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A Study on Quantum Mechanics in Toroidal Coordinate System

Jihan A. As-sya'bani[1], M.F. Rosyid*[1], M. Nur*[2]

[1]Research Group Cosmology, Astrophysics, Mathematical Physics & Particle Physics (KAMP)
Dept. of Physics, Universitas Gadjah Mada
[2]Centre for Plasma Research (CPR), Universitas Diponegoro
**Academic Supervisor*

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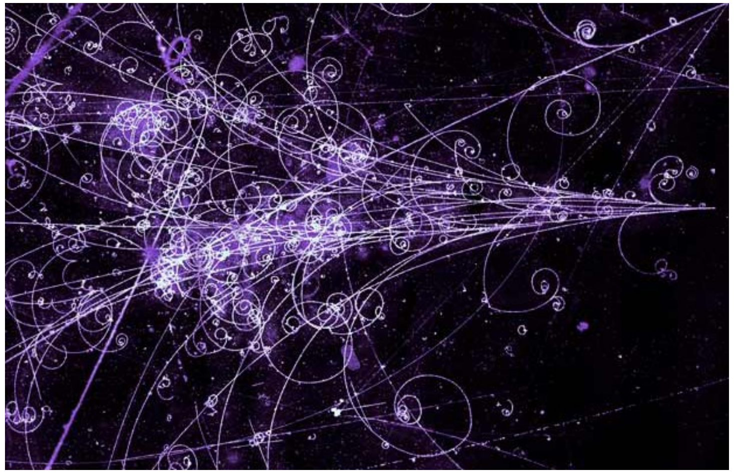
Once upon a time...

Motivation



Quantum Realm

Classical Realm

$$\lambda = \frac{h}{p}$$

- For 10 keV fusion plasmas in magnetic field of 3T

$$\lambda_{dB,e} \approx 1.24 \times 10^{-10} \text{ m}$$
$$\lambda_{dB,i} \approx 6.92 \times 10^{-12} \text{ m}$$

- Meanwhile:

$$r_i \approx 4.79 \text{ mm}$$
$$r_e \approx 1.12 \text{ cm}$$
$$\lambda_D \approx 74.3 \times 10^{-6} \text{ m}$$

Fusion plasmas is generally studied classically.

Motivation

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Why should bother to go quantum?

- Landau (1933) showed that the cyclotron energy of charged particle in uniform magnetic field is quantized:

$$E = \left(n + \frac{1}{2}\right)\hbar\omega_H + \frac{p_z^2}{2m} - \frac{\mu\sigma H}{s} \tag{1}$$

  resulted in oscillation of magnetic susceptibility, electrical resistivity of materials through de Haas-van Alphen effect.

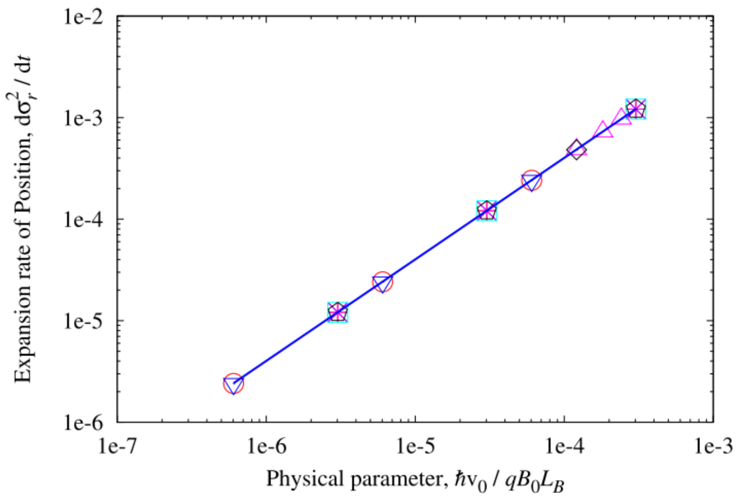
- de Jesus et al (1999) derived the quantized energy levels for charged particle in oscillating magnetic field (2)

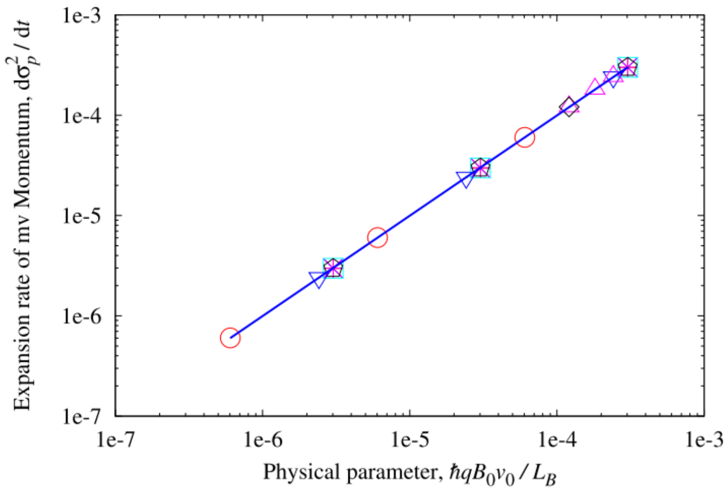
$$E_n = \frac{P'}{2m} + \left(n + \frac{1}{2}\right)\hbar\omega_c'; \qquad \omega_c = \gamma B_{eff} = \gamma\sqrt{B_0^2 + B_1^2}$$

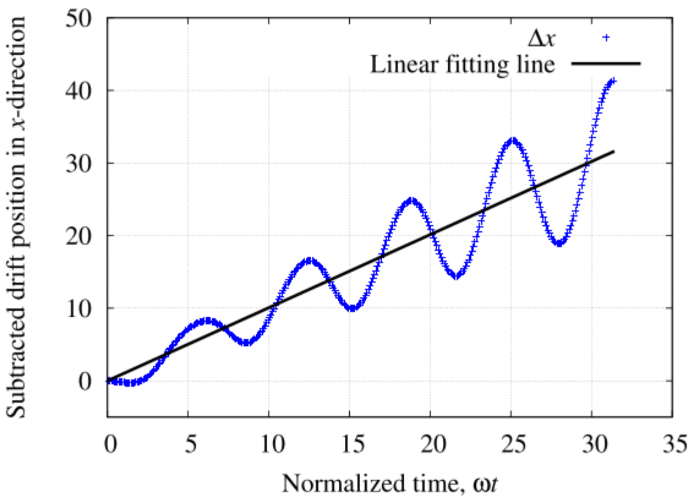
Landau, L. D., dan Lifshitz, E. M., 1977, *Quantum Mechanics, Non-relativistic Theory*, 3rd ed, Pergamon Press, New York
Holstein, T. D., Norton, R. E., Pincus, P (1973). *Physical Review B.* 8 (6): 2649.
de Jesus, V.L.B., Guimarães, A.P., Oliveira I.S., 1999, Classical and quantum mechanics of a charged particle in oscillating electric and magnetic fields, *Brazilian Journal of Physics*, **29**, pp.541-546.

Motivation

- Oikawa, Chan, and Kosaka showed (numerically) in plasma temperature of 10 keV and 3T magnetic field, quantum mechanical uncertainties behavior may starts show significance:
  - non-uniform $\mathbf{E} \times \mathbf{B}$ field (2014, 2017)
  - $\nabla \mathbf{B}$ drift in weakly non-uniform magnetic field (2016)







S. Oikawa, W. Kosaka and P.K. Chan, Plasma Fusion Res. **9**, 3401033 (2014).
P. K. Chan, S. Oikawa, W. Kosaka, Phys. Plasmas. **23**, 022104 (2016). doi: 10.1063/1.4941096
P. K. Chan, S. Oikawa, W. Kosaka, Phys. Plasmas. **24**, 072117 (2017). doi: 10.1063/1.4994075

Research Questions

Goal:

Simplify quantum mechanical properties evaluation of toroidal systems, such as charged particles in magnetic confinement fusion plasmas

- How does quantum mechanical operators look like in toroidal coordinate system?
  - *What is the quantization (or transformation) procedure?*
- How does the commutation relation between observables?
- What are the possible consequences from these findings?

Brief on Quantum Mechanics

- State of a system in QM is represented by its wavefunction

$$\psi(\mathbf{r}) \qquad \text{or} \qquad |\psi\rangle$$

Postulate:
Complete information regarding the system is contained in its wavefunction or ket vector.

- This information can be extracted from the wavefunction by means of operator that associated with a certain observables, e.g., position, momentum

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle = \int \psi^*(\mathbf{r}) \hat{A} \psi(\mathbf{r}) \, d\tau. \tag{3}$$

- An operator represents an observable **only and if only** it has real expectation value, i.e., Hermitian.

Brief on Quantum Mechanics

- In QM, multiple observables (unlike in classical mechanics) is not guaranteed can be found/measured simultaneously.

- Mathematically, this is evaluated by **commutator** between observables:

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \tag{4}$$

$$[\hat{A}, \hat{B}] = 0$$

Compatible Operators

$$[\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0$$

$$[\hat{A}, \hat{B}] \neq 0$$

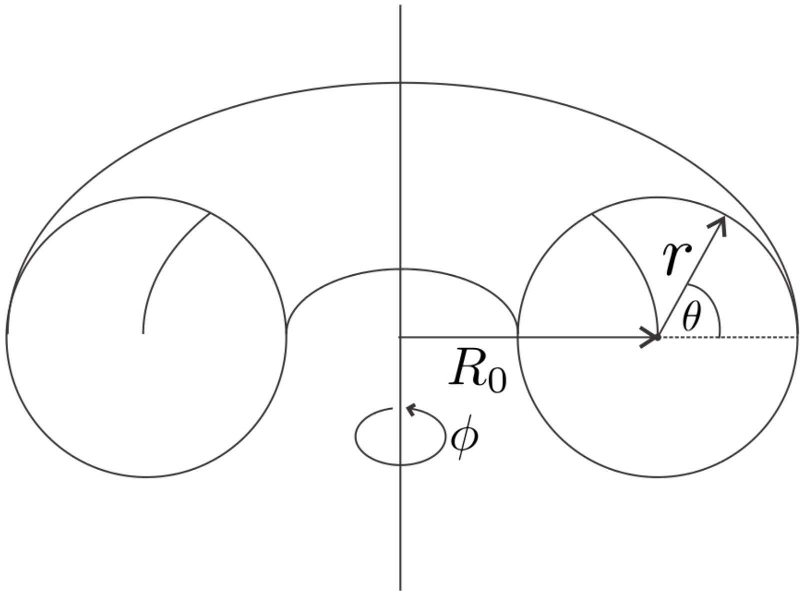
Incompatible Operators

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$$

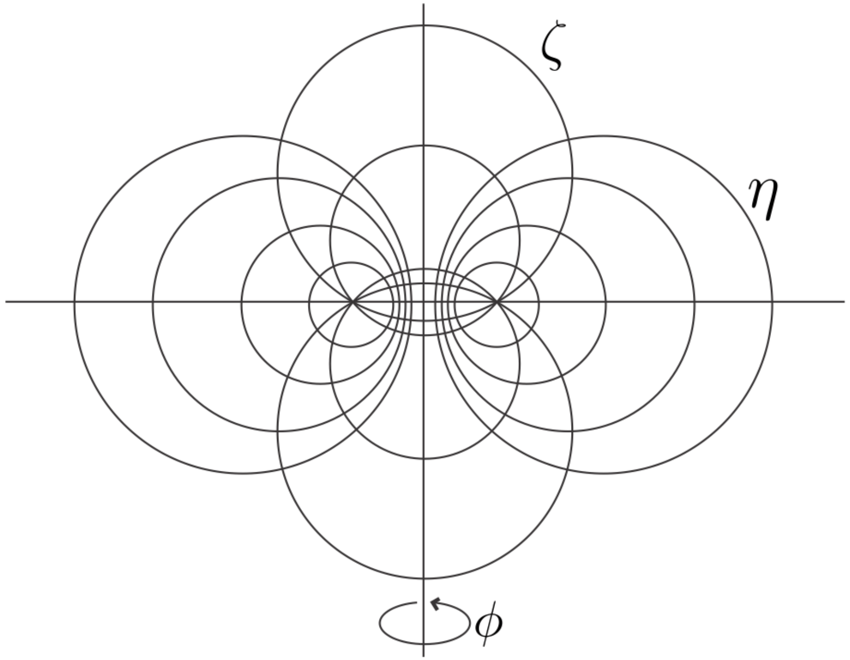
Heisenberg's Uncertainty Principle

Toroidal Coordinate System

- Mathematically, there are two ways to construct toroidal coordinate system



Simple/Primitive Toroidal Coordinate System

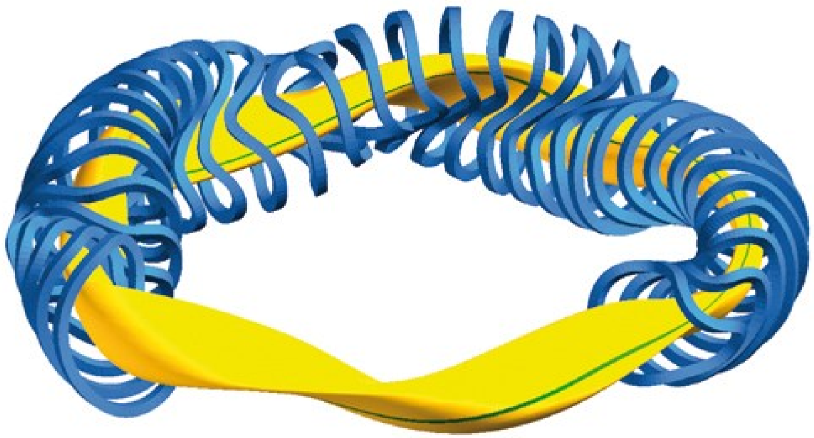


Proper Toroidal Coordinate System

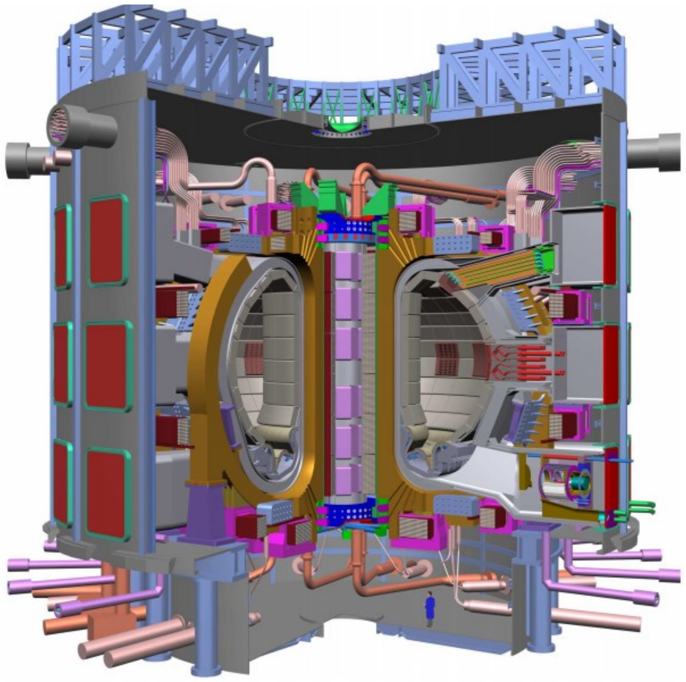
Arfken, G.B. dan Weber, H.J., 2005, *Mathematical Methods for Physicist*, edisi ke-6, Elsevier, London.
Margenau, H., dan Murphy, G.M., 1962, *The Mathematics of Physics and Chemistry*, 2nd ed, Affiliated East-West Press Private Ltd., New Delhi

Toroidal Coordinate System

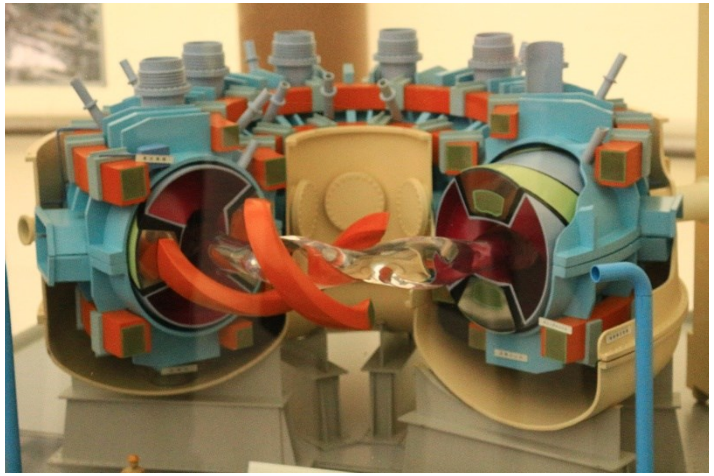
- Toroidal coordinate system, for instance, exists in magnetic confinement devices:



Wendelstein 7-X (ipp.mpg.de)



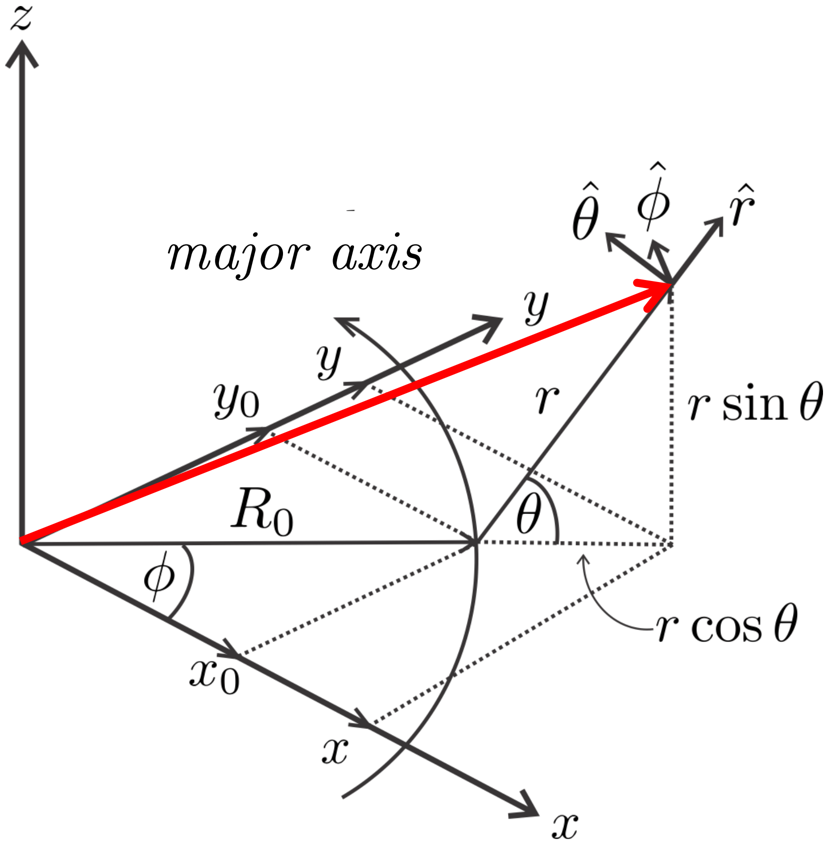
ITER (www.iter.org)



LHD

Toroidal Coordinate System

$$\mathbf{r} = (r + R_0 \cos\theta)\hat{\mathbf{r}} - R_0 \sin\theta\hat{\boldsymbol{\theta}}$$



- In Cartesian:

$$\begin{aligned} x &= (R_0 + r\cos\theta)\cos\phi, \\ y &= (R_0 + r\cos\theta)\sin\phi, \\ z &= r\sin\theta, \end{aligned} \tag{5}$$

- In toroidal:

$$\begin{aligned} r &= \left[(x - x_0)^2 + (y - y_0)^2 + z^2\right]^{1/2} \\ \tan\theta &= \frac{z}{\left[(x - x_0)^2 + (y - y_0)^2\right]^{1/2}} \\ \tan\phi &= \frac{y - y_0}{x - x_0}. \end{aligned} \tag{6}$$

Toroidal Coordinate System

- It can be proved from Eq. (5) that the square of distance in TCS is:

$$ds^2 = dr^2 + r^2 d\theta^2 + (R_0 + r\cos\theta)^2 d\phi^2 \quad (7)$$

- Since in general,

$$ds^2 = h_1^2 dq_1^2 + h_2^2 dq_2^2 + h_3^2 dq_3^2 \quad (8)$$

- We can obtain the scale factors for TCS:

$$h_r = 1, \quad h_\theta = r, \quad \text{and} \quad h_\phi = (R_0 + r\cos\theta) \quad (9)$$

- The volume element is therefore

$$d\tau = r(R_0 + r\cos\theta)\, dr\, d\theta\, d\phi \quad (10)$$

- And the del-operator is

$$\nabla f = \frac{\partial f}{\partial r}\hat{\boldsymbol{r}} + \frac{1}{r}\frac{\partial f}{\partial \theta}\hat{\boldsymbol{\theta}} + \frac{1}{(R_0 + r\cos\theta)}\frac{\partial f}{\partial \phi}\hat{\boldsymbol{\phi}} \quad (11)$$

Quantization Approach

- Quantization in Cartesian frame of reference (Hermiticity is guaranteed):

$$x_i \rightarrow \hat{x}_i = x_i \qquad p_i \rightarrow \hat{p}_i = \frac{\hbar}{i}\frac{\partial}{\partial x_i} \tag{12}$$

- Quantization in generalized curvilinear coordinate system has been studied by Zhan (1986):

$$\hat{p}_i = \frac{\hbar}{i}\left(\frac{\partial}{\partial q_i} + f(q_i)\right) \qquad f(q_i) = \frac{1}{2k_i}\frac{\partial k_i}{\partial q_i} \tag{13}$$

- For any operator F (e.g. Hamiltonian) the correspondence rule reads:

$$F(q_i, p_i) \longrightarrow \hat{F}(\hat{q}_i, \hat{p}_i) = \hat{F}'(\hat{q}_i, \hat{p}_i) + D(q_i) \tag{14}$$

$$D_{q_i} = -\frac{1}{2}\sum_i \left[\beta_1 \frac{\hbar}{i}\frac{\partial \hat{F}}{\partial \hat{p}_i}\left(\frac{1}{2k_i}\frac{\partial k_i}{\partial q_i}\right) - \beta_2 \frac{\hbar^2}{2!}\frac{\partial^2 \hat{F}}{\partial \hat{p}_i^2}\left(\frac{1}{2k_i}\frac{\partial k_i}{\partial q_i}\right)^2 + \cdots\right] \qquad \beta_1 = 1 \text{ dan } \beta_2 = 2$$

Quantization Approach

- The wavefunction is assumed to be **well-behaved**:

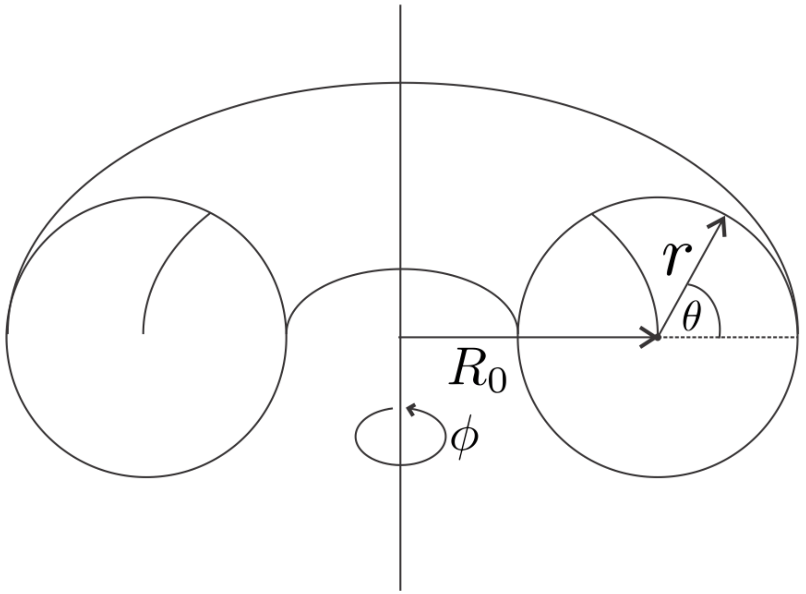
  - Periodic, both, poloidally and toroidally:

$$\psi(0) = \psi(2\pi) \tag{16}$$

  - If the torus major radius is R_0, then

$$\psi(r \to R_0) = 0 \tag{17}$$

  - The particle can be found inside the torus:



$$\int_0^{2\pi} \int_0^{2\pi} \int_0^{\boldsymbol{R}} |\psi(\mathbf{r})|^2 \, r(R_0 + r\cos\theta) \, dr \, d\theta \, d\phi = 1. \tag{18}$$

Free Particle

Position operators

- Direct quantization, yields:

$$\hat{r}\psi = (r + R_0\cos\theta)\psi$$
$$\hat{\theta}\psi = -R_0\sin\theta\psi \tag{19}$$

- Position operators are commute with each other:

$$[\hat{r}, \hat{\theta}] = 0 \tag{20}$$

Momentum operators

- Using quantization rule in Eq. (13)

$$\hat{p}_r = \frac{\hbar}{i}\left(\frac{\partial}{\partial r} + \frac{R_0 + 2r\cos\theta}{2r(R_0 + r\cos\theta)}\right) \qquad \hat{p}_\theta = \frac{\hbar}{i}\left(\frac{\partial}{\partial\theta} - \frac{r^2\sin\theta}{2r(R_0 + r\cos\theta)}\right) \qquad \hat{p}_\phi = \frac{\hbar}{i}\frac{\partial}{\partial\phi} \tag{21}$$

- Momentum operators of free particle also commute with each other:

$$[\hat{p}_r, \hat{p}_\theta] = [\hat{p}_\theta, \hat{p}_\phi] = [\hat{p}_\phi, \hat{p}_r] = 0, \tag{22}$$

Free Particle

- Position and momentum operators are incompatible

$$[\hat{r}, \hat{p}_r] = i\hbar \qquad [\hat{\theta}, \hat{p}_\theta] = i\hbar R_0 \cos\theta \qquad [\hat{r}, \hat{p}_\theta] = -i\hbar R_0 \sin\theta \tag{23}$$

- And the uncertainty relations are

$$\sigma_{\hat{\mathbf{r}}_\theta}\sigma_{\hat{p}_\theta} \geq \frac{\hbar}{2} R_0 |\langle\cos\theta\rangle| \qquad \sigma_{\hat{\mathbf{r}}_r}\sigma_{\hat{p}_\theta} \geq \frac{\hbar}{2} |\langle\hat{\mathbf{r}}_\theta\rangle| \tag{24}$$

- To find the Hamiltonian, momentum operators are written as follows

$$\hat{p}_r = \frac{\hbar}{i}\left(\frac{\partial}{\partial r} + \frac{R_0 + 2r\cos\theta}{2r(R_0 + r\cos\theta)}\right) \qquad \hat{p}_\theta = \frac{\hbar}{i}\left(\frac{\partial}{\partial\theta} - \frac{r^2\sin\theta}{2r(R_0 + r\cos\theta)}\right) \qquad \hat{p}_\phi = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$$

$$\hat{p}_r = \frac{\hbar}{i}\left(\partial_r + \frac{\mu}{2\gamma}\right) \qquad \hat{p}_\theta = \frac{\hbar}{i}\left(\partial_\theta + \frac{\nu}{2\gamma}\right) \qquad \hat{p}_\phi = \frac{\hbar}{i}\partial_\phi. \tag{25}$$

where $\quad \gamma = r(R_0 + r\cos\theta), \qquad \mu = R_0 + 2r\cos\theta, \qquad \nu = -r^2\sin\theta.$

Free Particle

- The classical Hamiltonian is

$$H = \frac{1}{2m}\left(p_r^2 + \frac{1}{r^2}p_\theta^2 + \frac{1}{(R_0 + r\cos\theta)^2}p_\phi^2\right) \tag{26}$$

- Using correspondence rule (14), the Hamiltonian operator reads

$$\hat{H} = \frac{1}{2m}\left[\hat{p}_r^2 + \frac{1}{r^2}\hat{p}_\theta^2 + \frac{1}{(R_0 + r\cos\theta)^2}\hat{p}_\phi^2 - \hbar^2\left(\frac{r^2 + (R_0 + r\cos\theta)^2}{4r^2(R_0 + r\cos\theta)^2}\right)\right]. \tag{27}$$

- Back substitution of momentum components in (21) to (27) yields Schrödinger's equation for free particle in TCS:

$$-\frac{\hbar^2}{2mr(R_0 + r\cos\theta)}\left[\frac{\partial}{\partial r}\left\{r(R_0 + r\cos\theta)\frac{\partial}{\partial r}\right\} + \frac{1}{r}\frac{\partial}{\partial\theta}\left\{(R_0 + r\cos\theta)\frac{\partial}{\partial\theta}\right\} + \frac{r}{(R_0 + r\cos\theta)}\frac{\partial^2}{\partial\phi^2}\right]\psi(\mathbf{r}) + V(r,\theta,\phi)\psi(\mathbf{r}) = E\psi(\mathbf{r}). \tag{28}$$

Charged Particle in Electromagnetic Field

- The classical Hamiltonian:

$$H = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 + eV, \tag{29}$$

- Following the same quantization yields:

$$\hat{H} = \frac{1}{2m}\left(\hat{\Pi}_r^2 + \frac{1}{r^2}\hat{\Pi}_\theta^2 + \frac{1}{(R_0 + r\cos\theta)^2}\hat{\Pi}_\phi^2 + D(q_i)\right) + e\hat{V}, \tag{30}$$

where

$$\Pi_r = p_r - \frac{e}{c}A_r, \qquad \Pi_\theta = p_\theta - \frac{er}{c}A_\theta, \qquad \Pi_\phi = p_\phi - \frac{e(R_0 + r\cos\theta)}{c}A_\phi. \tag{31}$$

Quantum Dynamics

- In QM, system dynamics can be evaluated through, either:
  - the time-evolution of its wavefunction (**Schrödinger's picture**)
  - the time-evolution of its operator (**Heisenberg's picture**)
- The two pictures are related by time-evolution operator:

$$\langle\psi_1|\hat{A}|\psi_2\rangle = \langle\psi_1|\hat{U}^\dagger\hat{A}\hat{U}|\psi_2\rangle \qquad \hat{U} = \exp\left(-\frac{iH}{\hbar}t\right) \tag{32}$$

- In Schrödinger's picture:

$$\psi(\mathbf{r},t) = \hat{U}(t,t_0)\psi(\mathbf{r},t_0) \tag{33}$$

- In Heisenberg's picture, we define the operator as:

$$\hat{A}_H = \hat{U}^\dagger\hat{A}\hat{U} \tag{34}$$

then the change of the operator in time can be found by

$$\frac{d\hat{A}_H}{dt} = \frac{1}{i\hbar}[\hat{A}_H,\hat{H}] \tag{35}$$

“Velocity” operator

- The rate of change of radial position operator in TCS can be proved as

$$\frac{d\hat{\mathbf{r}}_r}{dt} = \frac{1}{i\hbar}[\hat{\mathbf{r}}_r, \hat{H}] = \frac{i\hbar}{2m}\left(2\hat{p}_r + \frac{1}{r^2}\{\hat{\mathbf{r}}_\theta, \hat{p}_\theta\}\right) \tag{36}$$

  with $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ is called ***anti-commutator***.

- We can define “velocity” operator in TCS as
  - For **free particle**:

$$\hat{\mathbf{v}}_r = \frac{d\hat{\mathbf{r}}_r}{dt} = \frac{1}{2m}\left(2\hat{p}_r + \frac{1}{r^2}\{\hat{\mathbf{r}}_\theta, \hat{p}_\theta\}\right) \qquad \hat{\mathbf{v}}_\theta = \frac{d\hat{\mathbf{r}}_\theta}{dt} = -\frac{1}{2mr^2}\{R_0\cos\theta, \hat{p}_\theta\} \tag{37}$$

  - For **charged particle in electromagnetic field**:

$$\hat{\mathbf{v}}_r = \frac{1}{m}\left[\hat{\Pi}_r + \frac{1}{2r^2}\{\hat{\mathbf{r}}_\theta, \hat{\Pi}_\theta\}\right] + e[\hat{\mathbf{r}}_r, \hat{V}], \qquad \hat{\mathbf{v}}_\theta = -\frac{1}{2mr^2}\{R_0\cos\theta, \hat{\Pi}_\theta\} + e[\hat{\mathbf{r}}_\theta, \hat{V}]. \tag{38}$$

  while in the Cartesian system

$$\frac{d\hat{x}_i}{dt} = \frac{1}{m}\hat{p}_{x_i} \tag{39}$$

Conclusions

- The position, momentum, and Hamiltonian operators for TCS for the case of free-particle are obtained
  - It is possible to find all position (or momentum) components simultaneously
  - It is not possible to find position AND momentum of the same component simultaneously
- The Schrödinger's equation for free particle in toroidal coordinate system is obtained.
- Position, momentum, and Hamiltonian for the case of charged particle in electromagnetic field also obtained
  - Radial velocity of particle is 'tied' to its poloidal momentum
- Further study needed to evaluate the solution for Schrödinger's equation in TCS for, both, free-particle and charged particle in electromagnetic field.

UNIVERSITAS GADJAH MADA

Questions?

Contact:
jihan.ahmad.a@mail.ugm.ac.id
jihan.assyabani@uni-oldenburg.de

in **Jihan A. As-sya'bani**