# Quantum Mechanics

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## Table of Contents

**Abstract**

Quantum Mechanics Lecture Notes.

TODO:

- Language - Русский or English?
- Определиться с стилистикой доказательств - всякие новомодные ЧТД □ и прочее

**Dual language Example**

Двуязычность можно например реализовать вот так... blah blah blahy

And here some english text

# 1 Introduction

## 1.1 Schrödinger formalism

$$\hat{f}\Phi = E\Phi \tag{1.1}$$

$$\Phi \rightarrow dP = |\Phi|^2 dq \tag{1.2}$$

$$x \leftrightarrow \hat{x} \tag{1.3}$$

$$p_x \leftrightarrow -i\hbar\frac{\partial}{\partial x} \tag{1.4}$$

$$f \leftrightarrow \hat{f} \tag{1.5}$$

$$\bar{f} = \int \hat{f} dp = \int \Phi^* \hat{f} \Phi dq \tag{1.6}$$

$$[\hat{f}, \hat{g}] = \hat{f}\hat{g} - \hat{g}\hat{f} \tag{1.7}$$

$$\{\hat{f}, \hat{g}\} = \hat{f}\hat{g} + \hat{g}\hat{f} \tag{1.8}$$

[1]

## 1.2 Heisenberg formalism

Schrödinger was good at math, which is why his quantum mechanics formalism is full of complex mathematical constructs. Heisenberg, on the other hand, had a lot of difficulty with math, which is why his matrix quantum mechanics formalism is limited almost exclusively to linear algebra constructs

Roman ...

| Name | Schrödinger | Heisenberg |
|---|---|---|
| State Basis | Wave function of basis states $\{\Phi_n\}$ | Column vector of basis states $\begin{pmatrix}\phi_1\\ \dots\\ \phi_n\end{pmatrix}$ |
| Observables | Operator $\bar{f} = \int \Phi_n^* \hat{f} \Phi_m$ | Operator matrix $\begin{pmatrix}\phi_{11} & \dots & \phi_{n1}\\ & \dots & \\ \phi_{1n} & \dots & \phi_{nn}\end{pmatrix}$ |
| Shrödinger Equation | $\hat{f}\Phi = E\Phi$ | $\begin{pmatrix}\phi_{11} & \dots & \phi_{n1}\\ & \dots & \\ \phi_{1n} & \dots & \phi_{nn}\end{pmatrix}\begin{pmatrix}\psi_1\\ \dots\\ \psi_n\end{pmatrix} = \lambda\begin{pmatrix}\psi_1\\ \dots\\ \psi_n\end{pmatrix}$ |

**Building an operator's matrix**

For a system with a discrete state basis, $\{\Psi_n\}$, any state of the system can be described as a linear combination of the basis' wave functions:

$$\Psi = \sum_n a_n \Psi_n \tag{1.9}$$

Observable $\bar{f}$ for such a wave function can be decomposed into a sum over the basis state wave functions:

$$\begin{aligned}\bar{f} &= \int \Psi^* \hat{f} \Psi dq = \int \sum_n a_n^* \Psi_n^* \hat{f} \sum_m a_m \Psi_m dq \\ &= \sum_n \sum_m a_n^* a_m \int \Psi_n^* \hat{f} \Psi_m dq = \sum_n \sum_m a_n^* a_m f_{nm}(t) \\ &= \sum_n \sum_m a_n^* f_{nm}(t) a_m \end{aligned} \tag{1.10}$$

Where $f_{nm}$ is the operator matrix.

**$f_n m(t)$ time dependence**

Move to appendix?
Solutions to the time-independent Shrödinger equation:

$$\hat{H}\Psi_n = E_n \Psi_n \tag{1.11}$$

$$\Psi_n(t) = e^{-\frac{i}{\hbar}E_n t}\Phi_n \tag{1.12}$$

Which, in operator matrix terms translates into

$$\begin{aligned} f_{nm}(t) &= \int \Psi_n^* \hat{f} \Psi_m dq = \int \Phi_n^* (e^{-\frac{i}{\hbar}E_n t})^* \hat{f} \Phi_m e^{-\frac{i}{\hbar}E_m t} dq \\ &= e^{+\frac{i}{\hbar}E_n t} e^{-\frac{i}{\hbar}E_m t} \int \Phi_n^* \hat{f} \Phi_m dq = e^{i\frac{E_n - E_m}{\hbar}t} \int \Phi_n^* \hat{f} \Phi_m dq \\ &= f_{nm} e^{i\omega_{nm} t} \end{aligned} \tag{1.13}$$

**Operator matrix properties**

1. The operator matrix is hermitian [1] Transposed operator:

$$(\int \Phi \hat{f} \Psi dq \quad)^T = \int \Psi (\hat{f})^T \Phi dq \tag{1.14}$$

   Complex conjugate:

$$(\hat{f})^* = \hat{f}^* \tag{1.15}$$

   Hermitian conjugate:

$$\bar{f}^* = \int \Psi^* \hat{f}^\dagger \Psi dq \tag{1.16}$$

   In operator matrix terms:

$$\begin{aligned} (f_{nm}^*) &= \int \varphi_n^* \hat{f}^\dagger \varphi_m dq = \int \varphi_n^* (\hat{f}^*)^T \varphi_m dq \\ &= \int \varphi_m (\hat{f}^* \varphi_n^*) dq = (\int \varphi_m^* \hat{f}^\dagger \varphi_n dq)^* = (f_{mn})^* \end{aligned} \tag{1.17}$$

   Which means, if $f_{nm}$ is real, meaning $f_{nm}^* = f_{nm}$ that

$$f_{nm} = f_{mn}^* = f_{nm}^\dagger \tag{1.18}$$

2. The matrix' diagonal elements are time-independent and real

$$f_{nn} = \int \Psi_n \hat{f} \Psi_n dq \equiv \bar{f}_n \tag{1.19}$$

   Where $\bar{f}_n$ is the value of observable $f$ in basis state $n$.

3. The matrix of the product of two operators is the product of their matrices
   For operators $\hat{f}$ and $\hat{g}$, what is the operator matrix for operator $\hat{f} \times \hat{g}$ — $(\hat{f} \times \hat{g})_{nm}$?

[1] $H^\dagger = H = (H^*)^T$

Move to appendix?

$$\hat{f}\varphi_n = \sum_m f_{mn}\varphi_m \tag{1.20}$$

$$\int \varphi_k^* dq \times \hat{f}\varphi_n = \int \varphi_k^* dq \times \sum_m f_{mn}\varphi_m$$

$$\int \varphi_k^* \hat{f}\varphi_n dq = \sum_m f_{mn} \int \varphi_k^* \varphi_m dq f_{kn} = \sum_m f_{mn}\delta_{km} = f_{kn} \tag{1.21}$$

Because for state basis $\varphi_n$, $\varphi_n$ and $\varphi_m$ are orthogonal for all $m \neq n$.

Using 1.18, we can write:

$$\begin{aligned}\hat{f}\hat{g}\varphi_n = \hat{f}(\hat{g}\varphi_n) = \hat{f}\sum_k g_k n\varphi_k = \sum_k g_{kn}\hat{f}\varphi_k \\ = \sum_k g_{kn}\sum_m f_{mk}\varphi_m = \sum_{k,m} g_{kn}f_{mk}\varphi_m \\ = \sum_{k,m} f_{mk}g_{kn}\varphi_m\end{aligned} \tag{1.22}$$

And knowing that:

$$(\hat{f}\hat{g})\varphi_n = \sum_m (\hat{f}\hat{g})_{nm}\varphi_m \tag{1.23}$$

We end up with:

$$(\hat{f}\hat{g})_{mn} = \sum_k f_{mk}g_{kn} \tag{1.24}$$

4. The operator's matrix is equivalent to the operator

$$\Psi = \sum_m c_m\varphi_m \tag{1.25}$$

$$\hat{f}\Psi = f\Psi \tag{1.26}$$

$$\hat{f}\sum_m c_m\varphi_m = f\sum_m c_m\varphi_m$$

$$\int \varphi_n^* \hat{f}\sum_m c_m\varphi_m dq = \int \varphi_n^* f\sum_m c_m\varphi_m dq$$

$$\sum_m c_m \int \varphi_n^* \hat{f}\varphi_m dq = f\sum_m c_m \int \varphi_n^*\varphi_m dq$$

$$\sum_m c_m f_{nm} = f\sum_m c_m\delta_{nm}$$

$$\sum_m c_m f_{nm} = fc_n \tag{1.27}$$

(1.28)

$$\sum_m c_m f_{nm} = f c_n$$
$$\sum_m f_{nm} - f\delta_{nm} c_m = 0 \Rightarrow$$
$$|| \, f_{nm} - f\delta_{nm} \, || = 0 \tag{1.29}$$
$$\tag{1.30}$$

## 1.3 Switching to a different state basis

$\{\varphi_n(q)\}$ and $\{\varphi'_n(q)\}$ are two different basis's.

$$\varphi'_n(q) = \sum_m S_{mn}\varphi_n(q) \tag{1.31}$$
$$\varphi'_n = \hat{S}\varphi_n \tag{1.32}$$

Where $\hat{S}$ is the transition operator. If the new basis$\{\varphi'_n(q)\}$ is orthogonal, meaning:

$$\int \varphi'^*_m \varphi'_n dq = \delta_{mn} \tag{1.33}$$

then $\hat{S}^\dagger = \hat{S}^{-1}$.

$$\int \varphi'^*_m \varphi'_n dq = \delta_{mn}$$
$$\int \hat{S}^* \varphi^*_m \hat{S}\varphi_n dq = \delta_{mn}$$
$$\int \varphi^*_m (\hat{S}^*)^T \hat{S}\varphi_n dq = \delta_{mn}$$
$$\int \varphi^*_m \sum_l S^*_{ml} S_{ln}\varphi_n dq = \delta_{mn}$$
$$\sum_l S^*_{ml} S_{ln} \int \varphi^*_m \varphi_n dq = \delta_{mn}$$
$$\delta_{mn}(\sum_l S^*_{ml} S_{ln} - 1) = 0 \quad \Rightarrow$$
$$\hat{S}^\dagger = \hat{S}^{-1} \quad (S^\dagger_{mn} = S^*_{nm}) \tag{1.34}$$

Operators in the new basis can be written as:

$$\int \varphi'^*_m \hat{f} \varphi'_n dq = \int (\hat{S}^* \varphi^*_m)(\hat{f}\hat{S}\varphi_n) dq =$$
$$= \int \varphi^*_m \hat{S}^{*T} \hat{f}\hat{S}\varphi_n) dq = \int \varphi^*_m \hat{f}' \varphi_n dq \Rightarrow$$
$$\hat{f}' = \hat{S}^{*T}\hat{f}\hat{S} = \hat{S}^\dagger \hat{f}\hat{S} = \hat{S}^{-1}\hat{f}\hat{S} \tag{1.35}$$

**The operator's matrix's trace** is the sum of the operator matrix's diagonal elements:

$$Sp\hat{f} = \sum_n f_{nn} \tag{1.36}$$

1. The trace of the product of two operators is invariant to the order of the operators

$$Sp(\hat{f}\hat{g}) = Sp(\hat{g}\hat{f}) \tag{1.37}$$

According to 1.36, $Sp\hat{f} = \sum_n f_{nn}$, therefore (using 1.24):

$$\begin{aligned} Sp(\hat{f}\hat{g}) &= \sum_n (\hat{f}\times\hat{g})_{nn} \\ &= \sum_n \sum_k f_{nk}g_{kn} \quad \text{and} \end{aligned} \tag{1.38}$$

$$\begin{aligned} Sp(\hat{g}\hat{f}) &= \sum_n (\hat{g}\times\hat{f})_{nn} \\ &= \sum_n \sum_k g_{nk}f_{kn}, \quad n\to k; k\to n \\ = \sum_k \sum_n g_{kn}f_{nk} &= \sum_n \sum_k f_{nk}g_{kn} \end{aligned} \tag{1.39}$$

2. The trace of the product of three or more operators is invariant to the cyclic permutation of the operators

$$Sp(\hat{f}\hat{g}\hat{h}) = Sp(\hat{h}\hat{f}\hat{g}) = Sp(\hat{g}\hat{h}\hat{f}) \tag{1.40}$$

According to 1.37

$$Sp(\hat{f}(\hat{g}\hat{h})) = Sp((\hat{g}\hat{h})\hat{f}) \quad \text{and} \tag{1.41}$$

$$Sp((\hat{f}\hat{g})\hat{h}) = Sp(\hat{h}(\hat{f}\hat{g})) \tag{1.42}$$

Which is equivalent to 1.40 because matrix multiplication is associative.

The operator's matrix's trace is invariant to the basis.

$$Sp\hat{f}' = Sp\hat{S}^{-1}\hat{f}\hat{S} = Sp\hat{S}\hat{S}^{-1}\hat{f} = Sp\hat{f} \tag{1.43}$$

**Commutators** Two operators commute if and only if they share a set of basis states. Or, in other words, there exist as basis in which they are both diagonal.
If $\hat{f}$ and $\hat{g}$ commute, then:

$$[\hat{f},\hat{g}] = \hat{f}\hat{g} - \hat{g}\hat{f} = 0 \tag{1.44}$$

Which means that

$$\sum_k f_{mk}g_{kn} = \sum_k g_{mk}f_{kn} \tag{1.45}$$

If $\{\varphi_n\}$ are eigenfunctions of $\hat{f}$, then $f_{nm} \neq 0$ only if $n = m \to$

$$\begin{aligned} f_{mm}g_{mn} &= g_{mn}f_{nn} \\ g_{mn}(f_{mm} - f_{nn}) &= 0 \end{aligned} \tag{1.46}$$

Meaning that $g_{mn} = 0$ if $m \neq n$

## 1.4 Pauli uncertainty principle

The Pauli uncertainty principle states that if the operators of two observables do not commute, than we cannot measure both observables with arbitrary precision at the same time. In other words, that to more certain are we about one observable, the more uncertain we are about the other. For example:

$$[\hat{x}, \hat{p_x}] = i\hbar \tag{1.47}$$

$$\Delta x \Delta p_x \geq \hbar \tag{1.48}$$

or, for an exact relation,

$$\sigma_x \sigma_{p_x} \geq \frac{\hbar}{2} \tag{1.49}$$

$$\sigma_x = \sqrt{< \Delta x^2 >} \quad \sigma_{p_x} = \sqrt{< \Delta p_x^2 >} \tag{1.50}$$

$$\tag{1.51}$$

**Single-slit electron diffraction**

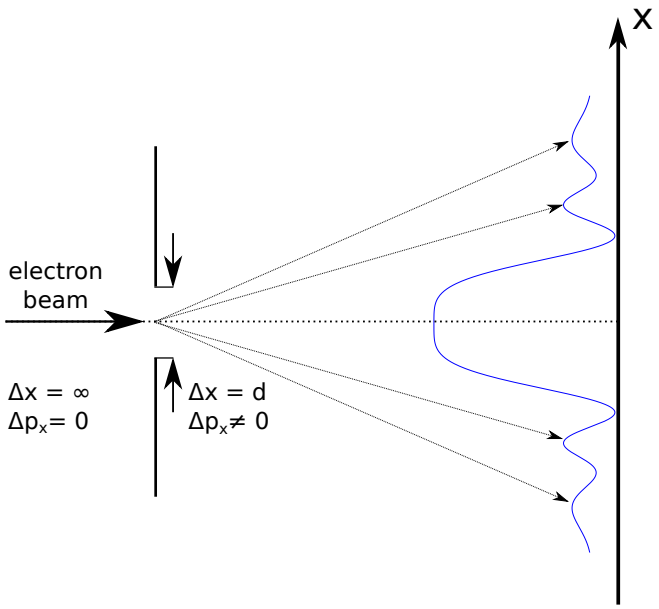


**Figure 1.1:** Single-slit electron diffraction

$$b \sin(\theta) = \lambda \tag{1.52}$$

$$\Delta p_x = p \sin(\theta) \tag{1.53}$$

$$\Delta x = d \tag{1.54}$$

Using the relation for the de Broglie wavelength

$$\lambda = \frac{h}{p} = \frac{2 * \pi * \hbar}{p} \tag{1.55}$$

We get, considering

$$\Delta x \Delta p_x = d \sin(\theta) \frac{2\pi\hbar}{\lambda} = 2\pi\hbar \tag{1.56}$$

$$\Delta x \Delta p_x \approx \hbar \tag{1.57}$$

**Black holes**

> And now let's talk about black holes
>
> Ivan Iorsh

For an white dwarf star we can say that it's electrically neutral, has about the name number of protons as neutrons and is approximately spherical:

$$\bar{e} \rightarrow N \tag{1.58}$$

$$\bar{p} \rightarrow N \tag{1.59}$$

$$\bar{n_0} \rightarrow N \tag{1.60}$$

$$V = \frac{4}{3}\pi R^3 \tag{1.61}$$

$$M_{\odot} = 2 m_p N \tag{1.62}$$

Knowing the total volume we can estimate the average volume occupied by each electron, $d_e$:

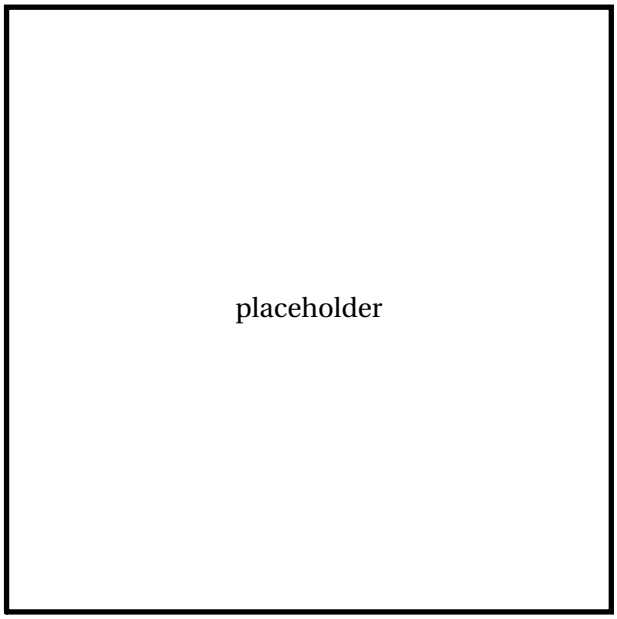


**Figure 1.2:** Spherical horse in a vacuum

$$d_e = \left(\frac{\frac{4}{3}\pi R^3}{N}\right)^{\frac{1}{3}} = \frac{R}{N^{\frac{1}{3}}}\left(\frac{4}{3}\pi\right)^{\frac{1}{3}} \tag{1.63}$$

TODO: MOVE TO END: Average electron position, taking into account the fact that the electrons are confined:

$$\langle \Delta d^2 \rangle = \langle d^2 \rangle + \cancelto{0}{\langle \Delta d \rangle^2} = \langle d^2 \rangle \tag{1.64}$$

And considering that electron positions $d$ are of the same order as their dispersion $\Delta d \approx d$; and the same for their momentum, $\Delta p \approx p$ the Pauli uncertainty principle can be written as (for one electron):

$$\Delta p \Delta d \gtrsim \frac{\hbar}{2}; \qquad v = \frac{p}{m_e} \tag{1.65}$$

$$\Delta p \approx= \frac{\hbar}{2\Delta d} = \frac{\hbar}{2d} \tag{1.66}$$

$$E_{kinetic} = \frac{m_e v^2}{2} = \frac{p^2}{2m_e} = \frac{\hbar^2}{8d^2 m_e} \tag{1.67}$$

And for $N$ electrons:

$$E_{kN} = \frac{N\hbar^2}{8d^2 m_e} \tag{1.68}$$

For an average star,

$$M_\odot \approx 2 * 10^{33}\text{g} \tag{1.69}$$

$$R_\odot \approx 6 * 10^{5}\text{m} \tag{1.70}$$

$$m_p \approx 10^{-27}\text{kg} \tag{1.71}$$

$$m_e \approx 10^{-30}\text{kg} \tag{1.72}$$

$$\hbar = 1.05 * 10^{-34}\text{J} * \text{s} \tag{1.73}$$

The average speed of an electron in the star isExplicit calc

$$V = \frac{p}{m_e} = \frac{\hbar}{m_e}\frac{N^{\frac{1}{3}}}{R}\left(\frac{4}{3}\pi\right)^{-\frac{1}{3}} = \frac{\hbar}{m_e}\left(\frac{M}{2m_p}\right)^{\frac{1}{3}}\frac{1}{R}\left(\frac{4}{3}\pi\right)^{-\frac{1}{3}} = \tag{1.74}$$

$$= \quad \ldots \tag{1.75}$$

$$\approx 10^8 \frac{\text{m}}{\text{s}} \approx \frac{1}{3}c \tag{1.76}$$

Which is highly relativistic. /hlEnd Part to move
Energy of a star:

$$E_{full} = E_{kinetic} + U_{gravitational} \tag{1.77}$$

$$F = \frac{Gm_1 m_2}{r^2} - \frac{\partial d}{\partial r} \tag{1.78}$$

$$U = -\frac{Gm_1 m_2}{r} \tag{1.79}$$

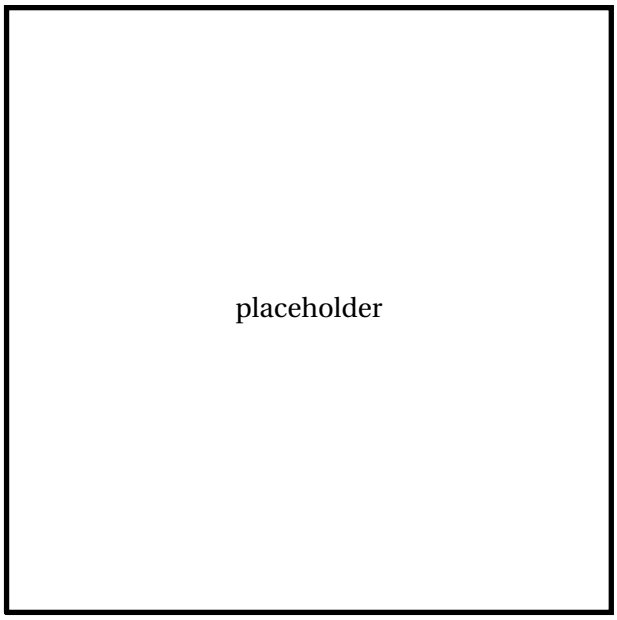


**Figure 1.3:** Forces integration schematic

The potenetial energy of the star:

$$dU = \frac{-G(\frac{4}{3}\pi r^3\rho)(4\pi r^2 dr\rho)}{r} = -\frac{16}{3}G\pi^2\rho^2 r^4 \tag{1.80}$$

$$U = \int_0^R dU = -\int_0^R \frac{16}{3}G\pi^2\rho^2 r^4 = -\frac{16}{15}G\pi^2\rho^2 r^5 \,|_0^R = -\frac{16}{15}G\pi^2\rho^2 R^5 \tag{1.81}$$

$$M = \frac{4}{3}\pi\rho R^5 \tag{1.82}$$

$$\frac{M^2}{R} = \frac{16}{9}\pi^2\rho^2 R^5 \tag{1.83}$$

$$U = -G\frac{9}{15}\frac{M^2}{R} \tag{1.84}$$

The kinetic energy of the star's electrons: For a single electron:

$$\Delta p\Delta d \gtrsim \frac{\hbar}{2}; \qquad v\frac{p}{m_e} \tag{1.85}$$

$$\Delta p \approx= \frac{\hbar}{2\Delta d} = \frac{\hbar}{2d} \tag{1.86}$$

$$E_{kinetic} = \frac{m_e v^2}{2} = \frac{p^2}{2m_e} = \frac{\hbar^2}{8d^2 m_e} \tag{1.87}$$

And for $N$ electrons:

$$E_{kN} = \frac{N\hbar^2}{8d^2 m_e} \tag{1.88}$$

Now the total energy of the star is:

$$E = \frac{N\hbar^2}{8d^2 m_e} - G\frac{9}{15}\frac{M^2}{R} = \tag{1.89}$$

$$= \frac{N^{\frac{5}{3}}\hbar^2}{8R^2 m_e (\frac{4}{3}\pi)^{\frac{2}{3}}} - G\frac{9}{15}\frac{M^2}{R} = \tag{1.90}$$

$$= \frac{M^{\frac{5}{3}}\hbar^2}{8R^2 m_e (\frac{4}{3}\pi)^{\frac{2}{3}}(2m_p)^{\frac{5}{3}}} - G\frac{9}{15}\frac{M^2}{R} \tag{1.91}$$

For a stable star, its stable radius should be in a minimum of energy,

$$\frac{\partial E}{\partial R} = 0 \tag{1.92}$$

For our star,

$$\frac{\partial E}{\partial R} = -\frac{M^{\frac{5}{3}}\hbar^2}{4R^3 m_e (\frac{4}{3}\pi)^{\frac{2}{3}}(2m_p)^{\frac{5}{3}}} + G\frac{9}{15}\frac{M^2}{R^2} \tag{1.93}$$

$$\frac{\partial E}{\partial R} = 0 \Rightarrow \tag{1.94}$$

$$\frac{M^{\frac{5}{3}}\hbar^2}{4R^3 m_e (\frac{4}{3}\pi)^{\frac{2}{3}}(2m_p)^{\frac{5}{3}}} = G\frac{9}{15}\frac{M^2}{R^2} \tag{1.95}$$

$$\frac{15}{36}\frac{GM^{-\frac{1}{3}}}{m_e (\frac{4}{3}\pi)^{\frac{2}{3}}(2m_p)^{\frac{5}{3}}} = R \tag{1.96}$$

Or simply,

$$M^{\frac{1}{3}}R = const \tag{1.97}$$

Which means that for every stellar mass there exists a certain stable radius. The problem with this equation is that it does not take into account that electrons in such a star a highly relativistic TODO: MOVE RELATIVISTIC THING HERE, meaning that the kinetic energy of the star cannot be accurately represented as in 1.88.
For a relativistic electron,

$$E_k = \sqrt{m^2c^4 + p^2c^2} \approx \tag{1.98}$$

$$pc \ll mc^2, \qquad \approx me^2 + \frac{p^2}{2m} \tag{1.99}$$

$$pc \gg mc^2, \qquad \approx cp \tag{1.100}$$

Taking into account that $v_e \approx \frac{1}{3}c$, and that $p = \frac{\hbar}{2d}$,

$$E_{kinetic} = \frac{c\hbar}{2d} = \frac{c\hbar N^{\frac{4}{3}}}{2R(\frac{4}{3}\pi)^{\frac{1}{3}}} = \frac{c\hbar M^{\frac{4}{3}}}{2R(\frac{4}{3}\pi)^{\frac{1}{3}}(2m_p)^{\frac{4}{3}}} \tag{1.101}$$

$$E = \frac{c\hbar M^{\frac{4}{3}}}{2R(\frac{4}{3}\pi)^{\frac{1}{3}}(2m_p)^{\frac{4}{3}}} - G\frac{9}{15}\frac{M^2}{R} = \tag{1.102}$$

$$= \frac{1}{R}\left(\frac{c\hbar M^{\frac{4}{3}}}{2(\frac{4}{3}\pi)^{\frac{1}{3}}(2m_p)^{\frac{4}{3}}} - GM^2\frac{9}{15}\right) \tag{1.103}$$

Which means that a stable $R$ doesn't exist for such stars - if the expression in parenthesis in 1.103 is greater than zero, than the star expands until its electrons are no longer relativistic, and it settles to a radius defined by 1.97, or if the expression in parenthesis in 1.103 is less than zero, the star's kinetic energy is insufficient to withstand its gravitational pull and it collapses into a black hole. The mass at which this happens, $M_{cr}$, is

$$M_{cr} = \left(\frac{15c\hbar}{9G2(2m_p)^{\frac{4}{3}}(\frac{4}{3}\pi)^{\frac{1}{3}}}\right)^{\frac{3}{2}} = \tag{1.104}$$

...explicit calc...

$$\approx 10^{30}\text{kg} \approx 1.4M_{\odot} \tag{1.105}$$

Where $M_{\odot}$ is the mass of our sun. Meaning that no white dwarf star with a mass over $1.4M_{\odot}$ can stably exist. Nobel Prize lecture, Subrahmanyan Chandrasekhar[2].

**Quantum Pencil**

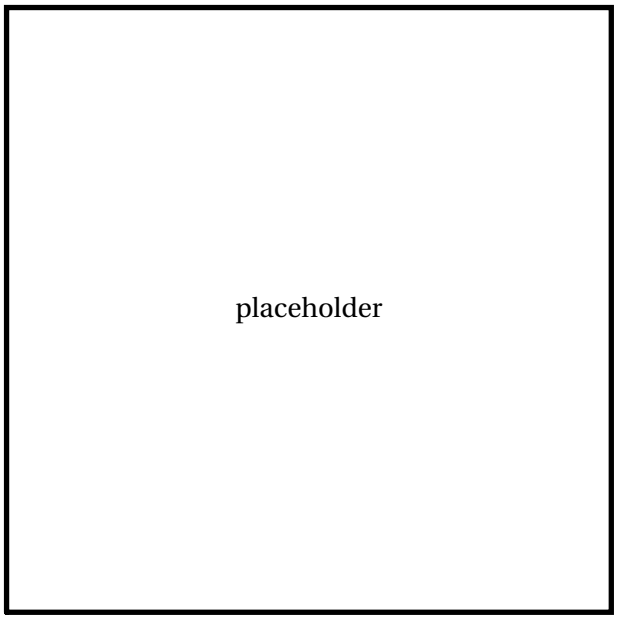


**Figure 1.4:** Vertical pencil diagram

If we place a pencil with mass $m = 10^{-6}\text{kg}$ on its tip $d_0 = 10^{-10}\text{m}$, because of the uncertainty principle, its center of

mass will start to move,

$$\Delta x \Delta \approx \frac{\hbar}{2} \tag{1.106}$$

$$\Delta x < d_0 \tag{1.107}$$

$$\Delta p > \frac{\hbar}{2d_0} \tag{1.108}$$

$$p \sim \Delta p \tag{1.109}$$

$$v = \frac{p}{m} = \frac{\hbar}{2d_0 m} \tag{1.110}$$

We can say that the pencil has fallen when its center of mass is no longer over the "tip" of the pencil (Fig,.1.4).

$$t \sim \frac{d_0}{v} = \frac{2d_0^2 m}{\hbar} \approx \frac{2 * (10^{-10})^2 * 10^{-6}}{10^{-34}} \approx 10^8 \text{s} \tag{1.111}$$

Which means that the pencil can stably exist in a vertical position for over 3 years (compared to other solutions, which give unrealistic estimates of about 3 seconds)[3].

## 1.5 Problems

# 2 Analytical Solutions

## 2.1 Rectangular quantum well

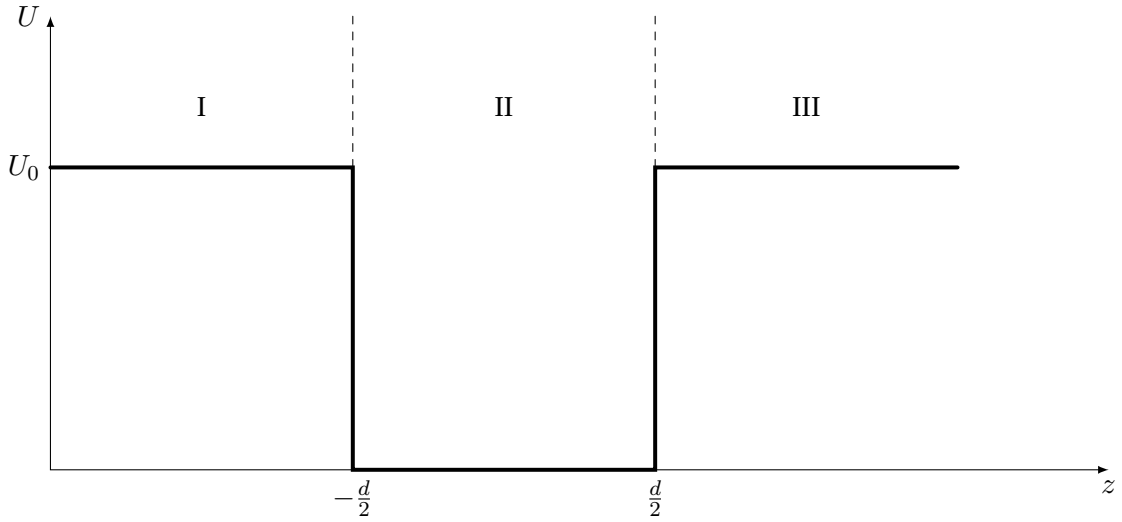


**Figure 2.1:** Finite rectangular quantum well

$$\hat{H} = \frac{\hbar}{2m}\frac{\partial^2}{\partial z^2} + U(z) \tag{2.1}$$

$$\text{II:} \qquad E\Psi = \frac{\hbar}{2m}\frac{\partial^2}{\partial z^2}\Psi \tag{2.2}$$

$$\text{I \& III:} \qquad E\Psi = \frac{\hbar}{2m}\frac{\partial^2}{\partial z^2}\Psi + U_0\Psi \tag{2.3}$$

Solutions for each area:

$$\text{I:} \qquad \Psi = Ae^{+ik'z} + Be^{-ik'z} \tag{2.4}$$

$$\text{II:} \qquad \Psi = Ce^{+ikz} + De^{-ikz} \tag{2.5}$$

$$\text{III:} \qquad \Psi = Fe^{+ik'z} + Ge^{-ik'z} \tag{2.6}$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}; \qquad k' = \sqrt{\frac{2m(E-U_0)}{\hbar^2}} \tag{2.7}$$

**Bound states**

For $E < U_0$, $k'$ is imaginary, meaning that

$$\lim_{z\to-\infty} Ae^{+ik'z} = \lim_{z\to-\infty} Ae^{-sz} = \infty \tag{2.8}$$

$$\lim_{z\to\infty} Ge^{-ik'z} = \lim_{z\to\infty} Ae^{sz} = \infty \tag{2.9}$$

Which is not physical, meaning that

$$A = G = 0 \tag{2.10}$$

We have bounadary conditions at $z = -\frac{d}{2}$ and $z = \frac{d}{2}$:

$$\Psi_I = \Psi_{II}|_{z=-\frac{d}{2}}; \qquad \Psi'_I = \Psi'_{II}|_{z=-\frac{d}{2}} \tag{2.11}$$

$$\Psi_{II} = \Psi_{III}|_{z=\frac{d}{2}}; \qquad \Psi'_{II} = \Psi'_{III}|_{z=\frac{d}{2}} \tag{2.12}$$

Which can be written as:

$$\kappa = ik' = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}} \tag{2.13}$$

$$Be^{-\kappa\frac{d}{2}} = Ce^{-ik\frac{d}{2}} + De^{+ik\frac{d}{2}} \tag{2.14}$$

$$-B\kappa e^{-\kappa\frac{d}{2}} = ikCe^{-ik\frac{d}{2}} - ikde^{+ik\frac{d}{2}} \tag{2.15}$$

$$Fe^{-\kappa\frac{d}{2}} = Ce^{+ik\frac{d}{2}} + De^{-ik\frac{d}{2}} \tag{2.16}$$

$$-F\kappa e^{-\kappa\frac{d}{2}} = ikCe^{+ik\frac{d}{2}} - ikde^{-ik\frac{d}{2}} \tag{2.17}$$

$$\tag{2.18}$$

Or in matrix form:

$$\begin{pmatrix} e^{-\kappa\frac{d}{2}} & -e^{-ik\frac{d}{2}} & -e^{ik\frac{d}{2}} & 0 \\ 0 & -e^{-ik\frac{d}{2}} & -e^{-ik\frac{d}{2}} & e^{-\kappa\frac{d}{2}} \\ -\kappa e^{-\kappa\frac{d}{2}} & -ike^{-ik\frac{d}{2}} & +ike^{ik\frac{d}{2}} & 0 \\ 0 & +ike^{ik\frac{d}{2}} & -ike^{ik\frac{d}{2}} & -\kappa e^{-\kappa\frac{d}{2}} \end{pmatrix} \begin{pmatrix} B \\ C \\ D \\ F \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{2.19}$$

Direct solution? Since our system is symmetric, we can simplify the system of equations:

$$|\Psi|^2_{-\frac{d}{2}} = |\Psi|^2_{\frac{d}{2}} \Rightarrow \tag{2.20}$$

$$\Psi(z) = \Psi(-z) \qquad \text{or} \qquad \Psi(z) = -\Psi(-z) \tag{2.21}$$

Which means that our system can have either symmetric or antisymmetric solutions:

$$\Psi_{II} = Ce^{ikz} + De^{-ikz} = C'\cos(kz) + D'\sin(kz) \tag{2.22}$$

$$\Psi_I = Be^{-\kappa z} \tag{2.23}$$

$$\Psi_{III} = Fe^{\kappa z} \tag{2.24}$$

$$\tag{2.25}$$

Where $C'\cos(kz)$ and $A = F$ correspond to symmetric solutions and $D'\sin(kz)$ and $A = -F$ — to antisymmetric solutions.

**Symmetric solutions**

$$Be^{-\kappa\frac{d}{2}} = C'\cos(\frac{kd}{2}) \tag{2.26}$$

$$\kappa Be^{-\kappa\frac{d}{2}} = kC'\sin(\frac{kd}{2}) \tag{2.27}$$

Or in matrix form:

$$\begin{pmatrix} e^{-\kappa\frac{d}{2}} & -\cos\frac{kd}{2} \\ \kappa e^{-\kappa\frac{d}{2}} & -k\sin\frac{kd}{2} \end{pmatrix} \begin{pmatrix} B \\ C' \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{2.28}$$

This system has non-trivial solutions when the determinant of the matrix is equal to zero:

$$\begin{vmatrix} e^{-\kappa\frac{d}{2}} & -\cos\frac{kd}{2} \\ \kappa e^{-\kappa\frac{d}{2}} & -k\sin\frac{kd}{2} \end{vmatrix} = -e^{-\kappa\frac{d}{2}} k\sin\frac{kd}{2} + \kappa e^{-\kappa\frac{d}{2}}\cos\frac{kd}{2} = \tag{2.29}$$

$$= -k\sin(\frac{kd}{2}) + \kappa\cos(\frac{kd}{2}) = 0 \tag{2.30}$$

$$\frac{k}{\kappa} = \cot(\frac{kd}{2}) \tag{2.31}$$

With solutions to 2.31 defining the number of bound states in the quantum well.

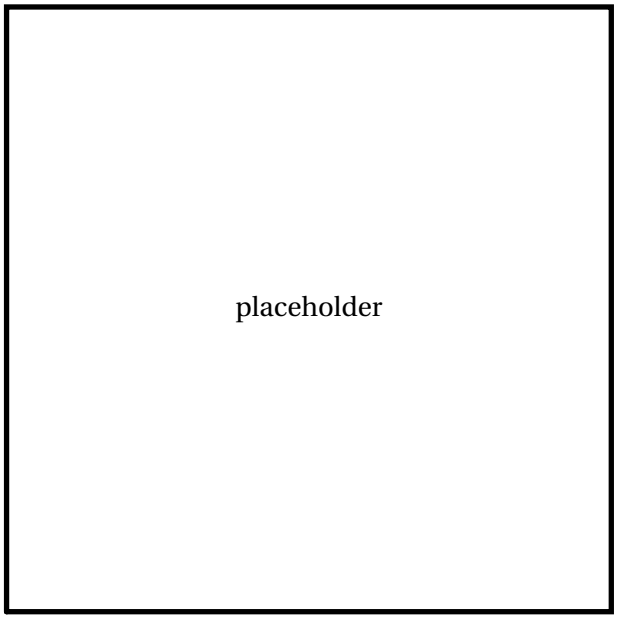


**Figure 2.2:** Graphical solution to 2.31

In the limit case of $U_0 \to \infty$,

$$\frac{k}{\kappa} = \cot(\frac{kd}{2}), \qquad \kappa \to \infty \Rightarrow \tag{2.32}$$

$$\cot(\frac{kd}{2}) = 0 \Rightarrow \qquad \cos(\frac{kd}{2}) = 0 \Rightarrow \tag{2.33}$$

$$\frac{kd}{2} = \frac{\pi}{2} + \pi n \tag{2.34}$$

$$k_n = \frac{\Pi + 2\pi n}{d} \tag{2.35}$$

$$E_n = \frac{\hbar^2}{2m}\frac{1}{d^2}(\pi + 2\pi n)^2 \tag{2.36}$$

Which corresponds to the symmetric solutions found earlier to the infinite quantum well problem.

**Antisymmetric solutions**

$$Be^{-\kappa\frac{d}{2}} = D'\sin(\frac{kd}{2}) \tag{2.37}$$

$$\kappa Be^{-\kappa\frac{d}{2}} = -kD'\cos(\frac{kd}{2}) \tag{2.38}$$

Or in matrix form:

$$\begin{pmatrix} e^{-\kappa\frac{d}{2}} & -\sin\frac{kd}{2} \\ \kappa e^{-\kappa\frac{d}{2}} & k\cos\frac{kd}{2} \end{pmatrix} \begin{pmatrix} B \\ D' \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{2.39}$$

This system has non-trivial solutions when the determinant of the matrix is equal to zero:

$$\begin{vmatrix} e^{-\kappa\frac{d}{2}} & -\sin\frac{kd}{2} \\ \kappa e^{-\kappa\frac{d}{2}} & k\cos\frac{kd}{2} \end{vmatrix} = e^{-\kappa\frac{d}{2}}k\cos\frac{kd}{2} + \kappa e^{-\kappa\frac{d}{2}}\sin\frac{kd}{2} = \tag{2.40}$$

$$= k\cos(\frac{kd}{2}) + \kappa\sin(\frac{kd}{2}) = 0 \tag{2.41}$$

$$\frac{k}{\kappa} = -\tan(\frac{kd}{2}) \tag{2.42}$$

With solutions to 2.42 defining the number of bound states in the quantum well.

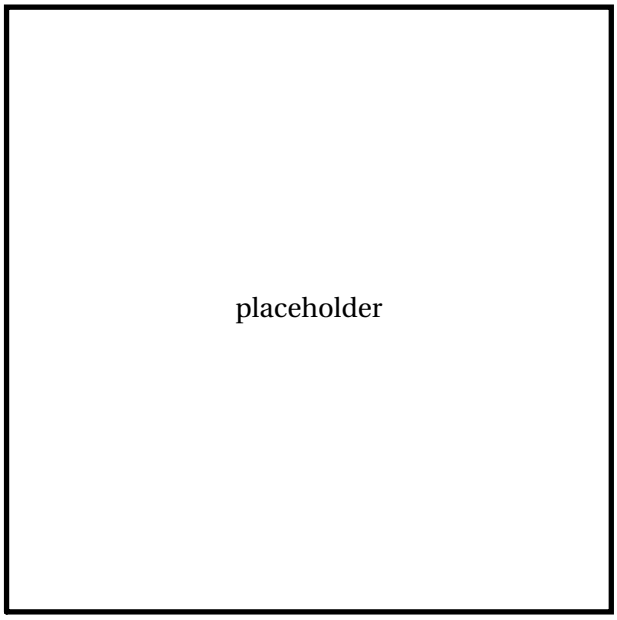


**Figure 2.3:** Graphical solution to 2.42

In the limit case of $U_0 \to \infty$,

$$\frac{k}{\kappa} = -\tan(\frac{kd}{2}), \qquad \kappa \to \infty \Rightarrow \tag{2.43}$$

$$\tan(\frac{kd}{2}) = 0 \Rightarrow \qquad \sin(\frac{kd}{2}) = 0 \Rightarrow \tag{2.44}$$

$$\frac{kd}{2} = \pi n \tag{2.45}$$

$$k_n = \frac{2\pi n}{d} \tag{2.46}$$

$$E_n = \frac{\hbar^2}{2m}\frac{1}{d^2}(2\pi n)^2 \tag{2.47}$$

Which corresponds to antisymmetric solutions found earlier to the infinite quantum well problem.

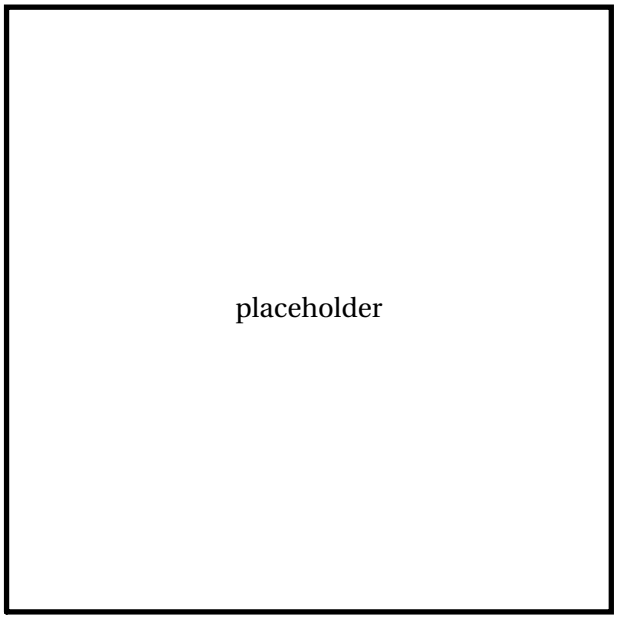


**Figure 2.4:** Quantum well bound state wave functions

For $E > U_0$, the states of the system form a continuous spectrum of waves propagating in either direction.

**Propagating states in a system of potential barriers**

The system and be separated into two cases: propagation through a region, and reflection/transmission through a barrier, these cases correspond to solutions of the Shrödinger equation in each of the regions and to the boundary conditions between the regions.
The wavefunction at each point of the system can be written as a sum of forward and backward propagating waves:

$$\Psi|_{z=z_0} = Ae^{ikz_0} + Be^{-ikz_0} \tag{2.48}$$

$$\Psi|_{z=z_0+d} = Ae^{ikz_0}e^{ikd} + Be^{-ikz_0}e^{-ikd} \tag{2.49}$$

or, in vector form:

$$\Psi = \begin{pmatrix} A_+ \\ A_- \end{pmatrix} \tag{2.50}$$

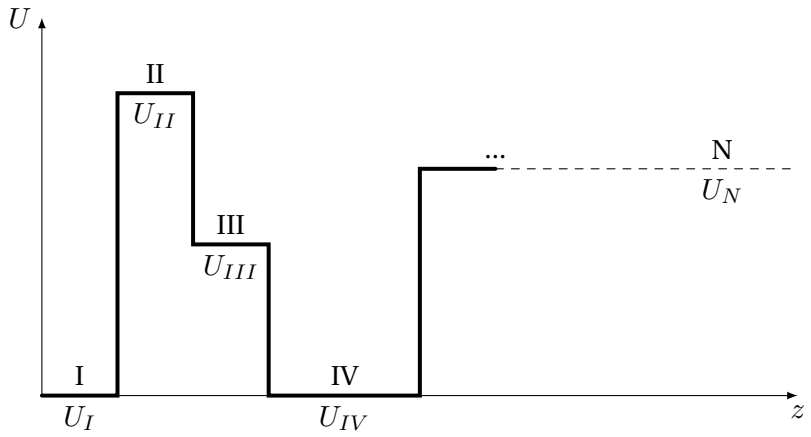


**Figure 2.5:** System of potential barriers

In that case, equations REF can be rewritten as a matrix equation:

$$\Psi|_{z=z_0} = \begin{pmatrix} A_+ \\ A_- \end{pmatrix} \tag{2.51}$$

$$\Psi|_{z=z_0+d} = \begin{pmatrix} A'_+ \\ A'_- \end{pmatrix} = \begin{pmatrix} A_+ \\ A_- \end{pmatrix} \hat{M} = \Psi|_{z=z_0} \hat{M} \tag{2.52}$$

If both $z_0$ and $z_0 + d$ correspond to the same region of the system of barriers, then matrix $\hat{M}$ is simply a propagation matrix:

$$\hat{P} = \begin{pmatrix} e^{ikd} & 0 \\ 0 & e^{-ikd} \end{pmatrix} \tag{2.53}$$

To build a matrix corresponding to the boundary between regions, he have to start with a different basis, in which we can easily write the boundary conditions:

$$\begin{pmatrix} \Psi_I \\ \frac{\partial \Psi_I}{\partial z} \end{pmatrix} = \hat{I} \begin{pmatrix} \Psi_{II} \\ \frac{\partial \Psi_{II}}{\partial z} \end{pmatrix} \tag{2.54}$$

$$\hat{I} = \begin{pmatrix} explicit & explicit \\ explicit & explicit \end{pmatrix} \tag{2.55}$$

The basis $\begin{pmatrix} \Psi_I \\ \frac{\partial \Psi_I}{\partial z} \end{pmatrix}$ can be easily written in terms of the basis $\begin{pmatrix} A'_+ \\ A'_- \end{pmatrix}$:

$$\Psi = A_+ e^{ikz} + A_- e^{-ikz} \tag{2.56}$$

$$\frac{\partial \Psi}{\partial z} = ikA_+ e^{ikz} - ikA_- e^{-ikz} \tag{2.57}$$

$$\begin{pmatrix} \Psi \\ \frac{\partial \Psi}{\partial z} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ ik & -ik \end{pmatrix} \begin{pmatrix} A_+ \\ A_- \end{pmatrix} = \hat{S} \begin{pmatrix} A_+ \\ A_- \end{pmatrix} \tag{2.58}$$

Meaning that

$$\begin{pmatrix} \Psi \\ \frac{\partial \Psi}{\partial z} \end{pmatrix} = \hat{S} \begin{pmatrix} A_+ \\ A_- \end{pmatrix} \qquad \& \qquad \begin{pmatrix} A_+ \\ A_- \end{pmatrix} = \hat{S}^{-}1 \begin{pmatrix} \Psi \\ \frac{\partial \Psi}{\partial z} \end{pmatrix} \tag{2.59}$$

$$\begin{pmatrix} \Psi_I \\ \frac{\partial \Psi_I}{\partial z} \end{pmatrix} = \hat{I} \begin{pmatrix} \Psi_{II} \\ \frac{\partial \Psi_{II}}{\partial z} \end{pmatrix} \tag{2.60}$$

$$\hat{S} \begin{pmatrix} A_{I+} \\ A_{I-} \end{pmatrix} = \hat{I}\hat{S} \begin{pmatrix} A_{II+} \\ A_{II-} \end{pmatrix} \tag{2.61}$$

$$\begin{pmatrix} A_{I+} \\ A_{I-} \end{pmatrix} = \hat{S}^{-1}\hat{I}\hat{S} \begin{pmatrix} A_{II+} \\ A_{II-} \end{pmatrix} \tag{2.62}$$

$$\begin{pmatrix} A_{I+} \\ A_{I-} \end{pmatrix} = \hat{M} \begin{pmatrix} A_{II+} \\ A_{II-} \end{pmatrix}, \qquad \hat{M} = \hat{S}^{-1}\hat{I}\hat{S} \tag{2.63}$$

$$\det \hat{M} = 1 \tag{2.64}$$

Meaning that we can represent a whole series of potential wells and barriers as a product of their *transfer* matricies:

$$\Psi_n = \hat{T_n}\hat{T_{n-1}}...\hat{T_2}\hat{T_1}\Psi_0, \qquad \hat{T_i} = \hat{M}_{i-1\to i}\hat{P}_i \tag{2.65}$$

Transfer matricies can also be used to find the bound states or eigenmodes of the system: Wait, what?

$$\hat{\Psi}_{\frac{d}{2}} = \hat{\Psi}_{-\frac{d}{2}} \tag{2.66}$$

$$\begin{pmatrix} Ae^{-\kappa\frac{d}{2}} \\ -\kappa Ae^{-\kappa\frac{d}{2}} \end{pmatrix} = \hat{T} \begin{pmatrix} Be^{-\kappa\frac{d}{2}} \\ \kappa Ae^{-\kappa\frac{d}{2}} \end{pmatrix} \tag{2.67}$$

Using transfer matricies, the calculation of an electron's probability of tunneling through a barrier is equivalent to solving the following matrix equation:

$$\begin{pmatrix} t \\ 0 \end{pmatrix} = \hat{M} \begin{pmatrix} 1 \\ r \end{pmatrix} \tag{2.68}$$

$$r = -\frac{M_{21}}{M_{22}} \tag{2.69}$$

$$t = \frac{1}{M_{22}} \tag{2.70}$$

## 2.2 Harmonic oscillator

## 2.3 Angular momentum

### Classical

$$\vec{L} = \vec{r} \times \vec{p} = \begin{vmatrix} \vec{e_x} & \vec{e_y} & \vec{e_z} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} \tag{2.71}$$

$$= \vec{e_x}(yp_z - zp_y) + \vec{e_y}(zp_x - xp_z) + \vec{e_z}(xp_y - yp_x) \tag{2.72}$$

$$= \vec{e_x}L_x + \vec{e_y}L_y + \vec{e_z}L_z \tag{2.73}$$

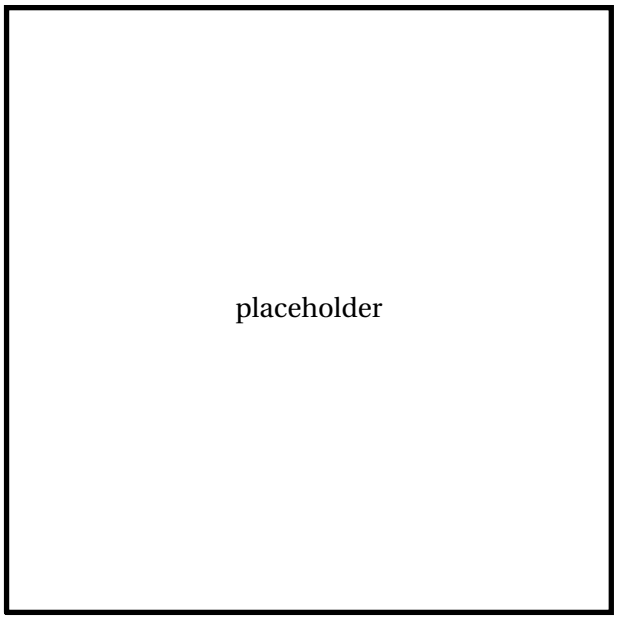


**Figure 2.6:** Classical angular momentum

**Quantum**

$$\hat{\vec{p}} = -i\hbar\vec{\nabla}, \qquad \vec{\nabla} = \vec{e_x}\frac{\partial}{\partial x} + \vec{e_y}\frac{\partial}{\partial y} + \vec{e_z}\frac{\partial}{\partial z} \tag{2.74}$$

$$p_x = -i\hbar\frac{\partial}{\partial x}, \quad p_y = -i\hbar\frac{\partial}{\partial y}, \quad p_z = -i\hbar\frac{\partial}{\partial z} \tag{2.75}$$

$$\hat{\vec{L}} = -i\hbar\vec{r}\times\vec{\nabla} \tag{2.76}$$

$$\hat{L_x} = -i\hbar(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}), \quad \hat{L_y} = -i\hbar(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}), \quad \hat{L_z} = -i\hbar(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}) \tag{2.77}$$

Proof! Commutators:

$$\left[\hat{L_x}, \hat{L_y}\right] = i\hbar\hat{L_z}, \quad \left[\hat{L_z}, \hat{L_x}\right] = i\hbar\hat{L_y}, \quad \left[\hat{L_y}, \hat{L_z}\right] = i\hbar\hat{L_x} \tag{2.78}$$

Uncertainty: Wait, what?

$$\Delta\hat{L_x} = \hat{L_x} - \left\langle\hat{L_x}\right\rangle, \quad \Delta\hat{L_y} = \hat{L_y} - \left\langle\hat{L_y}\right\rangle, \quad \Delta\hat{L_z} = \hat{L_z} - \left\langle\hat{L_z}\right\rangle \tag{2.79}$$

$$\left\langle(\Delta\hat{L_x})^2\right\rangle = \left\langle\hat{L_x}^2\right\rangle - \left\langle\hat{L_x}\right\rangle^2 \tag{2.80}$$

$$\left\langle(\Delta\hat{L_y})^2\right\rangle = \left\langle\hat{L_y}^2\right\rangle - \left\langle\hat{L_y}\right\rangle^2 \tag{2.81}$$

$$\left\langle\hat{L_x}\right\rangle = \int \Psi^*\hat{L_x}\Psi dV \tag{2.82}$$

$$\left\langle(\Delta\hat{L_x})^2\right\rangle\left\langle(\Delta\hat{L_y})^2\right\rangle \geq \frac{\hbar^2|\left\langle\hat{L_z}\right\rangle|^2}{4} \tag{2.83}$$

$$\left\langle(\Delta x)^2\right\rangle\left\langle(\Delta p_x)^2\right\rangle \geq \frac{\hbar^2}{4}$$

Generally it isn't possible to measure $L_x, L_y, L_z$ at once.
Total momentum:

$$\hat{L}^2 = \hat{L_x}^2 + \hat{L_y}^2 + \hat{L_z}^2 \tag{2.84}$$

$$\left[\hat{L}^2, \hat{L_x}^2\right] = \left[\hat{L}^2, \hat{L_y}^2\right] = \left[\hat{L}^2, \hat{L_z}^2\right] = 0 \tag{2.85}$$

$$|\vec{L}| = \sqrt{\hat{L_x}^2 + \hat{L_y}^2 + \hat{L_z}^2} \tag{2.86}$$

**Hydrogen atom** Using the definitions of $\hat{L_x}$ and $\hat{L}^2$ we can begin to solve the hydrogen atom:

$$\begin{cases} \hat{L}^2\Psi = L^2\Psi \\ \hat{L_z}\Psi = L_z\Psi \\ \Psi - ? \quad L - ? \quad L_z - ? \end{cases} \tag{2.87}$$

This system of equations is easy to solve in spherical coordinates:

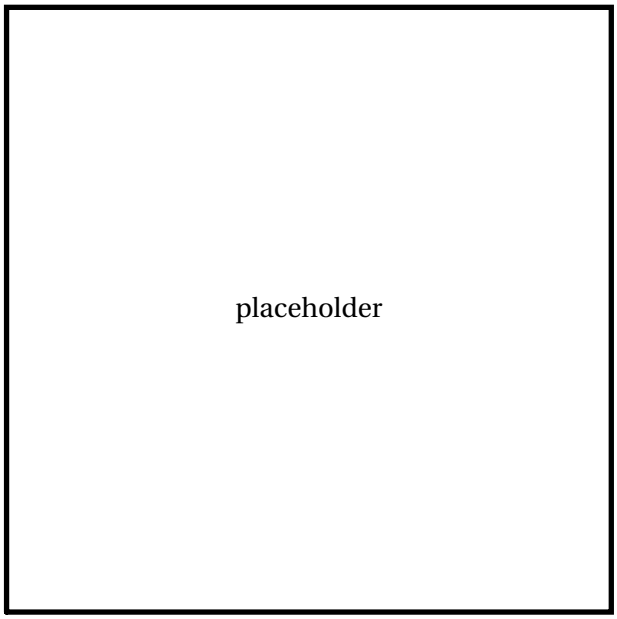


**Figure 2.7:** Spherical coordinates

$$z = r\cos(\theta) \tag{2.88}$$

$$x = r\cos(\theta)\sin(\phi) \tag{2.89}$$

$$y = r\cos(\theta)\cos(\phi) \tag{2.90}$$

$$\tag{2.91}$$

$$\begin{cases} \hat{L_x} = -i\hbar\left(\sin(\phi)\dfrac{\partial}{\partial\theta} + \cot(\theta)\cos(\phi)\dfrac{\partial}{\partial\phi}\right) \\ \hat{L_y} = -i\hbar\left(\cos(\phi)\dfrac{\partial}{\partial\theta} - \cot(\theta)\sin(\phi)\dfrac{\partial}{\partial\phi}\right) \\ \hat{L_z} = -i\hbar\dfrac{\partial}{\partial\phi} \end{cases} \tag{2.92}$$

Check

$$\hat{L}^2 = \hat{L_x}^2 + \hat{L_y}^2 + \hat{L_z}^2 = \tag{2.93}$$

$$= -\hbar^2\left(\frac{\partial^2}{\partial\phi^2} + \left(\sin^2(\theta) + \cos^2(\theta)\right)\frac{\partial^2}{\partial\theta^2} + \cot^2(\theta)\frac{\partial^2}{\partial\phi^2}\right) = \tag{2.94}$$

$$= -\hbar^2\triangle_{\theta,\phi} \tag{2.95}$$

$$\triangle_{\theta,\phi} = \frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2} \tag{2.96}$$

Which allows us to rewrite 2.88 as:

$$\begin{cases} -\hbar^2\triangle_{\theta,\phi}\Psi = L^2\Psi \\ -i\hbar\dfrac{\partial\Psi}{\partial\phi} = L_z\Psi \end{cases} \tag{2.97}$$

Since $\theta$ and $\phi$ are independent variables, we can first solve the equation for $L_z(\phi)$, and then use that solution to solve for $L(\theta,\phi)$. The whole hydrogen atom system is defined as follows (disregarding spin):

$$\begin{cases} \hat{H}\Psi = E\Psi \to n \\ \hat{L}^2\Psi = L^2\Psi \to l \\ \hat{L_z}\Psi = L_z\Psi \to m \end{cases} \tag{2.98}$$

$$\Rightarrow \Psi_{n,l,m} \tag{2.99}$$

## 2.4 Spherically symmetric potential

## 2.5 Problems

**Rectangular quantum well**

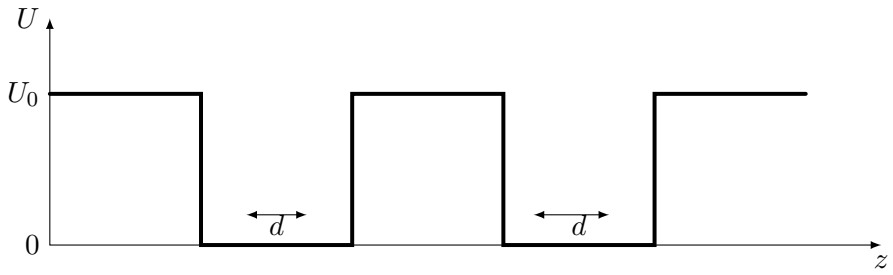


**Figure 2.8:** Double quantum well

**Double quantum well** Calculate the eigenstates.

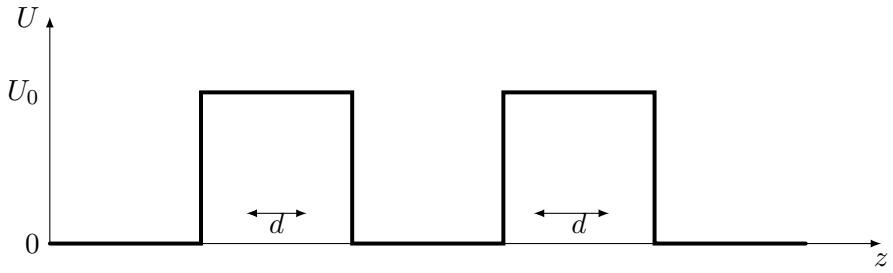


**Figure 2.9:** Double quantum barrier system

**Double quantum barrier** Calculate the probability of a an electron tunneling through a system of two potential barriers.

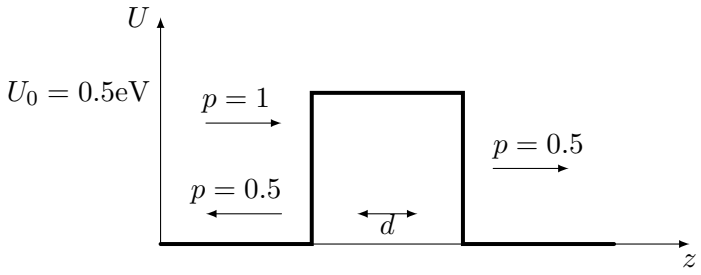


**Figure 2.10:** Model transistor

**Minimal transistor size** Calculate the size of a quantum barrier at which an electron's probability of tunneling through is equal to $0.5$.

$$m_{el} \approx 0.3 m_0 \tag{2.100}$$

$$m_0 \approx 10^{-30}\text{kg} \tag{2.101}$$

$$p = |\Psi|^2 \tag{2.102}$$

# 3 Quasi-classical approximation

## 3.1 Problems

# 4 Spin

## 4.1 Problems

# 5 Perturbation theory

## 5.1 Time-independent

## 5.2 Time-dependent

## 5.3 Problems

# 6 Problem Solutions

## 6.1 Introduction

## 6.2 Analytical solutions

## 6.3 Quasiclassical approximation

## 6.4 Spin

## 6.5 Petrubation theory

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