The spectral form factor for quantum graphs with spin-orbit coupling

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Abstract
We consider quantum graphs with spin-orbit couplings at the vertices. Time-reversal invariance implies that the bond S-matrix is in the orthogonal or symplectic symmetry class, depending on spin quantum number s being integer or half-integer, respectively. The periodic-orbit expansion of the spectral form factor is shown to acquire additional weights from spin rotations along orbits. We determine the spin contribution to the coefficients in an expansion of the form factor from properties of the representation of the group of spin transformations on the graph. Consistency with the Circular Orthogonal and Circular Symplectic Ensemble, respectively, of random matrices is obtained.

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1 Introduction

Since their introduction in the field of quantum chaos by Kottos and Smilansky [14, 15], quantum graphs have played an important role in efforts towards a deeper understanding of correlations in spectra of classically chaotic quantum systems. According to the conjecture of Bohigas, Giannoni, and Schmit [5], these correlations can be described by random matrix theory (RMT) [17]. Although overwhelming evidence supports this conjecture, until recently the theoretical understanding of the RMT connection remained rather poor.

Spectral two-point correlations are often measured in terms of the form factor $K(\tau)$. Its small-$\tau$ asymptotics have been the subject of recent studies, producing a considerably improved understanding of spectral correlations in terms of correlations among classical periodic orbits [21, 20, 18]. In this context quantum graphs have proven ideal models for detailed investigations into the duality between eigenvalue and periodic orbit correlations [3, 2, 1].

A guiding principle of the RMT conjecture is that symmetries of the quantum system determine the universality class of spectral correlations. Usually, the presence or absence of time-reversal invariance in quantum systems with integer or half-integer total spin is taken as an indicator whether an orthogonal, a unitary, or a symplectic universality class is appropriate. Since Berry’s pioneering semiclassical analysis of the form factor [4], however, a vast majority of investigations have concentrated on the orthogonal and the unitary case. (See [19] for exceptions where the symplectic case is considered.) Quantum graphs with spin 1/2 were introduced in [6] in the context of a realization of a Dirac operator on graphs. We demonstrated that in this way a quantum system in the symplectic universality class can be realized, and analyzed the form factor in the light of the recent developments [7].

Here we extend our previous studies of spin-orbit coupling on quantum graphs to the case of arbitrary values of the spin quantum number $s$. Since the use of Dirac operators is restricted to the case of $s = 1/2$, this extension is most conveniently performed with a Pauli operator. Starting from the case of spin zero, we introduce a spin-orbit coupling that is localized at the vertices, in terms of boundary conditions describing spin rotations at the vertices. We then continue to investigate the form factor for the spectrum of the bond $S$-matrix for a Pauli operator, following the diagrammatic method introduced in [3, 2]. We analyze the group of spin rotations on the graph generated by those at the vertices and show that properties of its irreducible representations fix the spin contribution to the form factor. In particular, it is found that a change from integer to half-integer spin induces the same transformation of the form factor as exists between the Circular Orthogonal Ensemble (COE) and Circular Symplectic Ensemble (CSE) in RMT.

This paper is organized as follows: After an introduction we recall basic facts about graphs in section 2. The construction of Pauli operators on graphs and the structure of the corresponding bond $S$-matrices is explained in section 3. The definition of the form factor and the removal of Kramers’ degeneracy is presented in section 4. Section 5 is then devoted to discussing the spin contribution to the form factor and in section 6 we evaluate the spin contribution. Group theoretic properties of representations used in the calculation
of the spin contribution are explained in an appendix.

2 Graphs

A compact graph $G$ consists of $V$ vertices connected by $B$ bonds. The topology of $G$ is encoded in the connectivity matrix $C$. This is a $V \times V$ matrix with entries

$$C_{ij} := \begin{cases} 1 & \text{if vertices } i \text{ and } j \text{ are connected}, \\ 0 & \text{otherwise}. \end{cases}$$  \hspace{1cm} (2.1)$$

The valency $v_i$ of a vertex $i$ is the number of bonds meeting in the vertex. Throughout we assume that $G$ possesses no loops so that the diagonal elements of $C$ vanish, and that any pair of vertices is connected by at most one bond. Hence $v_i = \sum_j C_{ij}$ and $2B = \sum_i v_i$. Paths on $G$ are sequences $(b_1, \ldots, b_t)$ of consecutive bonds, and periodic orbits are periodic sequences in which case $t$ is the period. We require the graph to be connected, i.e., any pair of vertices can be joined by a path.

By assigning lengths $L_b$ to bonds $b$ we turn $G$ into a metric graph. On each bond $b$ we then introduce a coordinate $x_b \in [0, L_b]$. The graph therefore becomes directed, since the coordinate on a bond $b = (ij)$ connecting the vertices $i$ and $j$ runs from $i$ to $j$. In order to avoid degeneracies in the length spectrum of periodic orbits we also demand that the lengths $L_b$ be rationally independent.

Functions $\psi = (\psi_1, \ldots, \psi_B)$ on the graph can now be defined in terms of functions $\psi_b : [0, L_b] \to \mathbb{C}$ on the bonds. The quantisation on graphs finally requires to introduce the Hilbert space

$$L^2(G) = \bigoplus_{b=1}^B L^2(0, L_b).$$  \hspace{1cm} (2.2)$$

Further spaces of functions on $G$ are defined analogously. E.g., the components of $\psi \in W^{2,2}(G)$ are functions in the $L^2$-Sobolev spaces $W^{2,2}(0, L_b)$.

3 Pauli operators on graphs

Usually metric, compact graphs $G$ are quantized in terms of a suitable realization of the Laplacian on $L^2(G)$. One thus describes a point-like quantum particle moving freely along the bonds of the graph, with local interactions at the vertices. These interactions are described in terms of the boundary conditions that specify a given self-adjoint realization of the Laplacian. We will closely follow the method of Kostrykin and Schrader [13], which we briefly now recall: As a differential expression the Laplacian reads $\Delta \psi = (\psi_1', \ldots, \psi_B')$. Any self-adjoint realization of this operator can be specified in terms of two complex $2B \times 2B$ matrices $A$ and $B$, when $\text{rank}(A, B) = 2B$ and $A B^\dagger$ is hermitian. In such a case an operator core consists of $\psi \in W^{2,2}(G)$ fulfilling

$$A \psi + B \psi' = 0.$$  \hspace{1cm} (3.1)$$
Here $\psi$ denotes the vector of the $2B$ boundary values of $\psi$, whereas $\psi'$ is the corresponding vector of inward derivatives at the vertices. In order for the boundary conditions to be local, we furthermore require a block structure of the matrices $A$ and $B$, such that only boundary values at the same vertex are related through (3.1).

The spectrum of $-\Delta$ on the graph is discrete, non-negative and has no finite accumulation point. Following Kottos and Smilansky [14, 15] this spectrum can most conveniently be characterized in terms of the so-called bond S-matrix $S(k)$, where $k \in \mathbb{R}$ is such that $\lambda = k^2$ is the spectral parameter of $-\Delta$: $k^2$ is an eigenvalue, iff $k$ is a solution of

$$\det \left( I_{2B} - S(k) \right) = 0 .$$

(3.2)

The bond S-matrix is a unitary, $2B \times 2B$ matrix defined in terms of the local transition matrices $T^{(i)}(k)$ that reflect the boundary conditions at the vertex $i$ prescribed by the blocks $A^{(i)}$ and $B^{(i)}$ of $A$ and $B$, respectively,

$$T^{(i)}(k) = - \left( A^{(i)} + ik B^{(i)} \right)^{-1} \left( A^{(i)} - ik B^{(i)} \right) .$$

(3.3)

More precisely, the entries of $S(k)$, labeled by the bonds $(ij)$ connecting the vertices $i$ and $j$, read

$$S^{(ij)(lm)} = \delta_{im} T_{(ij)(lm)}^{(i)} e^{ikL_{(lm)}} .$$

(3.4)

Time reversal is implemented by complex conjugation, so that a time-reversal invariant realization of the Laplacian is obtained when $A$ and $B$ are real. This implies that besides being unitary the bond S-matrix is symmetric, and hence possesses the symmetries of the Circular Orthogonal Ensemble (COE) of RMT.

We now introduce spin-orbit coupling on quantum graphs following the non-relativistic Pauli equation. In a first step we therefore consider the Laplacian realized on $L^2(G) \otimes \mathbb{C}^{2s+1}$, where $s \in \{1/2, 1, 3/2, \ldots \}$ denotes the spin quantum number. As long as the boundary conditions are taken over from the previous case without spin, through a trivial extension of the condition (3.1) to the $2s+1$ components of the functions on each bond, no spin-orbit coupling is present. A local spin-orbit interaction at the vertices can now be introduced in a very simple way: one merely has to allow for general $2B(2s+1) \times 2B(2s+1)$ matrices $A$ and $B$, with rank($A, B$) maximal and $AB^\dagger$ hermitian, to determine boundary conditions in analogy to (3.1). Locality furthermore requires, as above, that these condition be satisfied at each vertex separately.

For a spin-$s$ system the time reversal operator $T_s$ is anti-unitary, with $T_s^2 = (-1)^{2s}$, see [22]. In the case of integer spin, requiring time-reversal invariance of the Pauli operator therefore amounts to the same condition as in the case of the Laplacian: the bond S-matrix has to be unitary and symmetric. For half-integer spin, however, time-reversal invariance implies Kramers’ degeneracy [16], i.e., a twofold degeneracy in the spectrum of the Pauli operator. Moreover, the bond S-matrix possesses the symmetries of the Circular Symplectic Ensemble (CSE), see [17, 20]. The same conditions apply for the Dirac operator on a graph, corresponding to $s = 1/2$. This case was studied in [6]. In the general case of spin $s$ one merely has to replace the SU(2) matrices $u$ that provide the spin rotations at the
vertices by their \(2s+1\)-dimensional unitary irreducible representations \(R^s(u)\). Requiring invariance of the transition matrix (3.3) under a permutation of the bonds at the vertex as in [6], this yields

\[
T^{(i)} = \begin{pmatrix}
R^s(u_1) & & \\
& \ddots & \\
& & R^s(u_{v_i})
\end{pmatrix}(X \otimes I_{2s+1})
\begin{pmatrix}
R^s(u_1)^{-1} & & \\
& \ddots & \\
& & R^s(u_{v_i})^{-1}
\end{pmatrix}.
\] (3.5)

Here \(X\) is a \(v_i \times v_i\) matrix that is required to be unitary and invariant under simultaneous permutations of columns and rows. These conditions imply that this matrix must be of the form,

\[
X = e^{i\theta} \begin{pmatrix}
q & & \cdots & & q \\
\cdots & & \ddots & & \cdots \\
q & & \cdots & & q \\
\end{pmatrix} \quad \text{with} \quad q = \frac{1 + e^{i\omega}}{v_i},
\] (3.6)

where \(\omega\) and \(\theta\) are real parameters. It is easy to see that \(\omega = \pi\) corresponds to Dirichlet boundary conditions on the bonds. The most common choice, however, is \(\omega = 0\), leading to Neumann boundary conditions [14, 15]. The bond \(S\)-matrix constructed from (3.5) and (3.6) according to (3.4) therefore yields, for fixed \(k\), the general form of a unitary matrix that may serve as an \(S\)-matrix of a quantum graph with spin-orbit coupling.

4 The form factor

The purpose of this paper is to calculate the effect of spin in one particular, commonly studied, spectral statistic of a quantum graph, the form factor. We follow the approach taken in [3, 2] and consider the form factor derived from the spectrum of the \(S\)-matrix. For the \(S\)-matrix spectrum we replace \(e^{ikL_{(ij)}}\) in (3.4) with \(e^{i\phi_{(ij)}}\). The \(B\) phases \(\phi_{(ij)}\) are random variables uniformly distributed in \([0, 2\pi]\). They define an ensemble of matrices \(S_{\phi}\) over which we average, equivalent to averaging over bond lengths. With such a replacement the \(S\)-matrix is

\[
S_{\phi}^{(ij)(kl)} := \delta_{il} \sigma_{(ij)(ki)} R^s(u_{(ij)(ki)}) e^{i\phi_{(kl)}}.
\] (4.1)

The Kronecker-delta ensures transitions only occur between bonds connected at a vertex. \(\sigma_{(ij)(ki)}\) is the \((ij), (ki)\) element of the matrix \(X\) in (3.3) and \(R^s(u_{(ij)(ki)})\) is a spin-\(s\) representation of an element of \(SU(2)\) describing the spin transformation at the vertex \(i\). According to (3.5),

\[
R^s(u_{(ij)(ki)}) = R^s(u_{(ij)}^k) R^s(u_{(ij)}^{(i)})^{-1}.
\] (4.2)

Having defined the \(S\)-matrix, the form factor is introduced as in [9]. In the case of integer spin the \(S\)-matrix generically has \(N = 2B(2s+1)\) non-degenerate eigenvalues. Thus

\[
K_{\text{orth}}(\tau_{\text{orth}}) := \frac{1}{N} \langle |\text{tr} S_{\phi} |^2 \rangle_{\phi}, \quad \tau_{\text{orth}} = \frac{t}{2B(2s+1)}.
\] (4.3)
For half-integer spin the form factor is defined after first removing Kramers’ degeneracy as explained in [8]. The $S$-matrix then has $N = B(2s + 1)$ independent eigenvalues, and

$$K_{\text{symp}}(\tau_{\text{symp}}) := \frac{1}{4N} \langle |\text{tr} S_\phi^t|^2 \rangle_\phi, \quad \tau_{\text{symp}} = \frac{t}{B(2s + 1)}. \quad (4.4)$$

We distinguish the different definitions of the form factors and parameters $\tau$ with labels corresponding to the symmetry introduced by time-reversal invariance.

Expanding the trace of $S^t$ as a sum over the set $P_t$ of periodic orbits of period $t$ yields

$$\text{tr} S_\phi^t = \sum_{p \in P_t} \frac{t}{r_p} A_p e^{i\mu_p} \text{tr} (R_s^e(d_p)) e^{i\phi_p}. \quad (4.5)$$

The periodic orbit $p$ consists of a series of subsequently visited bonds $(b_1, b_2, \ldots, b_t)$. It has associated with it the quantities

$$A_p e^{i\mu_p} := \sigma_{b_t b_{t-1}} \sigma_{b_{t-1} b_{t-2}} \cdots \sigma_{b_2 b_1},$$

$$d_p := u_{b_t b_{t-1}} u_{b_{t-1} b_{t-2}} \cdots u_{b_2 b_1},$$

$$\phi_p := \sum_{j=1}^t \phi_{b_j}. \quad (4.6)$$

The phases $\mu_p$ are such that $A_p > 0$, and $r_p$ is the repetition number of $p$. $t/r_p$ is the number of equivalent starting positions of an orbit due to cyclic permutations.

Using the periodic orbit expansion,

$$\langle |\text{tr} S_\phi^t|^2 \rangle_\phi = t^2 \sum_{p,q \in P_n} \frac{A_p A_q}{r_p r_q} e^{i(\mu_p - \mu_q)} \chi_{R^e}(d_p) \chi_{R^e}(d_q) \delta_{\phi_p, \phi_q}, \quad (4.7)$$

where we have introduced character notation for the trace of a representation, $\chi_{R^e}(d) = \text{tr} R^e(d)$. The Kronecker-delta results from averaging over the phases $\phi$. It fixes contributing terms in the double sum to pairs of orbits in which each bond is visited the same number of times. On a metric graph with rationally independent bond lengths this is equivalent to requiring the lengths of $p$ and $q$ be equal.

For comparison the form factor of a graph quantized with the Laplacian (spin-0), as studied in [3, 2], is

$$K_{\text{zero}}(\tau_{\text{zero}}) := \frac{1}{2B} \langle |\text{tr} S_\phi^t|^2 \rangle_\phi = \frac{t^2}{2B} \sum_{p,q \in P_n} \frac{A_p A_q}{r_p r_q} e^{i(\mu_p - \mu_q)} \delta_{\phi_p, \phi_q}, \quad (4.8)$$

with $\tau_{\text{zero}} = t/2B$.

It was pointed out in [11] that the power series expansions of the CSE and COE form factors are closely connected, if one performs the same substitution that leads from (4.3) to (4.4),

$$K_{\text{CSE}}(\tau) = \frac{\tau}{2} + \frac{\tau^2}{4} + \frac{\tau^3}{8} + \frac{\tau^4}{12} + \ldots,$$

$$\frac{1}{2} K_{\text{COE}} \left( \frac{\tau}{2} \right) = \frac{\tau}{2} - \frac{\tau^2}{4} + \frac{\tau^3}{8} - \frac{\tau^4}{12} + \ldots. \quad (4.9)$$
Calling \( K^m \) the term containing \( \tau^m \) the relationship may be written

\[
K^m_{\text{CSE}}(\tau) = \left( -\frac{1}{2} \right)^{m+1} K^m_{\text{COE}}(\tau).
\]  

(4.10)

According to the conjecture of Bohigas, Giannoni, and Schmit [5] in the semiclassical limit we expect the form factors of quantum graphs to correspond to those of random matrices. In particular,

\[
K^m_{\text{sympl}}(\tau) = \left( -\frac{1}{2} \right)^{m+1} K^m_{\text{orth}}(\tau).
\]  

(4.11)

It is this relation we propose to establish in quantum graphs.

5 Spin contributions to the form factor

The form factor is usually studied in the semiclassical limit which for quantum graphs corresponds to \( B \to \infty \). For small but finite \( \tau = t/N \) the limit of long orbits, \( t \to \infty \), is also required. For details see [3, 2]. In this limit the proportion of orbits \( p \) with \( r_p \neq 1 \) tends to zero and these orbits can effectively be ignored in equations (4.7) and (4.8). Following [2] the sum over orbit pairs is organized in terms of diagrams. A diagram consists of all pairs of orbits related by the same pattern of permutations of arcs between self-intersections and time-reversal of arcs. Consequently such pairs of orbits have identical phases \( \phi_p = \phi_q \).

Figures 1 and 2 provide examples of diagrams.

We define the contribution to the form factor from a specific diagram \( D \) with \( n \) self-intersections to be \( K^n_{D} \),

\[
K^n_{\text{orth}}(\tau_{\text{orth}}) := \frac{t^2}{2B(2s+1)} \sum_{(p,q) \in D_t} A_p A_q e^{i\pi(\mu_p - \mu_q)} \chi_R(d_p)\chi^*_R(d_q),
\]  

(5.1)

\[
K^n_{\text{sympl}}(\tau_{\text{sympl}}) := \frac{t^2}{4B(2s+1)} \sum_{(p,q) \in D_t} A_p A_q e^{i\pi(\mu_p - \mu_q)} \chi_R(d_p)\chi^*_R(d_q).
\]  

(5.2)

Here \( D_t \) is the set of pairs of orbits \( (p,q) \) of period \( t \) contained in \( D \).

To separate spin contributions from the sum we assume that the elements \( R(d_p) \) are chosen randomly (independent of \( p \)) from a representation \( R(\Gamma) \) of a subgroup \( \Gamma \subseteq \text{SU}(2) \). This can be achieved by selecting the matrices \( R(u_{(i)}^{(j)}) \) randomly from \( R(\Gamma) \). Then

\[
K^n_{\text{orth/sympl}}(\tau_{\text{orth/sympl}}) = \frac{\alpha_{\text{orth/sympl}}}{(2s+1)} \left( \frac{1}{|D_t|} \sum_{(p,q) \in D_t} \chi_R(d_p)\chi^*_R(d_q) \right)
\times \left( \frac{t^2}{2B} \sum_{(p,q) \in D_t} A_p A_q e^{i\pi(\mu_p - \mu_q)} \right),
\]  

(5.3)
where $\alpha_{\text{orth}} = 1$ and $\alpha_{\text{sympl}} = 1/2$. The second term in (5.3) is the contribution to the form factor of the graph with spin zero (4.8),

$$K_{\text{zero}}^{n,D}(\tau_{\text{zero}}) := \frac{t^2}{2B} \sum_{(p,q) \in D_t} A_p A_q e^{i\pi(\mu_p - \mu_q)}.$$  \hspace{1cm} (5.4)

For a finite subgroup $\Gamma$ the matrices $R(u^{(i)}_j)$ are chosen independently with uniform probability $1/|\Gamma|$, where $|\Gamma|$ is the order of the subgroup. In the semiclassical limit the number and period of periodic orbits tends to infinity. Consequently, $\frac{1}{|\Gamma|} \sum_{u^1_1 \in \Gamma} \ldots \sum_{u^t_t \in \Gamma} \chi_R(d_p) \chi^*_R(d_q) \rightarrow \frac{1}{|\Gamma|} \sum_{u^1_1 \in \Gamma} \ldots \sum_{u^t_t \in \Gamma} \chi_R(d_p) \chi^*_R(d_q).$  \hspace{1cm} (5.5)

If the subgroup $\Gamma \subseteq SU(2)$ is continuous instead of finite the sums over $\Gamma$ are replaced with integrals over the subgroup. The elements $u^{(i)}_j \in \Gamma$ are then chosen randomly with respect to Haar measure on the subgroup.

We will show in section 6 that for $R$ an irreducible representation of $\Gamma$ of dimension $2s + 1$,

$$\frac{1}{|\Gamma|^t} \sum_{u^1_1 \in \Gamma} \ldots \sum_{u^t_t \in \Gamma} \chi_R(d_p) \chi^*_R(d_q) = \left( \frac{c_R}{2s + 1} \right)^n,$$  \hspace{1cm} (5.6)

where $n$ is the number of self-intersections at which arcs of the orbit $p$ have been rearranged to produce $q$. The constant $c_R$ takes the value $c_R = 1$ if the representation $R$ is real, and $-1$ if it is quaternionic. Consequently contributions to the form factor have the form,

$$K_{\text{orth/sympl}}^{n,D}(\tau_{\text{orth/sympl}}) = \frac{\alpha_{\text{orth/sympl}}}{(2s + 1)} \left( \frac{c_R}{2s + 1} \right)^n K_{\text{zero}}^{n,D}(\tau_{\text{zero}}).$$ \hspace{1cm} (5.7)

Let us first consider integer $s$, in this case the dimension of $R$ is odd. Quaternionic representations can only occur with even dimension (see [10] section 5-5) and therefore $c_R = 1$. For integer spin we use the form factor (4.3). Hence

$$K_{\text{orth}}^{n,D} \left( \frac{t}{2B(2s + 1)} \right) = \frac{1}{(2s + 1)^{n+1}} K_{\text{zero}}^{n,D} \left( \frac{t}{2B} \right).$$ \hspace{1cm} (5.8)

Conjecturing that $K^m(\tau)$, the term in the form factor expansion containing $\tau^m$, is generated by diagrams reordered at $n = m - 1$ self intersections, we have

$$K_{\text{orth}}^{m,D}(\tau_{\text{orth}}) = K_{\text{zero}}^{m,D}(\tau_{\text{orth}}).$$ \hspace{1cm} (5.9)

Introducing any irreducible representation of spin transformations for integer spin, the terms in the expansion of the form factor are the same as those for the graph quantized with spin zero.
If we consider half-integer spin the spectrum of $\mathbb{S}_\phi$ generically is doubly degenerate and the correct formula for the form factor is (4.4), i.e.,

$$K^{n,D}_{\text{symp}} \left( \frac{t}{B(2s+1)} \right) = \frac{c_R^n}{2(2s+1)^{n+1}} K^{n,D}_{\text{zero}} \left( \frac{t}{2B} \right).$$

Again, if we conjecture that the terms in the expansion containing $\tau^m$ are generated by diagrams with $n = m - 1$ self-intersections we find

$$K^{m,D}_{\text{symp}}(\tau_{\text{symp}}) = \frac{c_R^{m-1}}{2^{m+1}} K^{m,D}_{\text{zero}}(\tau_{\text{symp}}).$$

When $R$ is an irreducible quaternionic representation, $c_R = -1$, this would establish the same relationship between the expansion of the form factor for a system with half-integer spin and the graph quantized with spin zero as exists between the expansions of $K_{\text{CSE}}(\tau)$ and $K_{\text{CSE}}(\tau)$, see (4.10).

To conclude, an example of a finite subgroup $\Gamma$ of spin transformations are Hamilton’s quaternions, $\Gamma = \{ \pm 1, \pm i \sigma_x, \pm i \sigma_y, \pm i \sigma_z \}$, where $\sigma_j$ is a Pauli matrix. $\Gamma$ is itself a two dimensional irreducible quaternionic representation corresponding to transformations of spin-1/2. In [12] spin transformations from this subgroup are applied to the cat map and CSE statistics are observed. As $\Gamma$ is both irreducible and quaternionic CSE statistics are expected even with spin transformations taken from such a small subgroup of SU(2).

6 Spin correlations

Let $d_p = u_{b_t} u_{b_{t-1}} \ldots u_{b_2} u_{b_1}$ be a product of elements of $u_{b_j} \in \Gamma$, which corresponds to a periodic orbit $p = (b_1, b_2, \ldots, b_t)$. Here $u_{(ij)} = (u_i^{(j)})^{-1} u_i^{(j)} = u_{(ji)}^{-1}$ is the element of SU(2) that transforms spin when traversing the bond $(ij)$. This labeling of elements of SU(2) with bonds simplifies calculations. Let $d_q \in \Gamma$ be obtained from $d_p$ by taking the bonds of the periodic orbit $p$ in a different order. This corresponds to permuting and inverting the elements $u_{b_j}$ appropriately.

**Theorem 1**

$$\frac{1}{|\Gamma|} \sum_{u_{b_1} \in \Gamma} \cdots \sum_{u_{b_t} \in \Gamma} \chi_R(d_p) \chi_R^*(d_q) = \left( \frac{c_R}{2s+1} \right)^n,$$

where $n$ is the number of self-intersections at which the orbit $p$ has been rearranged to produce $q$.

**Proof.** We will apply properties of group representations to calculate average values of the product of the characters of $d_p$ and $d_q$. The properties we use, together with proofs where appropriate, are given in the appendix.
To begin, if the orbit $q = p$ we have $n = 0$. In this case
\[
\frac{1}{|\Gamma|^t} \sum_{u_b \in \Gamma} \chi_R(d_p) \chi_R^*(d_p) = \frac{1}{|\Gamma|^t} \sum_{u_b \in \Gamma} \chi_R(u_{b_1} \ldots u_{b_l}) \chi_R^*(u_{b_1} \ldots u_{b_l}) = \frac{1}{|\Gamma|^t} \sum_{u \in \Gamma} \chi_R(u) \chi_R^*(u) = 1. 
\] (6.1)

The sum over $u_b \in \Gamma$ is an abbreviation for the sum over all $u_{b_1}, \ldots, u_{b_l}$. The sum was evaluated by a simple change of variables $u = u_{b_1} \ldots u_{b_l}$ and character orthogonality. The rest of the proof is inductive. We consider two cases, firstly where $p$ and $q$ differ by reversing the direction of a section of $q$, and secondly where two sections of $q$ are permuted.

1. Reordering at a single intersection.

We assume the theorem holds for two orbits $p = (\alpha, \beta, l_1, \gamma, \delta, l_2)$ and $q = (\alpha, \beta, l_3, \gamma, \delta, l_4)$. The notation follows Figure 1, showing orbit $q$; $l_j$ denotes a loop of the orbit containing an unspecified number of bonds.

![Figure 1: The two orbits $q$ and $q'$ related by a change in the order of arcs at a single self-intersection.](image)

The order and direction in which bonds are traversed in the loops may differ between $p$ and $q$. The number of self-intersections at which the orbit $q$ differs from $p$ is $n$ by assumption. We will show that the theorem also holds when applied to an orbit $q' = (\alpha, \gamma, l_3, \beta, \delta, l_4)$, where $\bar{b}$ describes the bond or loop being traversed in the opposite direction. Figure 1 shows the relationship between $q$ and $q'$. By definition $n' = n + 1$, the order of bonds in $q'$ has been changed from the order in $q$ at a single self-intersection. Using $u_b^{-1} = u_b^{-1}$ and the definition of the orbit $q'$ we find
\[
\frac{1}{|\Gamma|^t} \sum_{u_b \in \Gamma} \chi_R(d_p) \chi_R^*(d_{q'}) = \frac{1}{|\Gamma|^t} \sum_{u_b \in \Gamma} \chi_R(u_{l_2} u_{\delta} u_{\gamma} u_{l_1} u_{\beta} u_{\alpha}) \chi_R^*(u_{l_4} u_{\delta} u_{\gamma}^{-1} u_{l_3}^{-1} u_{\gamma}^{-1} u_{\alpha}) = \frac{1}{|\Gamma|^t} \sum_{u_b \in \Gamma} \chi_R(u_{l_2} u_{y} u_{l_1} u_x) \chi_R^*(u_{l_4} u_{y} u_{l_3}^{-1} u_{x}) . 
\] (6.2)

Here $u_{l_j}$ is the product of elements $u_b$ picked up along the loop $l_j$, and $u_x = u_{\beta} u_{\alpha}, u_y = u_{\delta} u_{\gamma}$, $u_z = u_{\gamma}^{-1} u_{\beta}^{-1}$. Corollary 1 (see the appendix) can now be used to evaluate the sum on $u_z$, 
\[
\frac{1}{|\Gamma|^t} \sum_{u_b \in \Gamma} \chi_R(d_p) \chi_R^*(d_{q'}) = \left( \frac{c_R}{2s+1} \right) \frac{1}{|\Gamma|^t} \sum_{u \in \Gamma} \chi_R(u_{l_2} u_{y} u_{l_1} u_x) \chi_R^*(u_{l_4} u_{y} u_{l_3} u_x) . 
\] (6.3)
Returning to the original variables we find,
\[
\frac{1}{|\Gamma|} \sum_{u_b \in \Gamma} \chi_R(d_p) \chi_R^*(d_q) = \frac{c_R}{2s+1} \frac{1}{|\Gamma|} \sum_{u_b \in \Gamma} \chi_R(d_p) \chi_R^*(d_q), \tag{6.4}
\]

where we have introduced an extra dummy variable to account for the sum on \(u_z\) which was equivalent either to summing on \(u_\beta\) or \(u_\gamma\). Equation (6.4) shows that changing the orbit \(q\) by reordering the bonds at a single self-intersection introduces a factor \(\frac{c_R}{2s+1}\).

2. Reordering at a pair of self intersections.
The second way to reorder bonds in the orbit \(q\) is to permute two sections of the orbit. We consider a pair of orbits \(p\) and \(q\), where
\[
p = (\alpha_1, \beta_1, l_1, \alpha_2, \beta_2, l_2, \gamma_1, \delta_1, l_3, \gamma_2, \delta_2, l_4),
\]
\[
q = (\alpha_1, \beta_1, l_5, \alpha_2, \beta_2, l_6, \gamma_1, \delta_1, l_7, \gamma_2, \delta_2, l_8). \tag{6.5}
\]

Figure 2 shows the orbit \(q\).

![Figure 2: An orbit \(q\) with two self-intersections.](image)

The orbit \(q'\) is defined by exchanging two sections of \(q\),
\[
q' = (\alpha_1, \delta_1, l_7, \gamma_2, \beta_2, l_6, \gamma_1, \beta_1, l_5, \alpha_2, \delta_2, l_8). \tag{6.6}
\]

This changes the order of the arcs at two self-intersections. Thus, \(n' = n + 2\), and
\[
\frac{1}{|\Gamma|^p} \sum_{u_b \in \Gamma} \chi_R(d_p) \chi_R^*(d_{q'}) = \frac{1}{|\Gamma|^p} \sum_{u_b \in \Gamma} \chi_R(u_{l_4}u_{\delta_2}u_{\gamma_2}u_{l_3}u_{\delta_1}u_{\gamma_1}u_{l_2}u_{\beta_2}u_{l_1}u_{\beta_1}u_{\delta_1}) \\
\times \chi_R^*(u_{l_8}u_{\delta_2}u_{\alpha_2}u_{l_1}u_{\beta_1}u_{\gamma_1}u_{l_6}u_{\beta_2}u_{\gamma_2}u_{l_7}u_{\delta_1}u_{\alpha_1}) \\
= \frac{1}{|\Gamma|^p} \sum_{u_b \in \Gamma} \chi_R(u_{l_4}u_{y_2}u_{l_3}u_{y_1}u_{l_2}u_{x_2}u_{l_1}u_{x_1}) \\
\times \chi_R^*(u_{l_8}u_{y_2}u_{z_2}u_{l_1}u_{x_1}u_{z_1}^{-1}u_{l_6}u_{x_2}u_{z_2}^{-1}u_{l_7}u_{y_1}u_{z_1}), \tag{6.7}
\]

11
where \( u_{x_j} = u_{\beta_j} u_{\alpha_j}, u_{y_j} = u_{\delta_j} u_{\gamma_j} \) and \( u_{z_j} = u_{-1\gamma_j} u_{\alpha_j} \). This is in the form where we can apply Corollary 2, see the appendix, to evaluate the sums on \( z_1 \) and \( z_2 \),

\[
\frac{1}{|\Gamma|^t} \sum_{u_b \in \Gamma} \chi_R(d_p) \chi^*_R(d_{q'}) = \frac{1}{(2s + 1)^2} \frac{1}{|\Gamma|^{t-2}} \sum_{u \in \Gamma} \chi_R(u_{l_4} u_{y_2} u_{l_3} u_{y_1} u_{l_2} u_{x_2} u_{l_1} u_{x_1}) \\
\times \chi_R(u_{l_5} u_{y_2} u_{l_7} u_{y_1} u_{l_6} u_{x_2} u_{l_5} u_{x_1}) .
\] (6.8)

We can return to the original variables by including two dummy variables to account for the sums on \( z_1 \) and \( z_2 \). Taking \( c_R = \pm 1 \) for \( R(\Gamma), \Gamma \subset SU(2) \), into account we have thus shown that

\[
\frac{1}{|\Gamma|^t} \sum_{u_b \in \Gamma} \chi_R(d_p) \chi^*_R(d_{q'}) = \left( \frac{c_R}{2s + 1} \right)^2 \frac{1}{|\Gamma|^t} \sum_{u \in \Gamma} \chi_R(d_p) \chi^*_R(d_{q'}) .
\] (6.9)

Theorem 1 now follows by induction, since any orbit \( q \) can be constructed from \( p \) by permuting sections of the orbit between a pair of self-intersections or reversing a loop at a self-intersection.

We comment that at first sight it might not be obvious that all diagrams can be constructed via a combination of the two procedures described previously. Degenerate cases, in which a system of loops visits the same self-intersection more than once, allow both types of reordering. See Figure 3 for an example.

![Figure 3: An orbit with a degenerate self-intersection.](image)

To distinguish the cases it is necessary to follow the orbit counting each intersection when it is reached after determining whether the order of arcs at the intersection has been changed. The number of self-intersections for a given diagram is then \( n \). (Note our multiple counting of degenerate self-intersections differs from the definition in [2].)

It should also be noted that neither self-retracing loops or repeated bonds cause difficulties when evaluating the spin contribution. A self-retracing section of an orbit \( p = (\ldots, b_1, b_2, \overline{b_2}, \overline{b_1}, \ldots) \) does not contribute to \( d_p \) as \( u_{b_1} u_{b_2} u_{b_2}^{-1} u_{b_1}^{-1} = I \). Similarly, repeated bonds can be removed by a change of variables.

12
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Appendix: Group theoretic properties

The calculation of spin correlations uses the following properties of group representations.

**Lemma 1** Let $R(\Gamma)$ be a unitary irreducible representation of the finite group $\Gamma$, and let $a \in \Gamma$. Then

$$\frac{1}{|\Gamma|} \sum_{g \in \Gamma} \chi_R(a g^2) = \frac{c_R}{\eta_R} \chi_R(a) ,$$

where

$$c_R = \begin{cases} 
1 & \text{if } R \text{ is real} \\
-1 & \text{if } R \text{ is quaternionic} \\
0 & \text{if } R \text{ is not equivalent to } R^* 
\end{cases} .$$

Here $R^*$ is the complex-conjugate representation, $\eta_R$ is the dimension of $R(\Gamma)$, and $|\Gamma|$ is the order of the group.

For a proof see Hamermesh [10], section 5-5. This lemma will be applied in an alternate form.

**Corollary 1** For such a unitary irreducible representation $R(\Gamma)$, and $x, y \in \Gamma$,

$$\frac{1}{|\Gamma|} \sum_{g \in \Gamma} \chi_R(x g y g^{-1}) = \frac{c_R}{\eta_R} \chi_R(x y^{-1}) .$$

**Proof.** In lemma 1 replace $g$ with $y g$ and let $x = a y$. Summing over $y g$ is equivalent to a sum over $g$ for a fixed element $y \in \Gamma$. \qed

**Lemma 2** Let $R(\Gamma)$ be an irreducible representation of the finite group $\Gamma$, and let $x, y \in \Gamma$. Then

$$\frac{1}{|\Gamma|} \sum_{g \in \Gamma} \chi_R(x g y g^{-1}) = \frac{1}{\eta_R} \chi_R(x) \chi_R(y) .$$

**Proof.** The matrix $\sum_{g \in \Gamma} R(g) R(y) R(g^{-1})$ commutes with all elements of $R(\Gamma)$. For an irrep $R$, by Schur’s lemma,

$$\sum_{g \in \Gamma} R(g) R(y) R(g^{-1}) = \lambda I . \quad (6.10)$$
Taking traces yields $|\Gamma|\chi_R(y) = \eta_R\lambda$. Multiplying (6.10) by $R(x)$ we find,

$$
\sum_{g \in \Gamma} R(x)R(g)R(y)R(g^{-1}) = \frac{|\Gamma|}{\eta_R} R(x) .
$$

(6.11)

Then taking traces establishes the second lemma.

Lemma 3 Let $R(\Gamma)$ be an irreducible representation of the finite group $\Gamma$, and let $x, y \in \Gamma$. Then

$$
\frac{1}{|\Gamma|} \sum_{g \in \Gamma} \chi_R(xg)\chi_R(yg^{-1}) = \frac{1}{\eta_R} \chi_R(xy) .
$$

Proof. The matrix $\sum_{g \in \Gamma} R(g)XR(g^{-1})$ commutes with all elements of $R(\Gamma)$ for any matrix $X$. Again by Schur’s lemma,

$$
\sum_{g \in \Gamma} R(g)XR(g^{-1}) = \lambda I .
$$

(6.12)

Take $X$ to have all elements zero except $X_{lm} = 1$ and let $\lambda = \lambda_{lm}$. Equation (6.12) reads

$$
\sum_{g \in \Gamma} R_{il}(g)R_{mj}(g^{-1}) = \lambda_{lm}\delta_{ij} .
$$

(6.13)

Setting $i = j$ and summing over $i$,

$$
\lambda_{lm} = \frac{|\Gamma|}{\eta_R} \delta_{lm} .
$$

(6.14)

Consequently,

$$
\frac{1}{|\Gamma|} \sum_{g \in \Gamma} R_{il}(g)R_{mj}(g^{-1}) = \frac{1}{\eta_R} \delta_{lm}\delta_{ij} .
$$

(6.15)

Multiplying by $R_{li}(x)R_{jm}(y)$

$$
\frac{1}{|\Gamma|} \sum_{g \in \Gamma} R_{li}(x)R_{il}(g)R_{jm}(y)R_{mj}(g^{-1}) = \frac{1}{\eta_R} R_{li}(x)R_{jm}(y)\delta_{tm}\delta_{ij} .
$$

(6.16)

Summing on $i$ and $m$,

$$
\frac{1}{|\Gamma|} \sum_{g \in \Gamma} R_{il}(xg)R_{lj}(yg^{-1}) = \frac{1}{\eta_R} R_{lj}(x)R_{ij}(y) .
$$

(6.17)

Finally summing on $j$ and $l$ we obtain lemma 3.

Combining lemmas 2 and 3 we obtain a corollary that is useful when calculating spin correlations.

Corollary 2 For $R(\Gamma)$ an irreducible representation of the finite group $\Gamma$, and $a, b, c, d \in \Gamma$,

$$
\frac{1}{|\Gamma|} \sum_{g, h \in \Gamma} \chi_R(gah^{-1}bg^{-1}chd) = \frac{1}{\eta_R^2} \chi_R(cbad) .
$$
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