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Personal Notes
Internship under Dr Aparna Deshpande
Indian Institute of Science Education and Research

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1 Introduction

I have joined Dr Aparna Deshpande's lab for my summer internship May 2025. Her group researches on 2-D materials using the experimental techniques called Scanning Tunneling Microscopy (STM) and Atomic Force Microscopy (AFM). As my first assignment she asked me to go through a Reference Text called "Introduction to Scanning Tunneling Microscopy " by C Julian Chen. These are personal Notes/Diary I have written, while I am in her lab.

2 Notes from Chapter 2: "Principles"

I have gone through Bardeen's theory of tunneling and now have a basic understanding of the formalism. However, I still struggle with some of the mathematical steps—especially certain algebraic manipulations and approximations that appear during the derivation of the tunneling matrix element.

Since I am more inclined toward the experimental aspects of STM, I can manage without fully mastering every mathematical detail. That said, it is still essential to understand the physical meaning of each term** and the insight the formalism provides. Unlike the abstract study of quantum mechanics, the utility here is practical: understanding what the math is telling us about the tunneling process.

What Does the Tunneling Matrix Element Tell Us?

After working through the mathematics of the tunneling matrix elements, I found that simply reaching the final expression wasn't giving me much intuition. Here's the central formula

derived in Bardeen's approach:

$$M_{\mu\nu} = \frac{\hbar^2}{2m} \int_S \left(\psi_\mu^* \nabla \psi_\nu - \psi_\nu \nabla \psi_\mu^* \right) \cdot d\mathbf{S} \tag{1}$$

This integral is evaluated over a surface S located in the vacuum region between the tip and the sample. The matrix element $M_{\mu\nu}$ represents the tunneling amplitude from a state ψ_μ on one side (e.g., the tip) to a state ψ_ν on the other side (e.g., the sample).

Understanding this expression in terms of **wavefunction overlap** and **gradient matching** at the interface is critical for gaining physical insight. This matrix element is directly related to the tunneling current through Fermi's golden rule and forms the basis of the Tersoff–Hamann model and other approximations used in STM theory.

So in order understand I found some problems and solutions from the internet which I found reasonable and simple to suffice.

Problem Statement

Two wavefunctions near a flat vacuum interface at $z = 0$ are given by:

$$\psi_L(\mathbf{r}) = Ae^{-\kappa z}, \qquad \psi_R(\mathbf{r}) = Be^{\kappa z}, \quad \text{for } z < 0.$$

Evaluate the tunneling matrix element M_{LR} using Bardeen's formula:

$$M_{LR} = \frac{\hbar^2}{2m} \int_S \left(\psi_L^* \nabla \psi_R - \psi_R \nabla \psi_L^* \right) \cdot d\mathbf{S}$$

where the integral is taken over the plane $z = 0$, and amplitudes are assumed constant over the x-y surface.

Step-by-Step Solution

1. At $z = 0$:
$$\psi_L^* = A^*, \quad \nabla \psi_R = \hat{z}\kappa B, \quad \psi_R = B, \quad \nabla \psi_L^* = -\hat{z}\kappa A^*.$$

2. Substituting into Bardeen's expression:

$$M_{LR} = \frac{\hbar^2}{2m} \int_S \left[A^*(\kappa B) - B(-\kappa A^*) \right] \cdot \hat{z} \cdot d\mathbf{S}$$

$$= \frac{\hbar^2}{2m} \int_S 2\kappa A^* B \, dS = \frac{\hbar^2 \kappa}{m} A^* B \int_S dS$$

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3. If the surface area is S, then:

$$M_{LR} = \frac{\hbar^2 \kappa}{m} A^* B S$$

Matrix Representation of States

Suppose we define several orthonormal wavefunctions $\psi_L^{(i)}$ on the tip side and $\psi_R^{(j)}$ on the sample side. Then we can define a matrix $\mathbf{M}$ whose elements are:

$$M_{ij} = \frac{\hbar^2}{2m} \int_S \left(\psi_L^{(i)*} \nabla \psi_R^{(j)} - \psi_R^{(j)} \nabla \psi_L^{(i)*} \right) \cdot d\mathbf{S}$$

if we consider two states on each side, we get:

$$\mathbf{M} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}$$

Each element represents the tunneling amplitude from a specific tip state i to a specific sample state j.

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Physical Meaning of the Tunneling Matrix

The matrix $\mathbf{M}$ describes how different quantum states on the tip overlap and connect to those on the sample across the vacuum barrier. The larger the absolute value $|M_{ij}|$, the more likely an electron tunnels from state i on the tip to state j on the sample.

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What Do We Mean by "States" in STM?

Let us now consider a real STM setup with:

- **Tip material:** Tungsten (W)

- **Sample material:** Silicon (Si)

In this context:

- A **state** on the **tip** (W) could be a localized atomic orbital such as d_{z^2}, s, or d_{xz} centered at the apex atom.

- A **state** on the **sample** (Si) could be a surface state such as a dangling bond, a reconstructed band, or a conduction band orbital localized near the surface.

For example:

$$\psi_L^{(1)} \rightarrow d_{z^2} \text{ orbital of the W apex atom} \qquad \psi_R^{(1)} \rightarrow \text{dangling bond on the Si surface}$$

The element M_{11} in this context gives the tunneling amplitude between these two specific states.

Will think about it in much detail later.

3 The First Weekly Meeting 22 May

A short meeting, where she asked me some questions about the topics that I have covered. Those questions weren't that tricky nor complex—just a set of very basic questions for a student doing a Master's. But not surprisingly, I was blank as a new book. Nothing not even a word that made sense came out of my mind. She asked me,

"How do you define the wavelength of an electron which is initially known for its particle properties?"

Now, the question is very basic, but what happened was, I panicked. The simplest answer didn't appear in my stupid brain. I was so embarrassed in front of her. Her silence killed me. I lost all my confidence.

The Question and Answer:

So how do we define the wavelength of a particle?

To answer it, I would start from the Photoelectric Effect. Now, we found out we, as in our civilization—that light, which was initially known for its wave properties, suddenly started to behave like a particle, and the expression

$$E = h\nu$$

came into existence. From special relativity, we also know the expression for the energy of a particle moving near the speed of light.

Start from Planck's energy-frequency relation:

$$E = h\nu = \hbar\omega$$

For a photon (light), the frequency is related to the wavelength by:

$$\nu = \frac{c}{\lambda} \quad \Rightarrow \quad E = \frac{hc}{\lambda}$$

Now consider the relativistic energy-momentum relation:

$$E^2 = p^2c^2 + m^2c^4$$

For a photon, the rest mass is zero $(m = 0)$, so the equation simplifies to:

$$E^2 = p^2c^2 \quad \Rightarrow \quad p = \frac{E}{c}$$

Substitute $E = \frac{hc}{\lambda}$:

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

Using the identity $h = 2\pi\hbar$, we get:

$$p = \frac{2\pi\hbar}{\lambda}$$

Alternatively, if the angular wave number $k = \frac{2\pi}{\lambda}$, then:

$$p = \hbar k \quad \Rightarrow \quad \boxed{p = \frac{\hbar}{\lambda}}$$

The most interesting thing about this is that we just defined a particle property—momentum: mass times velocity—for an entity that has zero rest mass. Thanks to special relativity. Now we address the question: can we define a wave property like a wavelength for a particle—or more specifically, what is the wavelength of an electron? So I don't really know how exactly this happened historically—in the sense of what the exact chronology of events was—but my best guess would be that we took the same expression of momentum and wavelength from the previous derivation and simply applied it to the electron. Then we relied on experiment for confirmation. Other than that, I don't really think there is a theoretical way to understand it—at least I don't know about it so far.Now, what would be the wavelength of the electron, which is fundamentally thought of as pure matter?

Derivation of de Broglie Wavelength for an Electron

To derive the **de Broglie wavelength** of an electron (or any particle), we begin with the idea that particles can exhibit wave-like behavior, as proposed by Louis de Broglie.

Step 1: Start with Planck's relation for photons

From quantum theory (as seen in the photoelectric effect):

$$E = h\nu = \hbar\omega$$

Also, from the theory of relativity, the energy of a photon is related to its momentum:

$$E = pc \quad \Rightarrow \quad p = \frac{E}{c}$$

Since for photons:

$$\nu = \frac{c}{\lambda} \quad \Rightarrow \quad E = \frac{hc}{\lambda}$$

Substitute this into the expression for momentum:

$$p = \frac{E}{c} = \frac{hc/\lambda}{c} = \frac{h}{\lambda} \quad \Rightarrow \quad \boxed{\lambda = \frac{h}{p}}$$

Louis de Broglie hypothesized that this relation should hold not just for photons but for all matter particles.

Step 2: Apply to an Electron

For an electron of mass m moving with velocity v, the classical (non-relativistic) momentum is:

$$p = mv$$

Substitute into de Broglie's relation:

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

Hence, the **de Broglie wavelength** of an electron (non-relativistic case) is:

$$\boxed{\lambda = \frac{h}{mv}}$$

Relativistic Case

For high-speed electrons (relativistic), the momentum is given by:

$$p = \gamma m v = \frac{mv}{\sqrt{1 - \frac{v^2}{c^2}}}$$

Substitute this into de Broglie's relation:

$$\lambda = \frac{h}{p} = \frac{h}{\gamma m v}$$

So, the de Broglie wavelength for a relativistic electron becomes:

$$\boxed{\lambda = \frac{h}{\gamma m v}}$$

Of course, this is not a rigorous math derivation or a formal derivation, but more than that, this is just a way of representing certain ideas. The idea somehow is clear, and it's elegant too. For a completely wave like light, we defined a quantity which is completely of a particle. For a completely particle like electron, we just defined a completely wave quantity. When I say completely wave and particle, what I am referring to here is the previously known nature of the light or electron. From here, I might want to stop and think about the second question she asked: *"Why not use light to see atoms?"* You might think it would be easy to answer, but going a little deeper, it's actually hard, trust me.

Let that thought float around in your mind. Let's think about diffraction, since light and optics are now in the background. So, what is the necessary condition for diffraction to take place? I answered this one quickly: the slit width should be comparable to the wavelength of the light we are using.I've created this single slit diffraction setup, taken photographs, and even posted them on my LinkedIn page. Well, since we said that an electron, a matter particle, is also a wave and has a wavelength defined, what if we make a slit whose size is comparable to the wavelength of the incoming electron? Should we get a diffraction pattern? Apparently, yes! **Eureka!** That means we defined the wavelength correctly. How it is a wave, and so on that's philosophical, and I don't wanna go there. Anyway, our attempt to define the wavelength was a success. Now coming to the real question she asked: *"Why not use light to see the atoms?"*

Habits she asked me to develop

Apart from sticking to the core subject discussion, she asked me several other general questions. She wanted to know whether I have an exposure to journals, articles, and science magazines. Knowing that I have no habit of reading science articles or publications, she introduced me to some article publishing websites like IOP, ACS, APS, Science.org, Nature, ScienceNews.org, etc. The amazing thing I noticed about her is that she took my note and wrote the entire thing on my page. Thinking that she is ruining the page, she even asked me whether it's okay to write there. Also a new book is introduced to me and asked me to

read it parrallely. That one was " Scanning Probe Microscopy" by Bert Voigtländer. Those notes will be added to these diary too.

Additionally she wanted me to get a thorough understanding of two theories, W K B Approximation and Fowler Nordhein Tunneling / Field emission.

4   WKB Approximation

Of course, it is an approximation technique — but what kind?

Let's say we have a potential defined, and of course, we have our holy grail, the Schrödinger equation, which is again a differential equation just like Newton's second law. If solved, we will get the equation of motion. Now, the thing about differential equations is that they are so freaking hard to solve. There are only a limited number of differential equations that we can solve. Well, in other words, if we have a very straightforward potential defined for our particle, we have a chance of solving that differential equation and having a solution. On the other hand, if we have some weird-shaped potential—which would be more common because the universe loves complexity—it won't be that easy to solve the Schrödinger equation. It feels like, at the end of the day, physics is ultimately solving differential equations in different ways. Anyway, WKB is a special type of approximation that can be used to solve the Schrödinger equation for a very specific kind of potential. It's not a general trick or recipe to cook your solution right. Let's just put it here—no suspense—what kind of potentials are WKB-friendly? I'm just going to state that claim and will prove it later on. So, a potential that is slowly varying compared to the wavelength of the subject particle is the kind of potential that is WKB-friendly. For now, ignore the "compared to the wavelength of the particle" part and focus more on the slowly varying part. Let that thought be there—pin it. Now let's write the Schrödinger wave equation in momentum representation:

$$\hat{p}^2\psi(x) = p^2(x)\psi(x), \quad \text{where} \quad p^2(x) = 2m\big(E - V(x)\big). \tag{2}$$

Again, I love math and hate doing it, so this is not going to be a derivation, rather, well-framed arguments with the help of math. Now we need a potential to start with, and remember, it should be slowly varying. So what would be an extreme case of a slowly varying potential? Yep, a potential that is not varying at all. The slowest you can go on a bicycle is, well, not going anywhere at all. Sounds stupid, but it will work for my arguments, so moving on. We have a constant potential:

$$V(x) = V_0 \quad \text{(constant potential)} \tag{3}$$

and assume that

$$E > V_0. \tag{4}$$

Yes, classical region, I know. Why?? You will understand it in a bit. We well know that the solution will be in the form

$$\psi(x) = \exp\left(\frac{i}{\hbar}S(x)\right), \quad \text{where} \quad S(x) \in \mathbb{C}. \tag{5}$$

Free particle solution. Well, generally there is a plus or minus there; I am not putting it there for simplicity. Also, the reason for allowing $S(x)$ to be complex is to avoid loss of generality. If $S(x)$ were restricted to be purely real, the wavefunction

$$\psi(x) = \exp\left(\frac{i}{\hbar}S(x)\right)$$

would describe only wavefunctions with constant amplitude (pure oscillations). However, allowing $S(x) \in \mathbb{C}$ captures both the phase oscillations and amplitude variations:

$$S(x) = S_R(x) + iS_I(x),$$

so that

$$\psi(x) = \exp\left(\frac{i}{\hbar}S_R(x)\right)\exp\left(-\frac{1}{\hbar}S_I(x)\right),$$

where $S_R(x)$ controls the phase and $S_I(x)$ controls the amplitude decay or growth. Thus, by not restricting $S(x)$ to be real, we retain the full generality in describing any physically possible wavefunction. Well, let us substitute

$$\psi(x) = \exp\left(\frac{i}{\hbar}S(x)\right) \tag{6}$$

into the Schrödinger equation, where the momentum operator is

$$\hat{p} = -i\hbar\frac{d}{dx}. \tag{7}$$

Some pretty straightforward algebra gives us:

$$(S'(x))^2 - i\hbar S''(x) = p^2(x). \tag{8}$$

Now we know the free particle solution ψ is in the form

$$\psi(x) = \exp\left(\frac{i}{\hbar}Px\right) \tag{9}$$

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Comparing this with equation (6), we get

$$S(x) = Px \tag{10}$$

Then,

$$S'(x) = P \tag{11}$$

Now comes the crux of the WKB approximation. Substitute $S(x) = Px$ into equation (8), and we find an interesting observation: the term

$$i\hbar S''(x) = 0 \tag{12}$$

What do we infer from this? Simply, if the defined potential for a given system is varying slowly enough, then the term

$$i\hbar S''(x) \tag{13}$$

will tend to zero.

But hold on, our potential was not slowly varying; it was not varying at all. Big difference? Well, yes. But even if we made the potential infinitesimally slowly varying, it is simply absurd to think that suddenly this term would become significantly large. We can say that the term which has the $\hbar$ order is the culprit. If we change the potential from constant to varying, that is the term responsible for making the solution different when the potential varies in space rather than being constant. So we can say that if the potential is not changing, the $\hbar$-order term would be zero. If the potential is slowly varying, then the $\hbar$ term is negligible. So it is safe to assume that

$$i\hbar S''(x) \tag{14}$$

is negligible. This is the approximation we are talking about. Okay, but how is it helpful? Before going into a solid example, I would like to discuss the same thing but from the view point of Griffith. He is undoubtedly one of the best authors you can rely on to solidify your foundation on Quantum Mechanics. The approach Griffith took is much more general. While the above one is a lot of arguments, Griffith's is a general derivation (although not rigorous), making it suitable for beginners like me. So going on, as usual, we have the holy grail, Schrödinger's wave equation. Let us re-write the equation so the momentum is visible to us.

$$\hat{p}^2\psi = p^2\psi \quad \text{where } \hat{p} = -i\hbar\frac{d}{dx} \tag{15}$$

$$E > V_0 \quad \text{Yes, the classical region} \tag{16}$$

Let's assume that our wavefunction takes the form

$$\psi(x) = A(x) \exp\left(\frac{i}{\hbar}S(x)\right), \quad S(x) \in \mathbb{Z} \tag{17}$$

The assumption is reasonable, since we know the form of wavefunctions under classical region, which is of course oscillatory. While forbidden region must be a wavefunction which should be exponentially decaying. Now plug this assumed wavefunction into our particular form of Schrödinger equation. After some not-so-tricky algebra, we can easily obtain an expression which will give you some idea of the form of the amplitude varying and also the form of phase. The phase will be in the form

$$S(x) = \int p(x)\,dx \tag{18}$$

and our amplitude will be in the form

$$A(x) = \frac{C}{\sqrt{P(x)}} \tag{19}$$

Something to note here: see the probability would just be the square of the amplitude. If you think about it, the probability should always be inversely proportional to momentum. Why? The answer is pretty straightforward: If the particle is running away fast, you are not gonna see it a lot of time in your backyard; at the same time, if the particle is a lazy idiot then you're gonna see him everywhere, because bro is not moving anywhere. Moving on with Griffith, we again substitute these fantastic, super-useful forms of equations into our wavefunction $\psi(x)$. We get

$$\psi(x) = \frac{C}{\sqrt{P(x)}} \exp\left(\frac{i}{\hbar} \int P(x)\,dx\right) \tag{20}$$

Time to do some problems to get some idea of how WKB is useful.

Problems from WKB

1. Consider a one-dimensional infinite square well of width a, but with a non-flat ("bumpy") bottom. That is, the potential is given by

$$V(x) = \begin{cases} f(x), & 0 < x < a \\ \infty, & \text{otherwise} \end{cases} \tag{21}$$

where $f(x)$ is an arbitrary (possibly random) function. We assume that the energy of the

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particle satisfies $E > f(x)$ for all $x \in (0, a)$, so that the particle is in a classically allowed region throughout the well and the wavefunction is oscillatory inside. The time-independent Schrödinger equation inside the well is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + f(x)\psi(x) = E\psi(x), \quad \text{for } 0 < x < a \tag{22}$$

with boundary conditions

$$\psi(0) = \psi(a) = 0 \tag{23}$$

Now we have a boundary condition in play. We obtained a wave function which is an approximate wavefunction (one should be able to remember where exactly we did the approximation part—we assumed that $A(x)$ varies slowly, so we neglected the A'' term, which is the sole reason we got the WKB wavefunction). So what we can check is, how better we can do to find the energy eigenvalues with more information we got, like the boundary condition. So what we're gonna do is find out some form for the phase of the wave $S(x)$. Look at equation (20) We can express the same term using Sine cosine functions, thanks to Eulers Equation and yes that make sense remember we are dealing with oscillatory function. So we expect it to be a linear combination of sine and cosine function. Lets rewrite the same thing using Sine and Cosine function and then we can see what we can do with the boundary condition.

$$\psi(x) = \frac{1}{\sqrt{P(x)}}\left[C_1 \cos(\phi(x)) + C_2 \sin(\phi(x))\right] \tag{24}$$

Now remember that at $x = 0$ and $x = a$, the wavefunction should be zero. This means that the phase $\phi(x)$ must satisfy the condition:

$$\phi(0) = 0, \quad \phi(a) = n\pi, \quad n = 1, 2, 3, \ldots \tag{25}$$

This quantization condition ensures that the wavefunction vanishes at the boundaries, consistent with the infinite potential walls.

Since

$$\phi(x) = \frac{1}{\hbar}\int_0^x P(x')\,dx',$$

the condition $\phi(a) = n\pi$ leads to

$$\frac{1}{\hbar}\int_0^a P(x)\,dx = n\pi. \tag{26}$$

$$\int_0^a P(x)\,dx = \hbar\pi n \tag{26.2}$$

So using the new information, that is the boundary condition, we got a better knowledge about the wave function. The new information about the boundaries gave us more knowledge, Remember we still have ambiguity playing around of-course we don't yet know that the exact shape of the wavefunction. So its fair. The ambiguity lies in the difficulty of doing the integral inside since, we don't the V(x) we can never perform the integral. So this is the far we can go. Lets assume a simple case where the V(x) is 0, which is the infinite square well. But hey we already know the solution why should we bother about the infinite square well, yes we know the solution which gives us more reason to do it, if it matches we will have a little much more confidence on what we doing. Right ? So there is no need of Integral or something, the intergal will boil dowm to ,

$$E = \frac{n^2 \pi^2 \hbar^2}{2ma^2}, \quad n = 1, 2, 3, \ldots \tag{27}$$

Yes, we got it perfect.We gonna do one more problem.

2. Use the WKB approximation to find the allowed energies E_n of an infinite square well with a "shelf" of height V_0, extending halfway across the well:

$$V(x) = \begin{cases} V_0, & 0 < x < \frac{a}{2}, \\ 0, & \frac{a}{2} < x < a, \\ \infty, & \text{otherwise.} \end{cases}$$

Express your answer in terms of V_0 and

$$E_n^0 \equiv \frac{(n\pi\hbar)^2}{2ma^2},$$

the nth allowed energy for the infinite square well without the shelf. Assume that

$$E_1^0 > V_0,$$

but do not assume any relation between E_n and V_0.

Compare your result with the one obtained using first-order perturbation theory. This is from Griffith's text, he introduced perturbation before WKB, but we are going to look at that after. Note that the results agree if either V_0 is very small (the perturbation theory regime) or n is very large (the WKB semi-classical regime).

5 Field Emission and Fowler Nordheim

So Field Emission refers to the phenomenon of tunneling taking place under strong Electric field. An electron in front of the potential barrier might not be able to tunnel. If the potential barrier is too high, remember with the width of the potential barrier the transmission coefficient decreases exponentially. But one might think what happens if a strong external electric field is applied. To understand what happens think about the potential barrier height. What does it signifies. ? Think of it in this way, The height of the potential barrier is teh energy you have to give the electron to push it into the classical region. If F electric field is applied and is certainly strong that means one thing, you have an extra helping hand of electric field to push your electron in to the classical regime.so it is absolutely fine to think that that your potential is now not a flat line barrier but the same barrier width but with a slope on the top, a negative slope. As depicted in the below diagram.
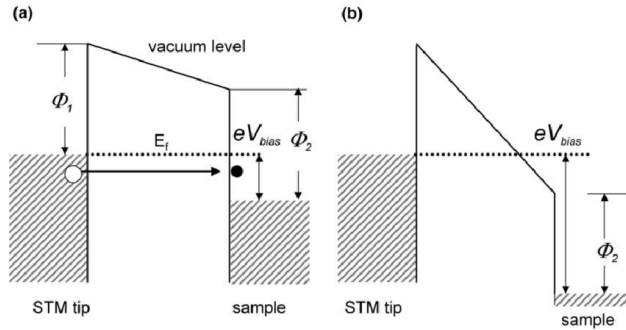

Figure 1: F N Barrier

Okay, the shape looks interesting, we already know, what the solution for the potential barrier which is flat. We spent a lot of time figuring about WKB and first order. one should think about applying those here, the shape of the potential barrier is now changing the height is changing it is not abruptly changing like an exponential decay.it is varying slowly, perfect example for a W K B friendly potential. If you check Griffiths text, there is a section called Tunneling under W K B. The derived expression for tunnelling is discussed there.

$$T \approx e^{-2\gamma}, \quad \text{with} \quad \gamma \equiv \frac{1}{\hbar} \int_{x_1}^{x_2} |p(x)| \, dx$$

So this is the W K B approximation for the tunneling, we can substitute the momentum, looking at the new kind of potential,we can obtain the T for the Fowler Nordheim and Field Emmission.

We now investigate how the semiclassical momentum p varies with the position-dependent quantity $P(x)$, within the context of field emission. The key to understanding this lies in examining the nature of the potential.

The reason the potential is sloped rather than flat is simply due to the presence of an external electric field. Suppose V_0 is the maximum height of the potential barrier. Then, due to this applied electric field, the potential decreases linearly with distance. This makes perfect sense—because the energy required for an electron to escape into the classical region is effectively reduced by the helping hand of the external field.

So, the potential takes the form:

$$V(x) = V_0 - eFx$$

For ease of calculation, we also perform a levelling procedure. When we write the Schrödinger equation, we encounter the term $E - V(x)$. We define this quantity as $M(x)$, and refer to it as the *motive energy* (a term used in some references):

$$M(x) = E - V(x) = E - V_0 - eFx$$

Now, define $h = E - V_0$. This gives:

$$M(x) = h - eFx$$

Then, the position-dependent momentum is:

$$P(x) = \sqrt{2mM(x)} = \sqrt{2m(h - eFx)}$$

Substituting $P(x)$ into the WKB tunneling formula and skipping intermediate algebra, the tunneling exponent becomes:

$$\gamma = \int_{x_1}^{x_2} P(x)\, dx$$

which yields the transmission probability:

$$T = \exp\left(-\frac{4}{3} \cdot \frac{\sqrt{2}}{eF\hbar} \cdot h^{3/2} \right)$$

Knowing T, we can then use Landau's theory or other emission models to calculate the absolute tunneling current and related physical observables.

6 Notes from Chapter 3 "Tunneling Matrix Elements"

7 P I D Control system : Control Theory

PID stands for **Proportional–Integral–Derivative** control. It's a general method used in control theory and can be applied to numerous automated dynamic systems.

General Architecture

PID is a **closed-loop system**, or in other words, a **feedback system**. Imagine a car that's automated using an open-loop system. Let's say you need to travel exactly 100 km. If the road is perfectly flat, we can set the accelerator using some complicated electronics, and it would work — even if we have no idea what the current speed of the vehicle is. Well, that's poorly stated. What I meant is: we do know the speed, because it's the speed we ourselves provided via the accelerator pedal. But that assumption breaks down if the car starts going downhill — now there's extra gravitational force accelerating the car, and we **no longer have any idea of the actual cruising speed**. That's where the open-loop system **fails**. So, the idea is simple:

> **Open loop — bad. Closed loop — good.**

But what kind of closed-loop system? We have an input value — the *setpoint* — that we want to reach. Suppose that's the total distance we want the car to travel. Then there's a **PID controller**, which has three separate sections: **P**, **I**, and **D**. These feed into a **summation block**, which adds together all the contributions from the P, I, and D components and gives the final **output**.

Proportional Control

Suppose you're driving a car and see an obstacle 1 km ahead. You don't need to release the gas pedal right away — you can afford to press it a little longer. But the closer you get to the obstacle, the more you need to ease off the pedal. Right?

That's your brain doing **proportional adjustment**.

Mathematically, we model this with:

$$y(t) = K_p \cdot (w(t) - x(t))$$

Here:

- K_p is a tunable constant (the proportional gain),

- $w(t)$ is the setpoint (what you want),

- $x(t)$ is the current value (what you have),

- The difference $e(t) = w(t) - x(t)$ is called the **error**,

- $y(t)$ is the output of the proportional controller.

Let's say we want to travel 10 kilometers, starting from zero. Let $K_p = 5$, and $w = 10$. Initially $x = 0$.

I've also included a table from which the intuition behind proportional control becomes obvious. You can clearly see how slowing the car down is modeled perfectly in that example.

Position [km]	e(t)	$K_p \cdot$e(t)
0	10 - 0 = 10	5 · 10 = 50 km/h
3	10 - 3 = 7	5 · 7 = 35 km/h
5	10 - 5 = 5	5 · 5 = 25 km/h
7	10 - 7 = 3	5 · 3 = 15 km/h
8	10 - 8 = 2	5 · 2 = 10 km/h
9	10 - 9 = 1	5 · 1 = 5 km/h
10	10 - 10 = 0	5 · 0 = 0 km/h

Analyzing the table, we see that the set point is 10 km and the initial position is 0 km. So, the error is:

$$\text{Error} = 10 - 0 = 10$$

Now, how fast should we go to correct this error? That's where the proportional adjustment comes in. Suppose our proportional gain, K_p, is 5. Then:

$$\text{Adjustment} = K_p \times \text{Error} = 5 \times 10 = 50$$

This means we press the gas pedal to go at 50 km/h.

Now, let's say we travel 3 km at that speed. The new error becomes:

$$10 - 3 = 7$$

According to our P-controller:

$$\text{New speed} = 5 \times 7 = 35 \text{ km/h}$$

We're told to slow down to 35 km/h. Repeating this process, the closer we get to 10 km, the smaller the error becomes. Eventually, at 10 km, the error is zero, and the controller tells us to stop. Simple and elegant, right?

Well... not quite.

If you think this alone will work perfectly, you are mistaken. Here's what can happen. Below is another table diagram of a possible scenario that can occur.

Speed [km/h]	e(t)	$K_p \cdot e(t)$
0	100 - 0 = 100	0.1 · 100 = 10 cm
30	100 - 30 = 70	0.1 · 70 = 7 cm
50	100 - 50 = 50	0.1 · 50 = 5 cm
60	100 - 60 = 40	0.1 · 40 = 4 cm
60	100 - 60 = 40	0.1 · 40 = 4 cm
⋮	⋮	⋮

Figure 2:

Carefully observe the table, notice that the Kp is too low now — the value of Kp is 0.1. Everything else is the same, but you will see our system is getting failed in the table. The point is: suppose our vehicle travels at the speed of 60 km while the gas pedal is at 4 cm. Something unfortunate happens. Understand that after our vehicle reaches 60, the error is again 40, which will give you the adjustment value to be again 4 cm, which is again 60, which will give you again the error of 40, which will again give you 4 cm... I can go on forever. But the idea is pretty much clear. We will end up in a loop if only proportional adjustment is used. This kind of deviation is called steady-state deviation. To overcome this kind of deviation, we use integral adjustment. The I in the PID. One more thing to note here, one may think that, increasing the value of Kp would solve the problem which is totally untrue because doing so, will introduce another problem of overshooting. Overshooting in simple words is when you take loner steps to reach a place, there is a chance of taking a wrong step where you will place your final step beyond the desired place.
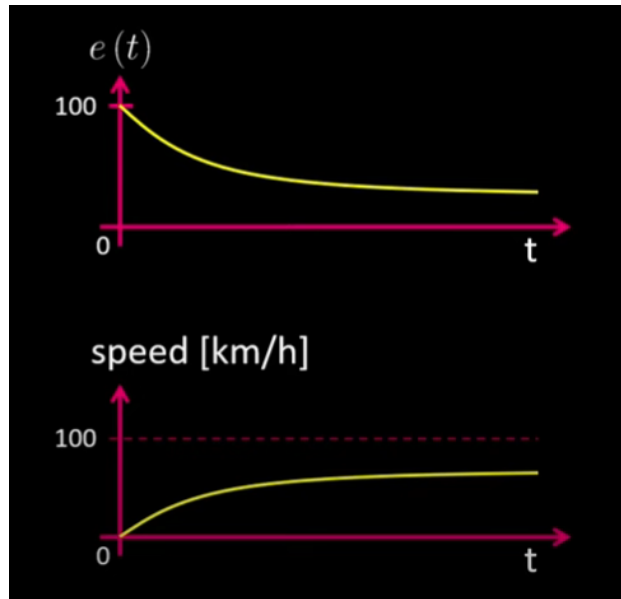
Figure 3:

Integral Control

We need a new system to overcome the steady-state deviation problem. So what is an integral adjustment? And how does this adjustment resolve the issue of steady-state deviation? Think about the real problem here — I mean the loop we fell into. Every time (from the previous example) our system knows that the vehicle is cruising at 60 km/h, the system adjusts the same way. No matter if it's the first time or 100th time. In other words, the system cannot distinguish between the first 60 and the 100th 60 coming back through its feedback. So we need some new adjustment that has some kind of "memory". When I say memory, I mean we need some new value or coefficient that depends on time. So yes — simple — we need a time-accumulated error correction term. So that next time our feedback system gives the information that the vehicle is going 60, it will also tell the system: "This is the 100th 60, goddammit — act on it.

$$y(t) = K_I \int_0^t (w - x(\tau)) \ d\tau$$

The expression says it all. Now let's look on to it. How exactly does this work.

Speed [km/h]	e(t)	$K_p \cdot e(t)$ K_p=0.1	$K_i \cdot \Sigma e(t)$ K_i=0.01	Sum
0	100	10.0 cm	$0.01 \cdot 100$ = 1.0 cm	11 cm
30	70	7.0 cm	$0.01 \cdot 170$ = 1.7 cm	8.7 cm
50	50	5.0 cm	$0.01 \cdot 220$ = 2.2 cm	7.2 cm
70	30	3.0 cm	$0.01 \cdot 250$ = 2.5 cm	5.5 cm
80	20	2.0 cm	$0.01 \cdot 270$ = 2.7 cm	4.7 cm
80	20	2.0 cm	$0.01 \cdot 290$ = 2.9 cm	4.9 cm
⋮	⋮	⋮	⋮	⋮

Figure 4:

8   Atomic Force Microscopy

AFM, unlike STM does not use tunnelling current inorder to extract information, rather atomic forces are exploited. There are two types of forces exists between two nuetral atoms. One is Van der Waal attraction and the replusive forces due to the Pauli Exclusion Principle. An AFM utilises both in order to extract information about the surface of the respective material. To understand the principle behind AFM, we might want to look into the nature of the forces or potential that exists between two atoms. Number of approximations to certain degree exists to describe this potential analytically, we here are going to talk about the Leonard jones potential which is a very common approximation taken in such fields and in AFM too. Leonard Jones' potential in a nutshell, will have two potential with opposite signs, which represents the attractive and replusive term. The order or range of both of these potential are very different.

$$V(r) = 4\varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^{6} \right]$$

The repulsive force is in the order of -12 which is a short range order and the attractive regime is much longer, order of -6. A natural question to ask, is why replusive regime is short termed and attractive regime is long range? The answer lies in the nature of these forces .A detailed derivation of those forces are out of the scope of my note. Hence, lets just state that, Pauli repulsion only become significant if the wavefunction of two particle starts to significantly overlaps, While van der waals force have much larger vicinity of action. The potential and force diagrams are given below.

$$U(r) = 4U_0 \left[\left(\frac{R_a}{r}\right)^{12} - \left(\frac{R_a}{r}\right)^{6} \right]$$

Repulsive interaction

Attractive interaction
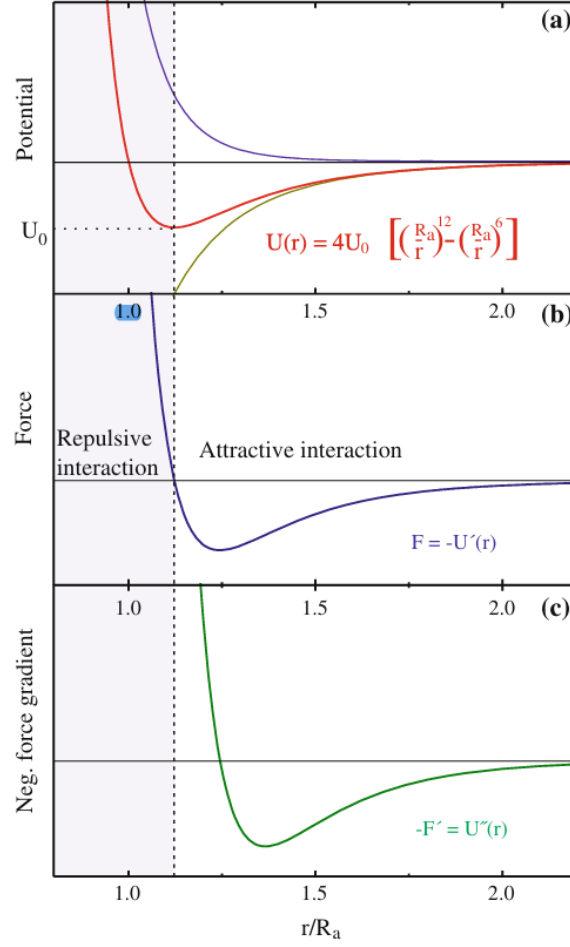
$$F = -U'(r)$$

$$-F' = U''(r)$$

r/R_a

Figure 5:

There are mainly two modes in AFM, Static Mode and Dynamic Mode. As the name suggests, in static mode, the cantilever of the AFM is kept static, and a scan in the XY plane is made. The cantilever deflection due to the force between the tip and sample is detected using a laser beam and a photo-detector. Static Mode can be done in both attractive and repulsive regimes. If the tip is picking up the deflection from the repulsive regime, it is called Contact Mode. In constant force mode, a particular setpoint force is fixed, and the surface is probed. If, suppose an edge came across the probe, the force between the tip and the sample changes. Essentially, a force F, let's say, which corresponds to a z height, will in turn gives a voltage V. Whenever there is a shift in the force is obtained a corresponding shift in the voltage detected by the photodiode is detected. This change in voltage goes through the feedback loop, and the cantilever is adjusted in a way that the new Z will correspond to the initial setpoint value. The feedback circuit is designed in such a way that it always makes sure, that the V is close to the setpoint value. While the feedback maintains a constant deflection, the Z contour gives you the height profile of the surface of the sample. To move

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further, an idea about the effect called "snap to contact" is essential. The example from Voightlander's text is the best to describe the snap-to-contact effect. Imagine a magnet at the end of the spring is hung, freely in the gravitational field. It will naturally find an equilibrium value, around which the magnet will oscillate if disturbed. Now, if a iron plate is brought near, the equilibruim point will change accordingly and the magnet will oscillate around a different point. But if the iron plate is brought too close, then there is a chance that the magnet will snap into the iron plate. This is effect is called snap to contact. The same effect can happen to the AFM tip, that implies certain Z values are not realizable.