The calculation of the Berry phase for spins with 1/2, 1, 3/2, and 2

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Here we discuss the Berry phase for the spins undergoing a precession around the *z* axis. We use the Mathematica for the calculation of the Berry phase. In general, the Berry phase is given by

$$\gamma_m(C) = -\mathrm{Im}\int d\mathbf{a}\cdot V_m(\mathbf{B}) = -\int d\mathbf{a}\cdot\frac{m(\mathbf{B})}{B^3}\mathbf{B} = \Omega(C)m(\mathbf{B}=0) = m\Omega(C)$$

where

$$\hat{S}_z\left|m(\boldsymbol{B}=0)\right\rangle = \hbar m\left|m(\boldsymbol{B}=0)\right\rangle$$

$$\gamma_m(C) = i\int d\boldsymbol{a}\cdot V_m(\boldsymbol{B}) = -\int d\boldsymbol{a}\cdot\frac{m(\boldsymbol{B})}{B^3}\boldsymbol{B} = \Omega(C)m(\boldsymbol{B}=0) = m\Omega(C)$$

$$\gamma_n(C) = -\mathrm{Im}\oint d\boldsymbol{a}\cdot[\nabla\times\left\langle n\middle|\nabla n\right\rangle]$$

1. Spin 1/2

The Example 10.2 (Griffiths)

Here we consider the eigenstate of a spin with 1/2 in the presence of a magnetic field

$$B = B_0(\sin\theta\cos\phi\,\boldsymbol{e}_x + \sin\theta\sin\phi\,\boldsymbol{e}_y + \cos\theta\,\boldsymbol{e}_z) = B_0\boldsymbol{n}.$$

The Hamiltonian is given by

$$\hat{H} = -(-\frac{2\mu_B}{\hbar}\hat{\boldsymbol{S}})\cdot\boldsymbol{B} = \mu_B B_0(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n}).$$

The eigenstates are given by

$$\left|\psi_{1/2}\right\rangle = \left|+\boldsymbol{n}\right\rangle = \begin{pmatrix} e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \\ e^{i\frac{\phi}{2}}\sin\frac{\theta}{2}\end{pmatrix}, \qquad \left|\psi_{-1/2}\right\rangle = \left|-\boldsymbol{n}\right\rangle = \begin{pmatrix} e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ -e^{i\frac{\phi}{2}}\cos\frac{\theta}{2}\end{pmatrix}.$$

Using the Mathematica we get

$$\nabla\times\langle +\boldsymbol{n}|\nabla(+\boldsymbol{n})\rangle = \frac{i}{2r^2}\boldsymbol{e}_r\,, \qquad \nabla\times\langle -\boldsymbol{n}|\nabla(-\boldsymbol{n})\rangle = -\frac{i}{2r^2}\boldsymbol{e}_r\,.$$

Thus we have

$$\gamma_{1/2}(C) = -\mathrm{Im}\oint d\boldsymbol{a}\cdot\frac{i}{2r^2}\boldsymbol{e}_r = -\mathrm{Im}\oint r^2 d\Omega_{1/2}\frac{i}{2r^2} = -\frac{1}{2}\Omega_{1/2} = -\pi(1-\cos\theta)$$

$$\gamma_{-1/2}(C) = -\mathrm{Im}\oint d\boldsymbol{a}\cdot\frac{-i}{2r^2}\boldsymbol{e}_r = \frac{1}{2}\Omega_{1/2} = \pi(1-\cos\theta)$$

or

$$\gamma_{-1/2}(C) = 2\pi-\pi(1-\cos\theta) = \pi(1+\cos\theta)\,, \qquad (\mathrm{mod}\ 2\pi).$$

2. Spin 1

The eigenstates for spin 1 are given by

$$|\psi_1\rangle = \begin{pmatrix} e^{-i\phi}\cos^2\frac{\theta}{2} \\ \frac{1}{\sqrt{2}}\sin\theta \\ e^{i\phi}\sin^2\frac{\theta}{2} \end{pmatrix}, \qquad |\psi_2\rangle = \begin{pmatrix} e^{-i\phi}\frac{1}{\sqrt{2}}\sin\theta \\ -\cos\theta \\ -e^{i\phi}\frac{1}{\sqrt{2}}\sin\theta \end{pmatrix}, \qquad |\psi_3\rangle = \begin{pmatrix} e^{-i\phi}\sin^2\frac{\theta}{2} \\ -\frac{1}{\sqrt{2}}\sin\theta \\ e^{i\phi}\cos^2\frac{\theta}{2} \end{pmatrix}.$$

$$\nabla\times\langle\psi_1|\nabla\psi_1\rangle = \frac{i}{r^2}\boldsymbol{e}_r\,, \qquad \nabla\times\langle\psi_0|\nabla\psi_0\rangle = 0$$

$$\nabla\times\langle\psi_{-1}|\nabla\psi_{-1}\rangle = -\frac{i}{r^2}\boldsymbol{e}_r$$

Thus we have

$$\gamma_1(C) = -\mathrm{Im}\oint d\boldsymbol{a}\cdot\frac{i}{r^2}\boldsymbol{e}_r = -\mathrm{Im}\oint r^2 d\Omega_1\frac{i}{r^2} = -\Omega_1 = -2\pi(1-\cos\theta)$$

$$\gamma_{-1}(C) = -\mathrm{Im}\oint d\boldsymbol{a}\cdot\frac{-i}{r^2}\boldsymbol{e}_r = \mathrm{Im}\oint r^2 d\Omega_1\frac{i}{r^2} = +\Omega_1 = 2\pi(1-\cos\theta)$$

or

$$\gamma_{-1}(C) = 4\pi - 2\pi(1-\cos\theta) = 2\pi(1+\cos\theta) \qquad (\text{mod } 2\pi)$$

3. Spin 3/2

$$\left|\psi_{3/2}\right\rangle = \begin{pmatrix} e^{-\frac{3i\phi}{2}}\cos^3\frac{\theta}{2} \\ \frac{\sqrt{3}}{4}e^{-\frac{i\phi}{2}}\csc\frac{\theta}{2}\sin^2\theta \\ \sqrt{3}e^{\frac{i\phi}{2}}(\cot\theta+\csc\theta)\sin^3\frac{\theta}{2} \\ e^{\frac{3i\phi}{2}}\sin^3\frac{\theta}{2} \end{pmatrix}$$

$$\left|\psi_{1/2}\right\rangle = \begin{pmatrix} \frac{\sqrt{3}}{2}e^{-\frac{3i\phi}{2}}\cos\frac{\theta}{2}\sin\theta \\ -\frac{1}{2}e^{-\frac{i\phi}{2}}\sin\frac{\theta}{2}(3\cos\theta-1) \\ -\frac{1}{2}e^{\frac{i\phi}{2}}(3\cos\theta+1)\sin\frac{\theta}{2} \\ -\frac{\sqrt{3}}{2}e^{\frac{3i\phi}{2}}\sin\frac{\theta}{2}\sin\theta \end{pmatrix}$$

$$\left|\psi_{-1/2}\right\rangle = \begin{pmatrix} \frac{\sqrt{3}}{2}e^{-\frac{3i\phi}{2}}\sin\frac{\theta}{2}\sin\theta \\ -\frac{1}{2}e^{-\frac{i\phi}{2}}(3\cos\theta+1)\sin\frac{\theta}{2} \\ \frac{1}{2}e^{\frac{i\phi}{2}}(3\cos\theta-1)\cos\frac{\theta}{2} \\ \frac{\sqrt{3}}{4}e^{\frac{3i\phi}{2}}\csc\frac{\theta}{2}\sin^2\theta \end{pmatrix}$$

$$\left|\psi_{-3/2}\right\rangle = \begin{pmatrix} e^{-\frac{3i\phi}{2}}\sin^3\frac{\theta}{2} \\ -\frac{\sqrt{3}}{2}e^{-\frac{i\phi}{2}}\sin\frac{\theta}{2}\sin\theta \\ \frac{\sqrt{3}}{4}e^{\frac{i\phi}{2}}\csc\frac{\theta}{2}\sin^2\theta \\ -e^{\frac{3i\phi}{2}}\cos^3\frac{\theta}{2} \end{pmatrix}$$

$$\nabla\times\left\langle\psi_{3/2}\middle|\nabla\psi_{3/2}\right\rangle = \frac{3i}{2r^2}\boldsymbol{e}_r, \qquad \nabla\times\left\langle\psi_{1/2}\middle|\nabla\psi_{1/2}\right\rangle = \frac{i}{2r^2}\boldsymbol{e}_r$$

$$\nabla\times\left\langle\psi_{-1/2}\middle|\nabla\psi_{-1/2}\right\rangle = -\frac{i}{2r^2}\boldsymbol{e}_r \qquad \nabla\times\left\langle\psi_{-3/2}\middle|\nabla\psi_{-3/2}\right\rangle = -\frac{3i}{2r^2}\boldsymbol{e}_r$$

4. Spin 1

$$\nabla\times\left\langle\psi_{2}\middle|\nabla\psi_{2}\right\rangle = \frac{2i}{r^2}\boldsymbol{e}_r, \qquad \nabla\times\left\langle\psi_{1}\middle|\nabla\psi_{1}\right\rangle = \frac{i}{r^2}\boldsymbol{e}_r$$

$$\nabla\times\left\langle\psi_{0}\middle|\nabla\psi_{0}\right\rangle = 0 \qquad \nabla\times\left\langle\psi_{-1}\middle|\nabla\psi_{-1}\right\rangle = -\frac{i}{r^2}\boldsymbol{e}_r$$

$$\nabla\times\left\langle\psi_{-2}\middle|\nabla\psi_{-2}\right\rangle = -\frac{2i}{r^2}\boldsymbol{e}_r$$

((**Mathematica**)) We use the Mathematica to get the above results.

```
Clear["Global`*"];
exp_* := exp /. {Complex[re_, im_] :> Complex[re, -im]};
j = 1;
Jx[j_, n_, m_] := ħ/2 Sqrt[(j - m) (j + m + 1)] KroneckerDelta[n, m + 1] +
   ħ/2 Sqrt[(j + m) (j - m + 1)] KroneckerDelta[n, m - 1];
Jy[j_, n_, m_] := -ħ/2 ⅈ Sqrt[(j - m) (j + m + 1)] KroneckerDelta[n, m + 1] +
   ħ/2 ⅈ Sqrt[(j + m) (j - m + 1)] KroneckerDelta[n, m - 1];
Jz[j_, n_, m_] := ħ m KroneckerDelta[n, m];
Jx = Table[Jx[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];
Jy = Table[Jy[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];
Jz = Table[Jz[j, n, m], {n, j, -j, -1}, {m, j, -j, -1}];
```

```
B1 = B0 { Sin[θ] Cos[ϕ], Sin[θ] Sin[ϕ], Cos[θ]};
A1 = (B1[[1]] Jx + B1[[2]] Jy + B1[[3]] Jz) // FullSimplify;
A1 // MatrixForm
```

$$\begin{pmatrix} B0\,\hbar\,\text{Cos}[\theta] & \frac{B0\,e^{-i\phi}\,\hbar\,\text{Sin}[\theta]}{\sqrt{2}} & 0 \\ \frac{B0\,e^{i\phi}\,\hbar\,\text{Sin}[\theta]}{\sqrt{2}} & 0 & \frac{B0\,e^{-i\phi}\,\hbar\,\text{Sin}[\theta]}{\sqrt{2}} \\ 0 & \frac{B0\,e^{i\phi}\,\hbar\,\text{Sin}[\theta]}{\sqrt{2}} & -B0\,\hbar\,\text{Cos}[\theta] \end{pmatrix}$$

```
eq1 = Eigensystem[A1] // FullSimplify
```

$$\Big\{\{0, -B0\,\hbar, B0\,\hbar\},\ \Big\{\Big\{-e^{-2 i\phi}, \sqrt{2}\,e^{-i\phi}\,\text{Cot}[\theta], 1\Big\}, \Big\{e^{-2 i\phi}\,\text{Tan}\Big[\frac{\theta}{2}\Big]^2, -\sqrt{2}\,e^{-i\phi}\,\text{Tan}\Big[\frac{\theta}{2}\Big], 1\Big\}, \Big\{e^{-2 i\phi}\,\text{Cot}\Big[\frac{\theta}{2}\Big]^2, \sqrt{2}\,e^{-i\phi}\,(\text{Cot}[\theta] + \text{Csc}[\theta]), 1\Big\}\Big\}\Big\}$$

```
ψ1 = eq1[[2, 3]]; ψ2 = eq1[[2, 1]]; ψ3 = eq1[[2, 2]];
```

```
N1 = ψ1*.ψ1 // FullSimplify
```

$$\text{Csc}\Big[\frac{\theta}{2}\Big]^4$$

N2 = ψ2*.ψ2 // FullSimplify

$$2\,\mathrm{Csc}[\theta]^2$$

N3 = ψ3*.ψ3 // FullSimplify

$$\mathrm{Sec}\left[\frac{\theta}{2}\right]^4$$

$$\phi 1 = e^{i\phi}\frac{\psi 1}{\mathrm{Csc}\left[\frac{\theta}{2}\right]^2} \text{ // Simplify; } \phi 1 \text{ // MatrixForm}$$

$$\begin{pmatrix} e^{-i\phi}\,\mathrm{Cos}\left[\frac{\theta}{2}\right]^2 \\ \frac{\mathrm{Sin}[\theta]}{\sqrt{2}} \\ e^{i\phi}\,\mathrm{Sin}\left[\frac{\theta}{2}\right]^2 \end{pmatrix}$$

$$\phi 2 = -e^{i\phi}\frac{\psi 2}{\sqrt{2}\,\mathrm{Csc}[\theta]} \text{ // Simplify; } \phi 2 \text{ // MatrixForm}$$

$$\begin{pmatrix} \frac{e^{-i\phi}\,\mathrm{Sin}[\theta]}{\sqrt{2}} \\ -\mathrm{Cos}[\theta] \\ -\frac{e^{i\phi}\,\mathrm{Sin}[\theta]}{\sqrt{2}} \end{pmatrix}$$

```
ϕ3 = e^(i ϕ) ψ3/Sec[θ/2]^2 // Simplify; ϕ3 // MatrixForm
```

$$\begin{pmatrix} e^{-i\phi}\,\mathrm{Sin}\left[\frac{\theta}{2}\right]^2 \\ -\frac{\mathrm{Sin}[\theta]}{\sqrt{2}} \\ e^{i\phi}\,\mathrm{Cos}\left[\frac{\theta}{2}\right]^2 \end{pmatrix}$$

```
Berry[ϕ1_] := Module[{P1, Pr, Pθ, Pϕ, Sr, Sθ, Sϕ, f1},
  Pr = 1/r D[ϕ1, r] // Simplify;
  Pθ = 1/r D[ϕ1, θ] // Simplify;
  Pϕ = 1/(r Sin[θ]) D[ϕ1, ϕ] // Simplify;
  Sr = ϕ1*.Pr // Simplify;
  Sθ = ϕ1*.Pr // Simplify;
  Sϕ = ϕ1*.Pϕ // Simplify;
  f1 = Curl[{Sr, Sθ, Sϕ}, {r, θ, ϕ}, "Spherical"] // Simplify]
Berry[ϕ1]
```

$$\left\{\frac{i}{r^2}, 0, 0\right\}$$

```
Berry[ϕ2]
```

$$\{0, 0, 0\}$$

```
Berry[ϕ3]
```

$$\left\{-\frac{i}{r^2}, 0, 0\right\}$$

REFERENCES

D.J. Griffiths, Introduction to Quantum Mechanics, second edition (Cambridge, 2017).
E.D. Commins, Quantum Mechanics An Experimentalist's Approach (Cambridge, 2014).