Time-Dependent $\mathcal{PT}$-Symmetric Quantum Mechanics [1]

Qing-hai Wang [王清海]

National University of Singapore

Non-Hermitian Operators in Quantum Physics XI
Paris, 27 August 2012

[1] Work in progress with Jiangbin Gong

Outline

Schrödinger eqn in conventional QM

- Stationary Schrödinger eqn (eigenvalue eqn)

$$h(t)|\phi_n(t)\rangle = E_n(t)|\phi_n(t)\rangle \tag{1}$$

- Time-dependent Schrödinger eqn (evolution eqn)

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\Phi(t)\rangle = h(t)|\Phi(t)\rangle \tag{2}$$

- Eq.(2) guarantees unitarity

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\Phi_1(t)|\Phi_2(t)\rangle = 0$$

- Remarks
  1. Any Hermitian evolution would be unitary.
  2. Eq.(2) cannot be derived from Eq.(1).
  3. The "dual-role" of $h(t)$ is a axiom in QM.

Unitary equivalence

- Stationary Schrödinger eqn is invariant under arbitrary unitary transformations

$$h'(t) = U(t)h(t)U^\dagger(t), \quad |\phi'_n(t)\rangle = U(t)|\phi_n(t)\rangle$$

$$h(t)|\phi_n(t)\rangle = E_n(t)|\phi_n(t)\rangle \rightarrow h'(t)|\phi'_n(t)\rangle = E_n(t)|\phi'_n(t)\rangle$$

- Time-dependent Schrödinger eqn is invariant under only time-independent unitary transformations.

$$h'(t) = Uh(t)U^\dagger, \quad |\Phi'(t)\rangle = U|\Phi(t)\rangle$$

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\Phi(t)\rangle = h(t)|\Phi(t)\rangle \rightarrow \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\Phi'(t)\rangle = h'(t)|\Phi'(t)\rangle$$

- For a time-dependent transformation, the full Schrödinger eqn becomes

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\Phi'(t)\rangle = \left[h'(t) - \mathrm{i}\hbar U\dot{U}^\dagger\right]|\Phi'(t)\rangle$$

Inner products

- Inner products in QM [Ballentine, *Quantum Mechanics*]
  1. (ψ, ϕ) is a complex number,
  2. $(\psi, \phi) = (\phi, \psi)^*$, where $*$ denotes complex conjugate,
  3. $(\psi, c_1\phi_1 + c_2\phi_2) = c_1(\psi, \phi_1) + c_2(\psi, \phi_2)$, where c_1 and c_2 are complex numbers,
  4. $(\phi, \phi) \geq 0$, with equality holding iff $\phi = 0$.
- In general, $(\psi, \phi) \equiv \langle\psi|W|\phi\rangle$.
  1. The metric operator is a Hermitian matrix: $W = W^\dagger$
  2. All the eigenvalues of W are positive: $\lambda^W > 0$.
  3. In some convention, one may choose $W = \mathcal{PC}$.
- A self-adjoint operator in finite dimensions

$$(\psi, H\phi) = (H\psi, \phi) \quad \Rightarrow \quad WH = H^\dagger W.$$

- A time-dependent $H(t)$ calls for a time-dependent $W(t)$.

Schrödinger-like eqn

- Stationary Schrödinger eqn is same as in QM

$$H(t)|\psi_n(t)\rangle = E_n(t)|\psi_n(t)\rangle$$

- Demand unitarity in evolution

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\Psi_1(t)|W(t)|\Psi_2(t)\rangle = 0.$$

- Schrödinger-like equation

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\Psi(t)\rangle = \Lambda(t)|\Psi(t)\rangle$$

with

$$\mathrm{i}\hbar\dot{W} = \Lambda^\dagger W - W\Lambda.$$

An axiom in PTQM

- Assume $\Lambda = \tilde{H} + A$, where

$$W\tilde{H} = \tilde{H}^\dagger W, \quad WA = -A^\dagger W.$$

- The partition is unique.
- A can be determined by unitarity,

$$A = -\tfrac{1}{2}\mathrm{i}\hbar W^{-1}\dot{W}.$$

- $\tilde{H}$ cannot be determined by the unitary condition.
- An axiom in PTQM: $H = \tilde{H}$.
- Evolution equation in PTQM

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle = \left(H - \frac{\mathrm{i}\hbar}{2}W^{-1}\dot{W}\right)|\Psi\rangle.$$

Dyson's map

- The metric is positive definite,

$$W = \eta^\dagger \eta.$$

- There are many square-roots of W,

$$W = \eta^\dagger \eta = (U\eta)^\dagger (U\eta) \quad \text{with} \quad U^{-1} = U^\dagger.$$

- Mapped Hamiltonian is Hermitian,

$$h \equiv \eta H \eta^{-1} = h^\dagger.$$

- Map on wavefunctions: $|\Phi\rangle \equiv \eta|\Psi\rangle$.
- Stationary Schrödinger eqn mapped accordingly,

$$H|\psi_n\rangle = E_n|\psi_n\rangle \quad \Rightarrow \quad h|\phi_n\rangle = E_n|\phi_n\rangle$$

Mapped evolution eqn

- Mapped evolution equation,

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\Phi\rangle = \tilde{h}|\Phi\rangle \quad \text{with} \quad \tilde{h} = h + \tfrac{1}{2}\mathrm{i}\hbar\left[\dot{\eta}\eta^{-1} - \left(\dot{\eta}\eta^{-1}\right)^{\dagger}\right].$$

- In general, $\tilde{h} \neq h$.
- "Proper mapping:"

$$\dot{\eta}_{\text{proper}}\eta_{\text{proper}}^{-1} = \left(\dot{\eta}_{\text{proper}}\eta_{\text{proper}}^{-1}\right)^{\dagger}.$$

- For an improper mapping, $\eta' = U\eta_{\text{proper}}$, U satisfies

$$\dot{U} = \tfrac{1}{2}\left[\left(\dot{\eta}'\eta'^{-1}\right) - \left(\dot{\eta}'\eta'^{-1}\right)^{\dagger}\right]U.$$

- The lack of the initial condition: Unitary equivalence.

Comments

- For a proper mapping, the evolution equation reduces to

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle = \left(H - \mathrm{i}\hbar\eta^{-1}\dot{\eta}\right)|\Psi\rangle.$$

  [Znojil PRD 2008, SIGMA 2009]
- Application in conventional QM
  - $W = \mathbf{1}$.
  - $\eta = U$ with $U^{-1} = U^{\dagger}$.
  - If $\eta = \mathbf{1}$ is a proper mapping, then the improper mapping $\eta' = U$ gives

$$\tfrac{1}{2}\left[\left(\dot{\eta}'\eta'^{-1}\right) - \left(\dot{\eta}'\eta'^{-1}\right)^{\dagger}\right] = \mathrm{i}\hbar\dot{U}U^{\dagger} = -\mathrm{i}\hbar U\dot{U}^{\dagger}.$$

Complex harmonic oscillator

- Hamiltonian

$$H = \frac{1}{2}\left[\left(X + 2\mathrm{i}\beta\frac{Y}{Z} - \beta^2\frac{Y^2}{Z}\right)\hat{q}^2 + (Y + \mathrm{i}\beta)\left(\hat{p}\hat{q} + \hat{q}\hat{p}\right) + Z\hat{p}^2\right].$$

- Real spectrum,

$$E_n = \left(n + \tfrac{1}{2}\right)\hbar\sqrt{ZX - Y^2}.$$

- The metric operator

$$W = \exp\left(-\frac{1}{\hbar}\frac{\beta}{Z}\hat{q}^2\right).$$

Dyson's map

- A Dyson's map $\eta = U\eta_0$
- with a Hermitian η_0,

$$\eta_0 = \exp\left(-\frac{1}{2\hbar}\frac{\beta}{Z}\hat{q}^2\right) = \eta_0^\dagger,$$

- and a unitary factor

$$U = \exp\left[-\frac{\mathrm{i}}{\hbar}\left(\frac{\xi}{2}\hat{q}^2 + \alpha\right)\right].$$

- Mapped Hamiltonian

$$\begin{aligned} h &= \eta H \eta^{-1} \\ &= \tfrac{1}{2}\left[\left(X + 2\xi Y + \xi^2 Z\right)\hat{q}^2 + (Y + \xi Z)(\hat{p}\hat{q} + \hat{q}\hat{p}) + Z\hat{p}^2\right]. \end{aligned}$$

Proper mapping

- Mapped evolution operator

$$\begin{aligned}\tilde{h} &= h + \tfrac{1}{2}\mathrm{i}\hbar\left[\dot{\eta}\eta^{-1} - \left(\dot{\eta}\eta^{-1}\right)^{\dagger}\right] \\ &= h + \tfrac{1}{2}\dot{\xi}\hat{q}^2 + \dot{\alpha}.\end{aligned}$$

- A proper mapping: $\xi = 0$ and $\alpha = 0$.
- The mapped Hermitian Hamiltonian is Berry's generalized harmonic oscillator

$$h_{\mathrm{GHO}} = \tfrac{1}{2}\left[X\hat{q}^2 + Y(\hat{p}\hat{q} + \hat{q}\hat{p}) + Z\hat{p}^2\right].$$

- The original $\mathcal{PT}$-symmetric H has the same Berry phase with this h_{GHO}.

Expansion by instantaneous eigenstates

- Instantaneous eigenstates of H

$$H[\mathbf{X}(t)]|\psi_n(t)\rangle = E_n[\mathbf{X}(t)]|\psi_n[\mathbf{X}(t)]\rangle$$

- Expanding the solution of the Schrödinger-like time evolution Eqn by the complete set,

$$|\Psi\rangle = \sum_n a_n \mathrm{e}^{\mathrm{i}\theta_n}|\psi_n\rangle,$$

  where the dynamical phase is $\theta_n(t) = -\frac{1}{\hbar}\int^t \mathrm{d}\tau\, E_n[\mathbf{X}(\tau)]$.

- The time-dependent coefficient,

$$\begin{aligned}\dot{a}_m &= -a_m\left(\langle\psi_m|W|\dot{\psi}_m\rangle + \frac{1}{2}\langle\psi_m|\dot{W}|\psi_m\rangle\right)\\ &\quad + \sum_{n\neq m} a_n\left(\frac{\langle\psi_m|W\dot{H}|\psi_n\rangle}{E_n - E_m} + \frac{1}{2}\langle\psi_m|\dot{W}|\psi_n\rangle\right).\end{aligned}$$

Adiabatic Approximation

- Adiabatic approximation: No contribution from $n \neq m$ terms.
- Adiabatic phase: $a_m(t) \approx a_m(0)\mathrm{e}^{\mathrm{i}\gamma_m(t)}$. where the phase satisfies

$$\dot{\gamma}_m = \mathrm{i}\left(\langle\psi_m|W|\dot{\psi}_m\rangle + \frac{1}{2}\langle\psi_m|\dot{W}|\psi_m\rangle\right).$$

- Geometry phase in PTQM:

$$\gamma_m^g = \mathrm{i}\int \mathrm{d}\mathbf{X}\cdot\left[\langle\phi_m|W\boldsymbol{\nabla}|\psi_m\rangle + \frac{1}{2}\langle\psi_m|(\boldsymbol{\nabla}W)|\psi_m\rangle\right].$$

- Berry phase in PTQM:

$$\gamma_m^B = \mathrm{i}\oint \mathrm{d}\mathbf{X}\cdot\left[\langle\psi_m|W\boldsymbol{\nabla}|\psi_m\rangle + \frac{1}{2}\langle\psi_m|\boldsymbol{\nabla}W|\psi_m\rangle\right].$$

2×2 $\mathcal{PT}$-symmetric H

- Hamiltonian

$$H_{2\times 2} = e\sigma_0 + \left(a\,\mathbf{n}^r + \mathrm{i}b\sin\delta\,\mathbf{n}^\theta + \mathrm{i}b\cos\delta\,\mathbf{n}^\varphi\right)\cdot\boldsymbol{\sigma}$$
$$= \begin{bmatrix} e + a\cos\theta - \mathrm{i}b\sin\theta\sin\delta & (a\sin\theta + \mathrm{i}b\cos\theta\sin\delta + b\cos\delta)\mathrm{e}^{-\mathrm{i}\varphi} \\ (a\sin\theta + \mathrm{i}b\cos\theta\sin\delta - b\cos\delta)\mathrm{e}^{\mathrm{i}\varphi} & e - a\cos\theta + \mathrm{i}b\sin\theta\sin\delta \end{bmatrix}$$

with

$$\begin{aligned} \mathbf{n}^r &\equiv (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta), \\ \mathbf{n}^\theta &\equiv (\cos\theta\cos\varphi, \cos\theta\sin\varphi, -\sin\theta), \\ \mathbf{n}^\varphi &\equiv (-\sin\varphi, \cos\varphi, 0). \end{aligned}$$

- Eigenvalues: $E_\pm = e \pm \sqrt{a^2 - b^2}$.

Metric and eigenstates

- Metric

$$W = \mu\left[a\sigma_0 + \left(\nu\,\mathbf{n}^r + b\cos\delta\,\mathbf{n}^\theta - b\sin\delta\,\mathbf{n}^\varphi\right)\cdot\boldsymbol{\sigma}\right],$$

where $a\mu > 0$ and $\nu^2 < a^2 - b^2$.

- Eigenstates

$$|\psi_\pm\rangle = \mathcal{N}_\pm\left[\begin{array}{c} \mathrm{e}^{-\mathrm{i}\varphi}(a\sin\theta + \mathrm{i}b\cos\delta\cos\theta + b\sin\delta) \\ -a\cos\theta + \mathrm{i}b\cos\delta\sin\theta \pm \sqrt{a^2-b^2} \end{array}\right]$$

- Since μ & ν can always be absorbed in $\mathcal{N}_\pm$, we choose $\mu = \mathrm{sign}(a)$ and $\nu = 0$. After μ & ν are fixed, $W(t) = W[\mathbf{X}(t)]$.
- Without loss of generality, assume that $a > 0$.
- The metric we used

$$W = a\sigma_0 + b\left(\cos\delta\,\mathbf{n}^\theta - \sin\delta\,\mathbf{n}^\varphi\right)\cdot\boldsymbol{\sigma}.$$

Geometry phase

- Parameters θ, φ, & δ change periodically in time.
- Geometry phase for $|\psi_\pm\rangle$

$$\gamma_\pm^g = \int \left[F_\pm^\varphi \, \mathrm{d}\varphi + F_\pm^\theta \, \mathrm{d}\theta + F_\pm^\delta \, \mathrm{d}\delta \right],$$

where

$$\begin{aligned} F_\pm^\varphi &= \frac{1}{2}\left(1 \pm \frac{a}{\sqrt{a^2-b^2}} \cos\theta\right) \\ F_\pm^\theta &= \frac{1}{2} \frac{b\sin\delta}{a + b\sin\theta\cos\delta \mp \sqrt{a^2-b^2}\cos\theta} \\ F_\pm^\delta &= \mp\frac{1}{2}\frac{b}{\sqrt{a^2-b^2}} \frac{b + a\sin\theta\cos\delta}{a + b\sin\theta\cos\delta \pm \sqrt{a^2-b^2}\cos\theta}. \end{aligned}$$

Fictitious magnetic field

- Berry phase $\gamma_{\pm}^{B} = \oint \left[F_{\pm}^{\varphi}\mathrm{d}\varphi + F_{\pm}^{\theta}\mathrm{d}\theta\right]$.
- Introduce a vector field by $\mathbf{A}_{\pm} \equiv \frac{\hbar}{e}\left(\frac{F_{\pm}^{\theta}}{r}\mathbf{n}^{\theta} + \frac{F_{\pm}^{\phi}}{r\sin\theta}\mathbf{n}^{\phi}\right)$.
- By Stokes' theorem,

$$\gamma_{\pm}^{B} = \frac{e}{\hbar}\oint \mathbf{A}_{\pm}\cdot\mathrm{d}\mathbf{r} = \frac{e}{\hbar}\iint \boldsymbol{\nabla}\times\mathbf{A}_{\pm}\cdot\mathrm{d}\mathbf{S}.$$

- In terms of solid angle and winding number,

$$\gamma_{\pm}^{B} = \mp\frac{1}{2}\frac{a}{\sqrt{a^2-b^2}}\Omega + \left(1 \pm \frac{a}{\sqrt{a^2-b^2}}\right)n\pi.$$

- Fictitious magnetic field:

$$\mathbf{B}_{\pm} = \left(1 \pm \frac{a}{\sqrt{a^2-b^2}}\right)\frac{\pi\hbar}{e}\delta(x)\delta(y)\mathbf{n}^{z} \mp \frac{a}{\sqrt{a^2-b^2}}\frac{\mathbf{r}}{r^3}\frac{\hbar}{2e}.$$

Improper (Hermitian) mapping

- Two square-roots of W:

$$\eta_\pm = \frac{1}{\chi_\pm\sqrt{2}} \begin{pmatrix} \chi_\pm^2 - b\sin\theta\cos\delta & b(\cos\theta\cos\delta + \mathrm{i}\sin\delta)\mathrm{e}^{-\mathrm{i}\varphi} \\ b(\cos\theta\cos\delta - \mathrm{i}\sin\delta)\mathrm{e}^{\mathrm{i}\varphi} & \chi_\pm^2 + b\sin\theta\cos\delta \end{pmatrix},$$

where $\chi_\pm \equiv \sqrt{a \pm \sqrt{a^2 - b^2}}$.

- Mapped Hamiltonian

$$h_\pm \equiv \eta_\pm H_{2\times 2}\eta_\pm^{-1} = e\sigma_0 \pm \sqrt{a^2 - b^2}\mathbf{n}^r \cdot \boldsymbol{\sigma}.$$

- A proper mapping is $\eta_{\text{proper}} = U^\dagger \eta_\pm$.

Only δ varies

- The eqn for U

$$\frac{\partial U}{\partial \delta} = \mathrm{i}\zeta \mathbf{n}^r \cdot \boldsymbol{\sigma} U, \quad \text{where} \quad \zeta \equiv \mp \frac{b^2}{\sqrt{a^2-b^2}\left(a \pm \sqrt{a^2-b^2}\right)}.$$

- Solution

$$\begin{aligned} U &= \exp(\mathrm{i}\zeta\delta \mathbf{n}^r \cdot \boldsymbol{\sigma}) U_0 \\ &= \begin{pmatrix} \cos(\zeta\delta) + \mathrm{i}\cos\theta \sin(\zeta\delta) & \mathrm{i}\sin\theta \sin(\zeta\delta) \mathrm{e}^{-\mathrm{i}\varphi} \\ \mathrm{i}\sin\theta \sin(\zeta\delta) \mathrm{e}^{\mathrm{i}\varphi} & \cos(\zeta\delta) - \mathrm{i}\cos\theta \sin(\zeta\delta) \end{pmatrix} U_0. \end{aligned}$$

- Mapped Hamiltonian: $U_0 h_\pm U_0^\dagger$.
- The mapping is a periodic function of δ with period $2\pi/\zeta$.

Only θ varies

- The eqn for U

$$\begin{aligned}\frac{\partial U}{\partial \theta} &= \mathrm{i}\zeta\cos\delta\begin{pmatrix}\sin\theta\sin\delta & (-\cos\theta\sin\delta+\mathrm{i}\cos\delta)\mathrm{e}^{-\mathrm{i}\varphi}\\ (-\cos\theta\sin\delta-\mathrm{i}\cos\delta)\mathrm{e}^{\mathrm{i}\varphi} & -\sin\theta\sin\delta\end{pmatrix}U\\ &= -\mathrm{i}\zeta\cos\delta\,\mathrm{e}^{-\mathrm{i}\varphi\sigma_3/2}\mathrm{e}^{-\mathrm{i}\theta\sigma_2/2}\mathrm{e}^{\mathrm{i}\delta\sigma_3/2}\sigma_2\mathrm{e}^{-\mathrm{i}\delta\sigma_3/2}\mathrm{e}^{\mathrm{i}\theta\sigma_2/2}\mathrm{e}^{\mathrm{i}\varphi\sigma_3/2}U.\end{aligned}$$

- Solution

$$U=\mathrm{e}^{-\mathrm{i}\varphi\sigma_3/2}\mathrm{e}^{-\mathrm{i}\theta\sigma_2/2}\exp\left[\mathrm{i}\left(-\zeta\cos\delta\,\mathrm{e}^{\mathrm{i}\delta\sigma_3/2}\sigma_2\mathrm{e}^{-\mathrm{i}\delta\sigma_3/2}+\tfrac{1}{2}\sigma_2\right)\theta\right]U_0.$$

Only θ varies

- Assume the mapped Hamiltonian has the form

$$h^{\theta} = e\sigma_0 + \sqrt{a^2 - b^2} \begin{pmatrix} \cos\Theta & \sin\Theta \ \mathrm{e}^{-i\Phi} \\ \sin\Theta \ \mathrm{e}^{i\Phi} & -\cos\Theta \end{pmatrix}.$$

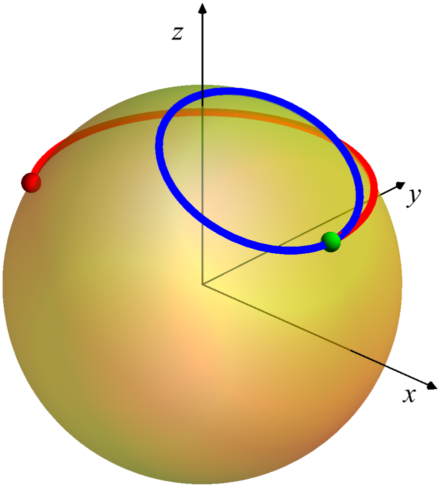
- Choose $U_0 = \sigma_0$ for simplicity.
- The mapped Hamiltonian has the parameters

$$\begin{aligned} \cos\Theta &= \cos\left[\theta\sqrt{1 - 4\zeta(1-\zeta)\cos^2\delta}\right], \\ \mathrm{e}^{\mathrm{i}\Phi} &= \frac{1 - 2\zeta\cos^2\delta + 2\mathrm{i}\zeta\sin\delta\cos\delta}{\sqrt{1 - 4\zeta(1-\zeta)\cos^2\delta}}. \end{aligned}$$

- Remarks
  1. It is independent of φ.
  2. Periodicity of θ is changed.
  3. Multiple-valued function for Θ & Φ.

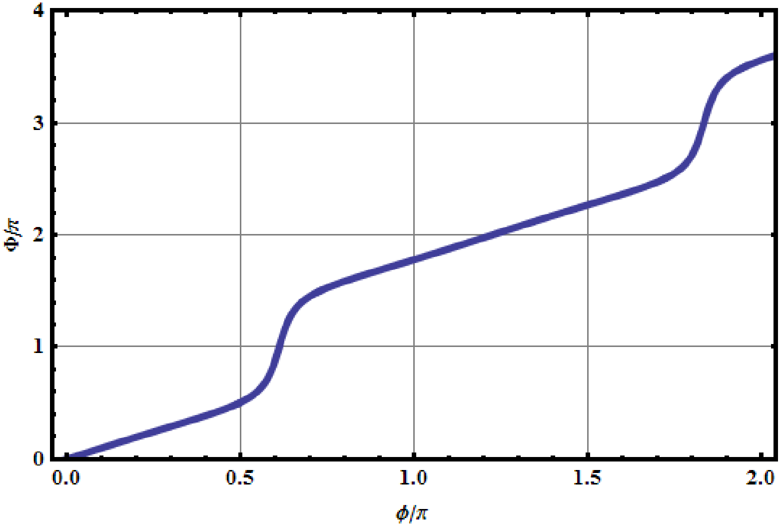
Only φ varies

The red line is a path in (θ, φ) space with $\zeta = -0.8$, $\theta = 1$, $\delta = 0$, & $\varphi : 0 \to 2\pi$. The blue line is the mapped curve in (Θ, Φ) space.



Only φ varies

Φ as a function of φ for $\zeta = -0.8$, $\theta = 1$, $\delta = 0$, & $\varphi : 0 \to 2\pi$.



Conclusions

- An axiom in PTQM is proposed.

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle = \left(H - \frac{i\hbar}{2}W^{-1}\dot{W}\right)|\Psi\rangle.$$

- Conventional full Schrödinger eqn is a special case of Schrödinger-like eqn in PTQM.
- A proper map links a PTQM Hamiltonian to a Hermitian Hamiltonian with "dual roles."
- Finding the proper map may be non-trivial.
- In PTQM, a new geometry phase is found. The associated fictitious magnetic field has a fractional and tunable magnetic monopole and an observable Dirac string.
- Experiments?