自旋系统的路径积分.

自旋 $\frac{1}{2}$

$$|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle = \begin{pmatrix}\alpha\\ \beta\end{pmatrix}, \quad |\alpha|^2+|\beta|^2=1.$$

自由度 其实有3个.

$$|\psi\rangle = |b,\theta,\varphi\rangle = e^{ib}\left(e^{-i\frac{\varphi}{2}}\cos\frac{\theta}{2}|\uparrow\rangle + e^{i\frac{\varphi}{2}}\sin\frac{\theta}{2}|\downarrow\rangle\right)$$

e^{ib} 为整体相因子. 无关乎物理. gauge 变换的自由度

$(\cdot)$ 中是 $\sigma_{\vec{n}}$ 的本征态. (本征值为 1). 完备:

$$\int_0^{\pi}\sin\theta\, d\theta\int_0^{2\pi}d\varphi\ |b,\theta,\varphi\rangle\langle b,\theta,\varphi| = |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| = \mathbb{1}$$

$$\langle b,\theta,\varphi|\frac{\hbar}{2}\vec{\sigma}|b,\theta,\varphi\rangle = \frac{1}{2}\langle\vec{n}|\vec{\sigma}|\vec{n}\rangle = \frac{1}{2}\vec{n} \qquad (\hbar=1)$$

但是不正交. $\langle\vec{n}'|\vec{n}\rangle \neq \delta(\vec{n}-\vec{n}')$

对路径积分而言, 完备性有了就 OK.

令 $|\tau\rangle = |b(\tau),\theta(\tau),\varphi(\tau)\rangle$

$$\langle\tau+\Delta\tau|e^{-\Delta\tau H}|\tau\rangle \cong \langle\tau+\Delta\tau|(1-\Delta\tau H)|\tau\rangle$$

$$= \langle\tau+\Delta\tau|\tau\rangle - \Delta\tau\langle\tau+\Delta\tau|H|\tau\rangle$$

$$\boxed{\text{由于 } 0=\frac{d}{d\tau}\langle\tau|\tau\rangle = \langle\dot{\tau}|\tau\rangle + \langle\tau|\dot{\tau}\rangle = 2\,\mathrm{Re}\langle\tau|\dot{\tau}\rangle}$$

$$\approx \left[\langle\tau| + \Delta\tau\frac{d}{d\tau}\langle\tau|\right]|\tau\rangle - \Delta\tau\langle\tau|H|\tau\rangle \qquad (\text{略去 } \Delta\tau^2)$$

$$= 1+\Delta\tau\left[\langle\dot{\tau}|\tau\rangle - \langle\tau|H|\tau\rangle\right]$$

$$= e^{\Delta\tau\left[\langle\dot{\tau}|\tau\rangle - \langle\tau|H|\tau\rangle\right]}$$

$\langle\dot{\tau}|\tau\rangle$ 纯虚数 $\rightarrow$ 相位.

反映 $|\tau\rangle$ 与 $|\tau+\Delta\tau\rangle$ 的"连络"

对应 单粒子空间运动.

$$\langle x(\tau+\Delta\tau)\,|\,x(\tau)\rangle = \int dp(\tau)\,\langle x(\tau+\Delta\tau)\,|\,p(\tau)\rangle\langle p(\tau)\,|\,x(\tau)\rangle$$

$$= \int \frac{dp(\tau)}{2\pi\hbar}\, e^{ip(\tau)[x(\tau+\Delta\tau)-x(\tau)]}$$

$$= \int \frac{dp(\tau)}{2\pi\hbar}\, e^{i\Delta\tau\, p(\tau)\,\dot{x}(\tau)}$$

$p(\tau)\,\dot{x}(\tau)$ 对应 $\langle \dot{\tau}\,|\,\tau\rangle$

$$\frac{d|\tau\rangle}{d\tau} = i\dot{b}\,|\tau\rangle + e^{ib}\Big[\Big(-\frac{i\dot{\varphi}}{2}\cos\frac{\theta}{2} - \frac{\dot{\theta}}{2}\sin\frac{\theta}{2}\Big)e^{-i\frac{\varphi}{2}}\,|\uparrow\rangle + \Big(\frac{i\dot{\varphi}}{2}\sin\frac{\theta}{2} + \frac{\dot{\theta}}{2}\cos\frac{\theta}{2}\Big)e^{i\varphi/2}\,|\downarrow\rangle\Big]$$

$$\langle\tau|\dot{\tau}\rangle = -\langle\dot{\tau}|\tau\rangle$$

$$= i\dot{b} + \cos\frac{\theta}{2}\Big(-\frac{i\dot{\varphi}}{2}\cos\frac{\theta}{2} - \frac{\dot{\theta}}{2}\sin\frac{\theta}{2}\Big) + \sin\frac{\theta}{2}\Big(\frac{i\dot{\varphi}}{2}\sin\frac{\theta}{2} + \frac{\dot{\theta}}{2}\cos\frac{\theta}{2}\Big)$$

$$= i\Big(\dot{b} - \frac{1}{2}\dot{\varphi}\cos\theta\Big)$$

现在 固定一个 规范:

边界条件 $\vec{n}(\beta) = \vec{n}(0)$. $\to$ ~~$\theta(0)=\theta(\beta),\ \varphi(0)=\varphi(\beta)$~~

但之 $\varphi \to \varphi \pm 2\pi$. $|\theta(\beta),\varphi(\beta)\rangle = |\theta(0),\varphi(0)\rangle$

我们选 $b = \pm\frac{\varphi}{2}$

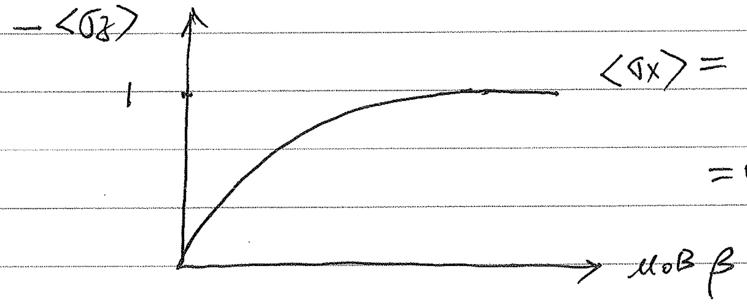
以磁场中一个自旋$\frac{1}{2}$粒子为例. $H=-\vec{\mu}\cdot\vec{B}$, $\vec{\mu}=-\mu_0\vec{\sigma}$

取磁场方向为z, 外界环境 T. $H=\mu_0 B\sigma_z$

$$\rho=\frac{e^{-\beta H}}{Z}, \quad Z=\mathrm{Tr}\, e^{-\beta H}$$

$$\langle\sigma_z\rangle=\mathrm{Tr}(\rho\sigma_z)=\frac{\mathrm{Tr}(e^{-\beta H}\sigma_z)}{Z}=\frac{\langle\uparrow|e^{-\mu_0 B\beta}|\uparrow\rangle-\langle\downarrow|e^{+\mu_0 B\beta}|\downarrow\rangle}{Z}$$

$=-\mathrm{th}\,x$, 令 $x=\beta\mu_0 B$.



$$\langle\sigma_x\rangle=\frac{\langle\uparrow|e^{-x}\sigma_x|\uparrow\rangle+\langle\downarrow|e^{x}\sigma_x|\downarrow\rangle}{Z}$$

$=0$.

理解: 粒子处于 $|\uparrow\rangle$ 的几率: $\frac{1}{Z}e^{-\mu_0 B\beta}$, 处于 $|\downarrow\rangle$ 的几率 $\frac{1}{Z}e^{\mu_0 B\beta}$

在 $|\uparrow\rangle$ 态. $\langle\sigma_z\rangle=+1$, 在 $|\downarrow\rangle$ 态, $\langle\sigma_z\rangle=-1$.

$\langle\sigma_x\rangle=0$, $\langle\sigma_x\rangle=0$.

$$Z=\langle\uparrow|e^{-\beta H}|\uparrow\rangle+\langle\downarrow|e^{-\beta H}|\downarrow\rangle$$

$$=e^{-x}+e^{x}$$

$$\langle\sigma_z\rangle=-\frac{\partial\ln Z}{\beta\mu_0\partial B}$$

在自旋相干态表象下 $|\vec{n}\rangle = e^{ib}\left(e^{-\frac{i\varphi}{2}}\cos\frac{\theta}{2}|\uparrow\rangle + e^{\frac{i\varphi}{2}}\sin\frac{\theta}{2}|\downarrow\rangle\right)$

$\sigma_{\vec{n}}|\vec{n}\rangle = 1\cdot|\vec{n}\rangle$, $\vec{\sigma}|\vec{n}\rangle = \vec{n}|\vec{n}\rangle$

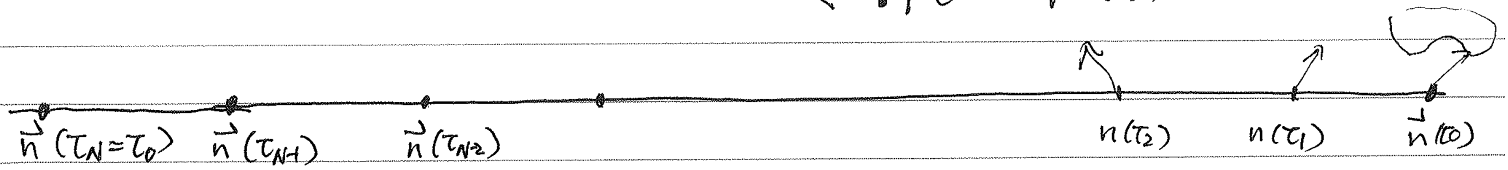
$$Z=\int_0^{\pi}\sin\theta d\theta\int_0^{2\pi}d\varphi\langle\vec{n}|e^{-\beta H}|\vec{n}\rangle$$ 对立体角积分.

$$e^{-\beta H} = e^{-\frac{\beta H}{N}\cdot N}, \quad \frac{\beta}{N}\equiv\Delta\tau,$$

插入完备关系:

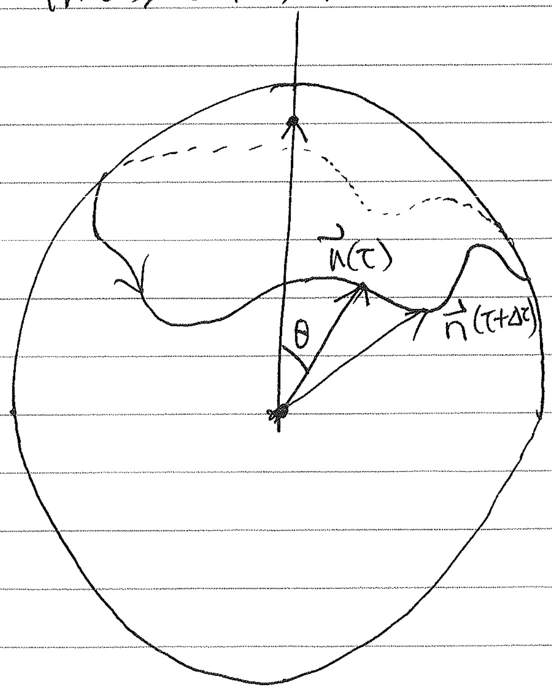
~~思~~ $\langle\vec{n}|e^{-\beta H}|\vec{n}\rangle = \langle\vec{n}|e^{-\Delta\tau H}|\vec{n}(\tau_{N-1})\rangle\langle\vec{n}(\tau_{N-1})|e^{-\Delta\tau H}|\vec{n}(\tau_{N-2})\rangle$

...... $\langle\tau_1|e^{-\Delta\tau H}|\vec{n}(0)\rangle$



"时间"方向上周期边界. $\underset{\downarrow\,\beta}{\vec{n}(\tau_N)} = \underset{\downarrow\,0}{\vec{n}(\tau_0)}$

简写: $|\vec{n}(\tau)\rangle\equiv|\tau\rangle$.



相邻两个时刻 $\langle\tau+\Delta\tau|e^{-\Delta\tau H}|\tau\rangle = e^{\Delta\tau[\langle\dot{\tau}|\tau\rangle - \langle\tau|H|\tau\rangle]}$

其中 $|\dot{\tau}\rangle\equiv\frac{d}{d\tau}|\tau\rangle$, $\langle\dot{\tau}|\tau\rangle$ 纯虚数. 给出相位

在上面例子中: $\langle\tau|H|\tau\rangle = \langle\tau|\mu_0\vec{\sigma}\cdot\vec{B}|\tau\rangle = \mu_0\vec{n}\cdot\vec{B}$ $\longrightarrow$ 经典自旋!

对应 单粒子空间运动.

$$\langle x(\tau+\Delta\tau) \mid x(\tau)\rangle = \int dp(\tau)\ \langle x(\tau+\Delta\tau) \mid p(\tau)\rangle\langle p(\tau) \mid x(\tau)\rangle$$

$$= \int \frac{dp(\tau)}{2\pi\hbar}\, e^{ip(\tau)[x(\tau+\Delta\tau)-x(\tau)]}$$

$$= \int \frac{dp(\tau)}{2\pi\hbar}\, e^{i\Delta\tau\, p(\tau)\, \dot{x}(\tau)}$$ 移到后面

$p(\tau)\dot{x}(\tau)$ 对应 $\langle \dot{\tau} \mid \tau\rangle$

直接计算:

$$\frac{d|\tau\rangle}{d\tau} = i\dot{b}\,|\tau\rangle + e^{ib}\Big[\Big(-\frac{i\dot{\varphi}}{2}\cos\frac{\theta}{2} - \frac{\dot{\theta}}{2}\sin\frac{\theta}{2}\Big)e^{-\frac{i\varphi}{2}}|\uparrow\rangle + \Big(\frac{i\dot{\varphi}}{2}\sin\frac{\theta}{2} + \frac{\dot{\theta}}{2}\cos\frac{\theta}{2}\Big)e^{i\varphi/2}|\downarrow\rangle\Big]$$

$$\langle\tau|\dot{\tau}\rangle = -\langle\dot{\tau}|\tau\rangle$$

$$= i\dot{b} + \cos\frac{\theta}{2}\Big(-\frac{i\dot{\varphi}}{2}\cos\frac{\theta}{2} - \frac{\dot{\theta}}{2}\sin\frac{\theta}{2}\Big) + \sin\frac{\theta}{2}\Big(\frac{i\dot{\varphi}}{2}\sin\frac{\theta}{2} + \frac{\dot{\theta}}{2}\cos\frac{\theta}{2}\Big)$$

$$= i\Big(\dot{b} - \frac{1}{2}\dot{\varphi}\cos\theta\Big)$$

现在 固定一个 规定:

θ, φ 要由 $\vec{n}$ 完全确定.

要求: 边界条件 $\vec{n}(\beta) = \vec{n}(0)$, ~~$\rightarrow \theta(0)=\theta(\beta),\ \varphi(0)=\varphi(\beta)$~~

边界条件 改为 $\boxed{|\theta(\beta),\varphi(\beta)\rangle = |\theta(0),\varphi(0)\rangle}$

然而: $|\vec{n}(\theta,\varphi)\rangle = e^{ib}\Big(e^{-\frac{i\varphi}{2}}\cos\frac{\theta}{2}|\uparrow\rangle + e^{\frac{i\varphi}{2}}\sin\frac{\theta}{2}|\downarrow\rangle\Big)$

设想 我们让 $\varphi \to \varphi \pm 2\pi$, 这不改变 $\vec{n}$, 但是

$|\vec{n}(\theta,\varphi\pm 2\pi)\rangle = -|\vec{n}(\theta,\varphi)\rangle$

选择 $b = \pm\frac{\varphi}{2}$. 让 $e^{\frac{i\varphi}{2}} = 1\ (\text{or } e^{-i\varphi})$, $e^{\frac{i\varphi}{2}} = -e^{-i\varphi}$ (或 1)

比如 $b=\frac{\varphi}{2}$. $\langle\vec n(\beta)|e^{-\beta H}|\vec n(0)\rangle$ 等于对所有路径的积分.

$\langle\vec n(\beta)| = \langle\vec n(0)|$

每一条路径对应单位圆上的一条封闭路径.

$$\langle\vec n(\beta)|e^{-\beta H}|\vec n(0)\rangle = \int \mathcal{D}\vec n(\tau)\, e^{-S} \qquad (\hbar=1.)$$

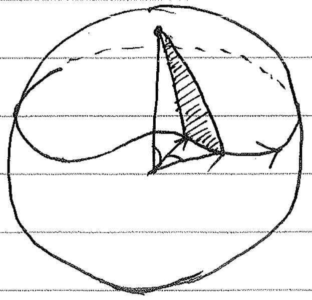
$$S = -\int_0^\beta \langle\dot\tau|\tau\rangle d\tau + \int_0^\beta \langle\tau|H|\tau\rangle d\tau$$

$$= i\int_0^\beta\left(\dot b-\frac{\dot\varphi}{2}\cos\theta\right)d\tau + \int_0^\beta H(\vec\sigma\to\vec n)\,d\tau$$

$b=\frac{\varphi}{2}$, $\dot b=\frac{\dot\varphi}{2}$,

$$= \underbrace{iI\int_0^\beta(1-\cos\theta)\dot\varphi\, d\tau}_{\text{Berry phase.}} + \int_0^\beta H(\vec n I)\,d\tau$$

$\boxed{\vec S = I\vec\sigma}$, $\hbar=1$ 也适用一般 $I=\frac12, 1, \frac32\cdots$



$(1-\cos\theta)\dot\varphi\,\Delta\tau$ 对应立体角 (从 z, $\vec n(\tau)$, $\vec n(\tau+\Delta\tau)$)

$$\int_0^{\theta(\tau)}\sin\theta\, d\theta = 1-\cos\theta(\tau).$$

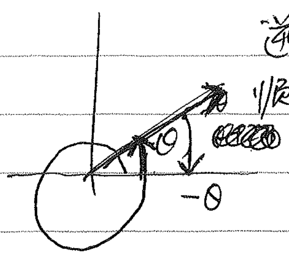
记封闭回路对应立体角为 Ω.

Berry phase $= iI\Omega$.

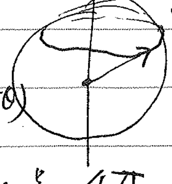
逆时针, 夹角为 θ.

顺时针, 夹角为 $-\theta$ 或 $(2\pi-\theta)$

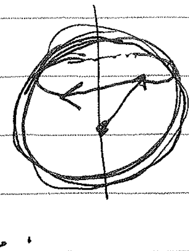
可理解为逆 $(2\pi-\theta)$



θ $-\theta$



Ω



右手法则:

$-\Omega$ 或 $4\pi-\Omega$

立体角 4π 为模

Ω 也可以是 $4\pi+\Omega$.

只要 $2I$ 是整数. $e^{iI(4\pi+\Omega)} = e^{iI\Omega}$ 不影响物理

这个要求说明 自旋量子数必须是 $\boxed{\text{整数或半整数}}$