The Gutzwiller Trace Formula for Quantum Systems with Spin

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Abstract. The Gutzwiller trace formula provides a semiclassical approximation for the density of states of a quantum system in terms of classical periodic orbits. In its original form Gutzwiller derived the trace formula for quantum systems without spin. We will discuss the modifications that arise for quantum systems with both translational and spin degrees of freedom and which are either described by Pauli- or Dirac-Hamiltonians. In addition, spectral densities weighted by expectation values of observables will be considered. It turns out that in all cases the semiclassical approximation yields sums over periodic orbits of the translational motion. Spin contributes via weight factors that take a spin precession along the translational orbits into account.

Thirty years ago, after several intermediate steps the Gutzwiller trace formula resulted from a detailed semiclassical investigation of the time evolution in quantum mechanics. It opened the way for the application of semiclassical methods to many problems that were so far believed to lie beyond the capability of semiclassics. The most prominent example being semiclassical quantisation rules for classically non-integrable systems, for which Einstein already in 1917 had shown that the usual Bohr-Sommerfeld type quantisation methods fail. Gutzwiller, however, devised a semiclassical expansion for the density of states in terms of a sum over the classical periodic orbits for a huge class of quantum systems, which in particular includes classically chaotic systems. Shortly afterwards, but seemingly independently, also mathematicians became interested in such trace formulae. They devised mathematical proofs for various versions of the trace formula, beginning with the work of Colin de Verdiere, and Duistermaat and Guillemin.

What was lacking so far, however, was a trace formula for quantum systems with a priori non-classical degrees of freedom as, e.g., spin. In such cases it is not immediately clear what the corresponding classical system is whose periodic orbits enter the trace formula, and how the non-classical degrees of freedom have to be taken into account. Even for systems with a classically integrable translational part there do not exist Bohr-Sommerfeld (or EBK) type quantisation rules for the eigenvalues of a Dirac-Hamiltonian, although already in 1932 Pauli began to generalise the WKB method to the Dirac equation. Pauli’s undertaking was only completed in 1963 by Rubinow and Keller, and it took again some 30 years before Emmrich and Weinstein proved that due to geometric obstructions for the Dirac equation EBK-
quantisation rules are generally impossible. It therefore seems to be especially
desirable to have a Gutzwiller trace formula for Dirac-Hamiltonians available.
Below we explain how one proceeds, if the Hamiltonian at hand describes a
quantum system with a spin 1/2 coupled to the translational motion, be it
a relativistic or a non-relativistic situation. The method that is used was de-
veloped in [9], where most of the details can be found that cannot be given
here.

1 Dirac- and Pauli-Hamiltonians

In the following we will consider relativistic and non-relativistic particles
with mass \( m \), charge \( e \) and spin 1/2 in external static electromagnetic fields
\( \mathbf{E}(x) = -\nabla \varphi(x) \) and \( \mathbf{B}(x) = \nabla \times \mathbf{A}(x) \). In the relativistic case the quantum
dynamics are generated by a Dirac-Hamiltonian

\[
\hat{H}_D = c \alpha \cdot \left( \frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A}(x) \right) + mc^2 \beta + e\varphi(x),
\]

(1)

where \( \alpha = (\alpha_1, \alpha_2, \alpha_3) \) and \( \beta = \alpha_0 \) are hermitian \( 4 \times 4 \) matrices satisfying
the algebraic relations \( \alpha_\mu \alpha_\nu + \alpha_\nu \alpha_\mu = 2 \delta_{\mu\nu} \). In Dirac representation they
read

\[
\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \quad \text{and} \quad \alpha_0 = \beta = \begin{pmatrix} 1_2 & 0 \\ 0 & -1_2 \end{pmatrix},
\]

(2)

where \( \sigma = (\sigma_1, \sigma_2, \sigma_3) \) denotes the Pauli matrices and \( 1_2 \) is a \( 2 \times 2 \) unit
matrix. As it is well known, in leading non-relativistic order \( \hat{H}_D \) is replaced
by the Pauli-Hamiltonian

\[
\hat{H}_P = \left[ \frac{1}{2m} \left( \frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A}(x) \right)^2 + e\varphi(x) \right] 1_2 - \frac{e\hbar}{2mc} \mathbf{B}(x) \cdot \sigma.
\]

(3)

For further information, see [10]. We remark that for the following the explicit
form of the right-most term in (3), describing a coupling of spin to the
translational degrees of freedom, is inessential. It can be any operator of the
form \( \hbar C(\frac{\hbar}{i} \nabla, x) \cdot \sigma \), where the components of \( C(p,x) \) are suitable functions
on phase space; e.g., \( C(p,x) = \frac{1}{4mc^2|p|} d\varphi(|x|)(x \times p) \) would yield a spin-orbit
coupling in a spherically symmetric potential.

In applications one is sometimes also interested in describing a coupling
of spin and translational degrees of freedom that is semiclassically strong. In
this case one would consider a (Pauli-) Hamiltonian of the form

\[
\hat{H}_{P'} = \left[ \frac{1}{2m} \left( \frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A}(x) \right)^2 + e\varphi(x) \right] 1_2 + D \left( \frac{\hbar}{i} \nabla, x \right) \cdot \sigma,
\]

(4)

where again the components \( D_k(p,x) \) are suitable functions on phase space
(independent of \( \hbar \)).
1.1 Weyl Representation

All of the above Hamiltonians can be represented as Weyl operators, i.e., their action on \( n \)-component spinors \( \psi(x) = (\psi_1(x), \ldots, \psi_n(x))^T \), where \( n = 4 \) applies to the case of Dirac spinors and \( n = 2 \) to Pauli spinors, can be given as

\[
\hat{H}\psi(x) = \frac{1}{(2\pi\hbar)^3} \int \int H\left(p, \frac{x+y}{2}\right) e^{ip\cdot(x-y)} \psi(y) \, dp \, dy .
\]

On the right-hand side the Weyl symbol \( H(p, x) \) is a function on phase space taking values in the hermitian \( n \times n \) matrices. For the Hamiltonians (1),(3) and (4) these arise upon replacing \( \frac{i}{\hbar} \nabla \) by \( p \).

In the case of the Dirac-Hamiltonian (1) the symbol \( H_D(p, x) \) is a hermitian \( 4 \times 4 \) matrix with the two doubly degenerate eigenvalues

\[
H^\pm(p, x) = e^{\varphi(x)} \pm \sqrt{(cp - eA(x))^2 + m^2c^2} .
\]

These eigenvalues can be recognized as the classical relativistic Hamiltonians for spinless particles (+) and anti-particles (−). The fact that the corresponding eigenspaces are two dimensional reflects the quantum mechanical spin 1/2 of the particles and anti-particles. More precisely, at each point \( (p, x) \) of phase space the eigenspaces of \( H_D(p, x) \) can be viewed as Hilbert spaces of a spin \( 1/2 \), one for particles and one for anti-particles. See [9] for further details.

The situation is similar for the Pauli-Hamiltonian (3), except for the absence of anti-particles: \( H_P(p, x) \) is a hermitian \( 2 \times 2 \) matrix,

\[
H_P(p, x) = \frac{1}{2m} \left( p - \frac{e}{c} A(x) \right)^2 + e\varphi(x) + \frac{\hbar}{2mc} B(x) \cdot \sigma ,
\]

whose classical part (independent of \( \hbar \)) is proportional to \( 1_2 \). This principal symbol therefore has one doubly degenerate eigenvalue, \( H_0(p, x) \), which simply is the factor multiplying \( 1_2 \). It can readily be identified as the classical non-relativistic Hamiltonian for spinless particles. As in the previous case spin is represented by the corresponding two dimensional eigenspace of the principal symbol, which in this case is trivial.

The Hamiltonian (4), however, leads to a different interpretation of its symbol,

\[
H_P'(p, x) = \frac{1}{2m} \left( p - \frac{e}{c} A(x) \right)^2 + e\varphi(x) + D(p, x) \cdot \sigma ,
\]

since this is independent of \( \hbar \) and thus has to be considered as a classical quantity in its entirety. Its two eigenvalues

\[
H^{1/2}(p, x) = \frac{1}{2m} \left( p - \frac{e}{c} A(x) \right)^2 + e\varphi(x) \pm |D(p, x)|
\]

(9)
are classical non-relativistic Hamiltonians of a particle with fixed spin up or down, respectively. Here ‘up’ and ‘down’ are defined with respect to the direction of \( \mathbf{D} \) at the respective point \((\mathbf{p}, \mathbf{x})\) in phase space. The eigenvalues are non-degenerate as long as they are different, i.e., away from mode conversion points where \( \mathbf{D}(\mathbf{p}, \mathbf{x}) = 0 \).

From the above discussions one may anticipate that in the semiclassical considerations of the Hamiltonians (1) and (3) to follow (see also [9]) there will occur classical translational dynamics that are uninfluenced by spin, and quantum mechanical spin dynamics driven by the classical translational motion. In contrast, in the case of the Hamiltonian (4) the classical translational motion will depend on the (fixed) direction of the spin and there will be no additional spin dynamics.

1.2 Spectra

Gutzwiller’s trace formula provides a semiclassical expansion for the quantum mechanical density of states. Since this quantity a priori requires a Hamiltonian with a discrete spectrum, we now want to discuss the spectra of the Hamiltonians (1), (3) and (4).

Dirac-Hamiltonians typically possess continuous spectra. Indeed, if the electromagnetic fields vanish as \(|\mathbf{x}| \to \infty\), \( \hat{H}_D \) has an essential spectrum consisting of two half axes, \((-\infty, -mc^2] \cup [+mc^2, +\infty)\), see [10] for precise statements. Thus, since we are interested in the discrete spectrum of a Hamiltonian, we have to localise in energy to within the gap \((-mc^2, +mc^2)\) of the essential spectrum. To this end one can choose a smooth function \( \chi(E) \) that vanishes outside of some interval contained in \((-mc^2, +mc^2)\) and then considers the Hamiltonian \( \chi(\hat{H}_D) \). This now has a purely discrete spectrum with eigenvalues \( \chi(E_n) \), if the \( E_n \)'s are the eigenvalues of \( \hat{H}_D \) with \(|E_n| < mc^2\).

The same procedure can be applied to the other Hamiltonians, if situations arise where their spectra are not purely discrete or when one is only interested in certain spectral stretches. For the purpose of deriving a semiclassical trace formula one then considers a truncated time evolution operator

\[
\hat{U}_\chi(t) = e^{-\frac{i}{\hbar} \hat{H}_\chi t} \chi(\hat{H}),
\]

whose spectral expansion in position representation reads

\[
K_\chi(\mathbf{x}, \mathbf{y}, t) = \langle \mathbf{x} | \hat{U}_\chi(t) | \mathbf{y} \rangle = \sum_n \chi(E_n) \psi_n(\mathbf{x}) \psi_n(\mathbf{y})^\dagger e^{-\frac{i}{\hbar} E_n t},
\]

where \( \psi_n(\mathbf{x}) \) denotes the eigenspinor of \( \hat{H} \) associated with \( E_n \).

The Gutzwiller trace formula has found many applications in the field of quantum chaos [2,11] in which the principal questions are associated with the distribution of eigenvalues and eigenfunctions of quantum Hamiltonians in relation to properties of the corresponding classical dynamics. In this context
one first confines oneself to some spectral interval $I$ that contains $N_I < \infty$ eigenvalues; universal statistical properties then emerge in the semiclassical limit $N_I \to \infty$. Here we implement this procedure by first choosing an interval

$$I = [E - \hbar \omega, E + \hbar \omega] ,$$

(12)

and then performing the limit $\hbar \to 0$; and although the length of $I$ shrinks to zero, $N_I$ diverges in this limit (see below). In this approach the localisation in energy described above hence appears to be very natural.

1.3 Observables

The quantum mechanical observables we consider are (bounded) Weyl operators, i.e., they can be represented as in (\textsuperscript{5}). Their symbols $B(p, x)$ are then functions on phase space taking values in the hermitian $n \times n$ matrices, and we suppose that they allow for asymptotic expansions in $\hbar$,

$$B(p, x) \sim \sum_{k \geq 0} \hbar^k B_k(p, x) .$$

(13)

The precise meaning of such expansions is explained in [12]. The $\hbar$-independent term $B_0(p, x)$, the principal symbol of the operator $\hat{B}$, represents the classical observable associated with $\hat{B}$, at least concerning the translational degrees of freedom. Expectation values of observables can be represented in terms of the symbol once one introduces a matrix valued Wigner transform of a spinor $\psi(x) = (\psi_1(x), \ldots, \psi_n(x))^T$ through

$$W[\psi]_{kl}(p, x) := \int e^{-\frac{i}{\hbar} p \cdot y} \psi_k(x - \frac{1}{2} y) \psi_l(x + \frac{1}{2} y) \, dy .$$

(14)

Then

$$\langle \psi, \hat{B} \psi \rangle = \frac{1}{(2\pi \hbar)^3} \int \int \text{tr} (W[\psi](p, x) B(p, x)) \, dp \, dx .$$

(15)

2 Trace Formula

Gutzwiller’s approach to the trace formula \textsuperscript{[2]} was to depart from a semiclassical expansion of the time evolution operator in position representation (\textsuperscript{11}). Expressing this in terms of a Feynman path integral and evaluating it in leading semiclassical order with the method of stationary phase, he arrived at a representation of the kernel $K(x, y, t)$ in terms of a sum over the classical trajectories connecting $y$ and $x$ in time $t$. In this context he made the important observation \textsuperscript{[13]} that for not too small times $t$ each term in this sum must contain an extra phase factor that essentially consists of the Morse index of this trajectory.
Here we are interested in a trace formula for quantum systems with spin that yields a semiclassical expansion of a weighted and smeared spectral density, where the weights are provided by the expectation values of an observable $\hat{B}$ in the eigenstates of the Hamiltonian and the smearing ensures convergence of the sums involved, see also [14]. To this end the 'spectral' side of the trace formula is given by

$$
\sum_n \chi(E_n) \langle \psi_n, \hat{B} \psi_n \rangle \rho \left( \frac{E_n - E}{\hbar} \right) = \text{Tr} \frac{1}{2\pi} \int_{-\infty}^{+\infty} \hat{\rho}(t) e^{\frac{\hbar}{i} E t} \hat{B} \hat{U} \chi(t) \, dt .
$$

In this expression $\rho(E)$ is a smooth, regularising function with Fourier transform $\tilde{\rho}(t)$ that is also smooth and vanishes outside of some compact interval.

The trace on the right-hand side will now be calculated in position representation, after the leading semiclassical order of (11), i.e., the appropriate Van Vleck-Gutzwiller propagator, has been introduced.

### 2.1 Van Vleck-Gutzwiller Propagator

In an alternative approach to Gutzwiller’s semiclassical expansion of the propagator ([13]), making use of a Feynman path integral, one represents the kernel in a way that is closely related to the WKB method. More precisely, one chooses the ansatz

$$
K(x, y, t) = \frac{1}{(2\pi \hbar)^3} \int \sum_{k \geq 0} \left( \frac{\hbar}{i} \right)^k a_k(x, y, t, \xi) \, e^{\frac{\hbar}{i} (S(x, \xi, t) - y \cdot \xi)} \, d\xi ,
$$

and determines the phase $S(x, \xi, t)$ and the coefficients $a_k(x, y, t, \xi)$ of the amplitude by requiring that $K(x, y, t)$ solves the Schrödinger (Dirac, Pauli) equation to arbitrary powers in $\hbar$ with an appropriate initial condition at $t = 0$. In the cases of the quantum Hamiltonians (1), (3) and (4) it turns out that the corresponding phases $S(x, \xi, t)$ have to be solutions of Hamilton-Jacobi equations with $H^\pm(p, x)$, $H_0(p, x)$ and $H^{1/2}(p, x)$, respectively, as classical Hamiltonians (see (6)–(9)). The matrix valued coefficients $a_k(x, y, t, \xi)$ of the amplitudes are determined by a hierarchy of (transport) equations that can be solved order by order in $\hbar$, starting with the leading expression $a_0(x, y, t, \xi)$, which apart from the contribution of the translational motion contains the leading order of the spin dynamics. Knowing the solutions $S(x, \xi, t)$ and $a_0(x, y, t, \xi)$, one then still has to evaluate the integral (17) over $\xi$ with the method of stationary phase. The details of this calculation can be found in [11].

Since $S(x, \xi, t)$ is a solution of a Hamilton-Jacobi equation, it is a generating function of a canonical transformation, $(p, x) \mapsto (\xi, z)$. Here $p = \nabla_x S(x, \xi, t)$ and $z = \nabla_\xi S(x, \xi, t)$, such that $(\xi, z)$ and $(p, x)$ are starting and end points, respectively, of a solution of the equations of motion generated by the respective classical Hamiltonian. The stationary points $\xi_{st}$ of the
phase in (15) are now uniquely related to classical trajectories from $y$ to $x$, since the condition of stationarity reads $y = \nabla \xi S(x, \xi_{st}, t)$. The stationary point $\xi_{st}$ itself hence is the momentum of the associated trajectory at time zero. Thus the sum over the stationary points leads to a sum over classical trajectories; see (7) for the explicit form of these sums. In the cases of the Dirac- and Pauli-Hamiltonians (1) and (3) the trajectories that contribute are purely translational without contributions from spin (since the respective classical Hamiltonians contain no spin). The latter only contributes through weight factors that come from the leading term $a_0(x, y, t, \xi_{st})$ of the amplitude. Since this is evaluated at the stationary point $\xi_{st}$, the spin contribution derives from a precession along the associated classical trajectory. For a further discussion see also the next subsection; more details are described in (9).

Only in the case of the Hamiltonian (4) is the spin already directly contained on a classical level, see (9). Here one has to deal with the (two) translational dynamics of a particle whose spin is tight to the direction of the external ‘field’ $D$, such that it follows this direction adiabatically along the trajectories of the particle. This adiabatic motion of the spin is reflected in the occurrence of a certain geometric phase, which has in the context of a Bohr-Sommerfeld quantisation been introduced by Littlejohn and Flynn (15), see also (9,16) for a discussion in the context of a trace formula.

### 2.2 Semiclassical Spin Transport

In the cases of the Dirac- and Pauli-Hamiltonians (1) and (3) there indeed is a dynamics of the spin degrees of freedom, which is driven by the classical translational motion. These driven dynamics derive from the transport equation for the lowest order amplitude $a_0(x, y, t, \xi_{st})$ after separation of the purely translational part. The spin transport equation that hence results reads

$$d(p, x, t) + i C(p(t), x(t)) \cdot \sigma d(p, x, t) = 0,$$

with initial condition $d(p, x, 0) = 1_2$. Its solution, the spin transport matrix $d(p, x, t) \in SU(2)$, propagates the (quantum) spin 1/2 along the classical trajectory $(p(t), x(t))$ starting at $(p, x)$. The vector $C(p, x)$ depends on which Hamiltonian one considers and contains the fields $E$ and $B$; for a Pauli-Hamiltonian $\hat{H}_P$ the quantity $C$ is precisely the one described below (3). Moreover, if the vector $s(t)$ denotes the expectation value of the (normalised) spin operator $\sigma$ in a two-component spinor $u(t) = d(p, x, t) u(0)$, this ‘classical’ spin obeys the equation

$$\dot{s}(t) = C(p(t), x(t)) \times s(t)$$

of classical spin precession and thus provides an Ehrenfest relation for the spin. In the relativistic case (16) yields the well known Thomas precession,
which Rubinow and Keller \cite{rubinow} were the first to derive semiclassically from the Dirac equation.

One can now combine the Hamiltonian translational motion and the spin dynamics that are driven by the former one into a single dynamical system on a combined phase space, \( \langle p(0), x(0), s(0) \rangle \mapsto \langle p(t), x(t), s(t) \rangle \). In ergodic theory such combinations are known as ‘skew products’ of the two types of dynamics. In applications to quantum chaos the ergodic properties of precisely these combined dynamics determine the ‘quantum chaotic’ properties of the quantum system, see \cite{berkolaiko, berthier, burak}.

### 2.3 Semiclassical Trace Formula

As mentioned earlier, the ‘semiclassical side’ of the trace formula emerges upon introducing the leading semiclassical order of the propagator \( \langle 1 \rangle \) on the right-hand side of \( (16) \) and evaluating all integrals, which involve the variables \( (\xi, x, t) \), with the method of stationary phase. Since this method requires all stationary points \( (\xi_{st}, x_{st}, t_{st}) \) to be non-degenerate, the trace formula can only be derived under appropriate conditions on the classical systems. In particular, since the stationary points are such that the phase space points \( (\xi_{st}, x_{st}) \) lie on a periodic orbit with energy \( E \) (that appears on the left-hand side of \( (16) \)) and period \( t_{st} \), the conditions have indeed to be imposed on the periodic orbits. One such condition is that \( E \) must not be a critical value of the relevant classical Hamiltonians, i.e., \( (\nabla_p H(p, x), \nabla_x H(p, x)) \neq 0 \) for all \( (p, x) \) on the energy shell \( \Omega_E = \{ (p, x); H(p, x) = E \} \). This condition ensures that all stationary points with \( t_{st} = 0 \) are non-degenerate. The corresponding points \( (\xi_{st}, x_{st}) \) make up all of the energy shell \( \Omega_E \) and the contribution of these stationary points yields the leading semiclassical term (also called Weyl term) on the right-hand side of the trace formula.

For the following we restrict our attention to the case where all non-trivial periodic orbits \( \gamma \) (i.e., \( T_\gamma = t_{st} \neq 0 \)) are isolated and non-degenerate. This means that their monodromy matrices \( M_\gamma \), describing the linear stability of the orbits, have no eigenvalues one. This does not exclude elliptic orbits, if these are isolated, but only parabolic (marginally stable) ones. Furthermore, we give the trace formula explicitly for the case of a Dirac-Hamiltonian \( \hat{H} \) and with the inclusion of an observable \( \hat{B} \). The other cases follow from this trace formula by specialising to the appropriate simplified situations; e.g., the Pauli-Hamiltonian \( \hat{H} \) has no contribution from anti-particles and therefore only contains one type of (translational) classical dynamics. In contrast, the Hamiltonian \( \hat{H} \) does lead to two types of classical dynamics, generated by \( \hat{B} \), but has no independent spin dynamics; there only is an additional
geometric phase as described in \[15,16,9\]. Now the trace formula reads

\[
\sum_n \chi(E_n) \langle \psi_n, \hat{B} \psi_n \rangle \rho \left(\frac{E_n - E}{\hbar}\right) = \tilde{\rho}(0)^2 / (2\pi) \chi(E) \left(\frac{2\pi \hbar}{2}\right)^3 (2 \text{ vol } \Omega_{\pm}^E + \text{tr } \hat{B}_0^E + 0 \text{E} - \text{tr } \hat{B}_0^E) + O(\hbar^{-1})
\]

\[+ \sum_{\gamma^\pm} \chi(E) \left(\frac{T_{\gamma^\pm}(T_{\gamma^\pm})}{2\pi} \text{tr } \hat{B}_0^\gamma^\pm A_{\gamma^\pm} e^{iS_{\gamma^\pm}(E)} (1 + O(\hbar))\right).\]

The first term on the right-hand side is the so-called Weyl term and yields the leading semiclassical approximation of the left-hand side. It essentially contains the averages \(\overline{B}_0^E\) of the principal symbol \(B_0(p, x)\) of the observable over the two energy shells \(\Omega_{\pm}^E\). The two contributions are weighted according to the relative volumes of the respective energy shells. The characteristic quantities appearing in the sum over the two types \(\gamma^\pm\) of periodic orbits are the same as in the case of the Gutzwiller trace formula for the spectral density of a quantum system without spin: there is an exponential factor with the actions \(S_{\gamma^\pm}(E)\), and an amplitude that contains the well known part

\[
A_{\gamma^\pm} = \frac{T_{\gamma^\pm}^{\text{prim}} e^{-i\Phi_{\mu_{\gamma^\pm}}}}{|\det(M_{\gamma^\pm} - 1)|^{1/2}},
\]

with the associated primitive period, the Maslov index \(\mu_{\gamma^\pm}\), and the stability denominator. The additional factors come from the regularisation and from the presence of the observable. In particular, \(\overline{B}_0^\gamma^\pm\) denotes an average of the projection of \(B_0(p, x)\) to one of the eigenspaces corresponding to the eigenvalues \(E\), weighted with the spin transport matrix \(d(p, x, t)\), along the periodic orbit \(\gamma^\pm\). Details of this average are described in \[14\].

A trace formula for a truncated spectral density, with only contributions from the discrete spectrum of \(\hat{H}_D\), can be obtained from (20) by choosing the observable \(\hat{B} = \text{id}\) and removing the regularisation provided by the function \(\rho\). The result is

\[
d\chi(E) = \sum_n \chi(E_n) \delta(E_n - E)
\]

\[
= \chi(E) \frac{2 \text{ vol } \Omega_{\pm}^E + 2 \text{ vol } \Omega_{-\pm}^E}{(2\pi \hbar)^3} + O(\hbar^{-2})
\]

\[+ \frac{\chi(E)}{2\pi \hbar} \sum_{\gamma^\pm} T_{\gamma^\pm}^{\text{prim}} \text{tr } d_{\gamma^\pm} e^{iS_{\gamma^\pm}(E) - i\Phi_{\mu_{\gamma^\pm}}} (1 + O(\hbar))\]

where here \(d_{\gamma^\pm}\) denotes the spin transport matrix associated with the transport of spin once along the periodic orbit. One immediately observes that in contrast to the Gutzwiller trace formula without spin two types of classical
dynamics (particles and anti-particles) occur, and spin contributes a factor of two in the Weyl term as well as weights $\text{tr} d_{\gamma}^2$ for the periodic orbits describing the effect of spin transport.

Obviously, the Weyl term in (22) yields the semiclassically leading contribution to the spectral density. This allows to derive the leading semiclassical asymptotics of the number $N_I$ of eigenvalues in the interval $[\omega]$, which is given by $2\hbar \omega$ times the Weyl term, and hence $N_I$ diverges as $\hbar^{-2}$ in the semiclassical limit.

3 Applications

Many applications of the Gutzwiller trace formula originate from problems in the field of quantum chaos (see, e.g., [2,11]). Apart from the question for semiclassical quantisation rules (see, e.g., [20]) one of the major successes in this field was Berry’s semiclassical analysis of spectral two-point correlations [21] based on the trace formula. In a certain range of validity, which stems from the so-called diagonal approximation Berry employed, he verified that the two-point correlations of energy levels of classically chaotic quantum systems (without spin) follow the predictions of random matrix theory (RMT). Subsequently, Bogomolny and Keating [22] extended Berry’s result in that they went one step beyond the diagonal approximation.

The first application of trace formula techniques, without, however, having a complete trace formula available, to quantum systems with spin goes back to Frisk and Guhr [14]. They considered a quantum Hamiltonian of the type (1) describing spin-orbit coupling in certain billiards. In spirit, they applied the trace formula in ‘reverse direction’ in that they used quantum energy levels in order to obtain information about the contribution of various types of periodic orbits. Similar studies can be found in [23].

A second type of applications concerns an extension of the semiclassical analysis of spectral two-point correlations to quantum systems with spin 1/2. If a time-reversal symmetry is present, Kramers’ degeneracy implies that all energy levels of a quantum system with half-integer spin are doubly degenerate. After removal of this systematic multiplicity, the spectral statistics should be described by the Gaussian symplectic ensemble (GSE) of RMT, if the corresponding classical system is chaotic. Without time-reversal symmetry Kramers’ degeneracy is absent, and the relevant ensemble of RMT is the Gaussian unitary one (GUE). In [17] Berry’s semiclassical approach is carried out with the trace formula (20), or (22), as a basis. It is shown that, within the same range of validity as in [21], indeed the two-point correlations agree with the GSE or GUE, respectively. Moreover, in [24] the Bogomolny-Keating method is carried over to the case of spin 1/2, with the same findings. In both studies, apart from a chaotic translational motion, ergodic properties of the combined dynamics described below (19) are needed in order to obtain an agreement with the RMT predictions.
The Weyl term of the trace formula (20) moreover allows to determine a semiclassical average of the expectation values \( \langle \psi_n, \hat{B} \psi_n \rangle \) in eigenstates of \( \hat{H}_D \) with \( E_n \in I \). The result is given by (14)

\[
\lim_{\hbar \to 0} \frac{1}{N_I} \sum_{E_n \in I} \langle \psi_n, \hat{B} \psi_n \rangle = \frac{1}{2} \frac{\text{vol} \Omega^+ E \text{tr} B^+_0 + \text{vol} \Omega^- E \text{tr} B^-_0}{\text{vol} \Omega^+ E + \text{vol} \Omega^- E},
\]

and does not require the classical system to be chaotic. The only requirement is that the set of periodic orbits on both energy shells must be of measure zero, which is a comparatively weak condition. Only if one requires individual expectation values to approach the expression on the right-hand side of (23) as \( \hbar \to 0 \) one needs a stronger condition on the classical side, since then no cancelations on the left-hand side are allowed. For the case of Pauli-Hamiltonians (3) it has been proven (18) (see also (19)) that almost all expectation values indeed converge to the equivalent of the right-hand side of (23), if the combined dynamics of translational and spin degrees of freedom are ergodic. For quantum systems without spin such a result had been known before under the notion of quantum ergodicity (see, e.g., (25)).

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