Schroedinger's Stationary Equation and Tunnel effect

1 Connection between Linear Algebra and Operators in Quantum Mechanics

Everything that follows assumes that wavefunctions $\psi \in \mathcal{H}$ are functions taken from the space of physical wave-function, that is, the Schwartz subset of the space $L^2(\mathbb{R})$ (square integrable) functions in 1D. All definitions can be generalized to other spaces like $\mathbb{R}^2$ or so on.

1.1 Inner product

I define the notation for the inner product between two wave-functions ψ_1 and ψ_2

$$\langle\psi_1|\psi_2\rangle = \int_{\mathbb{R}} \psi_1^\star(x)\psi_2(x)dx \tag{1}$$

from this follows that the norm of the wave-function is

$$\|\psi_1\| = \sqrt{\langle\psi_1|\psi_1\rangle} = \sqrt{\int_{\mathbb{R}} \psi_1^\star(x)\psi_1(x)dx} \tag{2}$$

We will refer to $|\psi\rangle$ as kets and $\langle\psi|$ as bras.

Linearity: From the definition above it is easy to prove that the inner product respects the linearity condition, therefore if $|\psi_2\rangle = a|\varphi\rangle + b|\gamma\rangle$

$$\langle\psi_1|\left(a|\varphi\rangle + b|\gamma\rangle\right) = a\langle\psi_1|\varphi\rangle + b\langle\psi_1|\gamma\rangle$$

Conjugation: One can also verify that

$$\left(\langle\psi_1|\psi_2\rangle\right)^\star = \langle\psi_2|\psi_1\rangle\,. \tag{3}$$

Positivity of the norm: One can also verify that

$$\|\psi\| \geq 0 \tag{4}$$

As mentioned during PC2, the attentive student will notice that those sums are just the continuous version of the standard inner product on finite-dimensional vector spaces $\langle v^1|v^2\rangle = \sum_i (v_i^{1,\star})v_i^2$. *We will see this in more detail in class 5, but for those of you that have a taste for the mathematical formalism, if we interpret the space of the wave-functions $\mathcal{H}$ as a vector space, $|\psi\rangle$ are vectors of this vector space and $\langle\psi|$ are co-vectors from the dual space $\mathcal{H}^\star$*[1] It is possible to show that this definition is a valid inner product as it satisfies all necessary requirements such as linearity, associativity, etc.

[1] A co-vector is an object

$$\langle\phi| : \mathcal{H} \to \mathbb{C} \tag{5}$$
$$|\psi\rangle \to \langle\phi|\psi\rangle \tag{6}$$

1.2 Linear operators

A **linear operator** $\hat{A}$, indicated by the hat, is a functional that takes wave-functions and returns wave-functions. In more mathematical terms, a linear operator takes vectors in $\mathcal{H}$ and returns vectors in $\mathcal{H}$, where we will use the following formalism:

$$\hat{A} : \mathcal{H} \to \mathcal{H} \tag{7}$$

$$|\psi\rangle \to |A\psi\rangle = \hat{A}\,|\psi\rangle \tag{8}$$

Notice that we indicate an operator by the hat, and that we tend to indicate with $|A\psi\rangle$ the wave-function ψ resulting from the application of the operator $\hat{A}$, where we drop the hat to stress the fact that A there does not indicate an operator anymore.

We define the **adjoint operator** or $\hat{A}^\dagger$ as the operator that associates to the bra $\langle\psi|$ corresponding to $|\psi\rangle$ the bra $\langle A\psi|$ corresponding to $|A\psi\rangle$, namely:

$$\hat{A}^\dagger : \mathcal{H}^\star \to \mathcal{H}^\star \tag{9}$$

$$\langle\psi| \to \langle A\psi| = \langle\psi|\,\hat{A}^\dagger \tag{10}$$

The **expectation value** of the operator $\hat{A}$ over a state ψ is defined to be

$$\langle A\rangle_\psi \equiv \langle\psi|\hat{A}|\psi\rangle = \langle\psi|A\psi\rangle = \int_{\mathbb{R}} \psi^\star(x)(A\psi)(x)dx \tag{11}$$

and the expectation value of an operator and its adjoint is related by a conjugation:

$$\left\langle A^\dagger\right\rangle = \langle A\rangle^\star \tag{12}$$

which can be rpoven by applying a few definitions

$$\left\langle A^\dagger\right\rangle = \langle\psi|\hat{A}^\dagger|\psi\rangle = \langle A\psi|\psi\rangle = \int_{\mathbb{R}} (A\psi)^\star(x)\psi(x)dx = \left(\int_{\mathbb{R}} (A\psi)(x)\psi^\star(x)dx\right)^\star = (\langle\psi|A\psi\rangle)^\star = \langle A\rangle^\star \tag{13}$$

Finally, we say that an **operator is Hermitian** or **self-adjoint** if and only if

$$\hat{A} = \hat{A}^\dagger \tag{14}$$

from which it is easy to prove that **the expectation value of hermitian operators is Real**. For a more complete analysis of linear operators and their properties in Quantum Mechanics, you can have a look at Chapter 2 of Cohen, Tannoudji Quantum Mechanics book.

1.3 Common Operators

In the previous classes we have defined the average position and momentum of a particle described by the wavefunction ψ as the expectation values

$$\langle x\rangle = \int_{\mathbb{R}} \psi^\star(x)x\psi(x)dx \qquad \langle p\rangle = \int_{\mathbb{R}} \psi^\star(x)(-i\hbar\frac{d}{dx})\psi(x)dx \tag{15}$$

it follows that we can define the **position operator** and the **momentum operator** as :

$$\hat{x} : \psi \to x\psi \qquad \hat{p} : \psi \to (-i\hbar\frac{d}{dx})\psi \tag{16}$$

and associate to the expectation value of those operators their respective expected physical quantities.

. an intuitive interpretation of co-vectors is the transposition of a vector, even though the mathematical interpretation is more subtle. If you are interested in a more through discussion of the topic, look at Chapter 1.2 of J.J. Sakurai, Modern Quantum Mechanics

Physical quantities are only described by real numbers, so it makes sense to require that all quantities of a quantum system that are physically observable must be associated to an **hermitian operators**. We assume this as a postulate of quantum mechanics (The weak version of the measurement postulate).

It is easy to show using the definition above that both the position, momentum operators and energy operators are hermitian.

1.4 Finite-dimensional interpretation of operators

If the space of wave-function was finite dimensional of dimension $N = \dim[\mathcal{H}]$, the wave-function would be a vector in $\mathbb{C}^N$. In that case, the infinite sum of the inner product defined in eq. (1) reduces to a simple sum, therefore we have that

$$\langle\phi|\psi\rangle = \sum_i \phi_i^\star \psi_i.$$

From linear algebra we recall that the space of linear operators acting on a vector space is isomorphic to the space of $\mathbb{C}^N \times \mathbb{C}^N$, and we can show that an operator $\hat{A}$ in this finite dimensional space can be represented as a matrix $A_{i,j}$. From this definition it follows that an expectation value is just a set of matrix-vector products:

$$\left\langle \hat{A} \right\rangle_\psi = \langle\psi|\hat{A}|\psi\rangle = \sum_{i,j} \psi_i^\star A_{i,j} \psi_j \tag{17}$$

and the *adjoint* $\hat{A}^\dagger$ *of the operator* $\hat{A}$ is the conjugate-transpose of the matrix A_{ij}, such that:

$$(A^\dagger)_{i,j} = (A^T)^\star_{i,j} = A^\star_{j,i}. \tag{18}$$

The proof can easily be derived from the equation above.

1.5 Spectral theorem and eigenvalues of Operators

If you recall from Linear algebra, matrices can be diagonalised and we can extract its eigenvalues and eigenvectors. In finite-dimensions Operators are represented by matrices, therefore they can also be diagonalised, and their eigenvectors form a basis of the space. In infinite-dimensional hilbert spaces, we can generalise the concepts of eigen-vectors to eigen-functions and obtain a similar decomposition. In the following, we try to discuss the physical interpretation of eigenvalues and eigenvectors, first in finite-dimensional spaces, and later in infinite-dimensional spaces.

We define the **eigen-function** or **eigen-state** (*fonction propre* in french) $\psi_n(x)$ of the operator $\hat{A}$, associated to the **eigen-value** a_n to be the function $\psi_n(x)$ (that is not zero everywhere) such that

$$\hat{A}\psi_n(x) = a_n\psi_n(x), \tag{19}$$

meaning that the operator $\hat{A}$ does not modify the state ψ_n other than multiplying it by a scalar. If every an eigenvalue corresponds to only one eigenfunction we say that it is **not degenerate**, otherwise we say that the eigenvalue is **degenerate**.

Spectral theorem (discrete version) : Given an operator $\hat{A}$, the operator can be diagonalised in an orthonormal basis such that

$$\hat{A}\psi_n(x) = a_n\psi_n(x), \tag{20}$$

If the spectrum is not degenerate, meaning that if $a_i \neq a_j$ for all i, j, then eigenvectors are orthonormal. If the spectrum is degenerate, the theorem is slightly more complex, but eigenvectors corresponding to different eigenvalues are still ortoghonal.

This theorem is only valid for discrete spaces. A version valid in infinite spaces exists, but to properly discuss it you'd need to know distribution theory. So we'll just say that for the operators we'll be working for now this is also valid.

Expectation value of an eigenstate: The expectation value of an operator $\hat{A}$ over a state that is an eigen-state ψ_n of the operator is trivially a_n. This can be easily proven by showing that:

$$\langle\psi_n|\hat{A}|\psi_n\rangle = \langle\psi_n| a_n |\psi_n\rangle = a_n \langle\psi_n|\psi_n\rangle = a_n. \tag{21}$$

As the expectation value of self-adjoint operators must be real, it follows that the spectrum of self-adjoint (or hermitian) operators must be real.

Note: This decomposition is in principle only valid in finite-dimensional spaces, but a very closely-related decomposition is valid in infinite-dimensional spaces as well. For the time being we will assume that the decomposition is valid in both cases, whether n labels a discrete basis or a continuous one.

1.5.1 Excercise: Eigendecomposition of the momentum operator

What are the eigenvalues of the momentum operator? We recall the definition

$$\hat{p}_x = -i\hbar\frac{d}{dx}$$

and to find its eigenvalues we can simply start from the eigenvalue equation, then substitute the definition of the operator

$$\begin{aligned}\hat{p}_x\psi(x) &= p\psi(x)\\ -i\hbar\frac{d\psi(x)}{dx} &= p\psi(x)\end{aligned}$$

(note that $\hat{p}$ is the operator, while p is a real valued scalar that indicates an eigenvalue) this way I obtain a standard first order differential equation

$$\frac{d\psi(x)}{dx} = i\frac{p}{\hbar}\psi(x)$$

which is solved by separation of variables finding the usual plane wave solution

$$\psi(x) = \psi_0 \exp\Big[i\frac{p}{\hbar}x\Big].$$

This means that plane-waves are the eigenstates ψ_p of the momentum operator $\hat{p}$, each with eigenvalue p.

Interpretation of the Fourier Transform: from this result, it follows that we can interpret the Fouerier transform

$$\psi(x) = \int \phi(p) \exp\Big[i\frac{p}{\hbar}x\Big] dp \tag{22}$$

as the decomposition of a wave-function $\psi(x)$ onto the eigen-basis of the momentum operator.

1.6 The Schroedinger's Equation for a generic system

Until now you we have considered the Schroedinger's equation of a particle in free space

$$\frac{d\psi(x,t)}{dt} = -\frac{i}{\hbar}\frac{\hat{p}^2}{2m}\psi(x),$$

If you notice that $p^2/2m$ has the dimensions of an energy and is nothing other than the kinetic energy, it is natural to **postulate** that when in presence of a potential the wavefunction must evolve according to

$$\frac{d\psi(x,t)}{dt} = -\frac{i}{\hbar}\left(\frac{\hat{p}^2}{2m} + V(x)\right)\psi(x) \tag{23}$$

$$\frac{d\psi(x,t)}{dt} = -\frac{i}{\hbar}\hat{H}\psi(x) \tag{24}$$

$$\tag{25}$$

where we have implicitly defined the **Hamiltonian operator** whose expectation value is associated to the energy of the system.

The eigenvalue equation for an Hamiltonian operator which does not depend on time is also known as the **time-independent Schroedinger's equation**, and it is defined by

$$\hat{H}\psi_n(x) = E_n\psi_n(x) \tag{26}$$

which can be rewritten by inserting the definition of the hamiltonian operator obtaining,

$$\left(\frac{\hat{p}^2}{2m} + V(x)\right)\psi_n(x) = E_n\psi_n(x) \tag{27}$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi_n(x) = E_n\psi_n(x) \tag{28}$$

In general it is very hard to solve this equation analytically if not in some relatively simple cases:

- The Harmonic potential (a.k.a., the harmonic oscillator), which is solved by the Hermite Polynomials
- The Coulomb potential
- a step-constant potential

2 Exercises

2.1 Exercise 1: Eigenstate of the Hamiltonian

In the case of a system with a time-independent Hamiltonian $\hat{H}$, meaning that $\partial\hat{H}/dt = 0$, we consider the spectral decomposition of the hamiltonian such that

$$\hat{H}\psi_\alpha(\boldsymbol{x}) = E_\alpha\psi_\alpha(\boldsymbol{x}) \tag{29}$$

where α labels the eigenstates and eigenvalues.

Q1 The Hamiltonian $\hat{H}$ is a *linear operator* that is also *self-adjoint*. What is the definition of those two properties?

A linear map must respect the property:

$$\hat{A}(\alpha\psi + \beta\phi) = \alpha\hat{A}\psi + \beta\hat{A}\phi \tag{30}$$

the self-adjoint property is verified if

$$\langle\psi|A\phi\rangle = \langle\psi A|\phi\rangle \tag{31}$$

Q2 Prove that the eigenvalues of $\hat{H}$ are real, namely that $E_\alpha \in \mathbb{R}$.

Taking $\psi \equiv \psi_\alpha$ and assuming that eigenvalues are normalized

$$\left\langle\psi_\alpha\middle|\hat{H}\psi_\alpha\right\rangle = \int_{\mathbb{R}} \psi^\star_\alpha(x)E_\alpha\psi_\alpha(x)dx = E_\alpha\int_{\mathbb{R}}|\psi_\alpha|^2dx = E_\alpha$$

but also

$$\left\langle\psi_\alpha\hat{H}\middle|\psi_\alpha\right\rangle = \int_{\mathbb{R}} \psi^\star_\alpha(x)E^\star_\alpha\psi_\alpha(x)dx = E^\star_\alpha\int_{\mathbb{R}}|\psi_\alpha|^2dx = E^\star_\alpha$$

therefore according to the self-adjoint property we have

$$E_\alpha = E^\star_\alpha$$

meaning that $E_\alpha \in \mathbb{R}$.

Q3 If the state at time $t = 0$ is an eigenstate of the hamiltonian, meaning that if $\psi(\boldsymbol{x}, t = 0) = \psi_\alpha(\boldsymbol{x})$, write the expression for $\psi(\boldsymbol{x}, t)$ by solving Schroedinger's equation.

- If you can't find a solution, try a solution of the form $\psi(\boldsymbol{x}, t) = \phi(\boldsymbol{x})\chi(t)$ where ϕ is a time-independent term and χ depends only on time.

The Schroedinger equation is

$$\frac{d\psi(x,t)}{dt} = -\frac{i}{\hbar}\hat{H}\psi(x,t)$$

I take as an ansatz the solution of the form

$$\psi(x,t) = \psi_\alpha(x)\chi(t)$$

where I assume a part takes on the spatial dependency and is time independent, while the other is time-dependent but not space-dependent. Plugging this into the Schroedinger's equation we obtain

$$\psi_\alpha(x)\frac{d\chi(t)}{dt} = -\frac{i}{\hbar}\chi(t)\hat{H}\psi_\alpha(x)$$
$$\psi_\alpha(x)\frac{d\chi(t)}{dt} = -\frac{i}{\hbar}\chi(t)E_\alpha\psi_\alpha(x)$$

meaning that we must verify

$$\frac{d\chi(t)}{dt} = -\frac{i}{\hbar}\chi(t)E_\alpha$$

and by separation of variable we can solve this integral finding

$$\chi(t) = \chi(0)\exp\left[-i\frac{E_\alpha}{\hbar}t\right]$$

and as the initial condition was $\psi(x, t = 0) = \psi_\alpha(x)$ we take $\chi(0) = 1$ and obtain the solution

$$\psi_\alpha(x,t) = \exp\left[-i\frac{E_\alpha}{\hbar}t\right]\psi_\alpha(x)$$

which will be valid for all x

Q4 Does the probability density $|\psi(\boldsymbol{x},t)|^2$ depend on the time?

The probability density for the state $\psi_\alpha(x,t)$ rotates with a complex phase which cancels out if we square it, therefore

$$|\psi_\alpha(x,t)|^2 = |\psi_\alpha(x)|^2$$

which does not depend on time.

Q5 Does the expectation value of a time-independent operator $\hat{A}$, computed for the $\psi(\boldsymbol{x},t)$ state obtained in Q3, depend on the time? Can you comment why?

Using the results from the following points we find that

$$\begin{aligned}\left\langle \hat{A}\right\rangle_{\psi_\alpha(t)} &= \langle\psi_\alpha(t)|\, A\psi_\alpha(t) = \int_{\mathbb{R}} \exp\left[i\frac{E_\alpha}{\hbar}t\right]\psi_\alpha^\star(x)\hat{A}\exp\left[-i\frac{E_\alpha}{\hbar}t\right]\psi_\alpha(x)dx \\ &= \int_{\mathbb{R}} \psi_\alpha^\star(x)\hat{A}\psi_\alpha(x)dx \\ &= \langle\psi_\alpha(t=0)|\hat{A}|\psi_\alpha(t=0)\rangle\end{aligned}$$

so expectation values are time-independent.

The underlying reason is that, if ψ is an eigenstate of the Hamiltonian, the action of the Hamiltonian on the state does not modify the vector, but merely give it a phase dependent on the eigenenergy. However, the phase is not observable.

Q6 Try to generalise the previous result to a superposition of eigenstates: assuming that

$$\psi(\boldsymbol{x}, t=0) = \sum_\alpha c_\alpha \psi_\alpha(\boldsymbol{x}) \tag{32}$$

such that $\sum_\alpha |c_\alpha|^2 = 1$, what is the form of $\psi(\boldsymbol{x}, t)$? (hint: use the linearity property starting from the solution of the previous question).

Because of linearity, the general solution will be a linear combination of the eigenstates of the Hamiltonian

$$\psi(x,t) = \sum_\alpha c_\alpha \exp\left[-i\frac{E_\alpha}{\hbar}t\right]\psi_\alpha(x)$$

Do notice that if we take $\hat{H} = \frac{\hat{p}^2}{2m}$, meaning the hamiltonian in free space without any potential, the eigenstates are plane waves and therefore we are back to the case studied in PC2. This, however, is more general, as will be valid also for arbitrary potentitals. We just need to find the eigenstates of the Hamiltonian.

Q7 What is the expression of the expectation value of the energy $\langle H\rangle(t)$ as a function of time? Can you comment on this result?

By applying the definition of the expectation value,

$$\begin{aligned}
\langle H\rangle(t) &= \sum_{\alpha,\beta}\int_{\mathbb{R}}\left(c_\alpha^\star \exp\left[i\frac{E_\alpha}{\hbar}t\right]\psi_\alpha^\star(x)\right)\hat{H}\left(c_\beta \exp\left[-i\frac{E_\beta}{\hbar}t\right]\psi_\beta(x)\right)dx \\
&= \sum_{\alpha,\beta}\left(c_\alpha^\star c_\beta \exp\left[i\frac{E_\alpha - E_\beta}{\hbar}t\right]\right)\int_{\mathbb{R}}\psi_\alpha^\star(x)\hat{H}\psi_\beta(x)dx \\
&= \sum_{\alpha,\beta}\left(c_\alpha^\star c_\beta \exp\left[i\frac{E_\alpha - E_\beta}{\hbar}t\right]\right)E_\beta\int_{\mathbb{R}}\psi_\alpha^\star(x)\psi_\beta(x)dx \\
&= \sum_{\alpha,\beta}\left(c_\alpha^\star c_\beta \exp\left[i\frac{E_\alpha - E_\beta}{\hbar}t\right]\right)E_\beta\langle\psi_\alpha|\psi_\beta\rangle
\end{aligned}$$

where in the last line I have applied the eigenvalue equation of the Hamiltonian. Now, we know that the eigenbasis of the hamiltonian is orthogonal, therefore

$$\langle\psi_\alpha|\psi_\beta\rangle = \delta_{\alpha,\beta} = \begin{cases}1 & \text{if } \alpha=\beta \\ 0 & \text{if } \alpha\neq\beta\end{cases}$$

where we call the $\delta_{\alpha,\beta}$ a Kronecker delta. Plugging this into the previous equation we obtain

$$\begin{aligned}\langle H\rangle(t) &= \sum_{\alpha,\beta}\left(c_\alpha^\star c_\beta \exp\left[i\frac{E_\alpha - E_\beta}{\hbar}t\right]\right)E_\beta\delta_{\alpha,\beta}\\ &= \sum_{\alpha}\left(c_\alpha^\star c_\alpha \exp\left[i\frac{E_\alpha - E_\alpha}{\hbar}t\right]\right)E_\alpha\\ &= \sum_\alpha |c_\alpha|^2 E_\alpha\\ &= \langle H\rangle(t=0)\end{aligned}$$

which is the expectation value on the initial state at $t = 0$ (as it is time-independent). This proves that the energy is conserved by the evolution according to the Schroedinger's equation.

Q8 Try to derive the same result of Q6 but without using the solution of a single eigenstate. Instead, assume that

$$\psi(x,t) = \sum_\alpha c_\alpha(t)\psi_\alpha(\boldsymbol{x}). \tag{33}$$

What differential equation do the coefficients $c_\alpha(t)$ have to obey? Prove that the solution you find is formally equivalent to

$$\psi(x,t) = \exp\left[-i\hat{H}t/\hbar\right]\psi(x,0), \tag{34}$$

(if you don't understand what the exponential of an operator is, try to replace the exponential with it's Taylor series, and see what happens)

2.2 Exercise 2: Step-constant Potential

We consider a particle of mass m moving in a 1-Dimensional space. A potential $V(x)$ affects the particle, where

$$V(x) = \begin{cases}0 & \text{if} \quad x < a\\ V_0 & \quad x \geq 0\end{cases} \tag{35}$$

where $V_0 \in \mathbb{R}^{>0}$. We will look at eigenstates $\psi_\alpha(x)$ of the Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x) \tag{36}$$

such that their eigenenergies will be $E_\alpha > 0$.

Q1 Show that the general solution to the time-independent Schroedinger's Equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\psi(x) \tag{37}$$

in the case where the energy of the particle is lower than the potential step, meaning that $E < V_0$, is

$$\psi(x) = \begin{cases}A_1 e^{ikx} + A_1' e^{-ikx} & \text{if} \quad x < 0\\ A_2 e^{-Kx} + A_2' e^{Kx} & \text{if} \quad x \geq 0\end{cases} \tag{38}$$

where $A_1, A_2, A'_1, A'_2 \in \mathbb{C}$ and $k, K \in \mathbb{R}^{>}$. Also find the expression for k and K. Try to give an intuitive explanation of what the four terms represent. (hint: if you consider only $x < 0$, $V(x)$ becomes a constant and you can write a solution in this interval, and the same is true in the other interval...)

Schroedinger's equation in a region where the potential is constant ($V(x) \equiv V$) is equivalent to

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = (E - V)\psi(x)$$

which has the same form of the one we studied in PC2 and we know is solved by a superposition of plane-waves. The solution is therefore

$$\psi(x) = Ae^{ikx} + A'e^{-ikx}$$

where $k = \sqrt{2m(E-V)}/\hbar$ and the solution is only valid in the region of constant potential.

If we have two regions of constant potential we can write

$$\psi(x) = \begin{cases} A_1 e^{ikx} + A'_1 e^{-ikx} & \text{if} \quad x < 0 \\ A_2 e^{ik'x} + A'_2 e^{-ik'x} & \text{if} \quad x \geq 0 \end{cases}$$

where $k = \sqrt{2m(E-0)}/\hbar = \sqrt{2mE}/\hbar$ and $k' = \sqrt{2m(E-V_0)}/\hbar$ and A_i are complex constants.

The problem asks us to consider the case where $E < V_0$, therefore

$$(E - V_0) < 0$$

and k' will be a purely imaginary number. We therefore define $k' = iK$ where $K = \sqrt{2m(V_0 - E)}/\hbar$ where K is now a real number. Substituting K into the expression for $\psi(x)$ we find

$$\psi(x) = \begin{cases} A_1 e^{ikx} + A'_1 e^{-ikx} & \text{if} \quad x < 0 \\ A_2 e^{-Kx} + A'_2 e^{Kx} & \text{if} \quad x \geq 0 \end{cases}$$

Q2 Based on the requirement of physicality of the solution (in this case, finite normalisation) what can you say about A_2 remembering that $E < V_0$? Why?

A solution to the time-dependent Schroedinger's equaiton will be a superposition of different plane waves like the ones shown above. However, if we take the limit for $x \to \infty$ we have that $\psi(x) \propto A'_2 \cdot \infty$ because of the diverging integral.

Instead, in the limit $x \to -\infty$ we have a constant amplitude.

For that reason, we will impose that $A'_2 = 0$.

In another terms, you can think that $|A_1|^2$ is the energy density coming from the left, $|A'_1|^2$ is the reflected energy density, and

$$|A_2|^2$$

is the energy coming from the right. But if we assume that $E < V_0$ there cannot be any energy coming from the right otherwise we'd have an energy higher than V_0.

Q3 If we require continuity of $\psi(x)$ and its first derivative at $x = 0$, what are the conditions that we must impose? Comment on the number of conditions and free variables.

We must ask that

$$\lim_{\epsilon \to 0} \left(\psi(x-\epsilon) = \psi(x+\epsilon)\right)$$
$$\lim_{\epsilon \to 0} \left(\frac{d\psi}{dx}(x-\epsilon) = \frac{d\psi}{dx}(x+\epsilon)\right)$$

which translates to

$$A_1 + A_1' = A_2$$
$$ikA_1 - ikA_1' = -KA_2$$

Q4 Take $A_1 = 1$ to be the normalisation of the incoming wave. And compute an expression for A_1', the reflected amplitude.

I will do the calculation without $A_1 = 1$ and instead try to find a ratio

$$A_1 + A_1' = A_2$$
$$ikA_1 - ikA_1' = -KA_2$$

we get

$$ikA_1 - ikA_1' = -KA_1 - KA_1'$$

giving

$$A_1(ik + K) = A_1'(ik - K)$$

giving

$$\frac{A_1'}{A_1} = \frac{ik + K}{ik - K}$$

and multiplying and dividing by $-i$ we get

$$\frac{A_1'}{A_1} = \frac{k - iK}{k + iK}$$

Q5 Compute the Reflected amplitude $R = |A_1'|^2$. Is this result consistent with classical mechanics?

Taking the definition

$$R = \left|\frac{A_1'}{A_1}\right|^2 = \left|\frac{k - iK}{k + iK}\right|^2 = \frac{k^2 + K^2}{k - K^2} = 1$$

We could also compute the Transmitted amplitude $T = 1 - R = 0$. This means that like in the classical case all power is reflected, even if we can measure the particle *inside* the potentital barrier in an expoenntially small interval proprtional to K^{-1}.

Q6 Discuss the wavefunction amplitude for $x > 0$ and for $x < 0$ in the limit of $\hbar \to 0$ and $m \to \infty$. What limit is this?

In the limit of $x < 0$ we have that the wave-function is solely described by the plane wave with amplitude A_1'. For $x > 0$ we have an exponentially small probability amplitude of detecting the particle inside the step (or forbidden region) where the length is determined by $L = K^{-1} \propto \hbar$ and therefore in the classical limit $\hbar \to 0$ we find that there is no "evanescent wave".

2.2.1 $E > V_0$ case

In the following we will now consider the case where $E > V_0$.

Q7 Show that the solution in this case has the form

$$\psi(x) = \begin{cases} A_1 e^{ikx} + A_1' e^{-ikx} & \text{if} \quad x < 0 \\ A_2 e^{ik'x} \quad \text{if} \quad x \geq 0 \end{cases} \tag{39}$$

can you give an intuitive explanation of why, given the problem description (a particle incoming from $x = -\infty$) we don't have a term $A_2' e^{-ik'x}$ for $x \geq 0$?

The proof is identical to before, but now $k' = \sqrt{2m(E - V_0)}/\hbar$ is real. We take $A_2' = 0$ because we assume that the particle is incoming from the left.

Q8 Set $A_1 = 1$. Compute the reflected amplitude A_1' and the transmission amplitued A_2', as well as the reflection and transmission probabilities $|A_1'|^2$ and $|A_2|^2$.

I will do the calculation without $A_1 = 1$ and instead try to find a ratio

$$A_1 + A_1' = A_2$$
$$ikA_1 - ikA_1' = ik'A_2$$

we get

$$ikA_1 - ikA_1' = ik'A_1 + ik'A_1'$$

and manipulating we get

$$A_1(ik - ik') = A_1'(ik + ik')$$

leading to

$$\frac{A_1'}{A_1} = \frac{k-k'}{k+k'}$$

and

$$\frac{A_2}{A_1} = \frac{A_1 + A_1'}{A_1} = 1 + \frac{k-k'}{k+k'} = \frac{2k}{k+k'}$$

From this we can compute the reflected and transmitted amplitudes which we can easily see are never 0 or 1

Q9 Is the result computed at the last question consistent with classical mechanics? What happens in the limit $\hbar \to 0$?

We can easily see that $\hbar$ disappears from the equations and therefore this result is independent of $\hbar$. Therefore this result is not consistent with Classical mechanics in the limit of $\hbar \to 0$.

This is due to the discontinuity at 0, and if we were to use a continuous potential, we would find a consistent result.

2.3 Exercise 3: Tunnel effect

We consider a particle of mass m moving in a 1-Dimensional space. A potential $V(x)$ affects the particle, where

$$V(x) = \begin{cases} V_0 & \text{if} \quad 0 < x < a \\ 0 & \text{otherwise} \end{cases} \tag{40}$$

and we consider $E < V_0$.

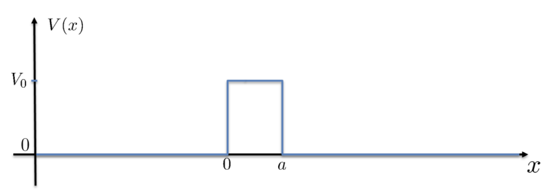

Figure 1: Sketch of the tunnel potential

Q1 Show that the solution to the time-independent schroedinger's equation can be written in the form

$$\psi(x) = \begin{cases} \alpha e^{ikx} + \beta e^{-ikx} & \text{if} \quad x < 0 \\ \gamma e^{Kx} + \delta e^{-Kx} & \text{if} \quad 0 \le x < a \\ \chi e^{ikx} & \text{if} \quad x \ge a \end{cases} \tag{41}$$

where $\alpha, \beta, \gamma, \delta, \chi \in \mathbb{C}$ and $K \in \mathbb{R}^{>0}$. Remember that $k = \frac{p}{\hbar}$.

Same reasoning as before. We have $k = \sqrt{2mE/\hbar}$ and $K = \sqrt{2m(V_0 - E)}/\hbar$.

Q2 Write down the continuity conditions for $\alpha, \beta, \gamma, \delta, \chi, K$ at the points $x = (0, a)$ to ensure that the wave-function and its first derivative are continuous.

$$\begin{cases} \alpha + \beta = \gamma + \delta \\ ik(\alpha - \beta) = K(\gamma - \delta) \\ \gamma e^{Ka} + \delta e^{Ka} = \chi e^{ika} \\ K(\gamma e^{Ka} - \delta e^{Ka}) = ik\chi e^{ika} \end{cases}$$

where the first two correspond to the continuity conditions in $x = 0$ and the last two to the conditions in $x = a$.

Q3 Assuming from the last point that

$$\chi = \frac{4ikKe^{-ika}}{(k + iK)^2 e^{Ka} - (k - iK)^2 e^{-Ka}}, \tag{42}$$

gives an expression for the transmission coefficient $T = |\chi|^2$, and show that if $Ka \gg 1$ we can approximate it with:

$$T = \frac{4E(V_0 - E)}{4E(V_0 - E) + V_0^2 \sinh^2(Ka)} \tag{43}$$

$$\approx \frac{16E}{V_0^2}(V_0 - E)e^{-2Ka}. \tag{44}$$

What experssion would have you expected in the case of a classical potential? What has changed?

From a classical calculation we would have expected that the transmitted power be an heavy-side theta $\theta(V_0 - E)$. In quantum mechanics, instead, we have an exponentially suppressed evanescent wave of length K^{-1} which crosses the potential barrier.

2.4 Exercise 4: The tunnel-effect microscope

A scanning tunneling microscope (STM) is a type of microscope used for imaging surfaces at the atomic level. Its development in 1981 earned its inventors, Gerd Binnig and Heinrich Rohrer, then at IBM Zurich, the Nobel Prize in Physics in 1986. STM senses the surface by measuring the current between an extremely sharp conducting tip and the surface of a material. While the tip does not touch the material, the tunnel effect guarantees a small flow of electrons (a current) which can be measured and therefore used to estimate the distance between the surface and the tip. By moving the tip along the x-y plane with high accuracy, the STM can distinguish features smaller than 0.1 nm with a 0.01 nm (10 pm) depth resolution.

We suppose that the tunneling current is proportional to the transmission factor given by eq. (43).

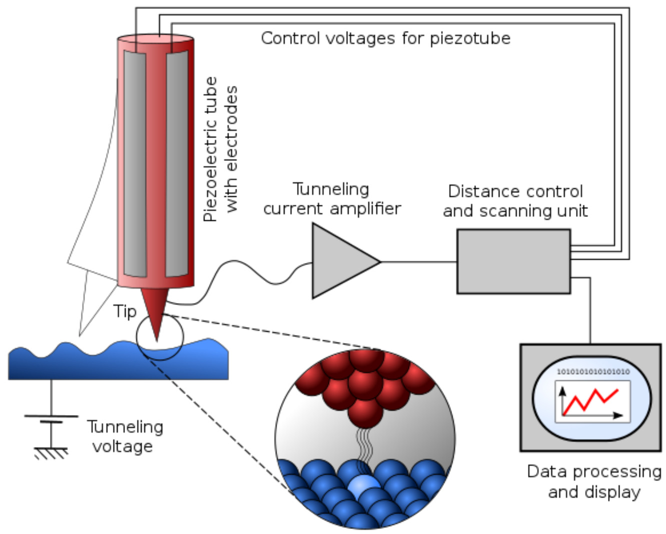

Figure 2: Schematic diagram of a STM.

Q1 We supposed that we want to keep fixed the tunneling current while we move along the x-y axis. Explain how the instrument can be used to measure the distance between the tip and the surface.

The tunneling current will be proportional to T. Assuming that we are in the vacuum and the potential barrier V_0 cannot be changed we can only move the tip distance a to keep the current constant.

Q2 If $E = 2eV$ and the tunneling barrier is $V_0 = 3eV$ compute the value of T for $a = 1nm$ and $a = 0.5nm$.

using $m_e = 9.1 \cdot 10^{-31}$ Kg, $\hbar = 1.05 \cdot 10^{-34}$ and $1eV = 1.6 \cdot 10^{-19}$ we can compute

$$K = \frac{\sqrt{2(9.1 \cdot 10^{-31} Kg)(1.6 \cdot 10^{-19} J)}}{1.05 \cdot 10^{-34} Js} \approx 5.1 \cdot 10^{9} m^{-1}$$

so $Ka = 2.6$ so the approximate formula is not extraordinarly good and we have to use the original formula. Plugging numbers inside we find

$$T \approx 10^{-4} \quad \text{for} \quad a = 1nm$$
$$T \approx 10^{-2} \quad \text{for} \quad a = 0.5nm$$

Q3 **Platform $9\frac{3}{4}$-tunneling effect:** we suppose that a magician named Harry Potter is a quantum particle weighting about 50kg and running at $3m/s$ against the wall enclosing train platform 10, described as a potential barrier 2 meters high and $0.5m$ thick.

- What is the probability that Harry makes it to his train?
- Now, assume that Harry is not a single quantum particle but is a composite object made up of $N_a \approx 10^{23}$ quantum particles. What is the probability that all the particles tunnel through the wall together?

We take the potentital barrier to be $U = mg\text{height} = 50 \cdot 9.8 \cdot 2 = 980J$. K is then

$$K = \frac{\sqrt{2 \cdot 50 \cdot 980}}{1.05 \cdot 10^{-34}} \approx 3 \cdot 10^{36} m^{-1}$$

so $Ka \gg 1$. The kinetic energy of Harry is $1\frac{1}{2}mv^2 = 225J$, therefore T

$$T = \frac{16(980 - 225)}{980^2} \exp\left[-2 \cdot 10^{36}\right] \approx \exp\left[-10^{36}\right]$$

which is abysmally small.tun
