NTNU – Trondheim
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Department of Physics

Examination paper for FY2045 Quantum Mechanics I

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09:00–13:00

Part I $(\sim 30\%)$

Answer the following questions in Inspera.

Problem 1 Multiple choice problems

Choose only **one** of the options for each problem.

a) Consider a system of two non-interacting particles. The first particle is in an eigenstate of its operator for the square of the total angular momentum, $\mathbf{J}_1^2$,

$$\mathbf{J}_1^2|j_1, m_1\rangle = \hbar^2 j_1(j_1+1)|j_1, m_1\rangle,$$

with $j_1 = 4$. The second particle is in an eigenstate of its operator for the square of the total angular momentum, $\mathbf{J}_2^2$,

$$\mathbf{J}_2^2|j_2, m_2\rangle = \hbar^2 j_2(j_2+1)|j_2, m_2\rangle,$$

with $j_2 = 3/2$. The possible values of the square of the total angular momentum operator of the two-particle system are given by $\hbar^2 j(j+1)$. What are the possible values of j?

A $j = 0, 1, \ldots, 4$

B $j = \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}$

C $j = \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}$

D $j = \frac{5}{2}, 3, \frac{7}{2}, 4, \frac{9}{2}, 5, \frac{11}{2}$

E $j = -4, -3, \ldots, 3, 4$

b) A particle in a harmonic oscillator potential is in the state

$$|\psi\rangle = A\big[|2\rangle + 2|4\rangle + |6\rangle\big], \tag{1}$$

where $|n\rangle$ are orthonormal energy eigenstates. What is the normalization constant A when chosen real and positive?

A $A = 1$

B $A = 6$

C $A = \frac{1}{6}$

D $A = \frac{1}{3}$

E $A = \frac{1}{\sqrt{6}}$

c) The energy eigenvalue of a harmonic oscillator eigenstate $|n\rangle$ is

$$E_n = \hbar\omega\left(n + \tfrac{1}{2}\right),$$

where $n = 0, 1, 2, \ldots$. What is the energy expectation value of the state $|\psi\rangle$ in Eq. (1)?

A $\langle E\rangle = \frac{3}{2}\hbar\omega$

B $\langle E\rangle = \frac{27}{2}\hbar\omega$

C $\langle E\rangle = \frac{11}{2}\hbar\omega$

D $\langle E\rangle = 4\hbar\omega$

E $\langle E\rangle = \frac{9}{2}\hbar\omega$

d) Consider the normalized state vector

$$|\psi\rangle = \frac{1}{3}\left[(1+2i)|1\rangle - 2i|2\rangle\right],$$

where $|1\rangle$ and $|2\rangle$ are orthonormal basis vectors. What is $\langle\psi|$, the dual vector of $|\psi\rangle$?

A $\langle\psi| = \frac{1}{3}\big[(1+2i)|1\rangle - 2i|2\rangle\big]$

B $\langle\psi| = \frac{1}{3}\big[\langle 1| + \langle 2|\big]$

C $\langle\psi| = \frac{1}{3}\big[(1+2i)\langle 1| - 2i\langle 2|\big]$

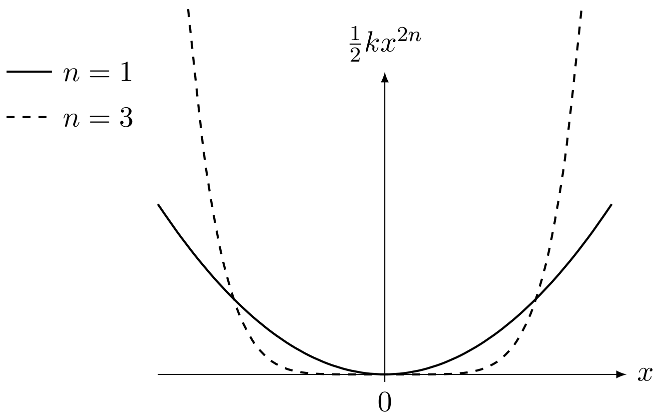
D $\langle\psi| = \frac{1}{3}\big[(1-2i)\langle 1| + 2i\langle 2|\big]$

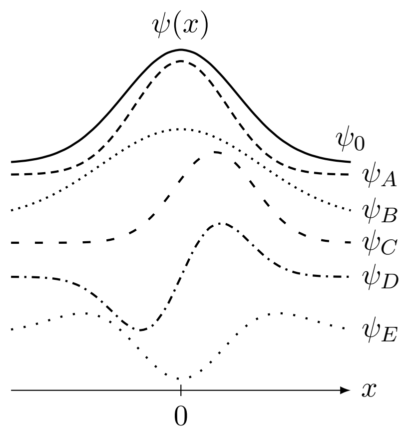
E $\langle\psi| = \frac{1}{3}\big[(1+2i)\langle 1| + 2i\langle 2|\big]$

e) Consider a system described by the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}_n,$$

with the potential function $\hat{V}_n = \frac{1}{2}k\hat{x}^{2n}$. The potentials for $n = 1$ and 3 are sketched in the left figure below.





The ground state wavefunction for the $n = 1$ case is ψ_0, illustrated in the right figure above together with other possible trial wavefunctions. The functions are not normalized and are shifted vertically for clarity.

Which of the functions is the best choice for trial wavefunction when using the variational method to estimate the ground state energy of a system with $n = 3$?

A ψ_A

B ψ_B

C ψ_C

D ψ_D

E ψ_E

f) A system described by a Hermitian Hamiltonian is in the state $|\psi\rangle$. Which **one** of the following statements is true:

A If $\langle n|\psi\rangle$ is nonzero only for $n = 1$, where $|n\rangle$ are energy eigenstates, then $|\psi\rangle$ is an energy eigenstate.

B $|\psi\rangle$ can only be written as a superposition of position eigenvectors $|\mathbf{r}\rangle$.

C The Heisenberg uncertainty principle tells us it is impossible to calculate the expectation values $\langle\psi|\hat{p}_x|\psi\rangle$ and $\langle\psi|\hat{x}|\psi\rangle$ simultaneously.

D If $|\psi\rangle$ is a superposition of two or more energy eigenstates with different energy eigenvalues, measuring the energy of the system will leave the system state unchanged.

E $\langle\psi|\psi\rangle$ can be time-dependent.

g) At time $t = 0$, a particle with spin $\frac{1}{2}$ is measured to be in the spin state

$$\chi(t=0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \tag{2}$$

a superposition of the energy eigenstates of the system Hamiltonian,

$$H = \hbar\omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3}$$

What is $\chi(t)$, that is, the spin state of the particle at time $t \geq 0$?

A $\chi(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

B $\chi(t) = \begin{pmatrix} e^{-i\omega t} \\ 0 \end{pmatrix}$

C $\chi(t) = \begin{pmatrix} 0 \\ e^{i\omega t} \end{pmatrix}$

D $\chi(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\omega t} \\ e^{i\omega t} \end{pmatrix}$

E $\chi(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\omega t} \\ e^{-i\omega t} \end{pmatrix}$

h) Again, consider the particle described by the Hamiltonian in Eq. (3), measured to be in the spin state in Eq. (2) at $t = 0$. Assuming no measurements have been made since $t = 0$, which **one** of the following statements is true?

A If you measure the spin along x, you will always get $S_x = \hbar/2$.

B At $t = \frac{\pi}{4\omega}$ you are guaranteed to measure $S_y = \hbar/2$.

C It is always impossible to know the outcome of a measurement of S_y.

D At $t = \frac{\pi}{4\omega}$ you are guaranteed to measure $S_x = -\hbar/2$.

E If you measure the energy of the particle, you lose all information about the spin state of the particle.

i) In the general formulation of quantum mechanics, the momentum representation is found by considering eigenstates of the momentum operator $\hat{p}$, defined by

$$\hat{p}|p\rangle = p|p\rangle,$$

where p is an eigenvalue. What is $\langle p_2|\hat{p}|p_1\rangle$?

A $\frac{\hbar}{i}\frac{\partial}{\partial p_1}\delta(p_2 - p_1)$

B $\delta(p_2 - p_1)$

C 0

D $-\frac{\hbar}{i}\frac{\partial}{\partial x}\delta(p_2 - p_1)$

E $p_2\delta(p_2 - p_1)$

Problem 2 Short answer questions

Give a short answer (maximum 2-3 sentences) to **only two** of the three questions below. If three answers are given, the **first two** will be graded. You may use simple equations in your answers.

a) Why do physical observables have to be represented by Hermitian operators?

b) What are the main differences between fermions and bosons?

c) How can probability densities be time-dependent even for time-independent Hamiltonians?

Part II $(\sim 70\%)$

Write your calculations and answers to the following problems on paper. Clearly mark each page and answer with the problem number.

Problem 3 Normalization condition

Show that if a state $|\psi\rangle$ is normalized, the corresponding position space wavefunction $\psi(x) = \langle x|\psi\rangle$ is also normalized.

Problem 4 Identical particles in a box

A rectangular box with dimensions L_x, L_y and L_z contains a particle with mass m. The potential is zero inside the box and infinite outside, giving the energy eigenfunctions

$$\psi_{n_x n_y n_z} = \sqrt{\frac{8}{L_x L_y L_z}} \sin\frac{\pi n_x}{L_x} x \cdot \sin\frac{\pi n_y}{L_y} y \cdot \sin\frac{\pi n_z}{L_z} z,$$

and eigenvalues

$$E_{n_x n_y n_z} = \frac{\hbar^2 \pi^2}{2m}\left[\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right],$$

where $n_x, n_y, n_z = 1, 2, 3, \ldots$.

a) One of the walls of the box is a piston that can move, meaning that L_x can vary while L_y and L_z remain fixed. Show that the force onto the piston from the particle is

$$F_x = \frac{\hbar^2 \pi^2}{m L_x^3}$$

when the particle is in the ground state.

Hint: The formula sheet might be useful.

b) Suppose now that the box instead contains 8 identical non-interacting spin-$\frac{3}{2}$ particles with mass m, and the many-particle system is in the ground state. What is the total force from the 8 particles onto the piston when $L_y = L_z = L$ and $L_x = 2L$?

Problem 5 Spin $\frac{1}{2}$

a) A spin-$\frac{1}{2}$ particle is subject to a static magnetic field with strength B_0, described by the Hamiltonian

$$\hat{H}_0 = -\frac{2\mu_B}{\hbar} B_0 \hat{S}_z. \tag{4}$$

Given that the eigenstates of the z-component of the spin operator, $\hat{S}_z$, satisfy

$$\hat{S}_z|\uparrow\rangle = +\frac{\hbar}{2}|\uparrow\rangle, \tag{5a}$$

$$\hat{S}_z|\downarrow\rangle = -\frac{\hbar}{2}|\downarrow\rangle, \tag{5b}$$

write down the energy eigenstates and eigenenergies of the system.

b) A general, normalized spin state for a spin-$\frac{1}{2}$ particle can be written

$$|\chi\rangle = \cos\alpha|\uparrow\rangle + e^{i\phi}\sin\alpha|\downarrow\rangle, \tag{6}$$

where α and ϕ are real numbers. Calculate the expectation values $\langle S_z\rangle$ and $\langle H_0\rangle$ using Eqs. (4) and (5). For what values of α and ϕ is the state $|\chi\rangle$ an energy eigenstate of the system?

c) At time $t = 0$ the particle is measured to be in the state $|\psi(t=0)\rangle = \left(|\uparrow\rangle + e^{i\phi}|\downarrow\rangle\right)/\sqrt{2}$. Assuming that no other measurement is made, the state at $t > 0$ is given by

$$|\psi(t)\rangle = \frac{e^{i\mu_B B_0 t/\hbar}}{\sqrt{2}}|\uparrow\rangle + \frac{e^{i\phi - i\mu_B B_0 t/\hbar}}{\sqrt{2}}|\downarrow\rangle. \tag{7}$$

Use Eq. (7) and the definitions of the spin-$\frac{1}{2}$ ladder operators,

$$\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y, \tag{8}$$

where $\hat{S}_{x(y)}$ is the x (y) component of the spin operator, to show that the expectation values for the spin components at times $t > 0$ are

$$\langle S_x\rangle(t) = \frac{\hbar}{2}\cos(\phi - 2\mu_B B_0 t/\hbar),$$

$$\langle S_y\rangle(t) = \frac{\hbar}{2}\sin(\phi - 2\mu_B B_0 t/\hbar),$$

$$\langle S_z\rangle(t) = 0.$$

Which physical effect does this describe?

Hint: Operating with the ladder operators on the eigenstates of $\hat{S}_z$ gives

$$\hat{S}_+|\uparrow\rangle = \hat{S}_-|\downarrow\rangle = 0, \tag{9a}$$

$$\hat{S}_+|\downarrow\rangle = \hbar|\uparrow\rangle, \tag{9b}$$

$$\hat{S}_-|\uparrow\rangle = \hbar|\downarrow\rangle. \tag{9c}$$

Problem 6 Perturbation theory

Consider a system described by the Hamiltonian

$$\hat{H} = \hat{H}_0 + \lambda \hat{U},$$

for which we cannot find an exact solution of the Schrödinger equation, but for which we do know the exact solution for the unperturbed system described by the Hamiltonian $\hat{H}_0$. Namely, we know the solutions to

$$\hat{H}_0 |\phi_n\rangle = \epsilon_n |\phi_n\rangle,$$

but we are not able to find the exact solutions of

$$\hat{H} |\psi_n\rangle = E_n |\psi_n\rangle,$$

where the index n labels the energy levels, assuming non-degenerate states throughout. The parameter λ is a book-keeping device used to turn the perturbation on ($\lambda > 0$) and off ($\lambda = 0$). Assuming that the perturbing potential is sufficiently weak, the exact solutions can be expanded in powers of the perturbation strength λ:

$$\begin{aligned} |\psi_n\rangle &= |\psi_n^{(0)}\rangle + \lambda |\psi_n^{(1)}\rangle + \lambda^2 |\psi_n^{(2)}\rangle + \dots, \\ E_n &= E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots. \end{aligned}$$

These expansions can be used to derive expressions for the corrections to the state vectors and energies to some power λ^n.

a) What is the simple argument for arriving at the identities

$$\begin{aligned} |\psi_n^{(0)}\rangle &= |\phi_n\rangle, \\ E_n^{(0)} &= \epsilon_n \end{aligned}$$

for a non-degenerate state?

b) We now consider the spin system in Eq. (4) perturbed by the potential

$$\hat{U} = \frac{2\kappa}{\hbar} \hat{S}_x,$$

such that the total system Hamiltonian can be written

$$\hat{H} = \hat{H}_0 + \lambda \hat{U} = -\frac{2\epsilon}{\hbar} \hat{S}_z + \lambda \frac{2\kappa}{\hbar} \hat{S}_x. \tag{12}$$

The two states of the system are labeled $|\chi_-\rangle$ and $|\chi_+\rangle$, where $|\chi_-\rangle$ is the ground state. We then have

$$
\begin{aligned}
|\chi_-^{(0)}\rangle &= |\uparrow\rangle, \\
|\chi_+^{(0)}\rangle &= |\downarrow\rangle, \\
E_\mp^{(0)} &= \mp\epsilon.
\end{aligned}
$$

The first and second order corrections to the energy due to the perturbing potential is

$$
\begin{aligned}
E_n^{(1)} &= \langle\phi_n|\hat{U}|\phi_n\rangle, \\
E_n^{(2)} &= \sum_{k\neq n} \frac{|\langle\phi_k|\hat{U}|\phi_n\rangle|^2}{\epsilon_n - \epsilon_k},
\end{aligned}
$$

while the first-order correction to the state vector is given by

$$
|\psi_n^{(1)}\rangle = \sum_{k\neq n} \frac{\langle\phi_k|\hat{U}|\phi_n\rangle}{\epsilon_n - \epsilon_k}|\phi_k\rangle,
$$

where the sums run over all states $k \neq n$ of the system. For the system in Eq. (12) the first-order corrections to the energies, $E_\mp^{(1)}$, are zero.

Calculate the first-order *state* correction $|\chi_-^{(1)}\rangle$ and second-order *energy* correction $E_-^{(2)}$ for the ground state of the system. Write down the state $|\chi_-\rangle$ and energy E_- to first and second order in λ, respectively.

Hint: Use either the algebraic formulation, see the ladder operators in Eqs. (8) and (9), or the matrix formulation for spin $\frac{1}{2}$, where

$$
|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix},
$$

and $\hat{S}_i = \frac{\hbar}{2}\sigma_i$ with $i = x, y, z$.

c) Rewrite the full Hamiltonian Eq. (12) to read

$$
\hat{H} = -\frac{2\xi}{\hbar}\hat{\mathbf{S}} \cdot \hat{n},
$$

where $\hat{\mathbf{S}} = \hat{S}_x\hat{e}_x + \hat{S}_y\hat{e}_y + \hat{S}_z\hat{e}_z$ and $\hat{n}$ is a vector depending on the relative size of ϵ and κ. Use this to show that the exact eigenenergies are

$$
E_\mp = \mp\sqrt{\epsilon^2 + \lambda^2\kappa^2} \equiv \mp\xi.
$$

Does this agree with the results from perturbation theory for small λ?

A Formula sheet

Schrödinger equation (time-dependent and time-independent)

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle$$
$$\hat{H}|\psi\rangle = E|\psi\rangle$$

Thermodynamics

$$dW = PdV$$

Eigenvalues and eigenvectors

$$\det(A - \lambda I) = 0$$
$$(A - \lambda I)\mathbf{v} = 0$$

Some properties of the Dirac delta function and Heaviside step function

$$\int dx\ f(x)\delta(x-a) = f(a)$$
$$\frac{1}{2\pi}\int dx\ e^{i(k-k_0)x} = \delta(k-k_0)$$
$$\Theta(x) = \begin{cases} 1, & x > 0, \\ 0, & x \leq 0. \end{cases}$$
$$\frac{d}{dx}\Theta(x) = \delta(x)$$
$$\int_{-\infty}^{\infty} dx\ \left[\frac{d}{dx}\delta(x)\right] f(x) = -\int_{-\infty}^{\infty} dx\ \delta(x)\left[\frac{d}{dx}f(x)\right]$$

Various physical constants

$$\hbar = 1.054\,571\,817 \times 10^{-34}\,\mathrm{J\,s} = 6.582\,119\,569 \times 10^{-16}\,\mathrm{eV\,s}$$
$$m_e = 9.109\,383\,701\,5 \times 10^{-31}\,\mathrm{kg}$$
$$e = 1.602\,176\,634 \times 10^{-19}\,\mathrm{C}$$
$$c = 299\,792\,458\,\mathrm{m\,s^{-1}} \approx 3 \times 10^{8}\,\mathrm{m\,s^{-1}}$$
$$\mu_0 = \frac{1}{\epsilon_0 c^2} = \frac{4\pi\alpha}{e^2}\frac{\hbar}{c} = 1.256\,637\,062\,12 \times 10^{-6}\,\mathrm{N\,A^{-2}}$$
$$\alpha = \frac{e^2}{4\pi\epsilon_0\hbar c} \approx \frac{1}{137}$$
$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{e^2 m_e} = 5.29 \times 10^{-11}\,\mathrm{m}$$

$$\mu_B = \frac{\hbar e}{2m_e} = 9.274\,010\,078\,3 \times 10^{-24}\,\mathrm{J\,T^{-1}} = 5.788\,381\,806\,0 \times 10^{-5}\,\mathrm{eV\,T^{-1}},$$

Commutators and anticommutators

$$\begin{aligned}
[A,B] &\equiv AB - BA \\
[AB,C] &= [A,C]B + A[B,C] \\
[A+B,C] &= [A,C] + [B,C] \\
\{A,B\} &\equiv AB + BA \\
[\hat{x},\hat{p}_x] &= i\hbar \\
[\hat{S}_x,\hat{S}_y] &= i\hbar\hat{S}_z
\end{aligned}$$

Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Taylor expansion

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{d}{dx}\right)^n f(x)\bigg|_{x=a} (x-a)^n$$

Some potentially useful integrals

$$\begin{aligned}
\int_{-\infty}^{\infty} dx\ e^{-a(x+b)^2} &= \sqrt{\frac{\pi}{a}} \\
\int_{-\infty}^{\infty} dx\ e^{-ax^2+bx+c} &= \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}+c} \\
\int_{-\infty}^{\infty} dx\ x^{2n} e^{-ax^2} &= \left(-\frac{\partial}{\partial a}\right)^n \int_{-\infty}^{\infty} dx\ e^{-ax^2}
\end{aligned}$$

Cylindrical coordinates

$$\begin{aligned}
x = r\cos\phi, \quad y &= r\sin\phi, \quad z = z \\
\boldsymbol{\nabla} f &= \frac{\partial f}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial f}{\partial \phi}\hat{\phi} + \frac{\partial f}{\partial z}\hat{z} \\
\boldsymbol{\nabla} \cdot \mathbf{A} &= \frac{1}{r}\frac{\partial}{\partial r}(rA_r) + \frac{1}{r}\frac{\partial A_\phi}{\partial \phi} + \frac{\partial A_z}{\partial z} \\
\nabla^2 f &= \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial f}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 f}{\partial \phi^2} + \frac{\partial^2 f}{\partial z^2} \\
\int d\mathbf{r} &= \int dz\ d\phi\ dr\ r
\end{aligned}$$

Spherical coordinates

$$
\begin{aligned}
x = r\sin\theta\cos\phi, \quad y &= r\sin\theta\sin\phi, \quad z = r\cos\theta \\
\boldsymbol{\nabla} f &= \frac{\partial f}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial f}{\partial \theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial f}{\partial \phi}\hat{\phi} \\
\boldsymbol{\nabla}\cdot\mathbf{A} &= \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 A_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(A_\theta\sin\theta\right) + \frac{1}{r\sin\theta}\frac{\partial A_\phi}{\partial\phi} \\
\nabla^2 f &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial f}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 f}{\partial\phi^2} \\
\int d\mathbf{r} &= \int d\phi\ d\theta\ dr\ \ \sin\theta r^2
\end{aligned}
$$