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Semiclassical form factor for chaotic systems with spin $\frac{1}{2}$

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Abstract. We study the properties of the two-point spectral form factor for classically chaotic systems with spin $\frac{1}{2}$ in the semiclassical limit, with a suitable semiclassical trace formula as our principal tool. To this end we introduce a regularized form factor and discuss the limit in which the so-called diagonal approximation can be recovered. The incorporation of the spin contribution to the trace formula requires an appropriate variant of the equidistribution principle of long periodic orbits as well as the notion of a skew product of the classical translational and spin dynamics. Provided this skew product is mixing, we show that generically the diagonal approximation of the form factor coincides with the respective predictions from random matrix theory.

1. Introduction

One of the major paradigms of quantum chaos is the conjecture of Bohigas, Giannoni and Schmit (BGS) [1] which states that the local statistics of energy spectra of (generic) individual quantum systems, whose classical analogues exhibit (strongly) chaotic behaviour, can be well described by that of ensembles of large random matrices. The symmetry properties of the relevant matrix ensembles have to be chosen according to the symmetries of the quantum system under consideration. In the case where the system is invariant under time reversal and has integer total angular momentum, its local eigenvalue statistics are conjectured to be that of the Gaussian orthogonal ensemble (GOE). If time-reversal invariance is broken one expects local statistics according to the Gaussian unitary ensemble (GUE).

However, if the total angular momentum of the system is half-integer and the system is invariant under time reversal all eigenvalues show Kramers' degeneracy [2, 3] and their statistics have to be compared with the Gaussian symplectic ensemble (GSE). In the GOE and in the GUE case there is plenty of numerical evidence available in favour of the BGS conjecture (see, e.g., [1, 4, 5]), whereas only a few examples have been studied in the GSE case (such as, e.g., in [6, 7]). For quantum systems whose classical limit is integrable, i.e. which shows regular behaviour, one expects the local eigenvalue statistics to follow the laws of a Poisson process [8]. For the analytical treatment semiclassical methods, in particular semiclassical trace formulae, have become the most important tools since Berry and Tabor [8] investigated the behaviour of the spectral form factor for classically integrable systems by means of an

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appropriate trace formula. By making use of the Gutzwiller trace formula [5, 9–12], Berry provided a semiclassical theory for the spectral form factor [13] of classically chaotic systems without spin. Based on the so-called diagonal approximation, and on the periodic-orbit sum rule of Hannay and Ozorio de Almeida [14], he could explain the semiclassical asymptotics of the form factor for small values of its argument, thus recovering the GOE and GUE behaviour, respectively.

In this paper our aim is to show that Berry's semiclassical treatment of the two-point form factor can be carried over to quantum systems with spin $\frac{1}{2}$, whose classical translational dynamics are chaotic. We base our analysis on the semiclassical trace formula for the Dirac equation that we developed recently [15, 16]. In this trace formula the presence of spin is reflected in a modification of the amplitudes with which the periodic orbits of the translational dynamics contribute. This modification arises from a spin dynamics that involves a 'classical' spin precessing along the periodic orbits. The central part of this paper therefore consists of calculating the effect of this spin contribution to the semiclassical form factor. For our analysis we use a two-point form factor whose definition differs slightly from the one that is more commonly used in spectral statistics (such as, e.g., in [13]). We rather prefer the point of view adopted in [17, 18]. Both definitions, however, are equivalent in the limit where infinitely many eigenvalues are taken into account. We also stress that both the form factor and the associated correlation function are distributions and hence have to be evaluated on suitable test functions. This approach makes a spectral average obsolete and enables one to state the BGS conjecture, specialized to the form factor, in a precise manner. Moreover, the lacking self-averaging property discussed in [19] poses no difficulty in this context.

This paper is organized as follows. In section 2 we introduce our definition of the spectral form factor for a finite part of the spectrum and discuss in which sense one can expect to recover the form factors given by random matrix theory. Section 3 is devoted to the definition of a regularized form factor which we evaluate semiclassically using trace formulae for the Dirac as well as for the Pauli equation [15, 16]. We also invoke the diagonal approximation and briefly discuss its range of validity. In section 4 a suitable version of the equidistribution principle of long periodic orbits is used in order to obtain the semiclassical asymptotics of the diagonal form factor. In this context we employ the notion of a skew product of the translational and the spin dynamics, the ergodic properties of which determine the semiclassical asymptotics. Our principal results are then summarized in section 5. Namely, depending on the presence or absence of quantum mechanical time-reversal invariance, and provided the dynamics of the skew product is mixing, we can recover a GSE or GUE behaviour of the diagonal form factor, respectively. The relation between classical and quantum mechanical time reversal as well as the equidistribution of long periodic orbits are discussed in two appendices.

2. The form factor for quantum systems with half-integer spin

The two-point correlations of a discrete quantum spectrum are conveniently measured by either the two-point correlation function R_2 or by the two-point form factor K_2, which is related to R_2 through a Fourier transform. Before defining these quantities one usually *unfolds* the spectrum, i.e. the eigenvalues E_k are rescaled to x_k such that the unfolded eigenvalues have a mean separation of one. This means that the spectral density $d(x)$ of the unfolded spectrum allows for a separation

$$d(x) := \sum_k \delta(x - x_k) = 1 + d_{fl}(x) \tag{2.1}$$

such that

$$\frac{1}{2\Delta x}\int_{x-\Delta x}^{x+\Delta x} d_{fl}(y)\,\mathrm{d}y = \frac{1}{2\Delta x}\,\#\{k;\, x-\Delta x \leqslant x_k \leqslant x+\Delta x\} - 1 \tag{2.2}$$

vanishes as $x \to \infty$, $\Delta x \to \infty$, $\Delta x/x \to 0$. For a finite part of the spectrum, containing N unfolded eigenvalues enumerated as $x_1, \ldots, x_N$, one defines the two-level correlation function by

$$R_2(s;N) := \frac{1}{N}\sum_{k,l\leqslant N}\delta(s-(x_k-x_l)) - 1. \tag{2.3}$$

Accordingly, the two-level form factor is defined as

$$K_2(\tau;N) := \int_{\mathbb{R}} R_2(s;N)\,\mathrm{e}^{-2\pi\mathrm{i}\tau s}\,\mathrm{d}s = \frac{1}{N}\sum_{k,l\leqslant N}\mathrm{e}^{-2\pi\mathrm{i}\tau(x_k-x_l)} - \delta(\tau). \tag{2.4}$$

Since both quantities are distributions, which is most clearly seen in the case of the correlation function (2.3), one should evaluate these on smooth and compactly supported test functions, i.e. $\phi \in C_0^\infty(\mathbb{R})$,

$$\begin{aligned}\int_{\mathbb{R}} K_2(\tau;N)\,\phi(\tau)\,\mathrm{d}\tau &= \frac{1}{N}\sum_{k,l\leqslant N}\int_{\mathbb{R}}\phi(\tau)\,\mathrm{e}^{-2\pi\mathrm{i}\tau(x_k-x_l)}\,\mathrm{d}\tau - \phi(0)\\ &= \frac{1}{N}\sum_{k,l\leqslant N}\hat{\phi}(2\pi(x_l-x_k)) - \phi(0)\\ &= \int_{\mathbb{R}} R_2(s;N)\,\hat{\phi}(2\pi s)\,\mathrm{d}s. \end{aligned}\tag{2.5}$$

We remark that since the form factor is obviously even in τ, it suffices to consider only even test functions ϕ. The convention for the Fourier transform that was used, and that will be used in all of what follows, is

$$\hat{f}(k) = \int_{\mathbb{R}} f(x)\,\mathrm{e}^{\mathrm{i}xk}\,\mathrm{d}x \qquad \text{and} \qquad f(x) = \frac{1}{2\pi}\int_{\mathbb{R}}\hat{f}(k)\,\mathrm{e}^{-\mathrm{i}xk}\,\mathrm{d}k. \tag{2.6}$$

After smearing with a test function all expressions occurring in (2.5) are obviously finite. In this form a semiclassical analysis of either the form factor or the correlation function can be carried out. If ϕ is chosen as non-negative, the left-hand side of (2.5) can also be viewed as the mean value of $K_2(\tau;N)$ when τ is drawn randomly with probability density ϕ. Since we always understand the form factor in the above sense, the absence of a self-averaging property discussed in [19] is not essential for our further considerations.

For a given quantum Hamiltonian $\hat{H}$ the unfolding of its discrete spectrum shall proceed in the following manner. We consider a spectral interval

$$I = I(E,\hbar) := [E-\hbar\omega, E+\hbar\omega] \qquad \omega > 0 \tag{2.7}$$

that has no overlap with a possible essential spectrum of $\hat{H}$. Then the condition $E_k \in I$ is equivalent to

$$-\omega \leqslant \frac{E_k - E}{\hbar} \leqslant \omega. \tag{2.8}$$

The number of eigenvalues contained in I,

$$N_I := \#\{k;\, E_k \in I\} \tag{2.9}$$

can be estimated semiclassically as

$$N_I \sim 2\hbar\omega\bar{d}(E) = \frac{\omega}{\pi}\, T_H(E) \qquad \hbar \to 0 \tag{2.10}$$

where $\bar{d}(E)$ denotes an appropriate mean spectral density and $T_H(E) := 2\pi\hbar\bar{d}(E)$ is the *Heisenberg time*. A convenient definition of $\bar{d}(E)$ can be derived from the semiclassical trace formula for $\hat{H}$ in that it shall denote the contribution coming from the singularity of $\mathrm{Tr}\exp[-(\mathrm{i}/\hbar)\hat{H}t]$ at $t = 0$ to all polynomial orders in $\hbar$ (see, e.g., [10–12, 16, 20]). The spectra that we are going to consider below are such that in the semiclassical limit $\hbar \to 0$ the Heisenberg time tends to infinity, $T_H \to \infty$. For example, given E in the gap of the essential spectrum of a Dirac Hamiltonian $\hat{H}_D$, i.e. in typical cases $-mc^2 < E < mc^2$, the mean spectral density reads [15, 16]

$$\bar{d}(E) = 2\,\frac{\mathrm{vol}\,\Omega_E^+ + \mathrm{vol}\,\Omega_E^-}{(2\pi\hbar)^3}\,[1 + \mathrm{O}(\hbar)] \tag{2.11}$$

where $\Omega_E^\pm$ denote the hypersurfaces of energy E in phase space corresponding to the classical Hamiltonians

$$H^\pm(\boldsymbol{p}, \boldsymbol{x}) = e\varphi(\boldsymbol{x}) \pm \sqrt{(c\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{x}))^2 + m^2c^4} \tag{2.12}$$

for relativistic particles of positive and negative kinetic energy, respectively, in the static external electromagnetic fields generated by the potentials φ and $\boldsymbol{A}$. Therefore, in the semiclassical limit the number of eigenvalues in the interval I increases, although its length $|I| = 2\hbar\omega$ shrinks to zero. A completely analogous argument applies to Pauli Hamiltonians [16].

We now define the unfolded spectrum through

$$x_k := E_k\bar{d}(E) \qquad \text{and} \qquad x := E\bar{d}(E). \tag{2.13}$$

The condition $E_k \in I(E, \hbar)$ is hence equivalent to $x_k \in [x - \Delta x, x + \Delta x]$, where $\Delta x := (\omega/2\pi)T_H$. With this choice indeed $x \to \infty$, $\Delta x \to \infty$, such that $\Delta x/x = \hbar\omega/E \to 0$ in the semiclassical limit. In this context the quantity (2.2) reads

$$\frac{1}{2\Delta x}\,\#\{k; x - \Delta x \leqslant x_k \leqslant x + \Delta x\} - 1 = \frac{\pi}{\omega T_H}\, N_I - 1 \tag{2.14}$$

such that (2.10) ensures its vanishing in the semiclassical limit.

From now on we will choose the numbering of the eigenvalues E_k and x_k, respectively, in such a way that the eigenvalues in I are given by

$$E_1 \leqslant E_2 \leqslant \cdots \leqslant E_{N_I}. \tag{2.15}$$

Changing the value of $\hbar$ therefore alters the numbering of the eigenvalues. Consequently, the condition $E_k \in I$ is equivalent to $k \leqslant N_I$. At this point we recall that the semiclassical limit $\hbar \to 0$, or $T_H \to \infty$, implies $N_I \to \infty$. For the form factor (2.4) we now obtain

$$\begin{aligned} K_2(\tau; N_I) &= \frac{1}{N_I}\sum_{E_k, E_l \in I} \mathrm{e}^{-2\pi\mathrm{i}\tau\bar{d}(E)(E_k - E_l)} - \delta(\tau) \\ &= \left|\frac{1}{\sqrt{N_I}}\sum_k \chi_{[-\omega,\omega]}\left(\frac{E_k - E}{\hbar}\right)\mathrm{e}^{-(\mathrm{i}/\hbar)\tau T_H E_k}\right|^2 - \delta(\tau) \end{aligned} \tag{2.16}$$

where the k-sum extends over all eigenvalues of $\hat{H}$ and $\chi_{[-\omega,\omega]}$ denotes the characteristic function of the interval $[-\omega, \omega]$ that occurs due to the condition (2.8).

In the preceding discussion we tacitly assumed that the discrete spectrum of the quantum Hamiltonian carries no systematic degeneracies. In order to achieve such a situation one has to remove all symmetries. As opposed to geometric or internal symmetries that have to be realized by unitary representations of the respective symmetry groups, the time-reversal operation must be implemented by an anti-unitary operator $\hat{T}$ (see [3] and appendix A). For single particles of spin s the square of $\hat{T}$ depends on s being integer or half-integer in that $\hat{T}^2 = (-1)^{2s}$. In case the quantum system is time-reversal invariant, i.e. $[\hat{H}, \hat{T}] = 0$, and has half-integer spin this leads to *Kramers' degeneracy* [2]: since $\hat{T}^2 = -1$ implies that every vector $\psi \neq 0$ in the Hilbert space is orthogonal to $\hat{T}\psi$, all eigenvalues of $\hat{H}$ are (at least) twofold degenerate (see [21, 22] for details).

Following the usual practice, we will remove Kramers' degeneracy by replacing each degenerate pair $E_{2k} = E_{2k+1}$ of eigenvalues by one of its representatives. Thus the mean spectral density is lowered by a factor of two. In analogy to (2.13) the unfolding $E_k \mapsto \tilde{x}_k$ of the so modified spectrum can therefore be achieved through the choice $\tilde{x}_k := x_k/2$. The modified form factor then reads

$$\begin{aligned}\widetilde{K}_2(\tau; N) &= \frac{2}{N} \sum_{\substack{k,l \leqslant N \\ k,l\ odd}} \mathrm{e}^{-2\pi \mathrm{i} \tau (\tilde{x}_k - \tilde{x}_l)} - \delta(\tau) \\ &= \frac{1}{2N} \sum_{k,l \leqslant N} \mathrm{e}^{-2\pi \mathrm{i} \frac{1}{2} \tau (x_k - x_l)} - \tfrac{1}{2}\delta\big(\tfrac{1}{2}\tau\big) \\ &= \tfrac{1}{2} K_2\big(\tfrac{1}{2}\tau; N\big). \end{aligned} \tag{2.17}$$

In this setting the conjecture of Bohigas *et al* [1] states that for individual (generic) classically chaotic quantum systems of particles with half-integer total spin and no unitary symmetries one should obtain

$$\lim_{N\to\infty} \int_{\mathbb{R}} \widetilde{K}_2(\tau; N)\, \phi(\tau)\, \mathrm{d}\tau \overset{!}{=} \int_{\mathbb{R}} K_2^{GSE}(\tau)\, \phi(\tau)\, \mathrm{d}\tau \tag{2.18}$$

for all test functions $\phi \in C_0^\infty(\mathbb{R})$. Here K_2^{GSE} denotes the two-point form factor of the Gaussian symplectic ensemble of random matrix theory,

$$K_2^{GSE}(\tau) = \begin{cases} \frac{1}{2}|\tau| - \frac{1}{4}|\tau| \log|1 - |\tau|| & \text{for} \quad |\tau| \leqslant 2 \\ 1 & \text{for} \quad |\tau| \geqslant 2 \end{cases} \tag{2.19}$$

see, e.g., [22]. When time-reversal invariance is lacking, the respective conjecture reads

$$\lim_{N\to\infty} \int_{\mathbb{R}} K_2(\tau; N)\, \phi(\tau)\, \mathrm{d}\tau \overset{!}{=} \int_{\mathbb{R}} K_2^{GUE}(\tau)\, \phi(\tau)\, \mathrm{d}\tau \tag{2.20}$$

where now the form factor of the Gaussian unitary ensemble [22] should occur,

$$K_2^{GUE}(\tau) = \begin{cases} |\tau| & \text{for } |\tau| \leqslant 1 \\ 1 & \text{for } |\tau| \geqslant 1. \end{cases} \tag{2.21}$$

In our subsequent semiclassical investigations we will in both cases, i.e. with and without time-reversal invariance, consider the form factor $K_2(\tau; N_I)$ as it is given in (2.16). When dealing with the case of time-reversal invariance we appeal to the relation (2.17).

3. The semiclassical form factor

Since the work of Berry and Tabor [8] on the distribution of eigenvalues for classically integrable systems, semiclassical trace formulae have found numerous and fruitful applications in the analysis of spectral statistics. A prominent example is Berry's analysis of the spectral rigidity [13], which relies in an essential way on a semiclassical evaluation of the two-point form factor based on the Gutzwiller trace formula. In this work it already became apparent that present semiclassical methods at most allow one to study the form factor in the restricted range $|\tau| < 1$ (see also [20] for a review). Only recently have improved techniques been developed [23] that might allow one to extend the semiclassical analysis of spectral statistics. In this paper, however, we follow the more traditional path in that in the end we consider the so-called diagonal approximation for the form factor.

The two-point form factor as given in (2.16) requires to establish a trace formula for the sum

$$\sum_k \chi_{[-\omega,\omega]}\left(\frac{E_k - E}{\hbar}\right) \mathrm{e}^{-(\mathrm{i}/\hbar)\tau T_H E_k}. \tag{3.1}$$

However, the general structure of (convergent) semiclassical trace formulae (see, e.g., [10–12, 16, 20]), necessitates the use of a smooth test function $\rho \in C^\infty(\mathbb{R})$ with the Fourier transform $\hat{\rho} \in C_0^\infty(\mathbb{R})$. One therefore has to replace the sharp cut-off, provided by the characteristic function in (3.1), by a smoothed substitute. For this reason we now introduce the *regularized form factor*

$$K_2^{\chi,\eta}(\tau; T_H) := \left|\sqrt{\frac{\pi}{\omega T_H}} \sum_k \chi(E_k)\, \eta\left(\frac{E_k - E}{\hbar}\right) \mathrm{e}^{-(\mathrm{i}/\hbar)\tau T_H E_k}\right|^2 - \delta(\tau) \tag{3.2}$$

where $\eta \in C^\infty(\mathbb{R})$ is a test function with the Fourier transform $\hat{\eta} \in C_0^\infty(\mathbb{R})$, but that is otherwise arbitrary at the moment. Later we will introduce a further normalization condition. In the following we will consider both relativistic and non-relativistic particles with spin $\frac{1}{2}$. In the relativistic case, when one is dealing with a Dirac Hamiltonian $\hat{H}_D$, the function $\chi \in C_0^\infty(\mathbb{R})$, which is not to be confused with the characteristic function $\chi_{[-\omega,\omega]}$, is necessary to truncate the essential spectrum of $\hat{H}_D$. In typical situations χ should therefore be supported in the interval $(-mc^2, mc^2)$, where the eigenvalues E_k of $\hat{H}_D$ are located. When these do not accumulate at some point, one could also leave out the truncation χ from (3.2).

We are now in a position to use the test function

$$\rho(\varepsilon) := \eta(\varepsilon)\, \mathrm{e}^{-2\pi \mathrm{i}\bar{d}(E)\tau(\hbar\varepsilon + E)} \tag{3.3}$$

in the semiclassical trace formula for the Dirac equation that was developed in [15, 16],

$$\sum_k \chi(E_k)\, \rho\left(\frac{E_k - E}{\hbar}\right) = \chi(E)\, \frac{T_H(E)}{2\pi}\, \hat{\rho}(0)\, [1 + \mathrm{O}(\hbar)] + \chi(E) \sum_\gamma \sum_{k\neq 0} \frac{T_\gamma}{2\pi}\, \hat{\rho}(kT_\gamma)\, A_{\gamma,k}. \tag{3.4}$$

The outer sum on the right-hand side extends over all primitive periodic orbits γ of energy E, with periods T_γ, of the two classical flows generated by the Hamiltonians (2.12). The inner sum then is over all k-fold repetitions of primitive orbits, formally including negative ones. The weight attached to each pair (γ, k) reads

$$A_{\gamma,k} := \frac{\mathrm{tr}\, d_\gamma^k}{|\det(\mathbb{M}_\gamma^k - \mathbb{1})|^{1/2}}\, \mathrm{e}^{(\mathrm{i}/\hbar)kS_\gamma(E) - \mathrm{i}\frac{1}{2}\pi k \mu_\gamma}\, [1 + \mathrm{O}(\hbar)]. \tag{3.5}$$

Here $d_\gamma \in SU(2)$ denotes the semiclassical time evolution operator for the spin degrees of freedom along the primitive periodic orbit γ of the translational dynamics. Furthermore, $S_\gamma(E)$ denotes the action of γ and μ_γ is its Maslov index. The (monodromy) matrix $\mathbb{M}_\gamma$ is the linearized Poincaré map transversal to γ. In the form given in (3.4) the trace formula is valid for all cases where the classical flows have only isolated and non-degenerate periodic orbits. An analogous trace formula, with appropriate simplifications, is also available for Pauli Hamiltonians, see [16].

Upon choosing the test function (3.3) in the trace formula (3.4), its left-hand side reads

$$\sum_k \chi(E_k)\,\rho\left(\frac{E_k - E}{\hbar}\right) = \sum_k \chi(E_k)\,\eta\left(\frac{E_k - E}{\hbar}\right) \mathrm{e}^{-(\mathrm{i}/\hbar)\tau T_H E_k} \tag{3.6}$$

and is hence the appropriate starting point for a semiclassical analysis of the form factor (cf (3.2)). As a first ingredient on the right-hand side of (3.4) one requires the Fourier transform of the test function (3.3), which is given by

$$\hat{\rho}(t) = \mathrm{e}^{-(\mathrm{i}/\hbar)E\tau T_H}\,\hat{\eta}(t - \tau T_H). \tag{3.7}$$

For convenience we now choose η to be even and real-valued, which implies that $\hat{\eta}$ also shares these properties. Furthermore, the truncation χ of the essential spectrum shall be such that $\chi(E) = 1$. Thus, the trace formula yields the following semiclassical representation of the regularized form factor:

$$\begin{aligned} K_2^{\chi,\eta}(\tau; T_H) &= -\delta(\tau) + \frac{T_H}{4\pi\omega}\left[\hat{\eta}(\tau T_H)\right]^2 [1 + \mathrm{O}(\hbar)] \\ &\quad + \sum_\gamma \sum_{k\neq 0} \frac{T_\gamma}{4\pi\omega}\,\hat{\eta}(\tau T_H)\,\hat{\eta}(kT_\gamma - \tau T_H)\,A_{\gamma,k}\,[1 + \mathrm{O}(\hbar)] \\ &\quad + \frac{1}{T_H}\sum_{\gamma,\gamma'}\sum_{k,k'\neq 0} \frac{T_\gamma T_{\gamma'}}{4\pi\omega}\,\hat{\eta}(kT_\gamma - \tau T_H)\,\hat{\eta}(\tau T_H - k'T_{\gamma'})\,A_{\gamma,k}\,A_{\gamma',-k'}. \end{aligned} \tag{3.8}$$

In the next step we are going to test the semiclassical form factor with some $\phi \in C_0^\infty(\mathbb{R})$ (cf (2.5)). To this end one needs the integral

$$F(T, T') := \int_{\mathbb{R}} \phi(\tau)\,\hat{\eta}(T - \tau T_H)\,\hat{\eta}(\tau T_H - T')\,\mathrm{d}\tau \tag{3.9}$$

whose leading term in the semiclassical limit $T_H \to \infty$ can be calculated by introducing the Fourier representations for ϕ and $\hat{\eta}$. A straightforward calculation then yields

$$F(T, T') = \frac{1}{T_H}\int_{\mathbb{R}}\int_{\mathbb{R}}\int_{\mathbb{R}} \hat{\phi}(t)\,\eta(\varepsilon)\,\eta(\varepsilon')\,\mathrm{e}^{\mathrm{i}(\varepsilon T - \varepsilon' T')}\,\delta\left(\frac{t}{T_H} + \varepsilon - \varepsilon'\right) \mathrm{d}\varepsilon'\,\mathrm{d}\varepsilon\,\mathrm{d}t. \tag{3.10}$$

Changing variables from $\varepsilon, \varepsilon'$ to $u := \varepsilon' - \varepsilon$ and $v := (\varepsilon' + \varepsilon)/2$, and employing the expansions

$$\eta\left(v \pm \frac{t}{2T_H}\right) = \eta(v) + \mathrm{O}\left(\frac{t}{T_H}\right) \tag{3.11}$$

finally shows that

$$\begin{aligned} F(T, T') &= \frac{1}{T_H}\int_{\mathbb{R}}\int_{\mathbb{R}} \hat{\phi}(t)\,\exp\left[-\mathrm{i}t\left(\frac{T + T'}{2T_H}\right)\right]\eta(v)^2\,\mathrm{e}^{\mathrm{i}v(T - T')}\,\mathrm{d}v\,\mathrm{d}t + \mathrm{O}\left(\frac{1}{T_H^2}\right) \\ &= \frac{1}{T_H}\,\phi\left(\frac{T + T'}{2T_H}\right)\hat{\eta} * \hat{\eta}(T - T') + \mathrm{O}\left(\frac{1}{T_H^2}\right) \end{aligned} \tag{3.12}$$

where the convolution

$$\hat{\eta} * \hat{\eta}(t) := \int_{\mathbb{R}} \hat{\eta}(t-t')\,\hat{\eta}(t')\,\mathrm{d}t' = 2\pi \int_{\mathbb{R}} \eta(v)^2\,\mathrm{e}^{\mathrm{i}tv}\,\mathrm{d}v \tag{3.13}$$

enters. We therefore conclude that

$$\begin{aligned}\int_{\mathbb{R}} K_2^{\chi,\eta}(\tau;T_H)\,\phi(\tau)\,\mathrm{d}\tau &= \phi(0)\left[-1+\frac{1}{4\pi\omega}\,\hat{\eta}*\hat{\eta}(0)\right]+\mathrm{O}(\hbar)\\ &\quad+\frac{1}{T_H}\sum_{\gamma}\sum_{k\neq 0}\frac{T_\gamma}{4\pi\omega}\,\hat{\eta}*\hat{\eta}(kT_\gamma)\,A_{\gamma,k}\,\phi\left(\frac{kT_\gamma}{2T_H}\right)[1+\mathrm{O}(\hbar)]\\ &\quad+\frac{1}{T_H^2}\sum_{\gamma,\gamma'}\sum_{k,k'\neq 0}\frac{T_\gamma T_{\gamma'}}{4\pi\omega}\,\hat{\eta}*\hat{\eta}(kT_\gamma-k'T_{\gamma'})\phi\left(\frac{kT_\gamma+k'T_{\gamma'}}{2T_H}\right)A_{\gamma,k}\,A_{\gamma',-k'}.\end{aligned} \tag{3.14}$$

At this point we introduce the normalization of η announced previously. Guided by the simple observation

$$\int_{\mathbb{R}} [\chi_{[-\omega,\omega]}(\varepsilon)]^2\,\mathrm{d}\varepsilon = 2\omega \tag{3.15}$$

we require the same normalization for the smooth substitute η of the sharp cut-off $\chi_{[-\omega,\omega]}$,

$$\frac{1}{2\pi}\,\hat{\eta}*\hat{\eta}(0) = \int_{\mathbb{R}} \eta(\varepsilon)^2\,\mathrm{d}\varepsilon \overset{!}{=} 2\omega. \tag{3.16}$$

Consequently, the leading semiclassical order of the first line on the right-hand side of (3.14) vanishes. Furthermore, since the Fourier transform $\hat{\eta}$ of the test function η is required to be compactly supported, the second line is a finite sum, multiplied by $1/T_H$. A similar argument applies to the third line, apart from the *diagonal contribution* with $kT_\gamma = k'T_{\gamma'}$, where $\hat{\eta}*\hat{\eta}(0)$ occurs and thus no such cut-off is present.

Due to the above reasoning it is tempting to assume that in the semiclassical limit $T_H \to \infty$ the right-hand side of (3.14) is completely fixed by the contribution of the *diagonal form factor*

$$K_2^{diag}(\tau;T_H) := \frac{1}{T_H^2}\sum_{\gamma}\sum_{k\neq 0} g_{\gamma,k}\,T_\gamma^2\,|A_{\gamma,k}|^2\,\delta\left(\tau-\frac{kT_\gamma}{T_H}\right). \tag{3.17}$$

Here we have assumed that $k'T_{\gamma'} = kT_\gamma$ implies $A_{\gamma',k'} = A_{\gamma,k}$ (see appendix A for the spin contribution), and then $g_{\gamma,k}$ denotes the number of pairs (γ,k) such that kT_γ has a given value. It is, however, well known that the above assumption is not justified. The reason for this lies in the subtleties of the limits involved. In order to arrive at the left-hand side of (2.18), or of (2.20), one first has to remove the smoothing of the characteristic function $\chi_{[-\omega,\omega]}$ in that a sequence of functions $\eta \in C^\infty(\mathbb{R})$ approaching $\chi_{[-\omega,\omega]}$ has to be considered. Then, in the limit, $\hat{\eta}*\hat{\eta}$ is no longer compactly supported. Indeed, according to (3.13) one obtains $\hat{\eta}*\hat{\eta}(t) = 4\pi\,\sin(\omega t)/t$. Still, the periodic-orbit sums in (3.14) are truncated by the test function ϕ. However, in the semiclassical limit this cut-off is being removed. Moreover, for long periodic orbits the differences $kT_\gamma - k'T_{\gamma'}$ can become arbitrarily small so that $\hat{\eta}*\hat{\eta}(kT_\gamma - k'T_{\gamma'})$ only provides a modest truncation of near-diagonal contributions. The only example where it could be rigorously shown [17] that the diagonal form factor itself produces the correct limit, if the test functions ϕ are restricted to those that are supported in the interval $[-1,1]$, is that of the correlations of the non-trivial zeros of principal L-functions, including the case of the Riemann zeta function (see also [24]). Rudnick and Sarnak [17] even proved an analogous result for general n-point correlations.

As announced previously, we now invoke the diagonal approximation, i.e. we leave aside the contribution of $K_2^{\chi,\eta}(\tau; T_H) - K_2^{diag}(\tau; T_H)$ to (3.14). This procedure, which goes back to Hannay and Ozorio de Almeida [14], is generally supposed to reveal the correct behaviour of the form factor for small $|\tau|$, as was first pointed out by Berry [13]. The reason for this being that if the test function ϕ is supported in a small interval, the contribution of long periodic orbits to (3.14) is truncated. Furthermore, due to the normalization (3.16) the diagonal form factor is independent of the smoothing η. This convenient fact exempts one from the need to discuss the removal of this smoothing. In order to now test the range of small $|\tau|$ one should restrict the class of test functions ϕ to those supported in intervals $[-\tau', \tau']$, where $\tau' > 0$ is 'small enough'. Recalling that K_2^{diag} and ϕ are even in τ an integration by parts yields

$$\begin{aligned}\int_{\mathbb{R}} K_2^{diag}(\tau; T_H)\,\phi(\tau)\,\mathrm{d}\tau &= 2\int_0^\infty K_2^{diag}(\tau; T_H)\,\phi(\tau)\,\mathrm{d}\tau \\ &= -\int_0^{\tau'} \phi'(\tau)\,\frac{2}{T_H^2}\sum_\gamma \sum_{\substack{k\geqslant 1\\ kT_\gamma\leqslant\tau T_H}} g_{\gamma,k}\,T_\gamma^2\,|A_{\gamma,k}|^2\,\mathrm{d}\tau. \end{aligned} \tag{3.18}$$

What is now required is the asymptotic behaviour of the periodic-orbit sum in (3.18) as $T_H \to \infty$. Since the contributions of repetitions of primitive periodic orbits are asymptotically suppressed due to their stronger instabilities (compare also with (4.3) below), in the following we only take the $k = 1$ term of the sum over the repetitions into account. Consequently, we therefore have to study the asymptotics of the periodic-orbit sum

$$\sum_{\gamma,\,T_\gamma\leqslant\tau T_H} \frac{g_{\gamma,1}\,T_\gamma^2\,(\mathrm{tr}\,d_\gamma)^2}{|\det(\mathbb{M}_\gamma - \mathbb{1})|} \tag{3.19}$$

in the double limit $T_H \to \infty$, $\tau \to 0$, such that $\tau T_H \to \infty$. In order to simplify this task we now make two assumptions, which should be verified in all cases that could be considered as 'generic' in any reasonable sense.

(a) The periods T_γ of primitive periodic orbits shall be such that any finite subset of them is linearly independent over $\mathbb{Q}$. This implies that the multiplicities $g_{\gamma,k}$ are independent of k, i.e. $g_{\gamma,k} = g_\gamma$.

(b) The subset of primitive periodic orbits γ with $g_\gamma \neq \bar{g}$ is of density zero in the set of all primitive periodic orbits,

$$\lim_{T\to\infty} \frac{\#\{\gamma;\, g_\gamma \neq \bar{g},\, T_\gamma \leqslant T\}}{\#\{\gamma;\, T_\gamma \leqslant T\}} \stackrel{!}{=} 0 \tag{3.20}$$

where $\bar{g} = 2$ in the case where the classical dynamics are time-reversal invariant, and $\bar{g} = 1$ when time-reversal symmetry is absent. In this context time-reversal invariance does not only mean that an orbit γ is geometrically identical to its time-reversed partner, but also that both orbits yield the same contribution of the spin degrees of freedom to the trace formula, which then implies that $A_{\gamma,k}$ is invariant under time reversal. In appendix A we show that this condition is a consequence of quantum mechanical time-reversal invariance.

Under these assumptions the factors $g_{\gamma,k}$ can be replaced by $\bar{g}$ and can then be pulled out of the sum (3.19).

4. Classical periodic-orbit sums and the contribution of spin

The aim of this section is to obtain the leading semiclassical behaviour of the periodic-orbit sum (3.19). Apart from the appearance of the Heisenberg time only quantities related to the classical flow enter this expression. It therefore seems appropriate to invoke results about the distribution of periodic orbits in phase space. In order to retain a certain convenient generality, we will not specify the classical translational dynamics further, except for the following assumptions.

(a) The classical flow $\Phi_H^t : \Omega_E \to \Omega_E$ on the compact hypersurface Ω_E of energy E in the $2d$-dimensional phase space is generated by some Hamiltonian function $H(\boldsymbol{p}, \boldsymbol{x})$ and hence preserves the (normalized) Liouville measure

$$\mathrm{d}\mu_E(\boldsymbol{p}, \boldsymbol{x}) := \frac{1}{\mathrm{vol}\,\Omega_E}\,\delta(H(\boldsymbol{p}, \boldsymbol{x}) - E)\,\mathrm{d}^d p\,\mathrm{d}^d x \tag{4.1}$$

on Ω_E.

(b) Φ_H^t is *ergodic* with respect to the Liouville measure.

(c) Φ_H^t is *hyperbolic* on all of Ω_E.

In the case of the semiclassical form factor for a Dirac Hamiltonian these requirements shall apply to both classical flows, i.e. to those generated by the two classical Hamiltonians $H^\pm$ given in (2.12). Moreover, we now assume that for a given energy E there will only be either a contribution coming from the dynamics generated by H^+ or from the dynamics generated by H^-, but never from both at the same time. This is not a strong restriction since it only excludes situations in which Klein's paradox [25] can appear.

The hyperbolicity of the classical flows implies that, in particular, all periodic orbits are either hyperbolic or loxodromic. This means that all monodromy matrices $\mathbb{M}_\gamma$ have eigenvalues with moduli strictly different from one. Since the eigenvalues occur in pairs of mutually inverse numbers, we denote them as $\mathrm{e}^{\pm(u_{\gamma,j}+\mathrm{i}v_{\gamma,j})}$, $u_{\gamma,j} > 0$, $v_{\gamma,j} \in [0, 2\pi)$, $j = 1, \ldots, d-1$. Thus

$$\begin{aligned} |\det(\mathbb{M}_\gamma - \mathbb{1})| &= \prod_{j=1}^{d-1}\big|\big(\mathrm{e}^{u_{\gamma,j}+\mathrm{i}v_{\gamma,j}} - 1\big)\big(\mathrm{e}^{-u_{\gamma,j}-\mathrm{i}v_{\gamma,j}} - 1\big)\big| \\ &= \exp\Bigg(\sum_{j=1}^{d-1} u_{\gamma,j}\Bigg)\prod_{j=1}^{d-1}\big|1 - \mathrm{e}^{-u_{\gamma,j}-\mathrm{i}v_{\gamma,j}}\big|^2. \end{aligned} \tag{4.2}$$

The stability exponents $u_{\gamma,j}$ are related to the Lyapunov exponents $\lambda_{\gamma,j}$ of γ through $u_{\gamma,j} = \lambda_{\gamma,j} T_\gamma$ so that $u_{\gamma,j} \to \infty$ as $T_\gamma \to \infty$. Hence, in this limit one obtains the asymptotic relation

$$\frac{1}{|\det(\mathbb{M}_\gamma - \mathbb{1})|} \sim p_\gamma := \exp\Bigg(-\sum_{j=1}^{d-1} u_{\gamma,j}\Bigg). \tag{4.3}$$

Since the semiclassical limit of the periodic-orbit sum (3.19) is dominated by the contribution of long periodic orbits, equation (4.3) allows one to analyse (3.19) in terms of periodic-orbits sums that are familiar from equidistribution theorems of periodic orbits (see, e.g., [26]).

For the kind of Hamiltonian flows characterized above mean values of observables on Ω_E with respect to the Liouville measure can be calculated with the help of appropriate periodic-orbit sums. We postpone a detailed discussion of this matter to appendix B, from which we here only quote that for any continuous observable a one obtains the representation

$$\bar{a}^E := \int_{\Omega_E} a(\boldsymbol{p}, \boldsymbol{x})\,\mathrm{d}\mu_E(\boldsymbol{p}, \boldsymbol{x}) = \lim_{T\to\infty}\frac{1}{T}\sum_{\gamma,\,T_\gamma \leqslant T} T_\gamma\,\bar{a}^\gamma\,p_\gamma \tag{4.4}$$

where $\bar{a}^\gamma$ denotes an average of a along the periodic orbit γ,

$$\bar{a}^\gamma := \frac{1}{T_\gamma}\int_0^{T_\gamma} a\big(\Phi_H^t(\boldsymbol{p}, \boldsymbol{x})\big)\,\mathrm{d}t \qquad \text{with} \quad (\boldsymbol{p}, \boldsymbol{x}) \in \gamma. \tag{4.5}$$

We remark that a heuristic derivation of an analogous identity to (4.4) was given by Hannay and Ozorio de Almeida [14].

One can apply the relation (4.4) to determine the leading semiclassical behaviour of (3.19) once one has chosen a suitable observable a whose average $\bar{a}^\gamma$ yields the quantity $(\mathrm{tr}\, d_\gamma)^2$ appearing in (3.19). This, however, can only be achieved in an indirect manner. Our choice of the observable requires recalling the semiclassical time evolution of the spin degrees of freedom along the trajectories of the classical flow Φ_H^t. Let $d(\boldsymbol{p}, \boldsymbol{x}, t) \in SU(2)$ denote the solution of the spin transport equation [15, 16]

$$\dot{d}(\boldsymbol{p}, \boldsymbol{x}, t) + \mathrm{i}M(\Phi_H^t(\boldsymbol{p}, \boldsymbol{x}))\, d(\boldsymbol{p}, \boldsymbol{x}, t) = 0 \qquad d(\boldsymbol{p}, \boldsymbol{x}, 0) = \mathbb{1}_2 \tag{4.6}$$

where the time derivative is understood to be along the trajectory $\Phi_H^t(\boldsymbol{p}, \boldsymbol{x})$. M is a certain Hermitian and traceless 2×2 matrix valued function on Ω_E, whose precise form depends on the quantum Hamiltonian under consideration (see [16] for details). Geometrically, $d(\boldsymbol{p}, \boldsymbol{x}, t)$ can also be interpreted as a parallel transporter in some vector bundle so that $d(\boldsymbol{p}, \boldsymbol{x}, T_\gamma)$, with $(\boldsymbol{p}, \boldsymbol{x}) \in \gamma$, is the holonomy associated with the periodic orbit γ. Since its trace is invariant under a shift of the initial point $(\boldsymbol{p}, \boldsymbol{x}) \in \gamma$ along the orbit, one can introduce the notation $\mathrm{tr}\, d_\gamma := \mathrm{tr}\, d(\boldsymbol{p}, \boldsymbol{x}, T_\gamma)$. We are thus in a position to define the observable

$$a(\boldsymbol{p}, \boldsymbol{x}, t) := [\mathrm{tr}\, d(\boldsymbol{p}, \boldsymbol{x}, t)]^2 \tag{4.7}$$

which is a function on Ω_E that in addition depends on a parameter t. Due to the above remark concerning the interpretation of $d(\boldsymbol{p}, \boldsymbol{x}, T_\gamma)$ as a holonomy, the average (4.5) of this observable along a periodic orbit γ, when $t = T_\gamma$ is chosen, yields

$$\bar{a}^\gamma(T_\gamma) = \frac{1}{T_\gamma} \int_0^{T_\gamma} a\big(\Phi_H^{t'}(\boldsymbol{p}, \boldsymbol{x}), T_\gamma\big)\, \mathrm{d}t' = (\mathrm{tr}\, d_\gamma)^2 \tag{4.8}$$

for any $(\boldsymbol{p}, \boldsymbol{x}) \in \gamma$. Without the choice $t = T_\gamma$, however, $\bar{a}^\gamma(t)$ is not related to $(\mathrm{tr}\, d_\gamma)^2$. We can hence now employ (4.4) to deduce the asymptotic relation

$$\sum_{\gamma,\, T_\gamma \leqslant T} T_\gamma^2\, \bar{a}^\gamma(t)\, p_\gamma \sim \tfrac{1}{2} T^2\, \bar{a}^E(t) \qquad T \to \infty \tag{4.9}$$

which is valid for any t. Notice that here we have introduced an extra power of T_γ in the same manner as in (B.7) and (B.8). We now differentiate with respect to T,

$$\sum_\gamma T_\gamma^2\, \bar{a}^\gamma(t)\, p_\gamma\, \delta(T - T_\gamma) \sim T\, \bar{a}^E(t) \qquad T \to \infty \tag{4.10}$$

and then choose $t = T$. Together with (4.8) this allows one to conclude that

$$\sum_\gamma T_\gamma^2\, (\mathrm{tr}\, d_\gamma)^2\, p_\gamma\, \delta(T - T_\gamma) \sim T\, \bar{a}^E(T) \qquad T \to \infty. \tag{4.11}$$

Thus, at this point we have obtained the asymptotic relation

$$K_2^{diag}(\tau; T_H) \sim \bar{g}\, \tau\, \bar{a}^E(\tau T_H) \tag{4.12}$$

for the diagonal form factor (3.17) in the limit $T_H \to \infty$, $\tau \to 0$ such that $\tau T_H \to \infty$.

The remaining task therefore consists of determining the asymptotics of $\bar{a}^E(T)$ as $T \to \infty$. In order to achieve this one has to go back to the representation

$$\bar{a}^E(T) = \int_{\Omega_E} [\mathrm{tr}\, d(\boldsymbol{p}, \boldsymbol{x}, T)]^2\, \mathrm{d}\mu_E(\boldsymbol{p}, \boldsymbol{x}) \tag{4.13}$$

of $\bar{a}^E(T)$ as an average over phase space. Since the T dependence involves $d(\boldsymbol{p},\boldsymbol{x},T)$ one might anticipate that the limit $T\to\infty$ of (4.13) depends on certain ergodic properties of the spin dynamics. The latter being considered along trajectories of the translational dynamics, one hence has to combine both dynamics in a suitable way. In ergodic theory the relevant construction is known as a *skew product* (see, e.g., [27]). Appropriate ergodic properties of the skew product dynamics will then allow for a determination of the asymptotic behaviour of (4.13). Let us therefore now construct the skew product of translational and spin dynamics. To this end one defines a flow Y^t on the product phase space $\mathcal{M} := \Omega_E \times SU(2)$ in the following way:

$$Y^t((\boldsymbol{p},\boldsymbol{x}),g) := \left(\Phi^t_H(\boldsymbol{p},\boldsymbol{x}), d(\boldsymbol{p},\boldsymbol{x},t)g\right) \tag{4.14}$$

for $(\boldsymbol{p},\boldsymbol{x})\in\Omega_E$ and $g\in SU(2)$. The initial condition $Y^0((\boldsymbol{p},\boldsymbol{x}),g) = ((\boldsymbol{p},\boldsymbol{x}),g)$ is obviously fulfilled, and the composition law $Y^{t+t'} = Y^t\circ Y^{t'}$ immediately follows from the relation

$$d(\boldsymbol{p},\boldsymbol{x},t+t') = d(\Phi^{t'}_H(\boldsymbol{p},\boldsymbol{x}),t)\, d(\boldsymbol{p},\boldsymbol{x},t') \tag{4.15}$$

that can be concluded from (4.6). On $\mathcal{M}$ one then defines the direct product $\mu := \mu_E\times\mu_H$ of the Liouville measure μ_E and of the normalized Haar measure μ_H of $SU(2)$. We recall that the latter is the *unique* normalized left- and right-invariant positive Radon measure on the group manifold (see, e.g., [28]). Due to both the invariance of the Liouville measure under the Hamiltonian flow Φ^t_H and the left-invariance of the Haar measure, the product measure μ is invariant under Y^t. A dynamical system of this kind is known as an $SU(2)$ extension of Φ^t_H or, more generally, a skew product. The spin dynamics defined by (4.6) is then called a cocycle for Φ^t_H with values in $SU(2)$ (for further information see, e.g., [27]).

In addition to the assumptions made for Φ^t_H in section 3, in the following we will assume that Y^t is (strongly) mixing. This implies that for any $F\in L^2(\mathcal{M}\times\mathcal{M})$

$$\begin{aligned}\lim_{t\to\infty}\int_{\mathcal{M}} & F\left(Y^t((\boldsymbol{p},\boldsymbol{x}),g),((\boldsymbol{p},\boldsymbol{x}),g)\right)\mathrm{d}\mu((\boldsymbol{p},\boldsymbol{x}),g)\\ &= \int_{\mathcal{M}}\int_{\mathcal{M}} F(((\boldsymbol{p},\boldsymbol{x}),g),((\boldsymbol{\xi},\boldsymbol{y}),h))\,\mathrm{d}\mu((\boldsymbol{p},\boldsymbol{x}),g)\,\mathrm{d}\mu((\boldsymbol{\xi},\boldsymbol{y}),h).\end{aligned} \tag{4.16}$$

We remark that usually the mixing property is defined for pairs of functions $F_1, F_2\in L^2(\mathcal{M})$. However, if one views $L^2(\mathcal{M}\times\mathcal{M})$ as $L^2(\mathcal{M})\otimes L^2(\mathcal{M})$ and introduces a tensor-product basis, equation (4.16) follows immediately because every element of this basis fulfils the usual mixing property. If now the function F does not depend on the translational degrees of freedom, i.e. $F: SU(2)\times SU(2)\to\mathbb{R}$, the mixing property (4.16) yields

$$\lim_{t\to\infty}\int_{\mathcal{M}} F(d(\boldsymbol{p},\boldsymbol{x},t)g,g)\,\mathrm{d}\mu((\boldsymbol{p},\boldsymbol{x}),g) = \int_{SU(2)}\int_{SU(2)} F(g,h)\,\mathrm{d}\mu_H(g)\,\mathrm{d}\mu_H(h). \tag{4.17}$$

A suitable choice of the function F then allows one to determine the asymptotic behaviour of $\bar{a}^E(T)$ as $T\to\infty$ from (4.17). In order to achieve this we recall the representation (4.13) of $\bar{a}^E(T)$, which obviously can also be written as

$$\bar{a}^E(T) = \int_{SU(2)}\int_{\Omega_E}\left[\mathrm{tr}(d(\boldsymbol{p},\boldsymbol{x},T)gg^{-1})\right]^2\mathrm{d}\mu_E(\boldsymbol{p},\boldsymbol{x})\,\mathrm{d}\mu_H(g). \tag{4.18}$$

Upon now defining the function $F(g,h) := [\mathrm{tr}(gh^{-1})]^2$, $g,h\in SU(2)$, one can employ (4.17) to conclude that

$$\begin{aligned}\lim_{T\to\infty}\bar{a}^E(T) &= \lim_{T\to\infty}\int_{\mathcal{M}} F(d(\boldsymbol{p},\boldsymbol{x},T)g,g)\,\mathrm{d}\mu((\boldsymbol{p},\boldsymbol{x}),g)\\ &= \int_{SU(2)}\int_{SU(2)}[\mathrm{tr}(gh^{-1})]^2\,\mathrm{d}\mu_H(g)\,\mathrm{d}\mu_H(h).\end{aligned} \tag{4.19}$$

Substituting $g' = gh^{-1}$ in the inner integral and using the right-invariance of μ_H, the integrand no longer depends on h. Thus we obtain

$$\lim_{T\to\infty} \bar{a}^E(T) = \int_{SU(2)} [\operatorname{tr} g']^2 \, \mathrm{d}\mu_H(g') \tag{4.20}$$

i.e. in the limit $T \to \infty$ the expectation value of $[\operatorname{tr} d(\boldsymbol{p}, \boldsymbol{x}, T)]^2$, when averaged over phase space, can be computed by an average over the group $SU(2)$ with respect to the Haar measure.

The same obviously holds true for any moment of $\operatorname{tr} d(\boldsymbol{p}, \boldsymbol{x}, T)$ so that the asymptotic distribution of $\operatorname{tr} d(\boldsymbol{p}, \boldsymbol{x}, T)$, when the initial points $(\boldsymbol{p}, \boldsymbol{x}) \in \Omega_E$ are uniformly distributed with respect to μ_E, can be computed via

$$\lim_{T\to\infty} \mu_E\{(\boldsymbol{p}, \boldsymbol{x}) \in \Omega_E; \operatorname{tr} d(\boldsymbol{p}, \boldsymbol{x}, T) \in [a, b]\} = \int_a^b \int_{SU(2)} \delta(\operatorname{tr} g - w) \, \mathrm{d}\mu_H(g) \, \mathrm{d}w. \tag{4.21}$$

In order to evaluate the integral over $SU(2)$ explicitly we remark that any $g \in SU(2)$ can be represented as

$$g(u) = u_0 \mathbb{1}_2 + \mathrm{i}\boldsymbol{\sigma u} \qquad \text{with} \quad u = (u_0, \boldsymbol{u}) \in \mathbb{R}^4 \quad \text{and} \quad \sum_{j=0}^{3} u_j^2 = 1. \tag{4.22}$$

In this parametrization the Haar measure is given by (see, e.g., [28])

$$\mathrm{d}\mu_H(g(u)) = \frac{1}{\pi^2} \, \delta\left(\sum_{j=0}^{3} u_j^2 - 1 \right) \mathrm{d}^4 u. \tag{4.23}$$

A simple calculation now shows that the distribution (4.21) obeys a *semicircle law*, i.e. its density reads

$$p(w) = \int_{SU(2)} \delta(\operatorname{tr} g - w) \, \mathrm{d}\mu_H(g) = \begin{cases} \dfrac{1}{\pi} \sqrt{1 - \left(\frac{1}{2} w\right)^2} & -2 \leqslant w \leqslant +2 \\ 0 & \text{otherwise.} \end{cases} \tag{4.24}$$

What is required in (4.20) is the second moment of the distribution (4.21). With the help of (4.24) this can now easily be computed to yield one, i.e.

$$\bar{a}^E(T) \sim 1 \qquad \text{as} \quad T \to \infty. \tag{4.25}$$

The integrated version of (4.11) therefore reads

$$\sum_{\gamma,\, T_\gamma \leqslant T} T_\gamma^2 \, (\operatorname{tr} d_\gamma)^2 \, p_\gamma \sim \tfrac{1}{2} T^2 \qquad T \to \infty. \tag{4.26}$$

Furthermore, equations (4.12) and (4.25) imply the asymptotic behaviour

$$K_2^{diag}(\tau; T_H) \sim \bar{g}\tau \tag{4.27}$$

of the diagonal form factor in the regime $T_H \to \infty$, $\tau \to 0$, $\tau T_H \to \infty$.

5. Summary and conclusions

In section 3 we demonstrated how the two-point form factor for a quantum system with spin $\frac{1}{2}$ can be analysed semiclassically by making use of an appropriate trace formula. The diagonal approximation led us to the periodic-orbit sum (3.19) whose asymptotics determine the behaviour of the diagonal form factor for small τ in the semiclassical limit. Our conclusion (4.27) now has to be compared with the relevant random matrix results (2.19) and (2.21). To this end we have to distinguish time-reversal invariant quantum Hamiltonians from non-invariant ones. But let us first summarize our findings. In appendix A we show that quantum mechanical time-reversal invariance implies that not only the classical translational dynamics are time-reversal invariant but, moreover, the spin dynamics behave in such a way that the amplitudes $A_{\gamma,k}$ appearing in the semiclassical trace formula are also invariant under time reversal. This leads to the occurrence of the multiplicities $g_{\gamma,k}$ in the expression (3.19). Then, when the generic conditions stated at the end of section 3 are met, we can pull out the factors $g_{\gamma,k}$ from the sum and replace them by either $\bar{g} = 2$, if (quantum mechanical) time-reversal invariance is present, or else by $\bar{g} = 1$. If, furthermore, the translational dynamics are ergodic and hyperbolic, the equidistribution of periodic orbits allowed us to determine the spin contribution to the amplitudes $A_{\gamma,k}$. We further requested the skew product of the translational and the spin dynamics to be mixing. This then enabled us to identify the distribution of the traces of the spin-transport matrices and to calculate its second moment, which enters through the amplitudes $A_{\gamma,k}$.

Hence, if quantum mechanical time-reversal invariance is absent, the diagonal approximation (4.27) states that $K_2^{diag}(\tau; T_H) \sim \tau$, which is identical with the diagonal approximation in the case of Schrödinger operators [13] and coincides with the small-τ asymptotics of the GUE form factor (2.21). If, however, the quantum Hamiltonian is invariant under time reversal so that we have to choose $\bar{g} = 2$, the diagonal approximation becomes $K_2^{diag}(\tau; T_H) \sim 2\tau$. According to (2.17) Kramers' degeneracy then forces us to compare the random matrix form factor with the modified semiclassical result

$$\widetilde{K}_2^{diag}(\tau; T_H) = \tfrac{1}{2} K_2^{diag}\left(\tfrac{1}{2}\tau; T_H\right) \sim \tfrac{1}{2}\tau \tag{5.1}$$

which now coincides with the small-τ asymptotics of the GSE form factor (2.19). In both cases this is exactly the behaviour that is predicted by the conjecture of Bohigas, Giannoni and Schmit as stated in (2.20) and (2.18).

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Appendix A. Classical and quantum mechanical time reversal

In this appendix we are going to discuss the relation between classical and quantum mechanical time reversal for systems with spin $\frac{1}{2}$. We restrict our discussion to the conventional time-reversal operation that leaves the position coordinates unchanged and reverses momentum and spin coordinates as well as the time t. The discussion of generalized time-reversal operators that combine conventional time reversal with another unitary symmetry operation is analogous (see [21] for examples). To be specific we consider as a quantum Hamiltonian for a particle of mass m, charge e and spin $\frac{1}{2}$ either a Dirac Hamiltonian

$$\hat{H}_D = c\boldsymbol{\alpha}\left(\frac{\hbar}{\mathrm{i}}\nabla - \frac{e}{c}\boldsymbol{A}(\boldsymbol{x})\right) + \beta mc^2 + e\varphi(\boldsymbol{x}) \tag{A.1}$$

or a (generalized) Pauli Hamiltonian

$$\hat{H}_P = \hat{H}_S\,\mathbb{1}_2 + \hbar\,\boldsymbol{\sigma}\boldsymbol{C}\left(\frac{\hbar}{\mathrm{i}}\nabla, \boldsymbol{x}\right). \tag{A.2}$$

In the relativistic case (A.1) the Dirac algebra is realized by the 4×4 matrices

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix} \tag{A.3}$$

where $\boldsymbol{\sigma}$ denotes the vector of Pauli matrices and $\mathbb{1}_2$ is a 2×2 unit matrix. The non-relativistic Hamiltonian (A.2) is composed of a Schrödinger operator $\hat{H}_S$ and a coupling term of spin to the translational degrees of freedom. The latter has to be understood as the quantization of some $\mathbb{R}^3$-valued function $\boldsymbol{C}(\boldsymbol{p}, \boldsymbol{x})$ on phase space. For example, this can be a magnetic field, i.e. $\boldsymbol{C}_B(\boldsymbol{p}, \boldsymbol{x}) = -(e/2mc)\,\boldsymbol{B}(\boldsymbol{x})$, or a spin–orbit coupling term $\boldsymbol{C}_{so}(\boldsymbol{p}, \boldsymbol{x}) = [1/(4m^2c^2|\boldsymbol{x}|)][\mathrm{d}V(|\boldsymbol{x}|)/\mathrm{d}|\boldsymbol{x}|]\,(\boldsymbol{x} \times \boldsymbol{p})$.

For systems with spin $\frac{1}{2}$ the operator of time reversal is given by

$$\hat{T} := \mathrm{e}^{\mathrm{i}\frac{1}{2}\pi\sigma_y}\,\hat{K} = \mathrm{i}\,\sigma_y\hat{K} \tag{A.4}$$

where $\hat{K}$ is the operator of complex conjugation in position representation, see [21]. In the relativistic case, where $\hat{T}$ has to act on four-component spinors, equation (A.4) shall mean a block diagonal 4×4 matrix with two copies of (A.4) in the diagonal blocks. A quantum system with Hamiltonian $\hat{H}$ to be time-reversal invariant requires $\hat{T}\hat{H}\hat{T}^{-1} = \hat{H}$. Thus, in the case of a Dirac Hamiltonian (A.1)

$$\hat{T}\hat{H}_D\hat{T}^{-1} = c(-\boldsymbol{\alpha})\left(-\frac{\hbar}{\mathrm{i}}\nabla - \frac{e}{c}\boldsymbol{A}(\boldsymbol{x})\right) + \beta mc^2 + e\varphi(\boldsymbol{x}) \tag{A.5}$$

shows that conventional time-reversal invariance is equivalent to the absence of magnetic forces. For the Pauli Hamiltonian (A.2) to commute with $\hat{T}$ we first need the Schrödinger operator $\hat{H}_S$ to be time-reversal invariant, i.e. $\hat{K}\hat{H}_S\hat{K} = \hat{H}_S$. In addition, the condition

$$\hat{T}\boldsymbol{\sigma}\boldsymbol{C}\left(\frac{\hbar}{\mathrm{i}}\nabla, \boldsymbol{x}\right)\hat{T}^{-1} = -\boldsymbol{\sigma}\boldsymbol{C}\left(-\frac{\hbar}{\mathrm{i}}\nabla, \boldsymbol{x}\right) \stackrel{!}{=} \boldsymbol{\sigma}\boldsymbol{C}\left(\frac{\hbar}{\mathrm{i}}\nabla, \boldsymbol{x}\right) \tag{A.6}$$

has to be met, i.e. the coupling term $\boldsymbol{C}(\boldsymbol{p}, \boldsymbol{x})$ must be an odd function of momentum $\boldsymbol{p}$. This requirement is fulfilled by the spin–orbit coupling term $\boldsymbol{C}_{so}$, but is violated by the coupling $\boldsymbol{C}_B$ to an external magnetic field. In both the relativistic and the non-relativistic situation, however, even the presence of a magnetic field might allow for the existence of an anti-unitary operator representing a generalized time-reversal symmetry that commutes with the Hamiltonian (see [3, 21]).

We now want to investigate the implications of a quantum mechanical time-reversal invariance for the semiclassical analysis of the form factor. The first obvious consequence is a time-reversal invariance of the classical translational dynamics. But furthermore, also the spin dynamics, governed by the spin transport equation (4.6), exhibits a certain kind of symmetry under time reversal. In order to discuss the latter, one has to study the behaviour of the matrix M entering (4.6) under $\boldsymbol{x} \mapsto \boldsymbol{x}$, $\boldsymbol{p} \mapsto -\boldsymbol{p}$. For a Pauli Hamiltonian M is given by

$\boldsymbol{\sigma}\boldsymbol{C}(\boldsymbol{p},\boldsymbol{x})$, where $\boldsymbol{C}(\boldsymbol{p},\boldsymbol{x})$ is defined as above, and for a Dirac Hamiltonian with no magnetic field one finds $M = \boldsymbol{\sigma} g(|\boldsymbol{p}|)\, E(\boldsymbol{x}) \times \boldsymbol{p}$ (see [16] for details). In each case quantum mechanical time-reversal invariance therefore implies $M(-\boldsymbol{p},\boldsymbol{x}) = -M(\boldsymbol{p},\boldsymbol{x})$. Now substituting $t \mapsto -t$ and $\boldsymbol{p} \mapsto -\boldsymbol{p}$ in (4.6) one obtains

$$-\dot{d}(-\boldsymbol{p},\boldsymbol{x},-t) + \mathrm{i}M(\Phi_H^{-t}(-\boldsymbol{p},\boldsymbol{x}))\, d(-\boldsymbol{p},\boldsymbol{x},-t) = 0. \tag{A.7}$$

Since the translational dynamics are time-reversal invariant, M being odd in the momentum variable leads to

$$\dot{d}(-\boldsymbol{p},\boldsymbol{x},-t) + \mathrm{i}M(\Phi_H^{t}(\boldsymbol{p},\boldsymbol{x}))\, d(-\boldsymbol{p},\boldsymbol{x},-t) = 0 \tag{A.8}$$

and therefore $d(-\boldsymbol{p},\boldsymbol{x},-T_\gamma) = d(\boldsymbol{p},\boldsymbol{x},T_\gamma)$. Moreover, the fact that $d(\boldsymbol{p},\boldsymbol{x},T_\gamma) \in SU(2)$ is a holonomy implies $d(-\boldsymbol{p},\boldsymbol{x},-T_\gamma) = [d(-\boldsymbol{p},\boldsymbol{x},T_\gamma)]^{-1}$ so that finally $\operatorname{tr} d(-\boldsymbol{p},\boldsymbol{x},T_\gamma) = \operatorname{tr} d(\boldsymbol{p},\boldsymbol{x},T_\gamma)$. Altogether the above considerations confirm that the presence of a quantum mechanical time-reversal invariance implies that a primitive periodic orbit γ and its time-reversed partner share identical amplitudes $A_{\gamma,k}$.

Appendix B. Equidistribution of long periodic orbits

In this appendix we want to show how the periodic-orbit representation (4.4) of Liouville measure can be obtained from equidistribution properties of periodic orbits. The basic reference for the following is [26]. Our assumptions on the flow Φ_H^t are as stated in section 4.

In order to proceed further we first have to introduce some notation. Let $\mathcal{B}$ denote the set of all Φ_H^t-invariant Borel probability measures on Ω_E. Any $\mu \in \mathcal{B}$ can be associated with a metric entropy h_μ. Then for any Hölder-continuous observable $f \in C^\alpha(\Omega_E)$, with some $\alpha > 0$, the topological pressure is defined as

$$P(f) := \sup\left\{ h_\mu + \int_{\Omega_E} f\, \mathrm{d}\mu;\ \mu \in \mathcal{B} \right\}. \tag{B.1}$$

The supremum is attained for a unique measure μ_f, which is called the *equilibrium measure* for the observable f. The periodic orbits of the flow Φ_H^t are then equidistributed with respect to μ_f in the following sense:

$$\int_{\Omega_E} a(\boldsymbol{p},\boldsymbol{x})\, \mathrm{d}\mu_f(\boldsymbol{p},\boldsymbol{x}) = \lim_{T\to\infty} \frac{\sum_{\gamma,\,T_\gamma \leqslant T} T_\gamma\, \bar{a}^\gamma \exp(T_\gamma \bar{f}^\gamma)}{\sum_{\gamma,\,T_\gamma \leqslant T} T_\gamma \exp(T_\gamma \bar{f}^\gamma)} \tag{B.2}$$

for every $a \in C(\Omega_E)$. The averages over periodic orbits are defined as in (4.5).

In the next step one has to identify the Liouville measure as the equilibrium measure of some observable f. To this end we consider the tangential map $D\Phi_H^t$ restricted to the unstable sub-bundle E^u of the tangent bundle $T\Omega_E$ and define

$$f(\boldsymbol{p},\boldsymbol{x}) := -\frac{\mathrm{d}}{\mathrm{d}t} \log\det D\Phi_H^t(\boldsymbol{p},\boldsymbol{x})\Big|_{E^u,\,t=0}. \tag{B.3}$$

A direct calculation then yields

$$\bar{f}^\gamma = -\frac{1}{T_\gamma}\sum_{j=1}^{d-1} u_{\gamma,j} \qquad \text{so that} \quad \mathrm{e}^{T_\gamma \bar{f}^\gamma} = p_\gamma \tag{B.4}$$

(cf (4.3)). Furthermore, the equilibrium measure associated with the observable (B.3) is called the *Sinai–Ruelle–Bowen* measure μ_{SRB}, for which it is known that for every $a \in C(\Omega_E)$

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T a\big(\Phi_H^t(\boldsymbol{p},\boldsymbol{x})\big)\, \mathrm{d}t = \int_{\Omega_E} a(\boldsymbol{p}',\boldsymbol{x}')\, \mathrm{d}\mu_{SRB}(\boldsymbol{p}',\boldsymbol{x}') \tag{B.5}$$

holds for a set of initial conditions $(\boldsymbol{p}, \boldsymbol{x}) \in \Omega_E$ with positive Liouville measure (see [29] for more information). Since Φ_H^t is supposed to be ergodic with respect to μ_E, one concludes that $\mu_{SRB} = \mu_E$.

What is still lacking is an asymptotic estimate of the denominator on the right-hand side of (B.2). In order to obtain this we first have to introduce a regularization in that we multiply the observable (B.3) by some factor $\beta < 1$. Then we appeal to the relation

$$\sum_{\substack{\gamma \\ T-\varepsilon \leqslant T_\gamma \leqslant T+\varepsilon}} T_\gamma\, p_\gamma^\beta \sim \frac{\mathrm{e}^{P(\beta f)T}}{P(\beta f)} \left[\mathrm{e}^{P(\beta f)2\varepsilon} - 1\right] \qquad T \to \infty \tag{B.6}$$

(see [26]). Since $P(f) = 0$, in the limit $\beta \to 1$ one obtains for $k \in \mathbb{N}$

$$\sum_{\substack{\gamma \\ T-\varepsilon \leqslant T_\gamma \leqslant T+\varepsilon}} T_\gamma^k\, p_\gamma \sim 2\varepsilon\, T^{k-1} \qquad T \to \infty. \tag{B.7}$$

Now replacing ε by T, followed by the rescaling $2T \mapsto T$, this implies

$$\sum_{\substack{\gamma \\ T_\gamma \leqslant T}} T_\gamma^k\, p_\gamma \sim 2^{1-k}\, T^k \qquad T \to \infty. \tag{B.8}$$

Then introducing the relations (B.4) and (B.8) in (B.2) finally yields the periodic-orbit representation (4.4) of the Liouville measure.

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