin. This behavior extends towards higher-order resonances but vanishes at odd-order resonances. However, there is no guarantee that such resonances will be isolated and hence observable.

Conclusion.—In this work, we investigated adiabatic transitions in the Floquet Hamiltonian when varying the driving frequency, leading to a transition between the ground and highest excited state away from resonance. Applying a periodically varying magnetic field to a central spin model, it was shown how frequency sweeps and Floquet resonances can be used to prepare the system in a coherent superposition of the targeted states, leading to either a vanishing magnetization or a spin state exactly aligned with the magnetic field, depending on the order of the resonance. The latter effectively leads to a decoupling of the central spin from its environment, which can be used to purify the central spin. Integrability-based techniques were shown to be able to model this transition, which allows for an investigation of larger system sizes and presents a first step in applying techniques from integrability to interacting integrable systems subjected to periodic driving.

We are grateful to M. Bukov, A. Russomanno, S. E. Tapias Arze, and D. Van Neck for valuable discussions and/or comments. P. W. C. acknowledges support from a Ph.D. fellowship and a travel grant for a long stay abroad at the University of Amsterdam from the Research Foundation Flanders (FWO Vlaanderen). J.-S. C. acknowledges support from the Netherlands Organization for Scientific Research (NWO) and from the European Research Council under ERC Advanced Grant No. 743032 DYNAMINT. This work is part of the Delta ITP consortium, a program of the Netherlands Organisation for Scientific Research (NWO) that is funded by the Dutch Ministry of Education, Culture and Science (OCW).
[64] After shifting one of the two states into the first Brillouin zone \([-π/T, π/T]\).
[71] Provided the micromotion operator does not change; see Ref. [4].