TFY4205 Quantum Mechanics II
Problemset mandatory exercise 1 fall 2022

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SUGGESTED SOLUTION

Problem 1
This problem actually also shows that the Berry phase is a real number. Note that the momentum operator must be Hermitian since it corresponds to a physical quantity, meaning

$$\hat{p} = \hat{p}^\dagger \tag{1}$$
$$\frac{\hbar}{i}\nabla_R = \left(\frac{\hbar}{i}\nabla_R\right)^\dagger \tag{2}$$
$$\nabla_R = -\nabla_R^\dagger \tag{3}$$

A first-order derivative is thus anti-Hermitian. Inserting this relationship into the expression of $\mathbf{A}_n(\mathbf{R})$ we get that $\langle n;t|(\nabla_R|n;t\rangle) = -(\langle n;t|(\nabla_R|n;t\rangle))^*$, in which case it is a purely imaginary quantity. Therefore $\mathbf{A}_n(\mathbf{R})$ must be real.

Alternatively: Remember that a differential operator acts to the right, and that you can differentiate a ket (or a bra) with respect to the parameters on which it depends, and get a different ket (or bra). Begin very explicit to make this clear, we have

$$0 = \nabla_R[\mathbf{1}] \tag{4}$$
$$= \nabla_R[\langle n;t|n;t\rangle] \tag{5}$$
$$= \nabla_R[(\langle n;t|)(|n;t\rangle)] \tag{6}$$
$$= (\nabla_R\langle n;t|)|n;t\rangle + \langle n;t|(\nabla_R|n;t\rangle) \tag{7}$$

However, $(\nabla_R\langle n;t|)|n;t\rangle = (\langle n;t|(\nabla_R|n;t\rangle))^*$. This can be seen as follows. First, note that:

$$\frac{d}{dx}\langle\psi|\phi\rangle = \langle\psi|\frac{d}{dx}\phi\rangle + \langle\frac{d}{dx}\psi|\phi\rangle, \tag{8}$$

where the second term can be evaluated as

$$\begin{aligned}
\langle\frac{d}{dx}\psi|\phi\rangle &= \int\frac{d\psi^*}{dx}\phi dx = \psi^*\phi|_{\text{surface}} - \int\psi^*\frac{d\phi}{dx}dx \\
&= -\int\psi^*\frac{d\phi}{dx}dx \\
&= \langle\psi| -\frac{d}{dx}\phi\rangle \\
&= \langle\psi|\left(\frac{d}{dx}\right)^\dagger\phi\rangle \\
&= \left(\langle\phi|\frac{d}{dx}\psi\rangle\right)^*
\end{aligned} \tag{9}$$

Here, we assumed that the surface term in the partial integration vanishes as it should infinitely far away. So $\langle n;t|(\nabla_R|n;t\rangle) = -(\langle n;t|(\nabla_R|n;t\rangle))^*$, in which case it is a purely imaginary quantity. Therefore $\mathbf{A}_n(\mathbf{R})$ must be real.

Problem 2

a. The original Hamiltonian is

$$H_0 = \frac{\hbar\omega}{2}\left[P^2 + Q^2\right] = \hbar\omega\left[a^\dagger a + \frac{1}{2}\right] \tag{10}$$

where $a = \frac{1}{\sqrt{2}}\big(Q + iP\big)$, $a^\dagger = \frac{1}{\sqrt{2}}\big(Q - iP\big)$. Let

$$H = \frac{\hbar\omega}{2}\left[\left(P - \sqrt{2}x_1\right)^2 + \left(Q - \sqrt{2}x_2\right)^2\right] \tag{11}$$

$$= \hbar\omega\left[\left(a^\dagger - \alpha\right)\left(a - \alpha^*\right) + \frac{1}{2}\right] \tag{12}$$

where $\alpha = (x_1 + ix_2)$ and x_1, x_2 are two slowly varying real parameter that together describe a closed curve in the x_1x_2 plane. We now show that

$$H = D(\alpha)H_0D^\dagger(\alpha) \tag{13}$$

where

$$D(\alpha) = \exp\big(\alpha a^\dagger - \alpha^* a\big) \tag{14}$$

$$D^\dagger(\alpha) = \exp\big(\alpha^* a - \alpha a^\dagger\big) \tag{15}$$

To demonstrate (13) we use the identity

$$e^A B e^{-A} = B + \big[A,B\big] + \frac{1}{2!}\big[A,\big[A,B\big]\big] + \ldots \tag{16}$$

where $A = \alpha a^\dagger - \alpha^* a$ and $B = a^\dagger a$. Now,

$$[a^\dagger, a^\dagger a] = -a^\dagger \tag{17}$$

$$[a, a^\dagger a] = a \tag{18}$$

Hence,

$$\big[A,\big[A,B\big]\big] = -\big[\big(\alpha a^\dagger - \alpha^* a\big),\big(\alpha a^\dagger - \alpha^* a\big)\big] \tag{19}$$

$$= 2|\alpha|^2 \tag{20}$$

Thus (16) can be written

$$D(\alpha)a^\dagger a D^\dagger(\alpha) = a^\dagger a - \alpha a^\dagger - \alpha^* a + |\alpha|^2 \tag{21}$$

which proves (13). Now, the eigenstates of H_0 are obviously the number eigenstates $|n\rangle$, with the corresponding eigenvalues $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$. Thus we have

$$H_0|n\rangle = E_n|n\rangle \tag{22}$$

and therefore

$$D(\alpha)H_0D^\dagger(\alpha)D(\alpha)|n\rangle = HD|n\rangle = E_nD|n\rangle \tag{23}$$

Thus the eigenvalues of H corresponding to the energies E_n are

$$|n,\alpha\rangle = D(\alpha)|n\rangle \tag{24}$$

b. We have that

$$D^\dagger \nabla D = D^\dagger \frac{\partial D}{\partial x_1}\hat{x}_1 + D^\dagger \frac{\partial D}{\partial x_2}\hat{x}_2 \tag{25}$$

To evaluate the right hand side of (25), use choose $A = -i(\alpha a^\dagger - \alpha^* a)$. Then

$$D^\dagger \frac{\partial D}{\partial x_1} = e^{-iA}\frac{\partial}{\partial x}e^{iA} \tag{26}$$

It will soon be clear why we make this choice.

Let $g(\lambda) = e^{\lambda A}\frac{\partial}{\partial x_1}e^{-\lambda A}$, and Taylor expand around $\lambda = 0$:

$$g(\lambda) = g(0) + \lambda\frac{\partial g}{\partial \lambda}\Big|_{\lambda=0} + \frac{\lambda^2}{2!}\frac{\partial^2 g}{\partial \lambda^2}\Big|_{\lambda=0} + \frac{\lambda^3}{3!}\frac{\partial^3 g}{\partial \lambda^3}\Big|_{\lambda=0} + \ldots \tag{27}$$

Evaluating each partial derivative, we get

$$\frac{\partial g}{\partial \lambda} = e^{\lambda A}A\left(\frac{\partial}{\partial x}e^{-\lambda A}\right) - e^{\lambda A}\left(\frac{\partial}{\partial x}Ae^{-\lambda A}\right) \tag{28}$$

$$= e^{\lambda A}A\left(\frac{\partial}{\partial x}e^{-\lambda A}\right) - e^{\lambda A}\left(\frac{\partial A}{\partial x}\right)e^{-\lambda A} - e^{\lambda A}A\left(\frac{\partial}{\partial x}e^{-\lambda A}\right) \tag{29}$$

$$= -e^{\lambda A}\left(\frac{\partial A}{\partial x}\right)e^{-\lambda A} \tag{30}$$

such that

$$\frac{\partial g}{\partial \lambda}\Big|_{\lambda=0} = -\frac{\partial A}{\partial x} \tag{31}$$

Also,

$$\frac{\partial^2 g}{\partial \lambda^2} = -e^{\lambda A}A\left(\frac{\partial A}{\partial x}\right)e^{-\lambda A} + e^{\lambda A}\left(\frac{\partial A}{\partial x}\right)Ae^{-\lambda A} \tag{32}$$

such that

$$\frac{\partial^2 g}{\partial \lambda^2}\Big|_{\lambda=0} = -\left[A, \frac{\partial A}{\partial x}\right] \tag{33}$$

Similar,

$$\frac{\partial^3 g}{\partial \lambda^3}\Big|_{\lambda=0} = -\left[A, \left[A, \frac{\partial A}{\partial x}\right]\right] \tag{34}$$

and so forth...

Thus, we can then rewrite (27) as

$$e^{\lambda A}\frac{\partial}{\partial x_1}e^{-\lambda A} = -\lambda\frac{\partial A}{\partial x} - \frac{\lambda^2}{2!}\left[A, \frac{\partial A}{\partial x}\right] - \frac{\lambda^3}{3!}\left[A, \left[A, \frac{\partial A}{\partial x}\right]\right] + \ldots \tag{35}$$

Going back to (25) and let $\lambda = -i$, we obtain

$$D^\dagger \frac{\partial D}{\partial x_1} = e^{-iA}\frac{\partial}{\partial x_1}e^{iA} \tag{36}$$

$$= \frac{\partial}{\partial x_1}\left(\alpha a^\dagger - \alpha^* a\right) - \frac{1}{2!}\left[\left(\alpha a^\dagger - \alpha^* a\right), \frac{\partial}{\partial x_1}\left(\alpha a^\dagger - \alpha^* a\right)\right] + \ldots \tag{37}$$

$$= \left(a^\dagger - a\right) - \frac{1}{2!}\left[\left(\alpha a^\dagger - \alpha^* a\right), \left(a^\dagger - a\right)\right] + \ldots \tag{38}$$

$$= -ix_2 + \left(a^\dagger - a\right) \tag{39}$$

and similarly,

$$D^{\dagger}\frac{\partial D}{\partial x_2} = ix_1 + \left(a^{\dagger} + a\right) \tag{40}$$

Inserting (39) and (40) into (25) we obtain

$$D^{\dagger}\nabla D = [-ix_2 + \left(a^{\dagger} - a\right)]\hat{x}_1 + [ix_1 + \left(a^{\dagger} + a\right)]\hat{x}_2 \tag{41}$$

such that the geometric phase associated with the state $|n\rangle$ becomes

$$\gamma_n = \oint (x_2 dx_1 - x_1 dx_2) \tag{42}$$

which is the same for all values of n. The geometric interpretation can be obtained from Stokes' theorem. Given a vector field $\mathbf{V}$, we have

$$\oint_C \mathbf{V}\cdot d\mathbf{l} = \int \nabla\times\mathbf{V}\cdot\hat{n}dS \tag{43}$$

where C is a closed path, and the surface integral on the right hand side is taken over a surface bounded by C. Let $\mathbf{V} = x_2\hat{x}_1 - x_1\hat{x}_2$. Then the component of $\nabla\times\mathbf{V}$ in the direction normal to the x_1x_2 plane is

$$\frac{\partial V_2}{\partial x_1} - \frac{\partial V_1}{\partial x_2} = -2 \tag{44}$$

Hence, in (42) γ_n is equal to -2 times the area of the closed loop in the x_1x_2 plane.

Problem 3

The state vector in spherical coordinates is gives as

$$|n;t\rangle = \cos\left(\frac{\theta}{2}\right)|+\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|-\rangle \tag{45}$$

The state $|n;t\rangle$ depends on the direction of the magnetic field, and hence we identify the vector-of-parameters $\mathbf{R}(t)$ as the field itself. We set $\mathbf{R}(t) = \mathbf{B}(t)$ where the magnetic field has a constant magnitude and polar angle direction, but rotates in the ϕ-direction.

The gradient $\nabla_{\mathbf{R}}$ used to compute the Berry-connection is most conveniently expressed in spherical coordinates for this problem, due to the rotating motion of the magnetic field. We have:

$$\nabla_{\mathbf{R}}|n;t\rangle = \left[\hat{\theta}\frac{1}{R}\frac{\partial}{\partial\theta} + \hat{\phi}\frac{1}{R\sin\theta}\frac{\partial}{\partial\phi}\right]|n;t\rangle \tag{46}$$

$$= -\frac{1}{2}\sin\left(\frac{\theta}{2}\right)\hat{\theta}\frac{1}{R}|+\rangle + e^{i\phi}\frac{1}{2}\cos\left(\frac{\theta}{2}\right)\hat{\theta}\frac{1}{R}|-\rangle + \frac{i}{R\sin\theta}e^{i\phi}\sin\left(\frac{\theta}{2}\right)\hat{\phi}|-\rangle. \tag{47}$$

Here, R is the field magnitude $B = |\mathbf{B}|$, which is time-independent, while θ and ϕ are the angles defining the direction of the magnetic field $\mathbf{B}$. From the above calculation, we see that:

$$\langle n;t|[\nabla_R|n;t\rangle] = \frac{i}{R\sin\theta}\sin^2\left(\frac{\theta}{2}\right)\hat{\phi},$$

$$\mathbf{A}_n(\mathbf{R}) = i\langle n;t|[\nabla_R|n;t\rangle] = -\frac{1}{R\sin\theta}\sin^2\left(\frac{\theta}{2}\right)\hat{\phi} = \mathrm{A}_{\phi}(\theta)\hat{\phi}. \tag{48}$$

The Berry curvature is then:

$$\nabla_R \times \mathbf{A}_n(\mathbf{R}) = \hat{r}\frac{1}{R}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta A_\phi) = -\hat{r}\frac{1}{R^2\sin\theta}2\frac{1}{2}\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right) = -\hat{r}\frac{1}{2R^2} \tag{49}$$

The Berry-phase γ_n can now be obtained as from an integral over a path in parameter space at fixed θ from (θ, ϕ) to $(\theta, \phi + 2\pi)$:

$$\gamma_n(C) = \oint \mathbf{A} \cdot d\mathbf{R} = \pm\pi(1 - \cos\theta), \tag{50}$$

where we used that $d\mathbf{R} = \pm R\sin\theta d\phi\hat{\phi}$ and the $\pm$ is given by a clockwise or counterclockwise traversion of the cnotour C. We note that the solid angle swept out by the trajectory is given by

$$\Delta\Omega = \int_0^\theta \sin\theta d\theta \int_0^{2\pi} d\phi = 2\pi(1 - \cos\theta), \tag{51}$$

meaning that the Berry-phase is half of the solid angle subtended by the closed path as seen from the origo of parameter space. This is consistent with what we have discussed in the lectures, namely that the Berry phase is a geometrical (topological) phase.