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LETTER TO THE EDITOR

Spin phase-space semiclassics for weak spin–orbit coupling

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Abstract

We apply the semiclassical spin coherent state method for the density of states by Pletyukhov *et al* (2002 *Phys. Rev. Lett.* **89** 116601) in the weak spin–orbit coupling limit and recover the modulation factor in the semiclassical trace formula found by Bolte and Keppeler (1998 *Phys. Rev. Lett.* **81** 1987; 1999 *Ann. Phys.*, *NY* **274** 125).

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1. Introduction

A new solution to the problem of how to include spin–orbit interaction in the semiclassical theory was recently proposed by Pletyukhov *et al* [1]. They use the spin coherent states to describe the spin degrees of freedom of the system. Then a path integral that combines the spin and orbital variables can be constructed, leading to the semiclassical propagator (or its trace) when evaluated within the stationary phase approximation. In such an approach, the spin and orbital degrees of freedom are treated on equal footings. In particular, one can think of a classical trajectory of the system in the extended phase space, i.e., the phase space with two extra dimensions due to spin. (The spin part of the extended phase space can be mapped onto the Bloch sphere.) As in the pure orbital systems, it is possible to construct a classical Hamiltonian that will be a function of the phase-space coordinates. The trajectories of the system satisfy the equations of motion generated by this Hamiltonian.

In this letter, we apply the general theory [1] to the limiting case of weak spin-orbit coupling. This limit is naturally incorporated in the theory proposed by Bolte and Keppeler [2] based on the $\hbar \rightarrow 0$ expansion in the Dirac (or Pauli) equation. Bolte and Keppeler have shown that the semiclassical trace formula without spin-orbit interaction acquires an additional modulation factor due to spin, but otherwise remains unchanged. We obtain the same modulation factor using the spin coherent state method.

2. Classical dynamics and periodic orbits

We begin with the classical phase-space symbol of the Hamiltonian [1]

$$H(p,q,z) = H_0(p,q) + \kappa \hbar S \sigma(z) \cdot \mathbf{C}(p,q) \equiv H_0 + \hbar H_{so}.$$
(1)

It includes the spin-orbit interaction term $\hbar H_{so}$ which is linear in spin, but otherwise is an arbitrary function of (possibly multidimensional) momenta and coordinates p and q. The spin direction is described by a unit vector $\sigma(z) \stackrel{\text{def}}{=} \langle z | \hat{\mathbf{S}} | z \rangle / S$, where $\hat{\mathbf{S}}$ is the spin operator and the complex variable $z \equiv u - iv$ labels the spin coherent states of total spin S [3]. At the end of our calculations we will set $S = \frac{1}{2}$. The Planck constant appears explicitly in this classical Hamiltonian and is treated as the perturbation parameter in the weak-coupling limit. The spin-orbit coupling strength κ is kept finite. Thus, the condition $\hbar \to 0$ provides both the semiclassical (high energy) and the weak-coupling limits.

Hamiltonian (1) determines the classical equations of motion for the orbital and spin degrees of freedom [1]

$$\dot{p} = -\frac{\partial H}{\partial q} = -\frac{\partial H_0}{\partial q} - \kappa \hbar S \boldsymbol{\sigma} \cdot \frac{\partial \mathbf{C}}{\partial q}$$
(2)

$$\dot{q} = \frac{\partial H}{\partial p} = \frac{\partial H_0}{\partial p} + \kappa \hbar S \sigma \cdot \frac{\partial \mathbf{C}}{\partial p}$$
(3)

$$\dot{\sigma} = -\kappa \sigma \times \mathbf{C}.\tag{4}$$

Since

$$\sigma(z) = \frac{1}{1+|z|^2} (2u, 2v, |z|^2 - 1)^{\mathrm{T}}$$
(5)

in the 'south' gauge¹, equation (4) is equivalent to two Hamilton-like equations

$$\dot{a} = -\frac{(1+|z|^2)^2}{4\hbar S}\frac{\partial H}{\partial v} = -\frac{\kappa}{4}(1+|z|^2)^2\frac{\partial\sigma}{\partial v}\cdot\mathbf{C}$$
(6)

$$\dot{v} = \frac{(1+|z|^2)^2}{4\hbar S} \frac{\partial H}{\partial u} = \frac{\kappa}{4} (1+|z|^2)^2 \frac{\partial \sigma}{\partial u} \cdot \mathbf{C}.$$
(7)

In the leading order in \hbar we keep only the unperturbed terms in equations (2) and (3). It follows then that the orbital motion, in this approximation, is unaffected by spin. The spin motion is determined by the unperturbed orbital motion via equation (4), which does not contain \hbar . It describes the spin precession in the time-dependent effective magnetic field $C(p_0(t), q_0(t))$, where $(p_0(t), q_0(t))$ is an orbit of the unperturbed Hamiltonian H_0 .

In order to apply a trace formula for the density of states, we need to know the periodic orbits of the system, both in orbital and spin phase-space coordinates. The orbital part of a periodic trajectory is necessarily a periodic orbit of H_0 . Assume that such an orbit with period T_0 is given. Then equation (4) generates a map on the Bloch sphere $\sigma(0) \mapsto \sigma(T_0)$ between the initial and final points of a spin trajectory $\sigma(t)$. The fixed points of this map correspond to periodic orbits with the period T_0 . Since equation (4) is linear in σ , for any two trajectories $\sigma_1(t)$ and $\sigma_2(t)$, their difference also satisfies this equation. But this means that $|\sigma_1(t) - \sigma_2(t)| = \text{const}$, i.e., the angles between the vectors do not change during the motion. Hence, the map is a rotation by an angle α about some axis through the centre of the Bloch sphere. The points of intersection of this axis and the sphere are the fixed points of

¹ By the south gauge we mean the choice of parametrization of the spin coherent states by z such that $\sigma_z(|z| \to \infty) = 1$.



Figure 1. Axis of rotation and fixed points of the map $\sigma(0) \mapsto \sigma(T_0)$.

the map (figure 1). Thus, for a given periodic orbit of H_0 , there are two periodic orbits of H with opposite spin orientations (unless α is a multiple of 2π , by accident). The angle α was mentioned in [4].

3. Modulation factor

3.1. Correction to the action

In order to derive a modulation factor in the trace formula, we need to determine the correction to the action and the stability determinant due to the spin–orbit interaction. The action along a periodic orbit is [1]

$$S = \oint p \, \mathrm{d}q + 2S\hbar \oint \frac{u \, \mathrm{d}v - v \, \mathrm{d}u}{1 + |z|^2} \equiv S_{pq} + \hbar S_{\mathrm{spin}}.$$
(8)

While the spin part contains \hbar explicitly, we need to extract the leading order correction to the orbital action. This is the only place where we implicitly take into account the influence of spin on the orbital motion. It is convenient for the following calculation to parametrize both the perturbed and unperturbed orbits by a variable $s \in [0, 1]$, i.e.,

$$S_{pq} = \int_0^1 p \frac{\mathrm{d}q}{\mathrm{d}s} \,\mathrm{d}s. \tag{9}$$

The time parametrization would be problematic since the periods of the perturbed and the unperturbed orbits differ by order of \hbar (see appendix A). The correction to the orbital part due to the perturbation is

$$\delta \mathcal{S}_{pq} = \int_0^1 \left[\delta p \frac{\mathrm{d}q_0}{\mathrm{d}s} + p_0 \frac{\mathrm{d}}{\mathrm{d}s} (\delta q) \right] \mathrm{d}s = \int_0^1 \left(\delta p \frac{\mathrm{d}q_0}{\mathrm{d}s} - \delta q \frac{\mathrm{d}p_0}{\mathrm{d}s} \right) \mathrm{d}s + p_0 \delta q \Big|_0^1. \tag{10}$$

The boundary term vanishes for the periodic orbit, and the integration can be done over the period of the unperturbed orbit now:

$$\delta \mathcal{S}_{pq} = \int_0^{T_0} (\delta p \dot{q}_0 - \delta q \dot{p}_0) \, \mathrm{d}t = \int_0^{T_0} \left(\delta p \frac{\partial H_0}{\partial p} + \delta q \frac{\partial H_0}{\partial q} \right) \mathrm{d}t = \int_0^{T_0} \delta H_0 \, \mathrm{d}t. \tag{11}$$

Since the perturbed and unperturbed orbits have the same energy, the variation of the Hamiltonian is $\delta H_0 = -\hbar H_{so}$. Taking into account equation (5), we can express the change in the orbital action as

$$\delta S_{pq} = -\hbar\kappa S \int_0^{T_0} \mathbf{C} \cdot \boldsymbol{\sigma} \, \mathrm{d}t = -\hbar\kappa S \int_0^{T_0} \mathbf{C} \cdot \begin{pmatrix} 2u \\ 2v \\ |z|^2 - 1 \end{pmatrix} \frac{\mathrm{d}t}{1 + |z|^2}.$$
 (12)

We now turn to the spin action. Parameterizing the trajectory with time and then using the equations of motion (6), (7) and equation (5), we find

$$\hbar S_{\rm spin} = \frac{\hbar \kappa S}{2} \int_0^{T_0} \mathbf{C} \cdot \left(u \frac{\partial \sigma}{\partial u} + v \frac{\partial \sigma}{\partial v} \right) (1 + |z|^2) \, \mathrm{d}t$$
$$= \hbar \kappa S \int_0^{T_0} \mathbf{C} \cdot \begin{pmatrix} u(1 - |z|^2) \\ v(1 - |z|^2) \\ 2|z|^2 \end{pmatrix} \frac{\mathrm{d}t}{1 + |z|^2}. \tag{13}$$

Summing up the orbital and spin contributions, equations (12) and (13), we obtain the entire change in action as

$$\delta S = \delta S_{pq} + \hbar S_{\text{spin}} = \hbar S \int_0^{T_0} F(t) \, \mathrm{d}t \tag{14}$$

where

$$F(t) = \kappa \mathbf{C} \cdot \begin{pmatrix} -u \\ -v \\ 1 \end{pmatrix}.$$
 (15)

3.2. Stability determinant

The stability determinant is derived from the second variation of the Hamiltonian $H^{(2)}$ about the periodic orbit [1]. In the leading order in \hbar , the orbital and spin degrees of freedom in $H^{(2)}$ are separated. This means that the spin phase space provides an additional block to the unperturbed monodromy matrix of the orbital phase space, which results in a separate stability determinant due to spin. The linearized momentum and coordinate for spin

$$\binom{\xi}{\nu} = \frac{2\sqrt{\hbar S}}{1+|z|^2} \binom{\delta u}{\delta \nu} \tag{16}$$

satisfy the equations of motion

$$\begin{pmatrix} \dot{\xi} \\ \dot{\nu} \end{pmatrix} = \begin{pmatrix} -\frac{\partial H^{(2)}}{\partial \nu} \\ \frac{\partial H^{(2)}}{\partial \xi} \end{pmatrix} = F(t) \begin{pmatrix} -\nu \\ \xi \end{pmatrix}.$$
(17)

Solving these equations we find the spin block of the monodromy matrix to be (appendix B)

$$M = \begin{pmatrix} \cos\varphi & -\sin\varphi\\ \sin\varphi & \cos\varphi \end{pmatrix}$$
(18)

where the stability angle is

$$\varphi = \int_0^{T_0} F(t) \,\mathrm{d}t. \tag{19}$$

The proportionality between φ and δS (equation (14)) will be exploited in a moment but, first, we find the stability determinant

$$|\det(M-I)|^{1/2} = 2\left|\sin\frac{\varphi}{2}\right|$$
 (20)

where *I* is the 2×2 unit matrix.

3.3. Trace formula

As was explained at the end of section 2, for each unperturbed periodic orbit there are two new periodic orbits with opposite spin orientations $\sigma(t)$. It is easy to deduce, then, that for these two orbits both δS and φ have the same magnitude but opposite signs. Now we are ready to write the trace formula for the oscillatory part of the density of states

$$\delta g(E) = \sum_{po} \sum_{\pm} \frac{\mathcal{A}_0}{2\left|\sin\frac{\varphi}{2}\right|} \cos\left[\frac{1}{\hbar}(\mathcal{S}_0 \pm \delta \mathcal{S}) - \frac{\pi}{2}(\mu_0 + \mu_{\pm})\right]$$
(21)

where the first sum is over the unperturbed periodic orbits and the second sum takes care of the contribution of the two spin orientations; A_0 is the prefactor for the unperturbed orbit, which depends on the stability determinant and the primitive period; S_0 and μ_0 are the unperturbed action and the Maslov index, respectively; μ_{\pm} are the additional Maslov indices due to spin. The nature of spin requires an additional Kochetov–Solari phase correction [3] that results in the shift $S \longmapsto S + \frac{1}{2}$ of the total spin parameter in δS (appendix C). Setting $S = \frac{1}{2}$, we end up with

$$\delta \mathcal{S} \longmapsto \delta \tilde{\mathcal{S}} = \hbar \varphi. \tag{22}$$

With this relation and the additional Maslov index (appendix D)

$$u_{\pm} = 1 + 2\left[\pm\frac{\varphi}{2\pi}\right] \tag{23}$$

([x] is the largest integer $\leq x$) the sum over the spin orientations in equation (21) becomes

$$\sum_{\pm} \frac{\mathcal{A}_0}{2\sin\frac{\varphi}{2}} \cos\left[\left(\frac{\mathcal{S}_0}{\hbar} - \frac{\pi}{2}\mu_0\right) \pm \left(\frac{\delta\tilde{\mathcal{S}}}{\hbar} - \frac{\pi}{2}\right)\right] = 2\cos\left(\frac{\varphi}{2}\right)\mathcal{A}_0\cos\left[\frac{\mathcal{S}_0}{\hbar} - \frac{\pi}{2}\mu_0\right].$$
 (24)

This is our main result: each term in the periodic orbit sum is the contribution of an unperturbed orbit $A_0 \cos \left[\frac{S_0}{\hbar} - \frac{\pi}{2}\mu_0\right]$ times the modulation factor

$$\mathcal{M} = 2\cos\left(\frac{\varphi}{2}\right). \tag{25}$$

Note that no assumption was made on whether the unperturbed periodic orbits are isolated or not.

4. Comparison with another method

Bolte and Keppeler [2] derived the modulation factor in the weak-coupling limit by a different method. Their results² are expressed in terms of a spin trajectory with the initial condition

$$\sigma(0) = (0, 0, -1)^{\mathrm{T}} \tag{26}$$

that obeys equation (4). This trajectory, in general, is not periodic. As in our approach, the influence of spin on the orbital motion is neglected. The spin motion can be described by the polar angles $(\theta(t), \phi(t))$ with $\theta(0) = \pi$. The modulation factor is then

$$\mathcal{M}_{\rm BK} = 2\cos\left(\frac{\Delta\theta}{2}\right)\cos\chi\tag{27}$$

where $\Delta \theta = \pi - \theta(T_0)$ and³

$$\chi = -\frac{\kappa}{2} \int_0^{T_0} \mathbf{C} \cdot \boldsymbol{\sigma} \, \mathrm{d}t + \frac{1}{2} \int_0^{T_0} [1 + \cos\theta(t)] \dot{\boldsymbol{\phi}}(t) \, \mathrm{d}t.$$
(28)

 $\frac{2}{2}$ We reformulate the results of [2] for the south gauge.

³ Reference [2] defines the phase $\eta = -\chi$.

In order to show that our modulation factor (25) is equal to \mathcal{M}_{BK} , let us express φ in terms of the polar angles. From equation (5) follows the coordinate transformation

$$u = \cot \frac{\theta}{2} \cos \phi$$
 $v = \cot \frac{\theta}{2} \sin \phi.$ (29)

Since $\varphi \propto \delta S$, we can represent it as a sum of two terms (cf equations (12)–(14))

$$\frac{\varphi}{2} = -\frac{\kappa}{2} \int_0^{T_0} \mathbf{C} \cdot \boldsymbol{\sigma} \, \mathrm{d}t + \frac{1}{2} \int_0^{T_0} [1 + \cos\theta(t)] \dot{\boldsymbol{\phi}}(t) \, \mathrm{d}t.$$
(30)

There is a striking similarity between the expressions for χ and $\frac{\varphi}{2}$. The only difference is that in equation (28) the integration is, in general, along a non-periodic orbit with the initial condition (26), while in equation (30) the integration is along the periodic orbit. Since the modulation factor should not depend on the choice of the z-direction, we can choose the z-axis to coincide with the spin vector $\sigma(0)$ for the periodic orbit at t = 0, i.e., the z-axis will be the rotation axis in figure 1. Then one of the periodic orbits will satisfy the initial condition (26), and thus both χ and $\frac{\varphi}{2}$ can be calculated along this orbit and are equal. Moreover, $\Delta \theta = 0$ in this case. Therefore the modulation factors derived within the two approaches coincide,

$$\mathcal{M}_{\rm BK} = \mathcal{M}.\tag{31}$$

It was mentioned in [4] that $M_{BK} = 2 \cos \frac{\alpha}{2}$, where α is the rotation angle defined in section 2. Then, of course, we conclude that

$$\cos\frac{\alpha}{2} = \cos\frac{\varphi}{2}.\tag{32}$$

To see that this is indeed the case, we can go back to section 3.2 where we calculated the stability determinant. It follows from that calculation that the neighbourhood of the periodic orbit is rotated by an angle φ during the period (appendix B). Therefore the entire Bloch sphere is rotated by this angle. Clearly, the angle of rotation must be defined by mod 4π , i.e., it depends on the parity of the number of full revolutions of the Bloch sphere around the periodic orbit during the period. It would be desirable to prove equation (32) without referring to the small neighbourhood of the periodic orbit.

The same property can also be shown if one treats the spin quantum mechanically. The spin propagator for the choice of the *z*-axis along the rotation axis (so that $\chi = \frac{\varphi}{2}$) is [2]

$$d(T_0) = \begin{pmatrix} e^{-i\frac{\varphi}{2}} & 0\\ 0 & e^{i\frac{\varphi}{2}} \end{pmatrix}.$$
(33)

Applying this operator to a spinor $(\psi_+, \psi_-)^T$ at t = 0, we get the spinor $(\psi_+ e^{-i\frac{\varphi}{2}}, \psi_- e^{i\frac{\varphi}{2}})^T$ at $t = T_0$, which corresponds to the initial spin vector rotated by the angle φ about the z-axis, i.e., $\varphi = \alpha$.

5. Summary and conclusions

We have studied the case of weak spin-orbit coupling in the semiclassical approximation using the spin coherent state method. The limit is achieved formally by setting $\hbar \rightarrow 0$. The trajectories in the orbital subspace of the extended phase space then remain unchanged by the spin-orbit interaction. For each periodic orbit in the orbital subspace there are two periodic orbits in the full phase space with opposite spin orientations. The semiclassical trace formula can be expressed as a sum over unperturbed periodic orbits with a modulation factor. This agrees with the results of Bolte and Keppeler. The form of the modulation factor does not depend on whether the unperturbed system has isolated orbits or whether it contains families of degenerate orbits due to continuous symmetries. We remark that in the semiclassical treatment of pure spin systems, a renormalization procedure is necessary in order to correct the stationary phase approximation in the path integral for finite spin *S*. Such a renormalization is equivalent to the Kochetov–Solari phase correction that we employed here without justification for a system with spin–orbit interaction. Although this correction worked well in our case, it may be necessary to develop a general renormalization scheme when the interaction is not weak.

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Appendix A. Time parametrization

For pedagogical reasons we do the calculation in equation (10) with the time parametrization. In this case $S_{pq} = \int_0^T p\dot{q} \, dt$, where *T* is the exact period. Then the correction is

$$\delta S_{pq} = \int_{0}^{T_0} [\delta p \dot{q}_0 + p_0(\dot{\delta q})] dt + p_0(T_0) \dot{q}_0(T_0) \delta T$$

=
$$\int_{0}^{T_0} (\delta p \dot{q}_0 - \delta q \dot{p}_0) dt + p_0 \delta q \Big|_{0}^{T_0} + p_0(T_0) \dot{q}_0(T_0) \delta T.$$
(A.1)

Transforming the boundary term

$$p_{0}\delta q \Big|_{0}^{T_{0}} = p_{0}(T_{0})[q(T_{0}) - q_{0}(T_{0}) - q(0) + q_{0}(0)] = p_{0}(T_{0})[q(T_{0}) - q(0)]$$

= $p_{0}(T_{0})[q(T_{0}) - q(T)] \simeq -p_{0}(T_{0})\dot{q}_{0}(T_{0})\delta T$ (A.2)

we see that it cancels the period correction term.

Appendix B. Monodromy matrix

We derive the monodromy matrix (18). In order to solve the equations of motion (17) we define $\eta = \xi + i\nu$. Then $\dot{\eta} = i\eta F(t)$, which solves to

$$\eta(t) = \eta(0) \exp\left[i \int_0^t F(t') dt'\right]. \tag{B.1}$$

It then follows that

$$\xi(T_0) = \xi(0) \cos \varphi - \nu(0) \sin \varphi$$
(B.2)

$$\nu(T_0) = \xi(0) \sin \varphi + \nu(0) \cos \varphi$$

resulting in equation (18).

Note that according to equation (5),

$$\xi = \sqrt{\hbar S} \left(\delta \sigma_x + \frac{\sigma_x \delta \sigma_z}{1 - \sigma_z} \right) \qquad \nu = \sqrt{\hbar S} \left(\delta \sigma_y + \frac{\sigma_y \delta \sigma_z}{1 - \sigma_z} \right). \tag{B.3}$$

If we choose the z-axis in such a way that the periodic orbit starts and ends in the south pole, i.e., $\sigma(0) = \sigma(T_0) = (0, 0, -1)^T$, then at t = 0 and $t = T_0$ we have

$$\xi = \sqrt{\hbar S} \delta \sigma_x \qquad \nu = \sqrt{\hbar S} \delta \sigma_y. \tag{B.4}$$

Comparing with equations (B.2) we conclude that the neighbourhood of the periodic orbit is rotated by the angle φ after the period.

Appendix C. Kochetov-Solari phase shift

The Kochetov-Solari phase shift [3] is given by

$$\varphi_{\rm KS} = \frac{1}{2} \int_0^{T_0} A(t) \,\mathrm{d}t \tag{C.1}$$

where

$$A(t) = \frac{1}{2\hbar} \left[\frac{\partial}{\partial \bar{z}} \frac{(1+|z|^2)^2}{2S} \frac{\partial H}{\partial z} + \text{c.c.} \right].$$
(C.2)

The spin-dependent part of the Hamiltonian is (cf equation (1))

$$\hbar H_{\rm so}(z,\bar{z}) = \frac{\hbar\kappa S}{1+|z|^2} \mathbf{C} \cdot \begin{pmatrix} z+\bar{z}\\ {\rm i}(z-\bar{z})\\ |z|^2-1 \end{pmatrix}.$$
(C.3)

We find

$$\frac{\partial}{\partial \bar{z}} \frac{(1+|z|^2)^2}{2S} \frac{\partial H_{so}}{\partial z} = \kappa \mathbf{C} \cdot \begin{pmatrix} -\bar{z} \\ i\bar{z} \\ 1 \end{pmatrix}$$
(C.4)

therefore the phase shift becomes

$$\varphi_{\rm KS} = \frac{1}{2}\varphi. \tag{C.5}$$

Comparing to equation (14) we see that it effectively shifts the spin *S* by $\frac{1}{2}$. One should keep in mind that this phase correction was originally derived for a pure spin system. It has not been proved to have the same form for a system with spin–orbit interaction. In the special case of the weak-coupling limit we have a reason to believe that the result (C.5) is correct, since we were able to reproduce the modulation factor found with another method [2] (see section 4).

Appendix D. Maslov indices

The additional Maslov indices μ_{\pm} are determined by the linearized spin motion about the periodic orbit. The second variation of the Hamiltonian reads (cf equation (17))

$$H^{(2)}(\xi,\nu) = \frac{F(t)}{2}(\xi^2 + \nu^2).$$
(D.1)

Following Sugita [5] we define its normal form

$$H_{\rm norm} = \frac{\varphi}{2T_0} (\xi^2 + \nu^2) \tag{D.2}$$

that has a constant frequency and generates the same phase change φ as $H^{(2)}$ after the period T_0 . Then the spin block of the monodromy matrix can be classified as elliptic and its Maslov index is given by equation (23). φ is the stability angle of one of the two orbits with opposite spin orientations. Therefore, without loss of generality, we can assume that $\varphi > 0$. Then, explicitly,

$$\mu_{\pm} = \begin{cases} \pm 1 & \text{if } \varphi \in (0, 2\pi) \mod 4\pi \\ \pm 3 & \text{if } \varphi \in (2\pi, 4\pi) \mod 4\pi \end{cases}$$
(D.3)

On the other hand,

$$\operatorname{sign}\left(\sin\frac{\varphi}{2}\right) = \begin{cases} 1 & \text{if } \varphi \in (0, 2\pi) \mod 4\pi \\ -1 & \text{if } \varphi \in (2\pi, 4\pi) \mod 4\pi \end{cases}$$
(D.4)

Clearly, one can take $\mu_{\pm} = \pm 1$ and at the same time remove the absolute value sign from $\sin \frac{\varphi}{2}$, as was done in equation (24).

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