PHYS 525
Solution to HW 2

(Dated: January 24, 2019)

PROBLEM I

Berry's phase and curvature in a two-level system. *Consider a two-level system described by the Hamiltonian*

$$H = \boldsymbol{d} \cdot \boldsymbol{\sigma} \tag{1}$$

where $\boldsymbol{d}$ is a real vector and $\boldsymbol{\sigma}$ the vector of the Pauli matrices.
a) Using the spherical representation $\boldsymbol{d} = d(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ write the Hamiltonian and show that its normalized, orthogonal eigenstates corresponding to eigenvalues $\pm d$ can be written as

$$|+\rangle = \begin{pmatrix} \cos\frac{\theta}{2}e^{i\phi} \\ \sin\frac{\theta}{2} \end{pmatrix}, \qquad |-\rangle = \begin{pmatrix} \sin\frac{\theta}{2}e^{i\phi} \\ -\cos\frac{\theta}{2}. \end{pmatrix} \tag{2}$$

SOLUTION:
With $\boldsymbol{d}$ as given in the problem, we have

$$\boldsymbol{\sigma} = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right). \tag{3}$$

Therefore, the Hamiltonian can be written as

$$H = d \begin{pmatrix} \cos\theta & \sin\theta e^{i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix}. \tag{4}$$

The eigenvalues λ can be determined from

$$\det\left(H - \lambda \mathbf{1}_{2\times 2}\right) = 0 \Rightarrow \left(\cos\theta - \frac{\lambda}{2}\right)\left(-\cos\theta - \frac{\lambda}{2}\right) - \sin^2\theta = 0 \tag{5}$$

$$\Rightarrow \left(\frac{\lambda}{d}\right)^2 = \sin^2\theta + \cos^2\theta = 1. \tag{6}$$

The eigenvalues are

$$\lambda_\pm = \pm d. \tag{7}$$

We can check that $|\pm\rangle$ are eigenstates via direct substitution

$$H|+\rangle = d \begin{pmatrix} \cos\theta & \sin\theta e^{i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix} \begin{pmatrix} \cos\frac{\theta}{2}e^{i\phi} \\ \sin\frac{\theta}{2} \end{pmatrix} = d \begin{pmatrix} e^{i\phi}\left[\cos\theta\cos\frac{\theta}{2} + \sin\theta\sin\frac{\theta}{2}\right] \\ \sin\theta\cos\frac{\theta}{2} - \cos\theta\sin\frac{\theta}{2} \end{pmatrix} \tag{8}$$

$$= d \begin{pmatrix} \cos\frac{\theta}{2}e^{i\phi} \\ \sin\frac{\theta}{2} \end{pmatrix} = d|+\rangle, \tag{9}$$

where the formulas

$$\sin(x-y) = \sin x\cos y - \cos x\sin y \tag{10}$$

$$\cos(x-y) = \cos x\cos y + \sin x\sin y \tag{11}$$

were used. A similar calculation holds for $|-\rangle$.

b) Find the components of the Berry connection A_d, A_θ and A_ϕ for the negative-energy state. Show that only the non-zero component of the Berry curvature is $F_{\theta\phi} = \frac{1}{2}\sin\theta$.

SOLUTION:

We can work using two conventions. The first is defined by

$$A_d = i \langle\lambda| \frac{\partial}{\partial d} |\lambda\rangle \tag{12}$$
$$A_\theta = i \langle\lambda| \frac{\partial}{\partial \theta} |\lambda\rangle \tag{13}$$
$$A_\phi = i \langle\lambda| \frac{\partial}{\partial \phi} |\lambda\rangle \tag{14}$$
$$F_{ij} = (\partial_i A_j - \partial_j A_i) \tag{15}$$
$$n = \sum_{ij} \int\int dx_i dy_j F_{ij} \tag{16}$$

where n is a topological invariant.

The second involves using the canonical form of the ∇ operator in spherical coordinates:

$$\boldsymbol{A} = i \langle\lambda| \boldsymbol{\nabla} |\lambda\rangle \tag{17}$$
$$\boldsymbol{F} = \boldsymbol{\nabla} \times \boldsymbol{A} \tag{18}$$
$$n = \int d\boldsymbol{S} \cdot \boldsymbol{F} \tag{19}$$

where the standard expressions of the operators in spherical coordinates are

$$\boldsymbol{\nabla} f = \frac{\partial f}{\partial d}\hat{\boldsymbol{d}} + \frac{1}{d}\frac{\partial f}{\partial \theta}\hat{\boldsymbol{\theta}} + \frac{1}{d\sin\theta}\frac{\partial f}{\partial \phi}\hat{\boldsymbol{\phi}} \tag{20}$$
$$\boldsymbol{\nabla} \times \boldsymbol{A} = \frac{1}{d\sin\theta}\left(\frac{\partial}{\partial\theta}(A_\phi \sin_\theta) - \frac{\partial A_\theta}{\partial \phi}\right)\hat{\boldsymbol{d}} \tag{21}$$
$$+ \frac{1}{d}\left(\frac{1}{\sin\theta}\frac{\partial A_d}{\partial\phi} - \frac{\partial}{\partial d}(dA_\phi)\right)\hat{\boldsymbol{\theta}} \tag{22}$$
$$+ \frac{1}{d}\left(\frac{\partial}{\partial d}(dA_\theta) - \frac{\partial A_d}{\partial\theta}\right)\hat{\boldsymbol{\phi}} \tag{23}$$

Note that while both $\boldsymbol{A}, \boldsymbol{F}$ differ due to the different conventions, the topological invariant is the same.

Within the first convention we have

$$A_d = 0 \ \text{(trivially)} \tag{24}$$
$$A_\theta = i\left(\sin\tfrac{\theta}{2}e^{i\phi} \quad -\cos\tfrac{\theta}{2}\right)\begin{pmatrix}\frac{1}{2}\cos\frac{\theta}{2}e^{-i\phi} \\ -\frac{1}{2}\sin\frac{\theta}{2}\end{pmatrix} \tag{25}$$
$$= 0 \tag{26}$$
$$A_\phi = i\left(\sin\tfrac{\theta}{2}e^{i\phi} \quad -\cos\tfrac{\theta}{2}\right)\begin{pmatrix}-i\sin\frac{\theta}{2}e^{-i\phi} \\ 0\end{pmatrix} \tag{27}$$
$$= \sin^2\frac{\theta}{2} \tag{28}$$

with

$$F_{\theta\phi} = \frac{1}{2}\sin\theta \tag{29}$$

in the first convention.

Within the second convention we have

$$A_d = 0 \tag{30}$$
$$A_\theta = 0 \tag{31}$$
$$A_\phi = \frac{1}{2d}\tan\frac{\theta}{2} \tag{32}$$
$$\boldsymbol{F} = \frac{1}{2d^2}\hat{\boldsymbol{d}} \tag{33}$$

c) Repeat the calculation in part (b) in a different gauge obtained by the transformation $|\pm\rangle \to e^{i\phi}|\pm\rangle$. Show that although A changes, F stays the same.

SOLUTION:

Within the first convention we have

$$\begin{aligned}
A_d =& 0 \;\; \text{(trivially)} && (34)\\
A_\theta =& \frac{i}{2}\begin{pmatrix}\sin\frac{\theta}{2} & -\cos\frac{\theta}{2}e^{-i\phi}\end{pmatrix}\begin{pmatrix}\cos\frac{\theta}{2}\\ \sin\frac{\theta}{2}e^{i\phi}\end{pmatrix} && (35)\\
=& 0 && (36)\\
A_\phi =& i\begin{pmatrix}\sin\frac{\theta}{2} & -\cos\frac{\theta}{2}e^{i\phi}\end{pmatrix}\begin{pmatrix}0\\ -i\cos\frac{\theta}{2}e^{-i\phi}\end{pmatrix} && (37)\\
=& -\cos^2\frac{\theta}{2} && (38)\\
F_{\theta\phi} =& \frac{1}{2}\sin\theta && (39)
\end{aligned}$$

A similar calculation holds within the second convention.

d) Now calculate the Berry curvature directly from the Hamiltonian making use of the formula $F_{\theta\phi} = \frac{1}{2}\hat{\boldsymbol{d}}\cdot\left(\partial_\theta\hat{\boldsymbol{d}}\times\partial_\phi\hat{\boldsymbol{d}}\right)$

SOLUTION

$$\begin{aligned}
F_{\theta\phi} =& \frac{1}{2}\begin{vmatrix}\sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta\\ \cos\theta\cos\phi & \cos\theta\sin\phi & -\sin\theta\\ -\sin\theta\sin\phi & \sin\theta\cos\phi & 0\end{vmatrix} && (40)\\
=& \frac{1}{2}\left[-\sin\theta\cos\phi\left(-\sin^2\theta\sin\phi-\cos^2\theta\sin\phi\right)\right]-\sin\theta\cos\phi\left(-\sin^2\theta\cos\phi-\cos^2\theta\cos\phi\right) && (41)\\
=& \frac{1}{2}\sin\theta && (42)
\end{aligned}$$

e) On the basis of the above results show that the Berry phase acquired by the system when vector $\hat{\boldsymbol{d}}$ sweeps a closed contour on the unit sphere is equal to $(1/2)\Omega$, where Ω is the corresponding solid angle.

SOLUTION

Within the first convention we have

$$\gamma = i\oint_\Omega \langle -|\boldsymbol{\nabla}|-\rangle = \int\int_{\text{Area enclosed by}\Omega} d\theta d\phi F_{\theta\phi} = \frac{1}{2}\int\int d\theta d\phi\sin\theta = \frac{\Omega}{2} \tag{43}$$

Within the second convention

$$\gamma = \oint d\boldsymbol{l}\cdot\boldsymbol{A} = \int\int d\boldsymbol{S}\cdot(\boldsymbol{\nabla}\times\boldsymbol{A}) = \int\int d\theta d\phi d^2\sin\theta\frac{1}{d^2} = \frac{\Omega}{2} \tag{44}$$

PROBLEM II

Thouless charge pump. *Consider the Su-Schrieffer-Heeger(SSH) model discussed in class. Propose a time-dependent generalization of the SSH Hamiltonian $H(k,\tau)$, where τ is the time parameter, such that the system realizes a Thouless charge pump.*

SOLUTION:

We need to choose $H(k,\tau) = \boldsymbol{d}(k,\tau)\cdot\boldsymbol{\sigma}$ such that the spectrum remains gapped. As suggested in the problem, it is sufficient to choose terms such that over a period T, the vector $\hat{\boldsymbol{d}}$ covers the unit sphere an integer number of times. This is equivalent to the statement

$$\Delta P = \frac{e}{2\pi}\int_S F_{k\tau}dkd\tau = en \tag{45}$$

with

$$F_{k\tau} = \frac{1}{2}\hat{\boldsymbol{d}}\cdot\left(\partial_\tau\hat{\boldsymbol{d}}\times\partial_k\hat{\boldsymbol{d}}\right), \tag{46}$$

and $\Delta P = P(T) - P(0)$ is the change in polarization.

One choice for the Hamiltonian *valid for either* $\delta t < 0$ *or* $\delta t > 0$, which covers the sphere once is

$$d_x = \left(t + \delta t\cos\frac{2\pi\tau}{T}\right) + \left(t - \delta t\cos\frac{2\pi\tau}{T}\right)\cos ka \tag{47}$$

$$d_y = \left(t - \delta t\cos\frac{2\pi\tau}{T}\right)\sin ka \tag{48}$$

$$d_z = \delta t\sin\frac{2\pi\tau}{T} \tag{49}$$

Other simple choices, valid *only for* $\delta t < 0$, and covering the sphere twice and once respectively are

$$d_x = [(t+\delta t) + (t-\delta t)\cos ka]\cos\frac{2\pi\tau}{T} \tag{50}$$

$$d_y = [(t-\delta t)\sin ka] \tag{51}$$

$$d_z = [(t+\delta t) + (t-\delta t)\cos ka]\sin\frac{2\pi\tau}{T} \tag{52}$$

and

$$d_x = (t+\delta t) + (t-\delta t)\cos ka\cos\frac{2\pi\tau}{T} \tag{53}$$

$$d_y = (t-\delta t)\sin ka\cos\frac{2\pi\tau}{T} \tag{54}$$

$$d_z = \alpha\sin\frac{2\pi\tau}{T} \tag{55}$$

In the first of the above one can see that the $\hat{d}$-vector starts as a circle along the equator of the unit sphere at $\tau = 0$. The circle then rotates around the y-axis as a function of τ, eventually coming back to the equator after a 2π rotation. This covers the unit sphere twice, resulting in charge $2e$ being pumped.

The second choice instead moves the circle from the equator to the north pole where it shrinks to a single point, covering the upper hemisphere in the process. The point then moves to the south pole (not covering any area), expands to a circle again and moves back to the equator covering the southern hemisphere.

INCORRECT, COMMON GUESSES:

$$d_x = (t+\delta t) + (t-\delta t)\cos ka \tag{56}$$

$$d_y = (t-\delta t)\sin ka \tag{57}$$

$$d_z = \alpha\sin\frac{2\pi\tau}{T} \tag{58}$$

This is incorrect since the Berry curvature must change sign with $d_z(\tau)$, s.t. the contributions cancel.

Also, for choices with $d_z = 0$ vector $\hat{d}$ remains confined to the equator of the unit sphere and thus cannot cover the sphere.