PERIODIC ORBIT THEORY INCLUDING SPIN DEGREES OF FREEDOM *

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We summarize recent developments of the semiclassical description of shell effects in finite fermion systems with explicit inclusion of spin degrees of freedom, in particular in the presence of spin-orbit interactions. We present a new approach that makes use of spin coherent states and a correspondingly enlarged classical phase space. Taking suitable limits, we can recover some of the earlier approaches. Applications to some model systems are presented.

1. Introduction

The periodic orbit theory (POT), initiated over 30 years ago by Gutzwiller, is a semiclassical approach in which the level density of a quantum system is approximated in terms of the periodic orbits of the corresponding classical system through the so-called ‘trace formula’. It has provided a great stimulus to the research area of quantum chaos, but is also applicable to integrable and nearly integrable systems. Although originally developed to describe the motion of a particle bound in a given external potential or an ideally reflecting boundary (a so-called ‘quantum billiard’), the POT can also be applied to describe the quantum oscillations (shell-corrections) in many-fermion systems within the mean-field approximation. For a general introduction to the POT and its applications in nuclear, mesoscopic and nanostructure physics, we refer to a recent text book.

An early application to nuclear physics consisted in a successful semiclassical explanation of the systematics of ground-state deformations. An corresponding investigation was recently carried out also for metal clusters. The onset of the mass asymmetry in the fission of actinide nuclei could also be explained semiclassically. Fig. 1 shows the shell-correction energy around the outer fission

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barrier of $^{240}$Pu, plotted versus the elongation parameter $c$ and the mass asymmetry parameter $\alpha$. The 3d plot to the left and the contour plots to the extreme right were obtained within the POT in terms of the (few) shortest periodic orbits, modeling the nucleus by axially symmetric cavities (see shapes to the extreme left),\cite{12} whereas the contour plots next to the right are the old quantum-mechanical results using realistic deformed nuclear shell-model potentials.\cite{14}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Shell-correction energy of $^{240}$Pu near fission isomer and outer barrier vs. elongation $c$ and mass asymmetry $\alpha$. Left: 3d plot of semiclassical POT calculation,\cite{12} along with the shapes at isomer minimum (A), asymmetric saddle (B), and on the way towards scission (C) (perpendicular lines indicate planes containing the shortest periodic orbits). Right: contour plot for neck parameter $h = 0$ (upper panels) and $h = -0.075$ (lower panels). The left panels show the quantum-mechanical calculations with realistic Woods-Saxon potentials including pairing correlations and spin-orbit interaction;\cite{14} the right panels show the semiclassical POT calculation for simple cavities.\cite{12}}
\end{figure}

We can see that, in spite of the simplicity of the cavity model (with only one kind of nucleons, neglecting pairing and spin-orbit interactions), the semiclassical calculation reproduces almost quantitatively the correct topology of the deformation energy surface and, in particular, predicts correctly the mass-asymmetric adiabatic fission path. The latter, indicated by the white dotted line, is simply given by the principle of stationary action of the shortest periodic orbits. The wavefunctions of the single-particle states, which are quantum-mechanically responsible for the lowering of the barrier due to the asymmetry, were found to have their maxima exactly in the planes containing the shortest periodic orbits that dominate the asymmetry effect semiclassically.\cite{13}

That the classical motion of the nucleons at these deformations is almost chaotic can be seen in Fig. 2. Here we show Poincaré surfaces of section, obtained for angular momentum $L_z = 0$, taken at the symmetric outer barrier (left) and at the asymmetric saddle (right); the corresponding shapes with the planes containing the shortest periodic orbits are shown on top of each plot. The regular motion is confined to small islands, containing the relevant periodic orbits, surrounded by a chaotic sea. Note that the energetically favored asymmetric shape has much smaller regular islands than the symmetric shape. Nevertheless, the shell effect coming from
these small regular regions of the classical dynamics is sufficiently strong to cause
the collective asymmetry effect of the system.

Fig. 2. Poincaré surfaces of section $p$ (parallel momentum at reflection point) vs. $\phi$ (polar angle of reflection point) for angular momentum $L_z = 0$ of the cavities corresponding to the symmetric outer barrier (left, $c = 1.53$, $\alpha = 0$) and to the asymmetric saddle (right, $c = 1.53$, $\alpha = 0.13$). The corresponding shapes and the planes containing the shortest orbits (vertical lines) are shown above the corresponding Poincaré plots.\textsuperscript{13}

This example illustrates the strength of the semiclassical theory in explaining qualitatively (and, at times, even semi-quantitatively) important quantum effects, both in one-body and in many-body systems, in terms of classical dynamics.

One aspect has, however, been neglected so far in the applications of the POT to nuclei: the spin of the nucleons. We know well that the spin-orbit interaction dramatically modifies the shell effects – that is, after all, why it had to be introduced to make the nuclear shell model work in the first place.\textsuperscript{15} In the semiclassical calculations of the Refs.\textsuperscript{10,12,13} the neglect of the spin-orbit interaction was compensated by a simple readjustment of the Fermi energy, allowing one to locally reproduce the correct shell situations (or magic numbers). But this was only a temporary remedy, and a more rigorous semiclassical treatment of the spin-orbit interaction clearly remains highly desirable. The remainder of this paper is therefore devoted to some recent developments of the inclusion of spin degrees of freedom into the POT, which is by no means trivial since there is no classical analogon of the spin.
2. Semiclassical theories with spin

We limit the discussion here to systems of fermions with spin $s = 1/2$ with a (mean-field) Hamiltonian linear in the spin operators

$$\hat{H} = \hat{H}_0(\hat{r}, \hat{p}) + \hat{H}_{so}$$

(1)

with

$$\hat{H}_0(\hat{r}, \hat{p}) = \frac{\hat{p}^2}{2m} + V(\hat{r})$$

$$\hat{H}_{so} = \hbar \kappa \sigma \cdot \hat{C}(\hat{r}, \hat{p})$$

(2)

The second term is a general spin-orbit interaction, where $\hat{C}(\hat{r}, \hat{p})$ is an arbitrary vector function of coordinate $\hat{r}$ and momentum operators $\hat{p}$, and $\kappa$ is a coupling strength independent of $\hbar$. $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices defining the spin operators $\hat{s} = \frac{1}{2} \hbar \sigma$. In the non-relativistic reduction of the Dirac equation with an external electrostatic potential $V(\hat{r})$, one obtains

$$\hat{C}(\hat{r}, \hat{p}) = [\nabla V(\hat{r}) \times \hat{p}]$$

$$\kappa = 1/4m^2c^2$$

(3)

With the Coulomb potential this yields the familiar Thomas term for $\hat{H}_{so}$.

2.1. Earlier approaches

We first summarize two earlier semiclassical approaches.

(i) SCL: Littlejohn and Flynn\textsuperscript{16} developed a semiclassical theory for multi-component systems, treating the spin matrices quantum mechanically while Wigner transforming the matrix operator (1) to the classical phase space $(r, p)$, keeping the leading terms in an $\hbar$ expansion. Diagonalisation leads to a pair of Hamiltonians

$$H_{\pm}(r, p) = H_0(r, p) \pm \hbar \kappa |C(r, p)|, \quad (s = 1/2)$$

(4)

where $H_0(r, p)$ and $C(r, p)$ are the Wigner transforms (to lowest order in $\hbar$) of the corresponding quantum operators. $H_{\pm}$ can be considered as two classical adiabatic Hamiltonians with opposite spin polarizations. Their two sets of periodic orbits must be superposed in the final trace formula. This approach is often referred to as the “strong coupling limit” (SCL), since it becomes valid in the formal limit $\kappa \to \infty$ and $\hbar \to 0$ with $\hbar \kappa$ kept finite.\textsuperscript{16,17} The SCL approach suffers, however, from the problem of mode conversion (MC): whenever $C = 0$ at a given point in (or in a subspace of) phase space, the two Hamiltonians $H_{\pm}$ become degenerate and singularities arise both in the classical equations of motion and in the calculation of the stabilities of the periodic orbits. (A similar situation occurs in the chemistry of molecular reactions when two or more adiabatic surfaces intersect.) The MC poses a difficult problem in semiclassical physics and chemistry that has not been satisfactorily solved so far. It was further discussed within the SCL in Refs.\textsuperscript{18,19}

(ii) WCL: Bolte and Keppeler\textsuperscript{17} have derived a semiclassical theory from the Dirac equation. In the “weak coupling limit” (WCL) they arrive at a trace formula, in which the periodic orbits are given by the dynamics of the unperturbed Hamiltonian $H_0$ and the effect of spin precession around the local ‘magnetic field’
κ \mathcal{C}(\mathbf{r}, \mathbf{p}) \) appears through a simple modulation factor. This approach neglects terms of higher than first order in \( \hbar \kappa \) and therefore is valid in the limit of weak spin-orbit couplings. Furthermore, it yields only a trivial spin degeneracy factor of two in the trace formula whenever all periodic orbits of \( H_0 \) are self retracing (i.e., librating between two turning points) such as in the two systems illustrated below.

An instructive example is that of a two-dimensional electron gas with a Rashba type spin-orbit interaction \( \mathbf{\hat{C}} = (\mathbf{\hat{r}} y, \mathbf{\hat{r}} x, 0) \) in an external homogeneous magnetic field where \( \mathbf{\hat{r}} = \mathbf{\hat{p}} - e \mathbf{A}/c \). For this system the exact quantum spectrum is explicitly known, and analytical trace formulae have been given for both the exact quantum-mechanical level density and the semiclassical WC and SC limits, from which the limitations of these two approaches become evident.

In a successful application of the SCL, a model relevant for nuclear physics was investigated in Ref. It consists of a three-dimensional harmonic oscillator with Thomas-type spin-orbit interaction \( V(\mathbf{r}) = \sum_{i=x,y,z} \frac{1}{2} \omega_i^2 r_i^2, \quad \mathbf{\hat{H}}_{so} = \hbar \kappa \mathbf{\sigma} \cdot [\mathbf{\nabla} V(\mathbf{r}) \times \mathbf{\hat{p}}], \quad (5) \)

which defines a Nilsson type Hamiltonian appropriate for light nuclei (where the \( \ell^2 \) term can be neglected). We express the oscillator frequencies in terms of two deformation parameters \( \alpha, \beta \):

\[
\omega_x = \omega_0, \quad \omega_y = (1 + \alpha) \omega_0, \quad \omega_z = (1 + \alpha)^\beta \omega_0, \quad (6)
\]

and use \( \hbar \omega_0 \) as energy unit. For the general case of incommensurable frequencies (i.e., three-axial deformations), all periodic orbits of the unperturbed system \( H_0 \) are librations along the coordinate axes and the WCL yields only the trivial spin factor of two. The shortest periodic orbits of the Hamiltonians \( H_\pm \) in the SCL lie in the three coordinate planes and can be obtained analytically. For these orbits no mode conversion takes place, and the SCL can be used.

In Fig. 3 we show the shell correction to the level density of this system, with a deformation \( \alpha = 0.1212, \beta = 2 \) and a spin-orbit strength \( \kappa = 0.1 \omega_0^{-1} \). Both the quantum mechanical and the semiclassical \( \delta g(E) \) have been coarse grained by Gaussian convolution over an energy range \( \gamma = 0.5 \hbar \omega_0 \), in order to suppress the contribution of the longer orbits and hereby to emphasize the gross-shell structure. The quantum-mechanical result is shown by the solid lines (QM) and includes the spin-orbit interaction in both curves a) and b). The semiclassical SCL result (SC) is shown by the dashed lines; in a) without spin-orbit interaction, which demonstrates that the latter dramatically changes the level density, and in b) with spin-orbit interaction. Only the six primitive planar orbits have been used. We see that this already leads to an excellent agreement with quantum mechanics, except at very low energies where semiclassics usually cannot be expected to work. As dicussed in Ref., bifurcations of the planar orbits occur for other deformations and values of \( \kappa \). These can, in principle, be handled by suitable uniform approximations (see Ref. for an overview), but they complicate the semiclassical calculations numerically.
2.2. POT in an extended phase space

A new semiclassical approach has recently been presented in which the spin degrees of freedom were introduced through spin coherent states defined by

$$|z; s\rangle = (1 + |z|^2)^{-s} \exp(z \hat{s}_+ / \hbar) |s, -s\rangle, \quad \hat{s}_-|s, -s\rangle = 0, \quad \hat{s}_\pm = \hat{s}_x \pm i \hat{s}_y,$$

where $z = u - iv$ is a complex number. This allows one to define classical spin components $n = (n_x, n_y, n_z) = \langle z; s|\hat{z}|z; s\rangle / \hbar s$ and to enlarge the classical phase space by only one pair of canonical variables $(u, v)$, independently of the value of the spin $s$. Starting from the path integral in the SU(2) spin coherent state representation and making the usual stationary-phase approximation in its evaluation, the semiclassical dynamics of the system in the extended phase space (EPS) $(r, p, v, u)$ is then determined by the Hamiltonian

$$H(r, p, v, u) = H_0(r, p) + \hbar \kappa 2s n(v, u) \cdot C(r, p).$$

Solving the equations of motion following from (8), one can determine the periodic orbits in the EPS and their properties, yielding the required input into the
Gutzwiller trace formula. Special attention is required for the Maslov indices and other phases arising in connection with the spin degrees of freedom.

The EPS approach is free of the problem of mode conversion and, in principle, applicable for both weak and strong spin-orbit interactions. Note that the Hamiltonian explicitly couples the orbital degrees of freedom \((r, p)\) with the spin degrees of freedom \((u, v)\). This is illustrated for the following model Hamiltonian of a two-dimensional semiconductor quantum dot with Rashba interaction:

\[
\hat{H} = \frac{(\hat{p}_x^2 + \hat{p}_y^2)}{2m^*} + m^*(\omega_x^2x^2 + \omega_y^2y^2)/2 + \hbar\kappa (\sigma_y\hat{p}_x - \sigma_x\hat{p}_y),
\]

where \(m^*\) is the effective mass of the conduction electrons, and the deformation parameters were chosen as \(\omega_x = 1.56\omega_0\) and \(\omega_y = 1.23\omega_0\). (In the figures, units are chosen such that \(\hbar = m^* = \omega_0 = 1\) and \(E\) and \(\kappa\) become dimensionless.) Like in the three-dimensional system discussed above, the periodic orbits of \(H_0\) are pure librations, so that the WCL yields only trivial results. But here also the SCL cannot be used, due to the MC problem, so that a new treatment is required.

For \(0 < \kappa \lesssim 0.7\), the following set of 12 shortest periodic orbits in the EPS were found:

(i) Two pairs of orbits \(A^\pm_x\) and \(A^\pm_y\) librating along the \(x\) and \(y\) axes with fully polarized spin \(n_y = \pm 1\) and \(n_x = \pm 1\), respectively. (ii) Two pairs of orbits \(D^+_1\) and \(D^+_2\) oscillating around \(A^\pm_x\) with \(n_y \sim 0\), and two pairs of orbits \(D^-_1\) and \(D^-_2\) oscillating around \(A^\pm_y\) with \(n_x \sim 0\). For stronger couplings with \(\kappa \gtrsim 0.7\), new orbits bifurcate from the \(A\) orbits.

In Fig. 4 we show the \((x, y)\) shapes of the orbits \(A^+_x\), \(D^+_1\), and \(D^+_2\) (left panels), and the time dependence of their spin components \(n_x\), \(n_y\), and \(n_z\) over one period (right panels), all evaluated for \(\kappa = 0.67\) and \(E = 60\). We see that along the orbits \(D^+_1\) and \(D^+_2\), the spin rotates mainly near the \((n_x, n_z)\) plane (i.e., \(n_y \sim 0\)), but in a non-uniform way. This complicated spin motion, together with the wiggly orbital shapes of the D orbits, reveals the rather sophisticated dynamics which is obtained from the equations of motion in the EPS through the explicit coupling of spin and orbital degrees of freedom.

Fig. 5 shows the shell correction of the level density, obtained quantum-mechanically (solid lines) and semiclassically (dashed lines), both coarse-grained over an energy range \(\gamma = 0.6\). The upper panel contains the semiclassical EPS result, while the lower panel exhibits the WCL result which is identical to that obtained by ignoring the spin-orbit interaction and multiplying the level density by a spin factor of two. (Note that the semiclassical trace formula for the unperturbed harmonic oscillator is analytically known and quantum-mechanically exact.) We observe a reasonably good agreement of the EPS result with quantum mechanics. The semiclassical amplitudes are too large, which is attributed to close-lying bifurcations of the periodic orbits; suitable uniform approximations are expected to remedy this defect. The phases of the quantum oscillations are, however, very well reproduced, which is not achieved at all in the WCL.
Fig. 4. Periodic orbits in the two-dimensional quantum dot (9) (see text for parameters). *Left panels:* orbits in the \((x, y)\) plane. *Right panels:* Spin components \(n_x\), \(n_y\), and \(n_z\) versus time. From *top to bottom:* orbit \(A_x^+\) along \(x\) axis with polarized spin in \(y\) direction, and orbits \(D_{x1}^+\) and \(D_{x2}^+\) oscillating around the \(x\) axis with spin rotating near the \((n_x, n_z)\) plane.22,23

Fig. 5. Coarse-grained level density of quantum dot (9) for the same parameters as in Fig. 4. *Solid lines:* quantum-mechanical result. *Dashed lines:* semiclassical results; in upper panel: EPS result, in lower panel: WCL result.23
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3. Summary and Outlook

After a short review of the two earlier semiclassical approaches including spin-orbit interactions, corresponding to the weak coupling limit (WCL) and the strong coupling limit (SCL), we have presented a new approach that makes use of spin coherent states and leads to (semi)classical dynamics in an extended phase space (EPS). Both the WCL and the SCL (with the ‘no-name’ phase still lacking) could be recovered from the EPS approach taking suitable limits.

We have only discussed here Hamiltonians linear in spin and systems with spin \( s = 1/2 \). The EPS approach was formulated for arbitrary spin-dependent Hamiltonians and arbitrary values of \( s \). As is well known, semiclassical approximations work best in the limit of large quantum numbers. Whether they can be used for small quantum numbers is a matter of numerical experience and fortune (like for harmonic oscillators without spin). As to the spin, there are firm grounds to expect good semiclassical results also for \( s = 1/2 \) for Hamiltonians linear in spin.\(^{23}\)

The example shown in Figs. 4 and 5 suggests that the EPS approach has a good potential for a general semiclassical theory with spin. Practically, this approach suffers from a large number of bifurcations occurring for the periodic orbits under variations of both \( \kappa \), energy, and deformation parameters. It would therefore be desirable to use it as a formal starting point for further approximations.

Indeed, in the limit of a weak spin-orbit coupling such that \( H_{so} \ll H_0 \), the WCL trace formula of Ref.\(^{17}\) could be rigorously derived from the EPS approach.\(^{28}\) Hereby the equations of motion of the orbital and spin degrees of freedom were decoupled, and the effects of \( H_{so} \) were included in the phases of the trace formula in first-order perturbation theory.\(^{29}\) Pushing this treatment to second order, along the lines proposed in Ref.\(^{30}\) for spin-independent systems, might allow one to extend the WCL trace formula, so that it becomes valid for larger values of \( \kappa \) while still benefiting from a simpler determination of the periodic orbits. In particular, for the self-retracing orbits where the first-order result is trivial, the second-order treatment is expected\(^{30}\) only to lead to a phase correction while the amplitudes in the trace formula still are determined by the unperturbed orbits of \( H_0 \). This expectation is, indeed, strongly supported by the results shown in the lower part of Fig. 5.

On the other hand, a careful study\(^{23}\) of the situation \( H_{so} \sim H_0 \) reveals that the essential ingredients of the SCL approach of Refs.\(^{16,18}\) – without, however, the so-called ‘no-name phase’ – can also be retrieved from the EPS approach. Adding suitable corrections to this limit might help to overcome the mode conversion problem without going through the cumbersome task of finding all relevant periodic orbits in the extended phase space, including all possible bifurcations and their treatment by uniform approximations.

In a recent application of the EPS approach to mesoscopic transport theory, the effects of spin-orbit interaction on weak anti-localization have been investigated,\(^{31}\) and its application to semiclassical studies of nuclear shell structure including realistic shell-model potentials and spin-orbit interactions is in progress.\(^{32}\)
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