Berry phase

Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
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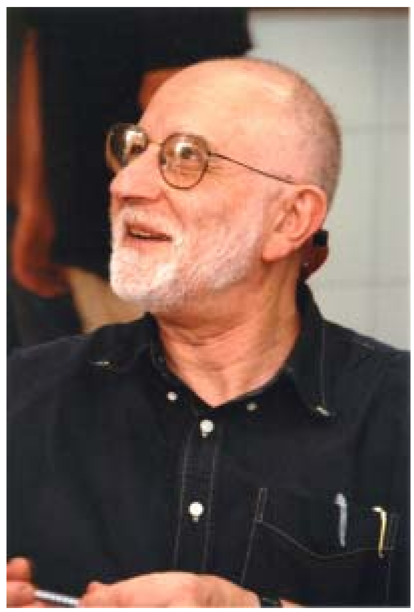
Sir Michael Victor Berry, FRS (born 14 March 1941), is a mathematical physicist at the University of Bristol, England. He was elected a fellow of the Royal Society of London in 1982 and knighted in 1996. From 2006 he has been editor of the journal, Proceedings of the Royal Society. He is famous for the Berry phase, a phenomenon observed e.g. in quantum mechanics and optics. He specializes in semi-classical physics (asymptotic physics, quantum chaos), applied to wave phenomena in quantum mechanics and other areas such as optics. He is also currently affiliated with the Institute for Quantum Studies at Chapman University in California.



Prof. Micheal Berry (Melville Wills Professor of Physics (Emeritus), University of Bristol)
https://michaelberryphysics.wordpress.com/

1. What is the Berry phase?

In classical and quantum mechanics, the **geometric phase**, **Pancharatnam–Berry phase** (named after S. Pancharatnam and Sir Michael Berry), **Pancharatnam phase** or most commonly **Berry phase**, is a phase difference acquired over the course of a cycle, when a system is subjected to cyclic adiabatic processes, which results from the geometrical properties of the parameter space of the Hamiltonian. The phenomenon was first discovered in 1956, and rediscovered in 1984. It can be seen in the Aharonov–Bohm effect and in the conical intersection of potential energy surfaces. In the case of the Aharonov–Bohm effect, the adiabatic parameter is the magnetic field enclosed by two interference paths, and it is cyclic in the sense that these two paths form a loop. In the case of the conical intersection, the adiabatic parameters are the molecular coordinates. Apart from quantum mechanics, it arises in a variety of other wave

systems, such as classical optics. As a rule of thumb, it can occur whenever there are at least two parameters characterizing a wave in the vicinity of some sort of singularity or hole in the topology; two parameters are required because either the set of nonsingular states will not be simply connected, or there will be nonzero holonomy.
http://en.wikipedia.org/wiki/Geometric_phase

2. General formula for phase factor

M.V. Berry, Quantum Phase Factors Accompanying Adiabatic Changes, Proc. R. London A392, 45-57 (1984).

Let the Hamiltonian $\hat{H}$ be changed by varying parameter $\boldsymbol{R}$ [$\boldsymbol{R}$ = (x, y, z)] on which it depends. Then the excursion of the system between times t = 0 and t = T can be pictured as transport round a closed path $\boldsymbol{R}(t)$ in parameter space, with Hamiltonian $\hat{H}(\mathbf{R}(t))$ and such that $\boldsymbol{R}(T) = \boldsymbol{R}(0)$. The path is called a circuit and denoted by C. For the adiabatic approximation to apply, T must be large.

The state vector $|\psi(t))\rangle$ of the system evolves according to Schrödinger equation given by

$$i\hbar\frac{\partial}{\partial t}|\psi(t))\rangle = i\hbar|\dot{\psi}(t))\rangle = \hat{H}(\boldsymbol{R}(t))|\psi(t))\rangle .$$

At any instant, the natural basis consists of the eigenstates $|n(\mathbf{R})\rangle$ (assumed discrete) of $\hat{H}(\mathbf{R})$ for $\boldsymbol{R} = \boldsymbol{R}(t)$, that satisfy

$$\hat{H}(\boldsymbol{R}(t))|n(\boldsymbol{R}(t))\rangle = E_n(\boldsymbol{R}(t))|n(\boldsymbol{R}(t))\rangle ,$$

with energies $E_n(\boldsymbol{R}(t))$. The eigenvalue equation implies no relation between the phases of the eigenstates $|n(\boldsymbol{R})\rangle$ at different $\boldsymbol{R}$.

Adiabatically, a system prepared in one of these states $|n(\boldsymbol{R}(0))\rangle$ will evolve with $\hat{H}$ and so be in the state $|n(R(t))\rangle$ at t

$$\begin{aligned}|\psi(t)\rangle &= \exp[-\frac{i}{\hbar}\int_0^t E_n(\boldsymbol{R}(t'))dt']\exp[i\gamma_n(t)]|n(\boldsymbol{R}(t))\rangle \\ &= \exp[i\theta_n(t)]\exp[i\gamma_n(t)]|n(\boldsymbol{R}(t))\rangle\end{aligned}$$

where $\gamma_n(t)$ is a geometric phase, and the dynamical phase factor $\theta_n(t)$ is defined by

$$\theta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(\boldsymbol{R}(t'))dt' . \qquad \dot{\theta}_n(t) = -\frac{1}{\hbar}E_n(t)$$

Plugging the solution form into the this Schrödinger equation, we get

$$i\hbar[\frac{\partial}{\partial t}\left|n(\boldsymbol{R}(t))\right\rangle - \frac{i}{\hbar}E_n(\boldsymbol{R}(t))\left|n(\boldsymbol{R}(t))\right\rangle + i\dot{\gamma}_n(t)\left|n(\boldsymbol{R}(t))\right\rangle] = E_n(\boldsymbol{R}(t))\left|n(\boldsymbol{R}(t))\right\rangle$$

or

$$\left|\dot{n}(\boldsymbol{R}(t))\right\rangle + i\dot{\gamma}_n(t)\left|n(\boldsymbol{R}(t))\right\rangle = 0 .$$

Taking the inner product with $\left\langle n(\boldsymbol{R}(t))\right|$ we get

$$\left\langle n(\boldsymbol{R}(t))\middle|\dot{n}(\boldsymbol{R}(t))\right\rangle + i\dot{\gamma}_n(t)\left\langle n(\boldsymbol{R}(t))\middle|n(\boldsymbol{R}(t))\right\rangle = 0 ,$$

Since $\left\langle n(\boldsymbol{R}(t))\middle|n(\boldsymbol{R}(t))\right\rangle = 1$, we have

$$\dot{\gamma}_n(t) = i\left\langle n(\boldsymbol{R}(t))\middle|\dot{n}(\boldsymbol{R}(t))\right\rangle$$

$\left|n(\boldsymbol{R}(t))\right\rangle$ depends on t because there is some parameter $\boldsymbol{R}(t)$ in the Hamiltonian that changes with time.

$$\left|\dot{n}(\boldsymbol{R}(t))\right\rangle = \left|\nabla_{\boldsymbol{R}} n(\boldsymbol{R}(t))\right\rangle \cdot \dot{\boldsymbol{R}}(t)$$

so that

$$\dot{\gamma}_n(t) = i\left\langle n(\boldsymbol{R}(t))\middle|\nabla_{\boldsymbol{R}} n(\boldsymbol{R}(t))\right\rangle \cdot \dot{\boldsymbol{R}}(t)$$

and thus

$$\gamma_n(t) = i\int_{\boldsymbol{R}_i}^{\boldsymbol{R}_f}\left\langle n(\boldsymbol{R}(t))\middle|\nabla_{\boldsymbol{R}} n(\boldsymbol{R}(t))\right\rangle \cdot d\boldsymbol{R}$$

3. Expression of $\gamma_n(C)$

We calculate the geometric phase $\gamma_n(C)$ as follows.

For $\langle n|n\rangle = 1$ (normalization), we have

$$\left\langle \frac{\partial n}{\partial x}\middle| n\right\rangle + \left\langle n \middle| \frac{\partial n}{\partial x}\right\rangle = 0,$$

$$\left\langle \frac{\partial n}{\partial y}\middle| n\right\rangle + \left\langle n \middle| \frac{\partial n}{\partial y}\right\rangle = 0,$$

$$\left\langle \frac{\partial n}{\partial z}\middle| n\right\rangle + \left\langle n \middle| \frac{\partial n}{\partial z}\right\rangle = 0.$$

For $\langle n|m\rangle = 0$ $\qquad (n \neq m)$ $\qquad$ (orthogonality)

$$\left\langle \frac{\partial n}{\partial x}\middle| m\right\rangle + \left\langle n \middle| \frac{\partial m}{\partial x}\right\rangle = 0,$$

$$\left\langle \frac{\partial n}{\partial y}\middle| m\right\rangle + \left\langle n \middle| \frac{\partial m}{\partial y}\right\rangle = 0,$$

$$\left\langle \frac{\partial n}{\partial z}\middle| m\right\rangle + \left\langle n \middle| \frac{\partial m}{\partial z}\right\rangle = 0.$$

The rotation of the vector $\boldsymbol{A}_0 = \langle n|\nabla n\rangle$ is given by

$$
\begin{aligned}
\nabla\times\boldsymbol{A}_0 &= \nabla\times\langle n|\nabla n\rangle \\
&= \begin{vmatrix} \boldsymbol{e}_x & \boldsymbol{e}_y & \boldsymbol{e}_z \\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \\ \left\langle n\middle|\dfrac{\partial n}{\partial x}\right\rangle & \left\langle n\middle|\dfrac{\partial n}{\partial y}\right\rangle & \left\langle n\middle|\dfrac{\partial n}{\partial z}\right\rangle \end{vmatrix} \\
&= [\frac{\partial}{\partial y}\left\langle n\middle|\frac{\partial n}{\partial z}\right\rangle - \frac{\partial}{\partial z}\left\langle n\middle|\frac{\partial n}{\partial y}\right\rangle]\boldsymbol{e}_x + [\frac{\partial}{\partial z}\left\langle n\middle|\frac{\partial n}{\partial x}\right\rangle - \frac{\partial}{\partial x}\left\langle n\middle|\frac{\partial n}{\partial z}\right\rangle]\boldsymbol{e}_y \\
&\quad + [\frac{\partial}{\partial x}\left\langle n\middle|\frac{\partial n}{\partial y}\right\rangle - \frac{\partial}{\partial y}\left\langle n\middle|\frac{\partial n}{\partial x}\right\rangle]\boldsymbol{e}_z
\end{aligned}
$$

$$
\begin{aligned}
(\nabla\times\boldsymbol{A}_0)_z &= \frac{\partial}{\partial x}\left\langle n\middle|\frac{\partial n}{\partial y}\right\rangle - \frac{\partial}{\partial y}\left\langle n\middle|\frac{\partial n}{\partial x}\right\rangle \\
&= \left\langle\frac{\partial n}{\partial x}\middle|\frac{\partial n}{\partial y}\right\rangle + \left\langle n\middle|\frac{\partial}{\partial x}\frac{\partial n}{\partial y}\right\rangle - \left\langle\frac{\partial n}{\partial y}\middle|\frac{\partial n}{\partial x}\right\rangle - \left\langle n\middle|\frac{\partial}{\partial y}\frac{\partial n}{\partial x}\right\rangle \\
&= \left\langle\frac{\partial n}{\partial x}\middle|\frac{\partial n}{\partial y}\right\rangle - \left\langle\frac{\partial n}{\partial y}\middle|\frac{\partial n}{\partial x}\right\rangle \\
&= \sum_m [\left\langle\frac{\partial n}{\partial x}\middle|m\right\rangle\left\langle m\middle|\frac{\partial n}{\partial y}\right\rangle - \left\langle\frac{\partial n}{\partial y}\middle|m\right\rangle\left\langle m\middle|\frac{\partial n}{\partial x}\right\rangle] \\
&= \sum_{m\neq n} [\left\langle\frac{\partial n}{\partial x}\middle|m\right\rangle\left\langle m\middle|\frac{\partial n}{\partial y}\right\rangle - \left\langle\frac{\partial n}{\partial y}\middle|m\right\rangle\left\langle m\middle|\frac{\partial n}{\partial x}\right\rangle] \\
&= \sum_{m\neq n} [-\left\langle n\middle|\frac{\partial m}{\partial x}\right\rangle\left\langle m\middle|\frac{\partial n}{\partial y}\right\rangle + \left\langle n\middle|\frac{\partial m}{\partial y}\right\rangle\left\langle m\middle|\frac{\partial n}{\partial x}\right\rangle]
\end{aligned}
$$

where we use the closure relation and the relations

$$
\left\langle\frac{\partial n}{\partial x}\middle|m\right\rangle = -\left\langle n\middle|\frac{\partial m}{\partial x}\right\rangle, \qquad \left\langle\frac{\partial n}{\partial y}\middle|m\right\rangle = -\left\langle n\middle|\frac{\partial m}{\partial y}\right\rangle.
$$

Then we obtain

$$
\begin{aligned}
(\nabla\times\boldsymbol{A}_0)_z &= \sum_{m\neq n}[-\left\langle n\left|\frac{\partial m}{\partial x}\right.\right\rangle\left\langle m\left|\frac{\partial n}{\partial y}\right.\right\rangle+\left\langle n\left|\frac{\partial m}{\partial y}\right.\right\rangle\left\langle m\left|\frac{\partial n}{\partial x}\right.\right\rangle] \\
&= \sum_{m\neq n}[-\frac{\langle n|\frac{\partial}{\partial x}\hat{H}|m\rangle}{E_m-E_n}\frac{\langle m|\frac{\partial}{\partial y}\hat{H}|n\rangle}{E_n-E_m}+\frac{\langle n|\frac{\partial}{\partial y}\hat{H}|m\rangle}{E_m-E_n}\frac{\langle m|\frac{\partial}{\partial x}\hat{H}|n\rangle}{E_n-E_m}] \\
&= \sum_{m\neq n}[\frac{\langle n|\frac{\partial}{\partial x}\hat{H}|m\rangle\langle m|\frac{\partial}{\partial y}\hat{H}|n\rangle-\langle n|\frac{\partial}{\partial y}\hat{H}|m\rangle\langle m|\frac{\partial}{\partial x}\hat{H}|n\rangle}{(E_m-E_n)^2}]
\end{aligned}
$$

where we use the relations

$$
\langle m|\partial_i n\rangle=\frac{\langle m|\partial_i\hat{H}|n\rangle}{E_n-E_m},\qquad \langle n|\partial_i m\rangle=\frac{\langle n|\partial_i\hat{H}|m\rangle}{E_m-E_n}
$$

with $i = x$, y, and z. We note that

$$
\boldsymbol{P}_{nm}\times\boldsymbol{P}_{mn}=\begin{vmatrix}\boldsymbol{e}_x & \boldsymbol{e}_y & \boldsymbol{e}_z \\ \langle n|\frac{\partial}{\partial x}\hat{H}|m\rangle & \langle n|\frac{\partial}{\partial y}\hat{H}|m\rangle & \langle n|\frac{\partial}{\partial z}\hat{H}|m\rangle \\ \langle m|\frac{\partial}{\partial x}\hat{H}|n\rangle & \langle m|\frac{\partial}{\partial y}\hat{H}|n\rangle & \langle m|\frac{\partial}{\partial z}\hat{H}|n\rangle\end{vmatrix}
$$

where

$$
\boldsymbol{P}_{nm}=\langle n|\nabla\hat{H}|m\rangle,\qquad \boldsymbol{P}_{mn}=\langle m|\nabla\hat{H}|n\rangle.
$$

Then we get

$$
\begin{aligned}
\nabla\times\boldsymbol{A}_0 &= \sum_{m\neq n}\frac{\boldsymbol{P}_{nm}\times\boldsymbol{P}_{mn}}{(E_m-E_n)^2} \\
&= \sum_{m\neq n}\frac{\langle n|\nabla\hat{H}|m\rangle\times\langle m|\nabla\hat{H}|n\rangle}{(E_m-E_n)^2}
\end{aligned}
$$

So we have

$$
\begin{aligned}
\gamma_n(C) &= i\oint d\boldsymbol{R}\cdot\boldsymbol{A}_0 \\
&= i\oint d\boldsymbol{R}\cdot\langle n|\nabla n\rangle \\
&= i\oint d\boldsymbol{R}\cdot[\mathrm{Re}(\langle n)|\nabla n\rangle) + i\,\mathrm{Im}(\langle n|\nabla n\rangle)] \\
&= -\mathrm{Im}\oint d\boldsymbol{R}\cdot\langle n|\nabla n\rangle
\end{aligned}
$$

since $\mathrm{Re}[\langle n)|\nabla n\rangle] = 0$. Using the Stokes' theorem, we get

$$
\begin{aligned}
\gamma_n(C) &= -\mathrm{Im}\oint d\boldsymbol{a}\cdot[\nabla\times\langle n|\nabla n\rangle] \\
&= -\oint d\boldsymbol{a}\cdot\boldsymbol{V}_n
\end{aligned}
$$

where da denotes are elements in *R* space

$$
\boldsymbol{V}_n(\boldsymbol{R}) = \mathrm{Im}\sum_{m\neq n}\frac{\langle n(\boldsymbol{R})|\nabla_{\boldsymbol{R}}\hat{H}(\boldsymbol{R})|m(\boldsymbol{R})\rangle\times\langle m(\boldsymbol{R})|\nabla_{\boldsymbol{R}}\hat{H}(\boldsymbol{R})|n(\boldsymbol{R})\rangle}{\left(E_m(\boldsymbol{R}) - E_n(\boldsymbol{R})\right)^2}
$$

The notation for $\boldsymbol{V}_n$ is the same used by Berry in the original paper (1984).

4. Spin in Magnetic Field (the adiabatic approximation)

A particle with the angular momentum $\hat{\mathbf{J}}$ interacts with a magnetic field ***B*** via the Hamiltonian:

$$
\hat{H}(\boldsymbol{B}) = -\frac{g_J\mu_B}{\hbar}\hat{\boldsymbol{J}}\cdot\boldsymbol{B},
$$

where g_J is the Lande-g factor. Note that

$$
\hat{J}_z|m(\boldsymbol{B})\rangle = \hbar m(\boldsymbol{B})|m(\boldsymbol{B})\rangle,
$$

where $|m(\boldsymbol{B})\rangle$ is the eigenstate of $\hat{J}_z$ with the eigenvalue $\hbar m(\boldsymbol{B})$.

For any fixed value of ***B***, we have

$$
\hat{H}(\boldsymbol{B})|m(\boldsymbol{B})\rangle = E_m(\boldsymbol{B})|m(\boldsymbol{B})\rangle
$$

Schrodinger equation:

$$i\hbar \frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \hat{H}[\boldsymbol{B}(t)]\left|\psi(t)\right\rangle = E_m(\boldsymbol{B}(t))\left|\psi(t)\right\rangle$$

with

$$\left|\psi(t=0)\right\rangle = \left|m(\boldsymbol{B}(t=0))\right\rangle$$

where $\left|m(\boldsymbol{B}(0))\right\rangle$ is the eigenstate of $\hat{H}(\boldsymbol{B}(t=0))$.

$$\begin{aligned}\left|\psi(t)\right\rangle &= \left|m(\boldsymbol{B}(t))\right\rangle \exp[-\frac{i}{\hbar}\int_0^t E_m(\boldsymbol{B}(t'))dt'] \exp[i\gamma_m(t)] \\ &= \left|m(\boldsymbol{B}(t))\right\rangle \exp[i\theta_m(t)] \exp[i\gamma_m(t)]\end{aligned}$$

where

$$\theta_m(t) = -\frac{1}{\hbar}\int_0^t E_m(\boldsymbol{B}(t'))dt'$$

Plugging the solution form into the this Schrodinger equation, we get

$$i\hbar[\frac{\partial}{\partial t}\left|m(\boldsymbol{B}(t))\right\rangle - \frac{i}{\hbar}E_m(\boldsymbol{B}(t))\left|m(\boldsymbol{B}(t))\right\rangle + \left|m(\boldsymbol{B}(t))\right\rangle i\frac{\partial \gamma_m(t)}{\partial t}] = E_m(\boldsymbol{B}(t))\left|m(\boldsymbol{B}(t))\right\rangle$$

or

$$i\left|\dot{m}(\boldsymbol{B}(t))\right\rangle = \left|m(\boldsymbol{B}(t))\right\rangle \frac{\partial \gamma_m(t)}{\partial t}$$

Taking the inner product with $\left\langle m(\boldsymbol{B}(t))\right|$ we get

$$i\left\langle m(\boldsymbol{B}(t))\middle|\dot{m}(\boldsymbol{B}(t))\right\rangle = \frac{\partial \gamma_m(t)}{\partial t}\left\langle m(\boldsymbol{B}(t))\middle|m(\boldsymbol{B}(t))\right\rangle,$$

Since $\left\langle m(\boldsymbol{B}(t))\middle|m(\boldsymbol{B}(t))\right\rangle = 1$, we have

$$\frac{\partial \gamma_m(t)}{\partial t} = i\langle m(\boldsymbol{B}(t)) | \dot{m}(\boldsymbol{B}(t))\rangle$$

or

$$\gamma_m(t) = i\int_0^t \langle m(\boldsymbol{B}(t')) | \dot{m}(\boldsymbol{B}(t'))\rangle dt'$$

Note that $\gamma_m(t)$ is real, since

$$\langle m(\boldsymbol{B}(t)) | \dot{m}(\boldsymbol{B}(t))\rangle + \langle \dot{m}(\boldsymbol{B}(t)) | m(\boldsymbol{B}(t))\rangle = \mathrm{Re}[\langle m(\boldsymbol{B}(t)) | \dot{m}(\boldsymbol{B}(t))\rangle] = 0$$

The geometrical character of the Berry phase emerges when the variation of the instantaneous energy eigenstates with time is restated as their variation with field;

$$|\dot{m}(\boldsymbol{B}(t))\rangle = \frac{\partial}{\partial t}|m(\boldsymbol{B}(t))\rangle = \frac{d\boldsymbol{B}(t)}{dt}\cdot\frac{\partial}{\partial \boldsymbol{B}}|m(\boldsymbol{B})\rangle = \dot{\boldsymbol{B}}\cdot|\nabla_{\boldsymbol{B}} m(\boldsymbol{B})\rangle$$

This expresses the phase as an integral over field values;

$$\begin{aligned}\gamma_m(C) &= i\oint d\boldsymbol{B}\cdot\langle m(\boldsymbol{B}) | \nabla_{\boldsymbol{B}} m(\boldsymbol{B})\rangle \\ &= i\oint d\boldsymbol{B}\cdot[\mathrm{Re}(\langle m(\boldsymbol{B}) | \nabla_{\boldsymbol{B}} m(\boldsymbol{B})\rangle) + i\,\mathrm{Im}(\langle m(\boldsymbol{B}) | \nabla_{\boldsymbol{B}} m(\boldsymbol{B})\rangle)] \qquad (1) \\ &= -\mathrm{Im}\oint d\boldsymbol{B}\cdot\langle m(\boldsymbol{B}) | \nabla_{\boldsymbol{B}} m(\boldsymbol{B})\rangle\end{aligned}$$

Note that

$$\langle m(\boldsymbol{B}) | \nabla_{\boldsymbol{B}} m(\boldsymbol{B})\rangle + \langle \nabla_{\boldsymbol{B}} m(\boldsymbol{B}) | m(\boldsymbol{B})\rangle = \mathrm{Re}[\langle m(\boldsymbol{B}) | \nabla_{\boldsymbol{B}} m(\boldsymbol{B})\rangle] = 0$$

Stokes’ theorem applied to Eq.(1) gives, in an abbreviated notation.

$$\begin{aligned}\gamma_m(C) &= -\mathrm{Im}\int d\boldsymbol{a}\cdot\nabla_{\boldsymbol{B}}\times\langle m(\boldsymbol{B}) | \nabla_{\boldsymbol{B}} m(\boldsymbol{B})\rangle \\ &= -\mathrm{Im}\int d\boldsymbol{a}\cdot\sum_{n\neq m}\langle \nabla_{\boldsymbol{B}} m(\boldsymbol{B}) | n(\boldsymbol{B})\rangle\times\langle n(\boldsymbol{B}) | \nabla_{\boldsymbol{B}} m(\boldsymbol{B})\rangle \\ &= -\mathrm{Im}\int d\boldsymbol{a}\cdot V_m(\boldsymbol{B})\end{aligned}$$

where

$$V_m(\boldsymbol{B}) = \sum_{n\neq m} \langle \nabla_{\boldsymbol{B}} m(\boldsymbol{B}) | n(\boldsymbol{B}) \rangle \times \langle n(\boldsymbol{B}) | \nabla_{\boldsymbol{B}} m(\boldsymbol{B}) \rangle$$

d$\boldsymbol{a}$ denotes area element in $\boldsymbol{B}$ space and exclusion in the summation is justified by $\langle n(\boldsymbol{B}) | \nabla_{\boldsymbol{B}} n(\boldsymbol{B}) \rangle$ being imaginary. The off-diagonal elements $\langle n(\mathbf{B}) | \nabla_{\mathbf{B}} m(\mathbf{B}) \rangle$ are obtained as follows. Since

$$\hat{H}(\boldsymbol{B}) | m(\boldsymbol{B}) \rangle = E_m(\boldsymbol{B}) | m(\boldsymbol{B}) \rangle, \qquad \text{(Eigenvalue problem)}$$

we get

$$\nabla_B \hat{H}(\boldsymbol{B}) | m(\boldsymbol{B}) \rangle + \hat{H}(\boldsymbol{B}) | \nabla_B m(\boldsymbol{B}) \rangle = \nabla_B E_m(\boldsymbol{B}) | m(\boldsymbol{B}) \rangle + E_m(\boldsymbol{B}) | \nabla_B m(\boldsymbol{B}) \rangle$$

But the $| n(\boldsymbol{B}) \rangle$ is an orthogonal set, so for $n \neq m$, we have

$$\langle n(\boldsymbol{B}) | \nabla_B \hat{H}(\boldsymbol{B}) | m(\boldsymbol{B}) \rangle + \langle n(\boldsymbol{B}) | \hat{H}(\boldsymbol{B}) | \nabla_B m(\boldsymbol{B}) \rangle = \langle n(\boldsymbol{B}) | \nabla_B E_m(\boldsymbol{B}) | m(\boldsymbol{B}) \rangle + \langle n(\boldsymbol{B}) | E_m(\boldsymbol{B}) | \nabla_B m(\boldsymbol{B}) \rangle$$

or

$$\langle n(\boldsymbol{B}) | \nabla_B \hat{H}(\boldsymbol{B}) | m(\boldsymbol{B}) \rangle + E_n(\boldsymbol{B}) \langle n(\boldsymbol{B}) | \nabla_B m(\boldsymbol{B}) \rangle = \langle n(\boldsymbol{B}) | \nabla_B E_m(\boldsymbol{B}) | m(\boldsymbol{B}) \rangle + E_m(\boldsymbol{B}) \langle n(\boldsymbol{B}) | \nabla_B m(\boldsymbol{B}) \rangle .$$

Since

$$\langle n(\boldsymbol{B}) | \nabla_B E_m(\boldsymbol{B}) | m(\boldsymbol{B}) \rangle = \nabla_B E_m(\boldsymbol{B}) \langle n(\boldsymbol{B}) | m(\boldsymbol{B}) \rangle = 0$$

we get

$$\langle n(\boldsymbol{B}) | \nabla_{\boldsymbol{B}} m(\boldsymbol{B}) \rangle = \frac{\langle n(\boldsymbol{B}) | \nabla_{\boldsymbol{B}} \hat{H}(\boldsymbol{B}) | m(\boldsymbol{B}) \rangle}{E_m(\boldsymbol{B}) - E_n(\boldsymbol{B})}$$

Hence

$$\boldsymbol{V}_m(\boldsymbol{B}) = \sum_{m\neq n} [\frac{\langle m(\boldsymbol{B}) | \nabla_{\boldsymbol{B}} \hat{H}(\boldsymbol{B}) | n(\boldsymbol{B}) \rangle \times \langle n(\boldsymbol{B}) | \nabla_{\boldsymbol{B}} \hat{H}(\boldsymbol{B}) | m(\boldsymbol{B}) \rangle}{(E_m(\boldsymbol{B}) - E_n(\boldsymbol{B})]^2}$$

where

$$\hat{H}(\boldsymbol{B}) = -\frac{g_J \mu_B}{\hbar}\hat{\boldsymbol{J}}\cdot\boldsymbol{B} = -\frac{g_J \mu_B B}{\hbar}\hat{\boldsymbol{J}}\cdot\boldsymbol{e}_B\,, \qquad \nabla_{\boldsymbol{B}}\hat{H}(\boldsymbol{B}) = -\frac{g_J \mu_B}{\hbar}\hat{\boldsymbol{J}}$$

Then we get

$$\boldsymbol{V}_m(\boldsymbol{B}) = \frac{1}{B^2\hbar^2}\sum_{m\neq n}[\frac{\langle m(\boldsymbol{B})|\hat{\boldsymbol{J}}|n(\boldsymbol{B})\rangle \times \langle n(\boldsymbol{B})|\hat{\boldsymbol{J}}|m(\boldsymbol{B})\rangle}{[m(\boldsymbol{B})-n(\boldsymbol{B})]^2}$$

$$\langle m(\boldsymbol{B})|\hat{\boldsymbol{J}}|n(\boldsymbol{B})\rangle \times \langle n(\boldsymbol{B})|\hat{\boldsymbol{J}}|m(\boldsymbol{B})\rangle = \begin{vmatrix} \boldsymbol{e}_1 & \boldsymbol{e}_2 & \boldsymbol{e}_3 \\ \langle m(\boldsymbol{B})|\hat{J}_1|n(\boldsymbol{B})\rangle & \langle m(\boldsymbol{B})|\hat{J}_2|n(\boldsymbol{B})\rangle & \langle m(\boldsymbol{B})|\hat{J}_3|n(\boldsymbol{B})\rangle \\ \langle n(\boldsymbol{B})|\hat{J}_1|m(\boldsymbol{B})\rangle & \langle n(\boldsymbol{B})|\hat{J}_2|m(\boldsymbol{B})\rangle & \langle n(\boldsymbol{B})|\hat{J}_3|m(\boldsymbol{B})\rangle \end{vmatrix}$$

$$\begin{aligned}\langle m(\boldsymbol{B})|\hat{J}_1|n(\boldsymbol{B})\rangle &= \frac{1}{2}\langle m(\boldsymbol{B})|\hat{J}_+ + \hat{J}_-|n(\boldsymbol{B})\rangle \\ &= \frac{1}{2}\langle m(\boldsymbol{B})|\hat{J}_+|n(\boldsymbol{B})\rangle + \frac{1}{2}\langle m(\boldsymbol{B})|\hat{J}_-|n(\boldsymbol{B})\rangle\end{aligned}$$

$$\langle m(\boldsymbol{B})|\hat{J}_2|n(\boldsymbol{B})\rangle = \frac{1}{2i}\langle m(\boldsymbol{B})|\hat{J}_+ - \hat{J}_-|n(\boldsymbol{B})\rangle$$

$$\langle m(\boldsymbol{B})|\hat{J}_3|n(\boldsymbol{B})\rangle = \hbar n\langle m|n\rangle = \hbar n\delta_{m,n}$$

$$\begin{aligned}\langle m(\boldsymbol{B})|\hat{J}_+|n(\boldsymbol{B})\rangle &= \hbar\sqrt{(j-n)(j+n+1)}\langle m|n+1\rangle \\ &= \hbar\sqrt{(j-n)(j+n+1)}\delta_{m,n+1} \\ &= \hbar\sqrt{(j-m-1)(j+m)}\delta_{m,n+1}\end{aligned}$$

$$\begin{aligned}\langle m(\boldsymbol{B})|\hat{J}_-|n(\boldsymbol{B})\rangle &= \hbar\sqrt{(j+n)(j-n+1)}\langle m|n-1\rangle \\ &= \hbar\sqrt{(j+n)(j-n+1)}\delta_{m,n-1} \\ &= \hbar\sqrt{(j+m+1)(j-m)}\delta_{m,n-1}\end{aligned}$$

So we get

$$[\,\mathrm{Im}[\boldsymbol{V}_{m1}(\boldsymbol{B})] = \frac{1}{B^2\hbar^2}\mathrm{Im}\sum_{m\neq n}[\frac{\langle m(\boldsymbol{B})|\hat{J}_2|n(\boldsymbol{B})\rangle\langle n(\boldsymbol{B})|\hat{J}_3|m(\boldsymbol{B})\rangle - \langle m(\boldsymbol{B})|\hat{J}_3|n(\boldsymbol{B})\rangle\langle n(\boldsymbol{B})|\hat{J}_2|m(\boldsymbol{B})\rangle}{[m(\boldsymbol{B})-n(\boldsymbol{B})]^2}$$

or

$$\mathrm{Im}\boldsymbol{V}_{m1}(\boldsymbol{B}) = 0 .$$

$$\mathrm{Im}\boldsymbol{V}_{m2}(\boldsymbol{B}) = \frac{1}{B^2\hbar^2}\mathrm{Im}\sum_{m\neq n}[\frac{\langle m(\boldsymbol{B})|\hat{J}_3|n(\boldsymbol{B})\rangle\langle n(\boldsymbol{B})|\hat{J}_1|m(\boldsymbol{B})\rangle - \langle m(\boldsymbol{B})|\hat{J}_1|n(\boldsymbol{B})\rangle\langle n(\boldsymbol{B})|\hat{J}_3|m(\boldsymbol{B})\rangle}{[m(\boldsymbol{B})-n(\boldsymbol{B})]^2}$$

or

$$\mathrm{Im}\boldsymbol{V}_{m2}(\boldsymbol{B}) = 0 .$$

$$\mathrm{Im}\boldsymbol{V}_{m3}(\boldsymbol{B}) = \frac{1}{B^2\hbar^2}\mathrm{Im}\sum_{m\neq n}[\frac{\langle m(\boldsymbol{B})|\hat{J}_1|n(\boldsymbol{B})\rangle\langle n(\boldsymbol{B})|\hat{J}_2|m(\boldsymbol{B})\rangle - \langle m(\boldsymbol{B})|\hat{J}_2|n(\boldsymbol{B})\rangle\langle n(\boldsymbol{B})|\hat{J}_1|m(\boldsymbol{B})\rangle}{[m(\boldsymbol{B})-n(\boldsymbol{B})]^2}$$

Since $[m(\boldsymbol{B})-n(\boldsymbol{B})]^2 = 1$, we have

$$\begin{aligned}
\mathrm{Im}[\boldsymbol{V}_{m3}(\boldsymbol{B})] &= \frac{1}{B^2\hbar^2}\mathrm{Im}\sum_{n=m\pm 1}[\langle m(\boldsymbol{B})|\hat{J}_1|n(\boldsymbol{B})\rangle\langle n(\boldsymbol{B})|\hat{J}_2|m(\boldsymbol{B})\rangle \\
&\quad - \langle m(\boldsymbol{B})|\hat{J}_2|n(\boldsymbol{B})\rangle\langle n(\boldsymbol{B})|\hat{J}_1|m(\boldsymbol{B})\rangle] \\
&= \frac{1}{B^2\hbar^2}\mathrm{Im}\langle m(\boldsymbol{B})|\hat{J}_1\hat{J}_2 - \hat{J}_2\hat{J}_1|m(\boldsymbol{B})\rangle \\
&= \frac{1}{B^2\hbar^2}\mathrm{Im}\langle m(\boldsymbol{B})|i\hbar\hat{J}_3|m(\boldsymbol{B})\rangle \\
&= \frac{m(\boldsymbol{B})}{B^2} \\
&= \frac{m(\boldsymbol{B})}{B^2}
\end{aligned}$$

Here we use the commutation relation

$$\hat{J}_1\hat{J}_2 - \hat{J}_2\hat{J}_1 = i\hbar\hat{J}_3 .$$

We can put this in a form that does not depend on choice of the 3-axis to lie along $\boldsymbol{B}$:

$$\mathrm{Im}[\mathbf{V}_m(\mathbf{B})] = \frac{m(\mathbf{B})}{B^3}\mathbf{B}$$

We note that is

$$\nabla \cdot \nabla_{\mathbf{B}} \frac{1}{B} = -4\pi\delta(\mathbf{B})$$

where

$$\nabla_{\mathbf{B}} \frac{1}{B} = -\frac{\mathbf{B}}{B^3}$$

This singularity is spherically symmetric. 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 $\Omega(C)$ is the solid angle subtended by C as seen from the origin in field space .

$$\int d\mathbf{a}\cdot \frac{1}{B^3}\mathbf{B} = \int B^2 d\Omega(\mathbf{e}_B \cdot \frac{1}{B^2}\mathbf{e}_B) = \int d\Omega = \Omega(C)$$

((**Note**)) Vector analysis: Gauss' law

$$\int d\mathbf{B}[\nabla_{\mathbf{B}}{}^2 \frac{1}{B})] = \int d\mathbf{B}[\nabla_{\mathbf{B}}\cdot(\nabla_{\mathbf{B}}\frac{1}{B})] = \int d\mathbf{a}\cdot\nabla_{\mathbf{B}}\frac{1}{B} = -\int d\mathbf{a}\cdot\frac{B}{B^3} = -4\pi$$

where

$$\nabla_{\mathbf{B}} \frac{1}{B} = -\frac{\mathbf{B}}{B^3}.$$

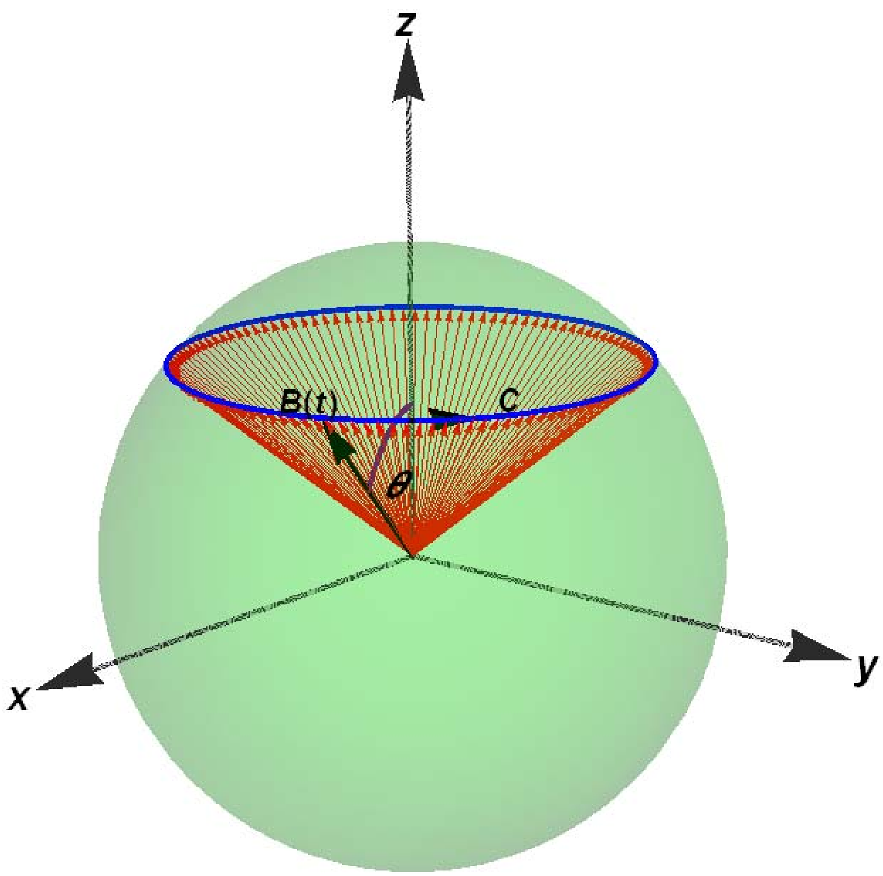
We have

$$\nabla_{\boldsymbol{B}}\cdot(\nabla_{\boldsymbol{B}}\frac{1}{B}) = \nabla_B{}^2\frac{1}{B} = -4\pi\delta(\boldsymbol{B})$$

where $\delta(\mathbf{B})$ is the Dirac delta function.

$$\Delta\Omega = \int_0^{\pi}\sin\theta d\theta\int_0^{2\pi}d\phi = 2\pi(1-\cos\theta)$$

5. Example: spin ½ under the magnetic field which undergoes a precession adiabatically



The magnetic field is given by

$$\boldsymbol{B} = B_0 \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}$$

with

$$\phi = \omega t\,.$$

Spin magnetic moment: $\hat{\boldsymbol{\mu}}_s = -\dfrac{2\mu_B}{\hbar}\hat{\boldsymbol{S}} = -\mu_B\hat{\boldsymbol{\sigma}}$.

where

$$\mu_B = \frac{e\hbar}{2mc}. \qquad \text{(Bohr magneton)}$$

The spin Hamiltonian is given by

$$\hat{H}(t) = -\hat{\boldsymbol{\mu}}_s \cdot \boldsymbol{B}(t) = \mu_B \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{B}(t) = \mu_B B(t) \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n}$$

where $\hat{\boldsymbol{\sigma}}$ is the Pauli spin operator. The eigenstates are given by

$$\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n}(t) \left| +\boldsymbol{n}(t) \right\rangle = + \left| +\boldsymbol{n}(t) \right\rangle, \qquad \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{n}(t) \left| -\boldsymbol{n}(t) \right\rangle = - \left| -\boldsymbol{n}(t) \right\rangle$$

where

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\left| +\mathbf{n}(t) \right\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi} \sin\frac{\theta}{2} \end{pmatrix}, \qquad \left| -\boldsymbol{n}(t) \right\rangle = \begin{pmatrix} -\sin\frac{\theta}{2} \\ e^{i\phi} \cos\frac{\theta}{2} \end{pmatrix}$$

The energy eigenstate:

$$\hat{H}(t) \left| +\boldsymbol{n}(t) \right\rangle = \mu_B B(t) \left| +\boldsymbol{n}(t) \right\rangle, \qquad \hat{H}(t) \left| -\boldsymbol{n}(t) \right\rangle = -\mu_B B(t) \left| -\boldsymbol{n}(t) \right\rangle$$

$\left| +\boldsymbol{n}(t) \right\rangle$ is the eigenstate of $\hat{H}(t)$ with the energy eigenvalue $E_+ = \mu_B B(t)$. $\left| -\boldsymbol{n}(t) \right\rangle$ is the eigenstate of $\hat{H}(t)$ with the energy eigenvalue $E_- = -\mu_B B(t)$.

We note that we change the parameters: $\theta \to \pi - \theta$ and $\phi \to \pi + \phi$ in

$$\left| +\boldsymbol{n}(t) \right\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi} \sin\frac{\theta}{2} \end{pmatrix},$$

Then we get

$$\left|-\mathbf{n}(t)\right\rangle = \begin{pmatrix} -\sin\dfrac{\theta}{2} \\ e^{i\phi}\cos\dfrac{\theta}{2} \end{pmatrix}$$

$$\rightarrow \begin{pmatrix} \cos\dfrac{(\pi-\theta)}{2} \\ e^{i(\phi+\pi)}\sin\dfrac{(\pi-\theta)}{2} \end{pmatrix} = -\begin{pmatrix} -\sin\dfrac{\theta}{2} \\ e^{i\phi}\cos\dfrac{\theta}{2} \end{pmatrix} = -\left|-\boldsymbol{n}(t)\right\rangle$$

except for the minus sign, when $\theta \to \pi - \theta$ and $\phi \to \pi + \phi$ (parity operation).

In the spherical co-ordinate,

$$\begin{aligned}
\nabla\left|+\boldsymbol{n}(t)\right\rangle &= \boldsymbol{e}_r \frac{\partial}{\partial r}\left|+\boldsymbol{n}(t)\right\rangle + \boldsymbol{e}_\theta \frac{1}{r}\frac{\partial}{\partial\theta}\left|+\boldsymbol{n}(t)\right\rangle + \boldsymbol{e}_\phi \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\left|+\boldsymbol{n}(t)\right\rangle \\
&= \boldsymbol{e}_\theta \frac{1}{r}\frac{\partial}{\partial\theta}\begin{pmatrix} \cos\dfrac{\theta}{2} \\ e^{i\phi}\sin\dfrac{\theta}{2} \end{pmatrix} + \boldsymbol{e}_\phi \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\begin{pmatrix} \cos\dfrac{\theta}{2} \\ e^{i\phi}\sin\dfrac{\theta}{2} \end{pmatrix} \\
&= \boldsymbol{e}_\theta \frac{1}{r}\begin{pmatrix} -\dfrac{1}{2}\sin\dfrac{\theta}{2} \\ e^{i\phi}\dfrac{1}{2}\cos\dfrac{\theta}{2} \end{pmatrix} + \boldsymbol{e}_\phi \frac{1}{r\sin\theta}\begin{pmatrix} 0 \\ ie^{i\phi}\sin\dfrac{\theta}{2} \end{pmatrix}
\end{aligned}$$

$$\begin{aligned}
\nabla\left|-\boldsymbol{n}(t)\right\rangle &= \boldsymbol{e}_r \frac{\partial}{\partial r}\left|-\boldsymbol{n}(t)\right\rangle + \boldsymbol{e}_\theta \frac{1}{r}\frac{\partial}{\partial\theta}\left|-\boldsymbol{n}(t)\right\rangle + \boldsymbol{e}_\phi \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\left|-\boldsymbol{n}(t)\right\rangle \\
&= \boldsymbol{e}_\theta \frac{1}{r}\frac{\partial}{\partial\theta}\begin{pmatrix} -\sin\dfrac{\theta}{2} \\ e^{i\phi}\cos\dfrac{\theta}{2} \end{pmatrix} + \boldsymbol{e}_\phi \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\begin{pmatrix} -\sin\dfrac{\theta}{2} \\ e^{i\phi}\cos\dfrac{\theta}{2} \end{pmatrix} \\
&= \boldsymbol{e}_\theta \frac{1}{r}\begin{pmatrix} -\dfrac{1}{2}\cos\dfrac{\theta}{2} \\ -e^{i\phi}\dfrac{1}{2}\sin\dfrac{\theta}{2} \end{pmatrix} + \boldsymbol{e}_\phi \frac{1}{r\sin\theta}\begin{pmatrix} 0 \\ ie^{i\phi}\cos\dfrac{\theta}{2} \end{pmatrix}
\end{aligned}$$

Then we get

$$\left\langle +\boldsymbol{n}(t)\right|\nabla\left|+\boldsymbol{n}(t)\right\rangle = \boldsymbol{e}_\theta \frac{1}{r}\begin{pmatrix}\cos\frac{\theta}{2} & e^{-i\phi}\sin\frac{\theta}{2}\end{pmatrix}\begin{pmatrix}-\frac{1}{2}\sin\frac{\theta}{2}\\ e^{i\phi}\frac{1}{2}\cos\frac{\theta}{2}\end{pmatrix}$$

$$+\boldsymbol{e}_\phi \frac{1}{r\sin\theta}\begin{pmatrix}\cos\frac{\theta}{2} & e^{-i\phi}\sin\frac{\theta}{2}\end{pmatrix}\begin{pmatrix}0\\ ie^{i\phi}\sin\frac{\theta}{2}\end{pmatrix}$$

$$= \boldsymbol{e}_\phi \frac{i\sin^2\frac{\theta}{2}}{r\sin\theta}$$

where

$$\left\langle +\boldsymbol{n}(t)\right| = \begin{pmatrix}\cos\frac{\theta}{2} & e^{-i\phi}\sin\frac{\theta}{2}\end{pmatrix}.$$

$$\left\langle -\boldsymbol{n}(t)\right|\nabla\left|-\boldsymbol{n}(t)\right\rangle = \boldsymbol{e}_\theta \frac{1}{r}\begin{pmatrix}-\sin\frac{\theta}{2} & e^{-i\phi}\cos\frac{\theta}{2}\end{pmatrix}\begin{pmatrix}-\frac{1}{2}\cos\frac{\theta}{2}\\ -e^{i\phi}\frac{1}{2}\sin\frac{\theta}{2}\end{pmatrix}$$

$$+\boldsymbol{e}_\phi \frac{1}{r\sin\theta}\begin{pmatrix}-\sin\frac{\theta}{2} & e^{-i\phi}\cos\frac{\theta}{2}\end{pmatrix}\begin{pmatrix}0\\ ie^{i\phi}\cos\frac{\theta}{2}\end{pmatrix}$$

$$= \boldsymbol{e}_\phi \frac{i\cos^2\frac{\theta}{2}}{r\sin\theta}$$

where

$$\left\langle -\boldsymbol{n}(t)\right| = \begin{pmatrix}-\sin\frac{\theta}{2} & e^{-i\phi}\cos\frac{\theta}{2}\end{pmatrix}.$$

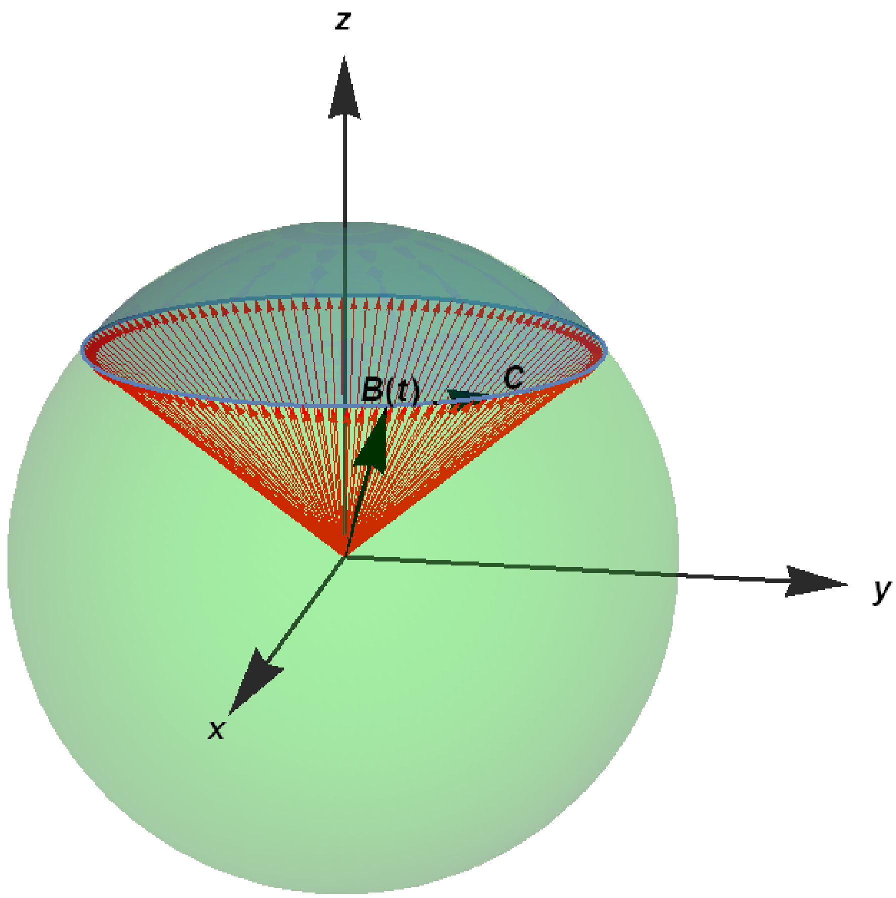
$$\begin{aligned}
\gamma_+(C) &= i\oint\left\langle +\boldsymbol{n}(t)\right|\nabla\left|+\boldsymbol{n}(t)\right\rangle\cdot d\boldsymbol{r}\\
&= i\int_0^{2\pi}\boldsymbol{e}_\phi\cdot\boldsymbol{e}_\phi \frac{i\sin^2\frac{\theta}{2}}{r\sin\theta} r\sin\theta d\phi\\
&= -2\pi\sin^2\frac{\theta}{2}\\
&= -\pi(1-\cos\theta)
\end{aligned}$$

$$
\begin{aligned}
\gamma_{-}(C) &= i\oint \langle -\boldsymbol{n}(t)|\nabla| -\boldsymbol{n}(t)\rangle \cdot d\boldsymbol{r} \\
&= i\int_{0}^{2\pi} \boldsymbol{e}_{\phi}\cdot\boldsymbol{e}_{\phi}\frac{i\cos^{2}\frac{\theta}{2}}{r\sin\theta} r\sin\theta d\phi \\
&= -2\pi\cos^{2}\frac{\theta}{2} \\
&= -\pi(1+\cos\theta)
\end{aligned}
$$

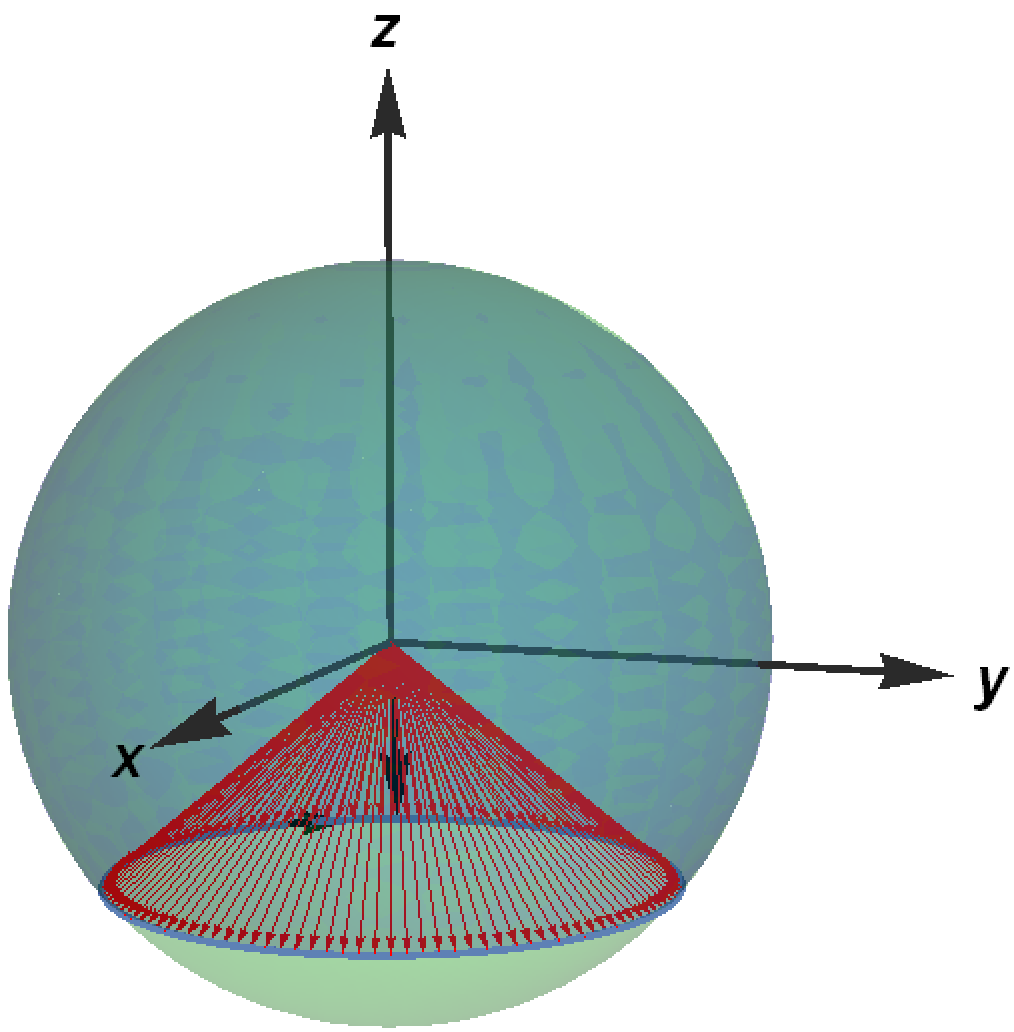
The solid angle

$$\Omega(C) = \int_{0}^{\theta} 2\pi\sin\theta d\theta = 2\pi(1-\cos\theta)$$

$$\theta_{\pm} = -\frac{1}{\hbar}\int_{0}^{T} E_{\pm}(t')dt' = \mp\frac{\mu_{B}}{\hbar}B_{0}T$$



z
B(t)
C
y
x



The final state after one rotation where $B(T) = B_0$ is then given by

$$\begin{aligned}|\psi_{\pm}(T)\rangle &= \exp[i\theta_n(T)]\exp[i\gamma_n(T)]|\pm n(T)\rangle \\ &= \exp[-i\pi(1\mp\cos\theta]\exp(\mp i\frac{\mu_B}{\hbar}B_0T)|\pm n(0)\rangle\end{aligned}$$

We see that the dynamical phase factor depends on the period T of the rotation, but the geometrical phase depends only on the special geometry of the problem. In this case it depends on the opening angle q of the cone that the magnetic field traces out.

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APPENDIX

Derivation of Green's function

$$\nabla^2 \frac{1}{r} = -4\pi\delta(\boldsymbol{r}),$$

where

$$\boldsymbol{r} = (x, y, z), \qquad r = \sqrt{x^2 + y^2 + z^2}\ .$$

We consider a sphere with radius ε ($\varepsilon \to 0$)

$$\int d\boldsymbol{r} \nabla \cdot \nabla \frac{1}{r} = \int d\boldsymbol{r} \Delta \frac{1}{r} = \int d\boldsymbol{a} \cdot \nabla \frac{1}{r} = \int da (\boldsymbol{n} \cdot \nabla \frac{1}{r})$$

where

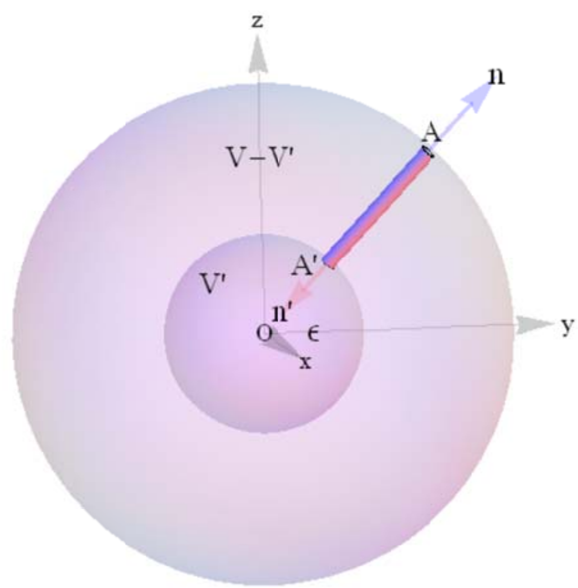
$$r = \sqrt{x^2 + y^2 + z^2}, \qquad \boldsymbol{n} = \frac{\boldsymbol{r}}{r} = \boldsymbol{e}_r = (\frac{x}{r}, \frac{y}{r}, \frac{z}{r}), \qquad d\boldsymbol{a} = \boldsymbol{n} da$$

and

$$\nabla \frac{1}{r} = -\frac{\boldsymbol{r}}{r^3}, \qquad \boldsymbol{n} \cdot \nabla \frac{1}{r} = \hat{r} \cdot (-\frac{\boldsymbol{r}}{r^3}) = -\frac{1}{r^2}$$

$\nabla \cdot \nabla(\frac{1}{r}) = 0$ except at the origin.

We now consider the volume integral over the whole volume (*V* - *V*') between the surface *A* and the surface of sphere *A*' (volume *V*', radius $\varepsilon \to 0)$. We note that the outer surface and the inner surface are connected to an appropriate cylinder.



Since $\nabla \cdot \nabla(\frac{1}{r}) = 0$ over the whole volume *V* - *V*' we have

Using the Gauss's law, we get

$$\int_{V-V'} d\mathbf{r}\nabla \cdot \nabla \frac{1}{r} = \int_{V-V'} d\mathbf{r}\nabla^2 \frac{1}{r}$$

$$= \int_A da(\mathbf{n} \cdot \nabla \frac{1}{r}) + \int_{A'} da'(\mathbf{n}' \cdot \nabla \frac{1}{r}) = 0$$

or

$$\int_A da(\boldsymbol{n} \cdot \nabla \frac{1}{r}) = -\int_{A'} da'(\boldsymbol{n}' \cdot \nabla \frac{1}{r}) = \int_{A'} da'(\boldsymbol{n} \cdot \nabla \frac{1}{r})$$

where $\boldsymbol{n}' = -\boldsymbol{n} = -\hat{r}$ and d$\boldsymbol{r}$ is over the volume integral. Then we have

$$\int_A da(\boldsymbol{n}\cdot\nabla\frac{1}{r}) = \int da(-\frac{1}{r^2}) = -4\pi\varepsilon^2\frac{1}{\varepsilon^2} = -4\pi = -4\pi\int d\boldsymbol{r}\delta(\boldsymbol{r})$$

Using the Gauss's law, we have

$$\int_A da(\boldsymbol{n}\cdot\nabla\frac{1}{r}) = \int_V d\boldsymbol{r}(\nabla\cdot\nabla\frac{1}{r}) = -4\pi\int_V d\boldsymbol{r}\delta(\boldsymbol{r})$$

or

$$\Delta\frac{1}{r} = -4\pi\delta(\boldsymbol{r}).$$

or

$$\Delta(\frac{1}{4\pi r}) = -\delta(\boldsymbol{r}).$$

((**Mathematica**))

```
Clear["Gobal`"];

Needs["VectorAnalysis`"]

SetCoordinates[Cartesian[x, y, z]]

Cartesian[x, y, z]

r1 = {x, y, z}; r = √r1.r1

√(x^2 + y^2 + z^2)

Grad[1/r] // Simplify

{-x/(x^2 + y^2 + z^2)^(3/2), -y/(x^2 + y^2 + z^2)^(3/2), -z/(x^2 + y^2 + z^2)^(3/2)}

Laplacian[1/r] // Simplify

0
```