Trace formula for spin chains

Daniel Waltner, Petr Braun, Maram Akila, Thomas Guhr
Faculty of Physics, University Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany;

Abstract. While detailed information about the semiclassics for single-particle systems is available, much less is known about the connection between quantum and classical dynamics for many-body systems. As an example, we focus on spin chains which are of considerable conceptual and practical importance. We derive a trace formula for coupled spin $j$ particles which relates the quantum energy levels to the classical dynamics. Our derivation is valid in the limit $j \to \infty$ with $j\hbar = \text{const.}$ and applies to time-continuous as well as to periodically driven dynamics. We provide a simple explanation why the Solari-Kochetov phase can be omitted if the correct classical Hamiltonian is chosen.

Keywords: Spin chain, trace formula, coherent states, Solari-Kochetov phase
1. Introduction

Connecting quantum properties such as the energy spectral distribution to the classical properties such as the periodic orbits is a central issue in the theory of quantum chaos. A milestone was here the derivation of the Gutzwiller trace formula \([1]\) for chaotic one-particle-systems in 1960s. Besides connecting classical dynamics and quantum properties for simple model systems with mixed dynamics such as the hydrogen atom in a strong magnetic field \([2]\), it also provided analytical understanding \([3]\) of the applicability of Random Matrix Theory \([4]\) to quantum systems with classically fully chaotic counterpart and thereby strongly corroborates the Bohigas-Giannoni-Schmit conjecture \([5]\).

Nowadays, the research focus switches more and more to interacting many particle systems. In this context, the trace formula for many particle systems consisting of indistinguishable particles was derived in \([6]\), the trace formula for Bose-Hubbard Models was obtained in \([7]\). A prominent many-particle system on which we focus in this paper, are spin chains. The existing investigations refer to the spin quantum number \(j = 1/2\) \([8, 9, 10, 11, 12, 13]\) and to larger spin quantum number both on the side of the theorists \([14, 15, 16, 17, 18]\) as well as experimentalists \([19]\).

We derive here a trace formula for the spin chains expressing their spectral density in terms of the classical periodic orbits. This formula is asymptotically valid in the limit of the spin quantum number \(j \rightarrow \infty\), where \(j \hbar\) is kept constant.

The investigations of the semiclassical spin evolution are usually performed in the basis of the spin coherent states, the motivation being that the angle eigenbasis does not provide states with well localized values of \(j\). Therefore the only alternative would be to use as the basis the eigenstates of the \(z\)-component of the angular momentum which would lead to the discrete semiclassics \([20, 21, 22, 23]\). A single spin is semiclassically a system with one degree of freedom such that the appropriate quantization condition is the Bohr-Sommerfeld rule; it is given in the coherent state basis in \([24]\). In Ref. \([18]\) a trace formula was derived in the coherent state basis for one particle with an orbital and one spin degree of freedom with the energy dependence on the spin variable disregarded. We, however, consider systems of an arbitrary number of interacting spins where the trace formula is the adequate tool of investigation.

We start in section \([2]\) with the time dependent propagator in the coherent state basis as derived in Ref. \([15]\) and reformulated in terms of an intuitively obvious classical Hamiltonian. We give an elementary proof that this Hamiltonian is the correct one. Thus the Solari-Kochetov corrections \([25]\) that attracted a lot of attention in the last years \([14, 15, 16]\) are not needed provided one observes the elementary rules of semiclassics such as replacing \(\sqrt{j(j+1)}\) with \(j + 1/2\) instead of \(j\). In section \([3]\) we compute the trace of the propagator and finally perform the Fourier transform from time to energy domain to obtain the spectral density. We note that these steps are performed in an order different from the derivation of the famous Gutzwiller trace
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In section 3 we discuss how these results can be generalized to periodically driven systems. We conclude in section 5. Technical details are relegated to appendices.

2. Propagator

This section is devoted to the propagator for a spin chain consisting of \( N \) spins. In subsection 2.1 we recapitulate the known expression for the propagator in the limit \( j \to \infty \). In the subsection 2.2 we show that the Solari-Kochetov phase is not needed if the classical Hamiltonian is chosen in an appropriate way.

2.1. Semiclassical expression for the propagator

The propagator for a system of \( N \) spins in the coherent state basis is derived in [15] as a generalization of the propagator for one spin [14]. The Hamiltonian \( \mathcal{H} = \mathcal{H}(\mathbf{J}_1, \ldots, \mathbf{J}_N) \) with \( \mathbf{J}_i = (J_{i,1}, J_{i,2}, J_{i,3}) \) is a Hermitian polynomial in the Cartesian components of the spin operators \( \mathbf{J}_i, i = 1, \ldots, N \) with real coefficients. This is no restriction as every Hamiltonian can be expressed like that using the commutation relations for the spin operators. The matrix element of the propagator between the initial state \( |U'\rangle \) and the final state \( |V''\rangle \) where the star denotes complex conjugation, is given by

\[
K(U', V'', t) = \langle V''^* | e^{-i\mathcal{H}t/\hbar} | U'\rangle.
\]

We use here the convention that the primed variables refer to initial and double primed variables to final coordinates. Here \( |U'\rangle \) and \( |V''\rangle \) are the direct products of unnormalized single particle coherent states

\[
|U'\rangle = \bigotimes_{i=1}^N |U'_i\rangle, \quad |V''\rangle = \bigotimes_{i=1}^N |V''_i\rangle,
\]

where

\[
|U'_i\rangle = e^{U_i\mathcal{J}_{i,+}/\hbar} |j, -j\rangle_i
\]

with \( U'_i \) any complex number, \( \mathcal{J}_{i,+} = \mathcal{J}_{i,1} + i\mathcal{J}_{i,2} \) the spin raising operator and \( |j, -j\rangle_i \) the lowest eigenstate of \( \mathcal{J}_{i,3} \) and \( \mathcal{J}_{i,2} \) with magnetic quantum number \(-j\). Accordingly, \( |U'_i\rangle \) is an eigenstate with the eigenvalue \( \hbar j \) of the angular momentum component along the direction \( \mathbf{n}_i \) with the spherical angles \( \theta_i, \phi_i \). The spin coherent states fulfill

\[
\langle V''_i^* | U'_i \rangle = \left(1 + V_i'' U_i'\right)^{2j}
\]

and the overcompleteness relation

\[
\frac{2j+1}{\pi} \int \frac{d^2U'_i}{(1 + U''_i U'_i)^{2j+2}} |U'_i\rangle \langle U'_i| = 1
\]

holds. Here \( d^2U'_i \) is a shorthand for \( d\text{Re}U'_id\text{Im}U'_i \).

The asymptotic expression for the propagator in the semiclassical limit \( \hbar \to 0, \quad J^2 = \hbar^2 j (j + 1) = \text{const} \), is derived in [15] by slicing \( t \) into small intervals. This
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yields a Feynman path integral expression in which the dynamics in the short intervals is glued together by stationary phase. Here we give the result in a slightly reformulated version as compared to [14]. As derived there, the classical dynamics is determined by the equations

\[ \dot{U}_i = -\frac{i}{2J_{\text{class}}} (1 + U_i V_i)^2 \frac{\partial H}{\partial V_i}, \quad \dot{V}_i = \frac{i}{2J_{\text{class}}} (1 + U_i V_i)^2 \frac{\partial H}{\partial U_i}, \]  

(6)

where \( J_{\text{class}} \equiv \hbar (j + 1/2) \approx \sqrt{\hbar^2 j (j + 1)} \). In contrast to [14], the classical Hamilton function \( H(U, V) \) is obtained from the operator \( \hat{H}(\hat{J}_1, \ldots, \hat{J}_N) \) by the “naive” semiclassical substitution

\[ J_i \rightarrow J_{i, \text{class}} = J_{i, \text{class}} n_i. \]  

(7)

on which we elaborate more in the next subsection. Here \( n_i \) stands for the unit vector with the spherical angles \( \theta_i, \phi_i \). Expressing the latter in terms of \( U_i, V_i \) according to

\[ U_i = e^{-i\phi_i} \cot \frac{\theta_i}{2}, \quad V_i = e^{i\phi_i} \cot \frac{\theta_i}{2}, \]  

(8)

we get the explicit substitution rules,

\[ J_{i,1} \rightarrow J_{i,1} n_{i,1} = J_{i, \text{class}} \frac{U_i + V_i}{U_i V_i + 1}, \]

\[ J_{i,2} \rightarrow J_{i,2} n_{i,2} = J_{i, \text{class}} \frac{V_i - U_i}{i(U_i V_i + 1)}, \]

\[ J_{i,3} \rightarrow J_{i,3} n_{i,3} = J_{i, \text{class}} \frac{U_i V_i - 1}{U_i V_i + 1}. \]  

(9)

The asymptotic expression for the propagator is then

\[ K(U', V'', t) = \sum_{\gamma} \det^{1/2} \left( \frac{i}{2J_{\text{class}}} \frac{\partial^2 S_\gamma}{\partial U' \partial V''} \right) e^{iS_\gamma / \hbar}. \]  

(10)

The sum runs over all trajectories \( \gamma \) determined by Eq. (9) with the boundary conditions \( U(0) = U' \) and \( V(t) = V'' \). The quantity \( S_\gamma \) is the classical action

\[ S_\gamma(U', V'', t) = -iJ_{\text{class}} \sum_{i=1}^N \left[ \ln(1 + V_i'' U_i') + \ln(1 + V_i'' U_i') \right] \]

\[ - \int_0^t dt' \left[ iJ_{\text{class}} \sum_{i=1}^N \frac{\dot{V}_i U_i - V_i \dot{U}_i}{(1 + U_i V_i)^2} + H \right]. \]  

(11)

which solves the Hamilton Jacobi equations

\[ i \frac{\partial S_\gamma}{\partial V_i''} = \frac{2J_{\text{class}} V_i''}{1 + U_i'' V_i''}, \quad i \frac{\partial S_\gamma}{\partial U_i'} = \frac{2J_{\text{class}} V_i'}{1 + U_i' V_i'}. \]  

(12)

As \( U_i \) is mostly not equal to \( V_i^* \) the trajectory on the unit sphere \( \theta_i = \theta_i(t), \phi_i = \phi_i(t) \) is, according to (8), complex. This is natural since arbitrarily chosen initial \( U' \) and final \( V'' \) points are not connected by a classical trajectory at time \( t \). Indeed, the system of \( N \) spins has \( N \) degrees of freedom in the classical limit, implying that a real trajectory is
fixed by $2N$, not $4N$, real parameters. The Hamilton function and the action are then complex and the propagator is exponentially small. On the other hand, for classical trajectories which solve (6) we must have $U_i = V_i^*$ such that the solution of (6) must additionally obey $U_i(t) = V_i''$ and $U_i'(0) = V_i^*(0)$. Here the factor of $\hbar/2$ in the definition of $J_{\text{class}}$ becomes essential, otherwise an inadmissible error $O(\hbar^0)$ will be introduced in the exponent of the propagator.

2.2. Solari-Kochetov phase

In many papers on the propagator in the coherent state representation, including [15], the Hamilton function is defined as

$$h(U, V) = \frac{\langle V^* | H | U \rangle}{\langle V^* | U \rangle}. \quad (13)$$

Compared with the “naive” $H(U, V)$, it contains non-classical additional terms, namely,

$$h(U, V) = H(U, V) + \hbar Z + O(\hbar^2), \quad (14)$$

with

$$Z = \frac{1}{4 J_{\text{class}}} \sum_{i=1}^{N} (1 + U_i V_i)^2 \frac{\partial^2 H}{\partial U_i \partial V_i}. \quad (15)$$

If $h(U, V)$ is chosen as the Hamilton function the spurious contribution of $\hbar Z$ to the classical action needs to be compensated by the so called Solari-Kochetov (SK) correction phase [25],

$$\Delta \Phi_{SK} = \int_0^t Z dt'. \quad (16)$$

Relations equivalent to (14) formulated as the connection between the $Q$-representation and the Weyl symbol, were established for the translational Hamiltonians in [26] and for the spin Hamiltonians in [16, 27].

In the remainder of this subsection we give an elementary proof of the relation (14) by induction. To simplify the notation we restrict ourselves to $N = 1$. Compare the Hamilton functions $h(U, V) = \langle V^* | H | U \rangle / \langle V^* | U \rangle$ and

$$\tilde{h}(U, V) = \frac{\langle V^* | \tilde{H} | U \rangle}{\langle V^* | U \rangle}. \quad (17)$$

with the spin Hamiltonian $\tilde{H} = (J_m H + H J_m)/2$ containing an additional spin operator $J_m$, with fixed but arbitrary $m = 1, 2, 3$. The relations how angular momentum operators act on the coherent states [3] (see [28], Eqs. (4.1)-(4.3))

$$J_3 |U\rangle = \hbar \left( \frac{d}{dU} - j \right) |U\rangle,$$

$$J_- |U\rangle = \hbar \left( 2jU - U^2 \frac{d}{dU} \right) |U\rangle,$$

$$J_+ |U\rangle = \hbar \frac{d}{dU} |U\rangle.$$
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show that \( \langle V^* | \hat{H} | U \rangle \) can be obtained from \( \langle V^* | \mathcal{H} | U \rangle \) as a combination of its derivatives by \( U \) and \( V \). Combining the result with \( \langle V^* | U \rangle \) from (14) we derive the exact relation between the Hamiltonians (13) and (17)

\[
\tilde{h} = h j n_m h + \frac{\hbar}{2} \mathcal{R}_m h, \quad m = 1, 2, 3,
\]

with the differential operator

\[
\mathcal{R}_1 = \frac{1 - U^2}{2} \frac{\partial}{\partial U} + \frac{1 - V^2}{2} \frac{\partial}{\partial V},
\]

\[
\mathcal{R}_2 = \frac{1 + U^2}{2i} \frac{\partial}{\partial U} - \frac{1 + V^2}{2i} \frac{\partial}{\partial V},
\]

\[
\mathcal{R}_3 = V \frac{\partial}{\partial V} + U \frac{\partial}{\partial U}.
\]

acting on the Hamiltonian (13). The functions \( n_m(U, V) \) are defined in Eq. (9). Next we expand \( h \) and \( \tilde{h} \) in (18) with respect to \( \hbar \) for \( \hbar \to 0 \)

\[
h = h_0 \left( 1 + \frac{\hbar}{J_{\text{class}}} W + \ldots \right), \quad \tilde{h} = \tilde{h}_0 \left( 1 + \frac{\hbar}{J_{\text{class}}} \tilde{W} + \ldots \right),
\]

substitute \( \hbar j = J_{\text{class}} - \frac{\hbar}{2} \) and compare terms of the same order in \( \hbar \). The zeroth order yields the “naive” classical substitution,

\[
\tilde{h}_0 = J_{\text{class}} n_m h_0
\]

while the next order gives,

\[
\tilde{W} = W - \frac{1}{2} + \frac{1}{2n_m} \mathcal{R}_m \ln h_0, \quad m = 1, 2, 3.
\]

Now consider the quantities \( Z \) calculated using \( h_0 \) instead of \( H \) in (15) and analogously \( \tilde{Z} \) calculated using \( \tilde{h}_0 \). After defining \( W_{SK} \) and \( \tilde{W}_{SK} \) by

\[
Z \equiv h_0 \frac{\hbar}{J_{\text{class}}} W_{SK}, \quad \tilde{Z} \equiv \tilde{h}_0 \frac{\hbar}{J_{\text{class}}} \tilde{W}_{SK},
\]

the relation between \( W_{SK} \) and \( \tilde{W}_{SK} \) follows from Eqs. (15), (19),

\[
\tilde{W}_{SK} = W_{SK} + \frac{(1 + UV)^2}{4} \left( \frac{1}{n_m} \frac{\partial^2 n_m}{\partial U \partial V} + \frac{\partial \ln n_m \partial \ln h_0}{\partial U \partial V} + \frac{\partial \ln n_m \partial \ln h_0}{\partial V \partial U} \right).
\]

It is easy to check that after insertion of the explicit \( n_m \) from Eq. (9) the last relation becomes identical to Eq. (20).

Starting from \( \mathcal{H} = 1 \) when \( W = 0 \) and \( W_{SK} = 0 \) trivially coincide we can build any spin Hamiltonian by consecutive \( \mathcal{H} \to \tilde{\mathcal{H}} \) steps each time changing \( W \) and \( W_{SK} \) by the same amount. Therefore, for all spin Hamiltonians we have \( W = W_{SK} \) and the term \( Z \) in Eq. (14) is given by Eq. (15). The SK correction thus indeed cancels the non-classical terms in \( h(U, V) \) resulting in the “naive” Hamilton function \( H(U, V) \). Importantly, ordering of the angular momentum operators in the spin Hamiltonian \( \mathcal{H} \) is semiclassically insignificant as long as it is Hermitian and has real coefficients since various orderings differ then at most by \( O(\hbar^2) \).
3. Trace formula

The aim is to derive an expression in terms of a sum over classical orbits for the leading fluctuating part \( d_{osc}(E) \) of the density of states starting from the propagator introduced in the last section. In subsection 3.1 we give the density of states as multiple integral of the propagator. To perform these integrals within saddle point approximation we introduce canonical deviations from the saddle points in subsection 3.2. In subsection 3.3 we rotate the coordinate system such that the integral becomes especially simple. Finally, we give the resulting expression for \( d_{osc}(E) \) in subsection 3.4.

3.1. Trace of the propagator as a periodic orbit sum

The density of states \( d(E) \) is obtained from the propagator by

\[
 d(E) = -\frac{1}{\pi} \text{Im} \left[ \frac{1}{i\hbar} \int_0^\infty dt \text{Tr} K(t) e^{iEt/\hbar} \right].
\]  

(22)

The density \( d(E) \) splits into a mean and an oscillating part. The mean part can be related to orbits with zero period in (10). However, we will concentrate in this section on orbits with nonzero period and thus on the oscillating part of the density of states \( d_{osc}(E) \). We begin with computing the trace of the propagator,

\[
 \text{Tr} K(t) = \left( \frac{2J_{\text{class}}}{\pi \hbar} \right)^N \int_{-\infty}^{\infty} \left( \prod_{i=1}^N \frac{d^2U_i'}{1 + |U_i'|^2} \right)^{2j+2} K(U', V'', t) \bigg|_{V''=(U')^*}. 
\]  

(23)

Here \( V'' \) is a complex conjugate of \( U' \), as the trajectories are closed. Inserting the expression (10) in the last equation, we obtain a sum over closed classical trajectories \( \gamma \) from \( U' \) to \( (V'')^* = U' \) with duration \( t \). Concentrating on one element of the sum, which we write as

\[
 [\text{Tr} K(t)]_{\gamma} = \left( \frac{i 2J_{\text{class}}}{\pi^2 \hbar^2} \right)^{N/2} \int_{-\infty}^{\infty} \left( \prod_{i=1}^N \frac{d^2U_i'}{1 + |U_i'|^2} \right) \left. \det^{1/2} \left( \frac{\partial^2 S_{\gamma}}{\partial U_i \partial V''} \right) \right|_{V''=(U')^*} e^{iF_{\gamma}/\hbar},
\]  

(24)

we perform the integrals via saddle point approximation by computing the stationary points of

\[
 F_{\gamma}(U', V'', t) \equiv S_{\gamma}(U', V'', t) + 2iJ_{\text{class}} \sum_{i=1}^N \ln(1 + U_i' V''_i).
\]  

(25)

Together with Eq. (12) we find the conditions \( V_i' = V''_i \) and \( U_i' = U''_i \), i.e. a periodic orbit with the coordinates \( U' = s \) and \( V'' = s^* \). Below the subscript \( \gamma \) of \( F \) is suppressed. We note that on the periodic orbit \( \gamma \) all logarithms in \( F(s, s^*, t) \) cancel and \( F(s, s^*, t) \) does not depend on the concrete choice of the initial and final point \( s \) along \( \gamma \). Thus, on \( \gamma \)

\[
 S(t) = -\int_0^t dt' \left[ iJ_{\text{class}} \sum_{i=1}^N \frac{\dot{V}_i U_i - V_i \dot{U}_i}{1 + U_i V_i} + H \right]
\]  

(26)

equals \( F(s, s^*, t) \).
3.2. Canonical variables for small deviations

In order to perform the integrals in Eq. (24) by saddle point approximation, we consider the motion in the vicinity of the saddle point $s$ described by small deviations $\delta U = U - s$ and $\delta V = \delta U^* = V - s^*$. However, we prefer to use deviations that fulfill canonical equations, but are no longer complex conjugate to each other. As shown in Appendix A, they are given by

$$\delta \tilde{U} = B \delta U, \quad \delta \tilde{V} = \delta V$$

where $B$ is the diagonal matrix

$$B = \text{diag} \left( \frac{2i J_{\text{class}}}{1 + |s_1|^2}, \ldots, \frac{2i J_{\text{class}}}{1 + |s_N|^2} \right).$$

Next we introduce the $2N$-component vector $\delta \tilde{v} = (\delta \tilde{U}', \delta \tilde{V}'^*)$, where primes again refer to initial and double primes to final deviations, express $F(U', V'', t)$ in terms of $\delta \tilde{U}', \delta \tilde{V}''$ and expand around the point $s$ of the periodic orbit up to second order

$$F(U', V'', t) \approx S(t) + \frac{1}{2} \delta \tilde{v}^T H_F \delta \tilde{v}. \quad (27)$$

Here $H_F$ is the $2N \times 2N$ Hessian matrix containing the second derivatives of $F(s + B^{-1} \delta \tilde{U}', s^* + \delta \tilde{V}'^*)$ with respect to $\delta \tilde{U}'$ and $\delta \tilde{V}''$. The analogous expansion can be done for the action $S(U', V'', t)$. Between the Hessians of $F$ and $S$ the relation

$$H_F = H_S + \begin{pmatrix} A & 1_N \\ 1_N & D \end{pmatrix} \quad (28)$$

holds with the $N \times N$ diagonal matrices

$$D = -\text{diag} \left( \frac{2i J_{\text{class}} s_1^2}{1 + |s_1|^2}, \ldots, \frac{2i J_{\text{class}} s_N^2}{1 + |s_N|^2} \right), \quad A = -B^{-2} D^* \quad (29)$$

The complex $2N \times 2N$ monodromy matrix $M$ consisting of the four $N \times N$ blocks $M_{aa}$, $M_{ab}$, $M_{ba}$ and $M_{bb}$ relates the initial and final deviations,

$$\begin{pmatrix} \delta \tilde{U}'' \\ \delta \tilde{V}'' \end{pmatrix} = \begin{pmatrix} M_{aa} & M_{ab} \\ M_{ba} & M_{bb} \end{pmatrix} \begin{pmatrix} \delta \tilde{U}' \\ \delta \tilde{V}' \end{pmatrix} \quad (30)$$

it is symplectic because the deviations obey canonical equations. Variation of (12) with respect to $U'$, $V'$, $U''$ and $V''$ yields

$$\begin{pmatrix} H_S + \begin{pmatrix} A & 0 \\ 0 & D \end{pmatrix} \end{pmatrix} \begin{pmatrix} \delta \tilde{U}' \\ \delta \tilde{V}'' \end{pmatrix} = -\begin{pmatrix} 1_N & 0 \\ 0 & 1_N \end{pmatrix} \begin{pmatrix} \delta \tilde{U}'' \\ \delta \tilde{V}' \end{pmatrix} \quad (31)$$

see the analogous relation for the non-canonical variables in (13). By partially inverting (30) such that it takes the form (31), $H_S$ is expressed in terms of the monodromy matrix

$$H_S = \begin{pmatrix} M_{bb}^{-1} M_{ba} - A & -M_{bb}^{-1} \\ M_{ab} M_{bb}^{-1} M_{ba} - M_{aa} & -M_{ab} M_{bb} - D \end{pmatrix} \quad (32)$$

yielding for $H_F$

$$H_F = \begin{pmatrix} H_{aa} & H_{ab} \\ H_{ba} & H_{bb} \end{pmatrix} = \begin{pmatrix} M_{bb}^{-1} M_{ba} & 1_N - M_{bb}^{-1} \\ 1_N + M_{ab} M_{bb}^{-1} M_{ba} - M_{aa} & -M_{ab} M_{bb}^{-1} \end{pmatrix}. \quad (33)$$
The symmetry of the Hessians can be checked using the symplectic property of $M$. In the sequel, “the three-determinants-identity”

$$\det M_{bb} \det H_F = \det(M - I_{2N}) \quad (34)$$

will be important. It is valid for any symplectic matrix $M$ with the subblock $M_{bb}$ and the symmetric matrix $H_F(M)$ connected with $M$ via (33). Although we can hardly believe that it is new, we could not find it in the literature and give the proof in Appendix B.

Equation (32) shows that the matrix of the second mixed derivatives of the action and its determinant are related to the monodromy matrix as,

$$\frac{\partial^2 S}{\partial U' \partial \bar{V}''} = B \frac{\partial^2 S}{\partial \bar{U}' \partial V''} = -BM_{bb}^{-1},$$

$$\det \frac{\partial^2 S}{\partial U' \partial \bar{V}''} = \frac{\det B}{\det(-M_{bb})}. \quad (35)$$

The contribution to the integral Eq. (24) of the vicinity of the point $s$ can be calculated using the real and imaginary parts of $\delta \bar{U}'$ as the integration variables with the Jacobian $1/\det B$.

Taking into account that

$$\prod_{i=1}^N \frac{1}{1 + |U'_i|^2} \approx \sqrt{\frac{\det B}{(2iJ_{\text{class}})^N}} \quad (36)$$

and collecting all $B$-dependent terms in Eq. (24) we obtain from Eq. (24),

$$[\text{Tr} K(t)]_\gamma = \left(\frac{1}{\pi \hbar}\right)^N \det^{-1/2}(-M_{bb}) e^{iS(t)/\hbar} \times \int_{-\infty}^{\infty} \prod_{i=1}^N d^2 \delta \bar{U}'_i \frac{1}{\det B} e^{i\bar{\delta} \bar{\delta}^T H_F \delta \bar{\delta}/2\hbar}. \quad (37)$$

The action $S(U', V'', t)$ does not change under the shift along the orbit and as a result the monodromy matrix has a double degenerate eigenvalue 1 while $H_F$ possesses a zero eigenvalue (see (34)). To get rid of it, we slightly perturb the problem, say, replacing $H_F$ for the moment by $H_\epsilon_F = H_F + \epsilon 1_{2N}$ with $\epsilon > 0$ and take the limit $\epsilon \to 0$ at the end. By inverting relation (33)

$$M = \left(\begin{array}{ccc} 1_N - H_{ab}^T & -H_{bb}Z - H_{bb}Z & -H_{bb}Z \\ ZH_{aa} & Z \end{array}\right) \quad (38)$$

with $Z \equiv (1_N - H_{ab})^{-1}$, we understand that this change preserves the symplectic property of the corresponding monodromy matrix $M^\epsilon$. The eigenvalue 1 is replaced in $M^\epsilon$ by a doublet with the splitting $\propto \sqrt{\epsilon}$.

Now the Gaussian integral in Eq. (37) can be performed. Remembering that the two parts of the vector $\delta \bar{v}$ are related as $\delta \bar{V}'' = B^{-1} \delta \bar{U}'$ we have,

$$\int_{-\infty}^{\infty} \prod_{i=1}^N d^2 \delta \bar{U}'_i e^{i\bar{\delta} \bar{\delta}^T H_\epsilon F \delta \bar{\delta}/2\hbar} = \frac{\pi^N \det B}{(-i)^N \sqrt{\det H_\epsilon F}}. \quad (39)$$

The integral (37) is thus obtained as const. $[\det (-M_{bb}) \det H_\epsilon F]^{-1/2}$. 

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3.3. Generalized eigensystem of the monodromy matrix

At the current stage it is unclear how to perform the limit $\epsilon \to 0$, therefore we introduce a system of variables for the deviations where $M$ is almost diagonal. We consider a linear symplectic transformation $\delta \mathbf{v} = W \delta \mathbf{x}$ introducing $2N$ real canonical variables $\delta \mathbf{x} = (\delta \mathbf{q}, \delta \mathbf{p})^T$ with the canonically conjugate

$$\delta \mathbf{q} = (\delta t, \delta \xi)^T, \quad \delta \mathbf{p} = (\delta E, \delta \pi)^T.$$ (40)

Here $\delta t$ is the time variation defining the shift along the direction of motion, $\delta E$ the variation of energy leading to the shift to a point of an infinitely close periodic orbit in the energy shell $H = E + \delta E$; the $N - 1$-componental $\delta \xi$ and $\delta \pi$ denote the shifts in the direction of the stable and unstable eigenvectors of the monodromy matrix corresponding to the eigenvalues $\Lambda_n$ with $|\Lambda_n| < 1$, and $1/\Lambda_n$, respectively, $n = 1, \ldots, N - 1$. For simplicity we assume that the periodic orbit is unstable. In these coordinates the monodromy matrix reads

$$m = \begin{pmatrix} m_{aa} & m_{ab} \\ 0_N & m_{bb} \end{pmatrix},$$ (41)

where the $N \times N$ blocks are diagonal matrices,

$$m_{aa} = \text{diag} \left(1, \Lambda_1, \ldots, \Lambda_{N-1}\right),$$

$$m_{bb} = \text{diag} \left(1, 1/\Lambda_1, \ldots, 1/\Lambda_{N-1}\right),$$

$$m_{ab} = \text{diag} \left(-k, 0, \ldots, 0\right).$$

It has a single non-zero off-diagonal element $-k$. One of the two eigenvalues equal to unity is associated with $\delta t$ and corresponds to the eigenvector tangent to the orbit in the phase space. The other one is connected with $\delta E$; in the assumption $k \neq 0$, it corresponds not to an eigenvector but to an associated eigenvector of the matrix $m$ which is then not diagonalizable.

To find $k$ we consider the change $T \to T + \delta T$ of the orbit period caused by the change of energy. After the time $T$ the point traveling along the infinitely close periodic orbit with the energy $E + \delta E$ will either not yet return to the initial position if $\delta T > 0$, or overrun it if $\delta T < 0$. Consequently after the time $T$ the energy shift $\delta E$ leads to the shift along the orbit described by $\delta t = -\delta T = -(dT/dE) \delta E$ such that

$$k = \frac{dT}{dE}.$$ (41)

The transformed Hessian $h_F \equiv H_F(m)$ consists of the subblocks,

$$(h_F)_{aa} = 0_N, \quad (h_F)_{bb} = \text{diag} \left(k, 0, \ldots, 0\right),$$

$$(h_F)_{ab} = (h_F)_{ba} = \text{diag} \left(0, 1 - \Lambda_1, \ldots, 1 - \Lambda_{N-1}\right).$$

Let $h_F^\epsilon$ be the Hessian resulting from the monodromy matrix $m^\epsilon = WM^\epsilon W^{-1}$ converging to $h_F$ for $\epsilon \to 0$. According to the three-determinants-relation the product $[\det(-M_{bb}) \det h_F^\epsilon]^{-1/2}$ is canonically invariant and can be replaced by $[\det(-m_{bb}^\epsilon) \det h_F^\epsilon]^{-1/2}$. Next the factor $(\det h_F^\epsilon)^{-1/2}$ can be replaced by a Gaussian
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integral in the coordinates $\delta x$. Now the limit $\epsilon \to 0$ can be performed. Collecting the prefactors we obtain,

$$[\text{Tr}K(t)]_\gamma \sim \left(\frac{1}{i\pi\hbar}\right)^N \frac{e^{iS_\gamma/\hbar}}{\det^{1/2}(-m_{bb})} \int_0^t \! \! d\delta t \int_{-\infty}^{\infty} \! \! d\delta E d\delta \xi d\delta \pi \exp \frac{i\delta x^T h_F \delta x}{2\hbar}. \quad (42)$$

The inner integrals are Gaussian, and the result of integration does not depend on the positions $s$ on the orbit, i.e., on the time variable. Therefore the integral with respect to $\delta t$ yields the primitive period of the orbit $t_P^\gamma = t/r_\gamma$, where $r_\gamma$ stands for the number of repetitions of the orbit $\gamma$. The Gaussian integral with respect to $\delta E$ brings about the factor $1/\sqrt{k}$.

### 3.4. Semiclassical expressions for the trace of the propagator and the density of states

Finally we obtain for the trace of the propagator in the semiclassical limit

$$\text{Tr}K(t) \sim \frac{1}{\sqrt{-2i\pi\hbar k}} \sum_\gamma \frac{t_P^\gamma}{\sqrt{|\det(m_{\gamma}^{\text{red}} - 1)|}} \exp \left[ i \left( \frac{S_\gamma(t)}{\hbar} + G_\gamma(t) \right) \right]. \quad (43)$$

with the sum running over all periodic orbits $\gamma$ of duration $t$. Here the reduced monodromy matrix $m_{\gamma}^{\text{red}}$ is obtained from the matrix $m_\gamma$ of the orbit $\gamma$ by omitting the directions related to variations of $\delta t$ and $\delta E$. It is obtained from combining the result of the Gaussian integrals in Eq. (42) with respect to $\xi$ and $\pi$ with the prefactor $\det^{-1/2}(-m_{bb})$. The symbol $G_\gamma(t)$ stands for the Maslov phase resulting from the saddle point integrations.

The final Fourier transform from the time to the energy domain in Eq. (22) yields the Gutzwiller sum over periodic orbits $\gamma'$ at energy $E$ which extends the result of [18] to several interacting spins,

$$d_{\text{osc}}(E) \sim \frac{1}{\pi\hbar} \sum_{\gamma'} \frac{t_P^\gamma}{\sqrt{|\det(m_{\gamma'}^{\text{red}} - 1)|}} \cos \left[ \frac{S_{\gamma'}(E)}{\hbar} + G_{\gamma'}(E) \right] \quad (44)$$

where $S_{\gamma'}(E)$ is the Legendre transform of the action $S_{\gamma'}(t)$ and $G_{\gamma'}(E)$ the Maslov phase.

### 4. Trace formula for periodically driven systems

The dynamics in periodically driven systems is governed by an explicitly time dependent Hamiltonian, thus the energy is no longer conserved. The conserved quantity in the quantum system is in this case the quasienergy, i.e. the eigenphase of the Floquet (one period time evolution) operator. Prominent examples of periodically driven systems are kicked maps like the kicked rotor or the kicked top in the one particle domain, see for example [29] for an overview, or the kicked Ising chain [30, 31] that serves as a model system to simulate effects in many particle systems.

To obtain the trace formula for the density of eigenphases of the quantum system, one starts from the time evolution operator for the period of driving $t_0$. Its semiclassical
expression is again of the form (10). In contrast to the last section the monodromy matrix for a fully chaotic system does not possess eigenvalues equal to one as in general energy is not conserved and a $\delta t$-translation does not leave the orbit invariant. Thus, no special action to separate these directions is needed when evaluating the Gaussian integral resulting from the saddle point approximation in (24).

Performing this integral and combining the result with the prefactor of the exponential in (10) and the factor $\prod_{i=1}^{N} \frac{1}{(1 + |U_i'|^2)^{-1}}$ resulting from the trace integrals, we obtain for the trace of the propagator at time $t = nt_0$ with $n \in \mathbb{N}$ in the limit $\hbar \to 0$

$$\text{Tr}K(t) \sim \sum_{\gamma} \frac{n^P_{\gamma}}{\sqrt{\text{det}(M_{\gamma} - 1)}} \exp \left[i \left( \frac{S_{\gamma}(t)}{\hbar} + G_{\gamma}(t) \right) \right]$$

with the sum running over all periodic orbits $\gamma$ of duration $t$. Here $n^P_{\gamma} \in \mathbb{N}$ is the discrete primitive period of the orbit, that means $n^P_{\gamma} = n/r_{\gamma}$ for an orbit that repeats a shorter periodic orbit $r$ times and $M_{\gamma}$ the $2N \times 2N$-dimensional monodromy matrix for a system consisting of $N$ spins. Other quantities in the last equation have the same meaning as in Eq. (43). We note that the expression given in [29] for particles is of the same form as the one in Eq. (45) for spins. Given that the variables $U_i, V_i$ are not canonically conjugate and that the trace (3) involves an additional factor $\prod_{i=1}^{N} (1 + |U_i'|^2)^{-2j-2}$, this is a nontrivial result.

In order to obtain a periodic orbit expansion for the density of eigenphases $\rho(\theta)$, the resulting expression for the trace (45) needs to be inserted in the following expression for the eigenphases $\theta_n$ for a $N$ particle spin system [29]

$$\rho(\theta) = \frac{1}{(2j)^N} \sum_{n=1}^{(2j)^N} \delta(\theta - \theta_n) = \frac{1}{2\pi} + \frac{1}{(2j)^N \pi} \text{Re} \sum_{n=1}^{\infty} \frac{e^{in\theta}}{nt_0}. \quad (46)$$

5. Conclusions

We studied a spin chain consisting of $N$ spin-$j$ particles. Currently there is a considerable interest in such systems both from theoretical and from experimental side. The goal is to investigate the properties of many particle systems, which are still small enough that finite size effects are important. For such a system we derived a trace formula connecting the classical dynamics obtained in the limit of large $j$ and the quantum energy levels for time-continuous as well as for periodically driven dynamics.

Similar to the trace formula for particles it can be used to predict the properties of the quantum spectra of the spin chains following from their classical dynamics. It can work also in the opposite direction and give information on the particular classical orbits responsible for the non-universal features of the quantum spectra. We restricted ourselves to distinguishable spins but it would be interesting as well to consider the non-distinguishable ones and their coupling to the bosonic particles.
Appendix A. Canonical Variables

We consider deviations $\delta U$ and $\delta V$ from a trajectory obtained as a solution of the equation of motion \( \dot{U} = \frac{\partial H}{\partial V} \). Such deviations fulfill up to linear order in the deviations the equations

\[
\begin{align*}
\delta \dot{U}_i &= \frac{\partial H}{\partial V_i} \left( \frac{\partial k_i}{\partial U_i} \delta U_i + \frac{\partial k_i}{\partial V_i} \delta V_i \right) + k_i \left( \frac{\partial^2 H}{\partial V_i \partial V_k} \delta U_k + \frac{\partial^2 H}{\partial U_k \partial V_i} \delta V_k \right), \\
\delta \dot{V}_i &= - \frac{\partial H}{\partial U_i} \left( \frac{\partial k_i}{\partial U_i} \delta U_i + \frac{\partial k_i}{\partial V_i} \delta V_i \right) - k_i \left( \frac{\partial^2 H}{\partial U_i \partial U_k} \delta U_k + \frac{\partial^2 H}{\partial U_i \partial V_k} \delta V_k \right) \quad (A.1)
\end{align*}
\]

with

\[
k_i = \frac{(1 + U_i V_i)^2}{2iJ_{\text{class}}} \quad (A.2)
\]

and the unperturbed trajectory determined by the complex coordinates $U_i$ and $V_i$ for the $i$-th spin. The aim of this appendix is to show that the variables $\delta \tilde{U}$ and $\delta \tilde{V}$ defined by

\[
\delta U_i = k_i \delta \tilde{U}_i, \quad \delta V_i = \delta \tilde{V}_i \quad (A.3)
\]

are canonical. This can be done by noting that they fulfill the canonical equations of motion

\[
\begin{align*}
\delta \dot{\tilde{U}}_i &= \frac{\partial \tilde{H}}{\partial \delta \tilde{V}_i}, \quad \delta \dot{\tilde{V}}_i &= - \frac{\partial \tilde{H}}{\partial \delta \tilde{U}_i} \quad (A.4)
\end{align*}
\]

with the Hamiltonian $\tilde{H} \left( \delta \tilde{U}, \delta \tilde{V} \right)$

\[
\begin{align*}
\tilde{H} &= \sum_{k,j=1}^{N} \left( \frac{1}{2} \frac{\partial^2 H}{\partial U_k \partial U_j} k_j k_j \delta \tilde{U}_k \delta \tilde{U}_j + \frac{\partial H}{\partial U_j} k_j \delta \tilde{U}_j \delta \tilde{V}_k + \frac{1}{2} \frac{\partial^2 H}{\partial V_k \partial V_j} \delta \tilde{V}_k \delta \tilde{V}_j \right) \\
+ \sum_{j=1}^{N} \frac{1}{1 + U_j V_j} \left( \frac{\partial H}{\partial V_j} U_j \delta \tilde{V}_j^2 + 2 \frac{\partial H}{\partial U_j} U_j k_j \delta \tilde{U}_j \delta \tilde{V}_j + \frac{\partial H}{\partial U_j} V_j k_j^2 \delta \tilde{U}_j^2 \right) \quad (A.5)
\end{align*}
\]

Appendix B. The three-determinants-relation

Here we give the proof of the identity \( (34) \). Its left hand side can be obtained as determinant of the matrix

\[
H_F \left( \begin{array}{cc}
1_N & 0 \\
0 & M_{bb}
\end{array} \right) = \left( \begin{array}{cc}
M_{bb}^{-1} M_{ba} & M_{bb} - 1_N \\
1_N - M_{aa} + M_{ab} M_{bb}^{-1} M_{ba} & -M_{ab}
\end{array} \right). \quad (B.1)
\]

The right hand side of \( (34) \) can be written as

\[
det \left( M - 1_{2N} \right) = det \left( \begin{array}{cc}
M_{ba} & M_{bb} - 1_N \\
1_N - M_{aa} & -M_{ab}
\end{array} \right). \quad (B.2)
\]

The equality of \( (B.2) \) and the determinant of \( (B.1) \) becomes evident when adding the second column of Eq. \( (B.1) \) multiplied on the right by $M_{bb}^{-1} M_{ba}$ to the first column.

A direct consequence of the relation \( (34) \) is that $\det M_{bb} \det H_F$ is invariant under a symplectic transformation $M \rightarrow WMW^{-1}$. 

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