Spin polarization through Floquet resonances in a driven central spin model – Supplementary Material

Pieter W. Claeys, 1, 2, 3, Stijn De Baerdemacker, 2 Omar El Araby, 1 and Jean-Sébastien Caux 1

1 Institute for Theoretical Physics Amsterdam and Delta Institute for Theoretical Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands
2 Department of Physics and Astronomy, Ghent University, Krijgslaan 281 S9, B-9000 Ghent, Belgium
3 Center for Molecular Modeling, Ghent University, Technologiepark 903, 9052 Ghent, Belgium

Appendix A: Integrability of the central spin model

The integrability of the central spin model is a crucial element in our analysis of the transitions in the Floquet quasi-energy spectrum. In this Appendix we provide the necessary technicalities in order to be self-contained. Following the notation from the main text, a set of operators can be defined as

\[ Q_i = B_z S_i^z + \sum_{j \neq i}^{L} \varepsilon_j S_i^j S_j^i, \] (A1)

such that the central spin Hamiltonian corresponds to \( Q_0 \), and these operators mutually commute \([Q_i, Q_j] = 0, \forall i, j\). These are the so-called conserved charges of the central spin model and can be simultaneously diagonalized by (unnormalized) Bethe ansatz states

\[ |B_z; v_1 \ldots v_N \rangle = \prod_{a=1}^{N} \left( \sum_{j=0}^{L} \frac{S_j^+}{\varepsilon_j - v_a} \right) |\downarrow \ldots \downarrow \rangle, \] (A2)

with rapidities \( \{v_1 \ldots v_N\} \) satisfying the Bethe equations

\[ B_z^{-1} + \frac{1}{2} \sum_{j=0}^{L} \frac{1}{\varepsilon_j - v_a} = \sum_{b \neq a}^{N} \frac{1}{v_b - v_a}, \quad \forall a = 1 \ldots N. \] (A3)

Following a famous result by Slavnov [7, 8, 9], overlaps between Bethe states at different magnetizations can be calculated as

\[ \langle B_z; v_1 \ldots v_N | B_z; v_1 \ldots v_N \rangle = \frac{\prod_{a=1}^{L} \prod_{b \neq a}^{N} (v_a - w_b) \prod_{a < b}^{N} (v_b - v_a)}{\det S_N}, \] (A4)

with \( S_N \) an \( N \times N \) matrix defined as

\[ (S_N)_{ab} = \frac{1}{v_a - w_b} \left[ \sum_{j=0}^{L} \frac{1}{(v_a - \varepsilon_j)(w_b - \varepsilon_j)} - 2 \sum_{c \neq a}^{N} \frac{1}{(v_a - v_c)(w_b - v_c)} \right]. \] (A5)

Taking the limit where the two sets of rapidities coincide leads to an expression for the normalization of a Bethe state as the determinant of a Gaudin matrix

\[ \langle B_z; v_1 \ldots v_N | B_z; v_1 \ldots v_N \rangle = \det G_N, \] (A6)

with \( G_N \) an \( N \times N \) matrix defined as

\[ (G_N)_{ab} = \left\{ \begin{array}{ll} \frac{1}{2} \frac{1}{(v_a - v_b)} & \text{if } a = b \\ -2 \sum_{c \neq a}^{N} \frac{1}{(v_a - v_c)(v_b - v_c)} & \text{if } a \neq b \end{array} \right.. \] (A7)

This is sufficient for the evaluation of all terms in the Floquet operator. In order to calculate expectation values from the resulting wave function one more result needs to be used, namely that for the matrix elements of the spin projection \( S_N^z \) (see e.g. Refs. [10, 11]). From the Hellmann-Feynman theorem, it follows that

\[ \frac{\langle B_z; v_1 \ldots v_N | S_N^z | B_z; v_1 \ldots v_N \rangle}{\langle B_z; v_1 \ldots v_N | B_z; v_1 \ldots v_N \rangle} = \frac{\partial}{\partial B_z} E(B_z; \{v_1 \ldots v_N\}), \] (A8)

while the off-diagonal elements can be calculated as

\[ \langle B_z; v_1 \ldots v_N | S_N^b | B_z; v_1 \ldots v_N \rangle = \frac{\prod_{c=1}^{L} (v_c - \varepsilon_0)}{\prod_{c=1}^{N} (v_c - \varepsilon_0) \prod_{a < b}^{N} (v_b - v_a) \prod_{a < b}^{N} (v_a - v_b)} \] (A9)

with \( T_N \) following from \( S_N \) as

\[ (T_N)_{ab} = (S_N)_{ab} \prod_{c}^{N} (v_c - w_c), \] (A10)

and \( Q_N \) an \( N \times N \) matrix defined as

\[ (Q_N)_{ab} = \prod_{c \neq a}^{N} (w_c - w_b) \left( \varepsilon_0 - v_a \right)^2. \] (A11)

Given a set of Bethe states, it is now possible to calculate all necessary overlaps and expectation values. Furthermore, the Bethe ansatz approach reduces the problem of obtaining eigenvalues and eigenstates to solving a set of coupled nonlinear equations, instead of diagonalizing the Hamiltonian in the full (exponentially large) Hilbert space. Many techniques have been proposed for solving these equations, where we have implemented the so-called eigenvalue-based approach [10, 11].

The other necessary result for our approach was an efficient expansion of a Bethe state at given magnetic field \( B_z \) in a set of Bethe states at slightly different magnetic field. In Refs. [10] and [11] it was shown how such an expansion can be efficiently implemented by targeting relevant eigenstates in a systematic way. This targeting can
be insufficient and the error exceeds a certain threshold. If this initial truncation would prove to be insufficient, a measure for the error is easily calculated as 

\[ \sum_{i=1}^{n} S_{i(\alpha)}^+ |\downarrow \ldots \downarrow \rangle. \]  

(A12)

In this limit, all states reduce to simple product states defined in terms of a set occupied spin levels \{\{1\} \ldots \{N\}\}. For the given parametrization, the ground state reduces to the initial state by simple spin-flip excitations in the limit \(B_z \rightarrow 0\). This results in a set of \(N(L + 1 - N)\) states for which the overlap needs to be calculated, which are again represented graphically in Figure 1.

When expanding an eigenstate at fixed \(B_z\) into eigenstates of a model at different \(B_z\), it is often sufficient to restrict the expansion to states which can be related to the initial state by simple spin-flip excitations in the limit \(B_z \rightarrow 0\). This results in a set of \(N(L + 1 - N)\) states for which the overlap needs to be calculated, which are again represented graphically in Figure 1.

When expanding an initial state \(\phi_i(B_z)\) in such a restricted basis, a measure for the error is easily calculated as \(1 - \sum_{n} |\langle \phi_i(B_z) | \phi_n \rangle|^2\), which reduces to zero for a complete basis. If this initial truncation would prove to be insufficient and the error exceeds a certain threshold (when e.g. there are large differences between the time-averaged Hamiltonian and the driving Hamiltonians), this summation can be extended in a systematic way by including higher-order spin-flip excitations.

Appendix B: Perturbation expansion of the Floquet operator

In order to better understand the behaviour of the Floquet eigenstates near resonance, we perform a perturbative expansion of the Floquet operator when the model is being driven in such a way that there are only small deviations from the average magnetic field. Then within each matrix element all non-diagonal overlaps in the summation will be of order \(B_{z,i} - B_z \approx \mathcal{O}(\Delta)\), allowing the summation to be severely restricted. For corrections up to \(\mathcal{O}(\Delta^2)\), only the initial and final state are relevant as intermediate states in the summation. The diagonal elements can easily be found as

\[
\langle \phi_0(B_z) | U_F | \phi_0(B_z) \rangle = e^{-ikE_0(T_z)} + \mathcal{O}(\Delta^2), \tag{B1}
\]

\[
\langle \phi_f(B_z) | U_F | \phi_f(B_z) \rangle = e^{-ikE_f(T_z)} + \mathcal{O}(\Delta^2), \tag{B2}
\]

which holds for arbitrary values of the driving period. In the first element, the summation has been restricted to \((m,n) = (0,0), (f, f)\) and \((0, f)\) and \((f, 0)\), leading to

\[
\langle \phi_0(B_z) | U_F | \phi_f(B_z) \rangle = e^{-i(1-n)E_0(T_z)}T_z e^{-in\pi E_0(T_z)}T_z (B_{z,1} - B_z) \langle \partial B_z \phi_0 | \phi_f \rangle 
+ e^{-i(1-n)E_f(T_z)}T_z e^{-in\pi E_f(T_z)}T_z (B_{z,2} - B_z) \langle \phi_f \partial B_z | \phi_f \rangle 
+ e^{-i(1-n)E_0(T_z)}T_z e^{-in\pi E_f(T_z)}T_z \times [(B_{z,2} - B_z) \langle \partial B_z \phi_0 | \phi_f \rangle + (B_{z,1} - B_z) \langle \phi_0 \partial B_z | \phi_f \rangle] 
+ \mathcal{O}(\Delta^2), \tag{B3}
\]

and similar for \(\langle \phi_0(B_z) | U_F | \phi_f(B_z) \rangle\), where the inner products have been expanded as e.g. \(\langle \phi_0(B_{z,i}) | \phi_f(B_z) \rangle = |\phi_0(B_{z,i})\rangle + (B_{z,i} - B_z) |\partial B_z \phi_0(B_{z,i})\rangle + \mathcal{O}(\Delta^2)\), where the dependence on \(B_z\) has been made implicit in the final expressions. Evaluating these at \(T = k \cdot T_z\), \(k \in \mathbb{N}\) and explicitly setting \(E_f = E_0 + 2\pi / T_z\), the matrix elements can be rewritten as

\[
\langle \phi_0(B_z) | U_F | \phi_0(B_z) \rangle = e^{-ikE_0(T_z)}T_z, 
\]

\[
\langle \phi_f(B_z) | U_F | \phi_f(B_z) \rangle = e^{-ikE_f(T_z)}T_z = e^{-ikE_0(T_z)}T_z, 
\]

\[
\langle \phi_0(B_z) | U_F | \phi_f(B_z) \rangle = e^{-ikE_0(T_z)}T_z (B_{z,1} - B_{z,2}) \times \langle \partial B_z \phi_0 | \phi_f \rangle (1 - e^{-in\pi kT_z}), 
\]

\[
\langle \phi_f(B_z) | U_F | \phi_0(B_z) \rangle = e^{-ikE_0(T_z)}T_z (B_{z,1} - B_{z,2}) \times \langle \partial B_z \phi_f | \phi_0 \rangle (1 - e^{+in\pi kT_z}).
\]
For the central spin model, it is known that all overlaps are purely real and hence $\langle \partial_{B_z} \phi_0 | \phi_f \rangle = -\langle \partial_{B_z} \phi_f | \phi_0 \rangle$. Taking $k = 1$ and $\eta = 1/2$ then results in

$$U_F = e^{-iE_0(\mathcal{B}_z)T_c} \times \left( 1 + 2(B_{z,1} - B_{z,2}) \langle \partial_{B_z} \phi_0 | \phi_f \rangle \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \right) + \mathcal{O}(\Delta^2).$$  \hspace{2cm} (B4)

Diagonalizing the $2 \times 2$ perturbation matrix leads to eigenstates

$$|\phi_0(\mathcal{B}_z)\rangle \pm i |\phi_f(\mathcal{B}_z)\rangle,$$  \hspace{2cm} (B5)

corresponding to relative phases of $\pi/2$ or $3\pi/2$, as mentioned in the main text.

For the second resonance $(1 - e^{\pm i\eta k^2\pi}) = 0$ and the first-order correction vanishes, so higher-order terms need to be included. It is no longer possible to explicitly obtain the corrections without performing the summation over the Hilbert space, but symmetry arguments can be used to predict the relative phase. If the first-order correction vanishes, the Floquet operator can be written as

$$U_F = e^{-iE_0(\mathcal{B}_z)T} \left( 1 + (B_{z,1} - B_{z,2})^2 V(\mathcal{B}_z) + \mathcal{O}(\Delta^3) \right),$$  \hspace{2cm} (B6)

with $V(\mathcal{B}_z)$ a $2 \times 2$ matrix containing the second-order corrections on the matrix elements. Demanding $U_F$ to be unitary then results in the constraint that $V(\mathcal{B}_z)$ is anti-hermitian $V(\mathcal{B}_z) = -V^\dagger(\mathcal{B}_z)$. Hence, taking the transpose of $U_F$ with $\eta = 1/2$ and exchanging $B_{z,1}$ and $B_{z,2}$ leaves $U_F$ invariant, since

$$\langle U_F(B_{z,1}, B_{z,2}) \rangle^T = \left( e^{-iTH(B_{z,2})/2} e^{-i\eta TH(B_{z,1})/2} \right)^T = e^{-iTH(B_{z,1})/2} e^{-i\eta TH(B_{z,2})/2}.$$  \hspace{2cm} (B7)

This restricts $V(\mathcal{B}_z)$ to be symmetric, since exchanging $B_{z,1}$ and $B_{z,2}$ leaves the second-order contribution $(B_{z,1} - B_{z,2})^2 V(\mathcal{B}_z)$ invariant. Combining these restrictions allows this matrix to be rewritten as $V(\mathcal{B}_z) = iW(\mathcal{B}_z)$, with $W(\mathcal{B}_z)$ a purely real and symmetric matrix. Diagonalizing this perturbation matrix, the eigenstates will be purely real and result in relative phases of $0$ or $\pi$.

Perturbation theory thus explains the relative phases in both resonances, where it is important to note that the presented arguments can be extended to systems where the condition $|B_z| \ll |A_b S_0|$ does not hold. The orthogonal eigenstates of $H_{Avg}$ can be approximately constructed as

$$|\phi_0\rangle = \cos(\varphi) |\frac{1}{2}, \frac{1}{2}\rangle_0 |S_b, -\frac{1}{2}\rangle_b + \sin(\varphi) |\frac{1}{2}, -\frac{1}{2}\rangle_0 |S_b, \frac{1}{2}\rangle_b,$$
$$|\phi_f\rangle = \sin(\varphi) |\frac{1}{2}, \frac{1}{2}\rangle_0 |S_b, -\frac{1}{2}\rangle_b - \cos(\varphi) |\frac{1}{2}, -\frac{1}{2}\rangle_0 |S_b, \frac{1}{2}\rangle_b.$$  \hspace{2cm} (B8)

In the first-order resonance, it can easily be checked that a coherent superposition of these states with a relative phase of $\pi/2$ and $3\pi/2$ (like $|\phi_0\rangle \pm i |\phi_f\rangle$) always has a vanishing magnetization. In the second-order resonance, the
relative phases 0 or π result in Floquet eigenstates with real coefficients interpolating between these two states. This then necessitates a change in sign in one of the two components (either when going from + cos(ϕ) to + sin(ϕ) or from + sin(ϕ) to − cos(ϕ)), resulting in an intermediate state where only a pure state remains and the central spin is decoupled. While this might not always be exactly the state where only a pure state remains and the central state energy gap in the time-averaged Hamiltonian, and a resonance is expected at $T = 2\pi/(E_{\text{max}}^{\text{Avg}} - E_{\text{min}}^{\text{Avg}} - E_{\text{gap}}^{\text{Avg}})$. This is the relevant period discussed in the main text, leading to

$$\frac{T - T_c}{T_c} = \frac{E_{\text{Avg}}^{\text{gap}}}{E_{\text{max}}^{\text{Avg}} - E_{\text{min}}^{\text{Avg}} - E_{\text{gap}}^{\text{Avg}}} \approx \frac{E_{\text{Avg}}^{\text{gap}}}{W}. \quad (C1)$$

The relevant state can again be efficiently targeted from the $B_z \to \infty$ limit and is related to the ground state through a simple spin-flip excitation (e.g., for the previously mentioned example $|\circ\bullet\bullet\circ\bullet\bullet\rangle$). This allows the energy gap to be easily calculated, returning the results mentioned in the main text. For the chosen parametrization the bandwidth $W$ scales linearly with system size $L$, whereas the energy gap $E_{\text{gap}}^{\text{Avg}}$ quickly converges to a constant (non-zero) value with increasing system size $L$. The relevant range of periods for which no additional resonances are expected to occur then scales inversely with system size since $E_{\text{gap}}^{\text{Avg}}/W \propto L^{-1}$. For the second-order resonance, this region can similarly be shown to be approximately $2E_{\text{gap}}^{\text{Avg}}/W$.

Two effects hence combine to lead to a second-order resonance which is more isolated compared to the first-order one – it is a second-order perturbative effect and hence more narrow, and the subsequent region where no additional resonances are expected to occur is larger.

Appendix C: Range of validity of the approximation

As shown in the main text, the two-level approximation fails when other resonances occur. Starting from the ground state of $H_{\text{Avg}}$ and increasing the driving period across the first-order resonance with the highest excited state, the range of periods for which no other resonances are expected to occur can be estimated. Specifically, the next relevant resonance occurs when the highest excited state is quasi-degenerate with the first excited state. This state has energy $E_{\text{max}}^{\text{Avg}} + E_{\text{gap}}^{\text{Avg}}$, with $E_{\text{Avg}}^{\text{gap}}$ the ground-state energy gap in the time-averaged Hamiltonian, and a resonance is expected at $T = 2\pi/(E_{\text{max}}^{\text{Avg}} - E_{\text{min}}^{\text{Avg}} - E_{\text{gap}}^{\text{Avg}})$.

$$\frac{T - T_c}{T_c} = \frac{E_{\text{Avg}}^{\text{gap}}}{E_{\text{max}}^{\text{Avg}} - E_{\text{min}}^{\text{Avg}} - E_{\text{gap}}^{\text{Avg}}} \approx \frac{E_{\text{Avg}}^{\text{gap}}}{W}. \quad (C1)$$

The relevant state can again be efficiently targeted from the $B_z \to \infty$ limit and is related to the ground state through a simple spin-flip excitation (e.g., for the previously mentioned example $|\circ\bullet\bullet\circ\bullet\bullet\rangle$). This allows the energy gap to be easily calculated, returning the results mentioned in the main text. For the chosen parametrization the bandwidth $W$ scales linearly with system size $L$, whereas the energy gap $E_{\text{gap}}^{\text{Avg}}$ quickly converges to a constant (non-zero) value with increasing system size $L$. The relevant range of periods for which no additional resonances are expected to occur then scales inversely with system size since $E_{\text{gap}}^{\text{Avg}}/W \propto L^{-1}$. For the second-order resonance, this region can similarly be shown to be approximately $2E_{\text{gap}}^{\text{Avg}}/W$.

Two effects hence combine to lead to a second-order resonance which is more isolated compared to the first-order one – it is a second-order perturbative effect and hence more narrow, and the subsequent region where no additional resonances are expected to occur is larger.