

Internship Notes

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Chapter 1

Introduction.

Our internship had for end goal to study the quantum behavior of a particle in a quasi-periodic potential. Since when we started we had only basic notions of quantum mechanics we had first to read and treat simpler problems to make our way there. We started by studying the theory behind periodic potentials. These potentials are interesting in general because we can model solids with crystalline structures with them, and for example understand the fundamental differences between a conductor and an insulator. This also then leads to a more complex theory called *Anderson's Localization* that studies this kind of systems but with some added disturbances. In the following we are going to retrace the steps of our internship, maybe in a bit more proper and orderly manner.

Chapter 2

General theorems and definitions.

2.1 Bravais Lattice.

Definition 2.1.1. Given any linearly independent vectors $(\mathbf{a}_1, \dots, \mathbf{a}_n) \in \mathbb{R}^n$, which we will call primitive vectors, we call Bravais lattice the set

$$\mathbb{B}_n = \{\mathbf{r} \in \mathbb{R}^n \mid \mathbf{r} = l_1 \mathbf{a}_1 + \dots + l_n \mathbf{a}_n, \ l_1, \dots, l_n \in \mathbb{Z}\}.$$

Remark 1. We should in principle specify that \mathbb{B}_n depends on the vectors \mathbf{a}_i , but it's bad notation and the initial vectors will be clear from the context.

Definition 2.1.2. When we consider \mathbb{B}_2 (or \mathbb{B}_3) then we define Primitive Cell a closed surface (resp. volume) that, when translated through all the vectors in the Bravais lattice, just fills all of surface (space) without overlapping itself or leaving voids.

Proposition 2.1.1. A Primitive Cell contains one and only one point of the corresponding Bravais lattice.

Proposition 2.1.2. If we call n the density of points in \mathbb{B}_2 or \mathbb{B}_3 , then the surface (volume) of a Primitive Cell is $1/n$.

2.2 Reciprocal Lattice

Definition 2.2.1. Consider a Bravais lattice \mathbb{B}_n then we define the associated reciprocal lattice as:

$$\mathbb{RP}_n = \{\mathbf{K} \in \mathbb{R}^n \mid e^{\mathbf{K} \cdot \mathbf{R}} = 1, \ \forall \mathbf{R} \in \mathbb{B}_n\}.$$

Proposition 2.2.1. If we call:

$$\mathbf{a}_i^* := 2\pi \frac{\bigwedge_{l \in [1, n] \setminus \{i\}} \mathbf{a}_l}{\mathbf{a}_i \cdot \left(\bigwedge_{l \in [1, n] \setminus \{i\}} \mathbf{a}_l \right)}$$

then we have that

$$\mathbb{RP}_n = \{\mathbf{r} \in \mathbb{R}^n \mid \mathbf{r} = l_1 \mathbf{a}_1^* + \dots + l_n \mathbf{a}_n^*, \ l_1, \dots, l_n \in \mathbb{Z}\}.$$

Proof. Notice that $\mathbf{a}_i^* \cdot \mathbf{a}_j = 2\pi \delta_{ij}$. Then notice that the \mathbf{a}_i^* are linearly independent, hence they generate \mathbb{R}^n . Any vector of \mathbb{R}^n can thus be written as $\mathbf{k} = k_1 \mathbf{a}_1^* + \dots + k_n \mathbf{a}_n^*$. Then we have:

$$e^{\mathbf{k} \cdot \mathbf{R}} = 1, \ \forall \mathbf{R} \in \mathbb{B}_n \Leftrightarrow \mathbf{k} \cdot \mathbf{R} = 0 \pmod{2\pi}, \ \forall \mathbf{R} \in \mathbb{B}_n \Leftrightarrow k_1, \dots, k_n \in \mathbb{Z}.$$

Hence the proposition is proved.

Proposition 2.2.2. \mathbb{RP}_n is also a Bravais lattice.

Remark 2. In one dimension if we have that \mathbb{B}_1 is generated by a vector $a\vec{e}_x$, then the reciprocal lattice is generated by $\frac{2\pi}{a}\vec{e}_x$.

Proposition 2.2.3. When considering a Bravais lattice \mathbb{B}_3 whose primitive cells have volume v , then the primitive cell of the reciprocal lattice has volume $(2\pi)^3/v$.

Definition 2.2.2. Given a Bravais lattice \mathbb{B}_n then the Weigner-Seitz cell around a point of the lattice is the set of points that are closer to that point than to any other lattice point (distance is intended as the standard distance induced by the standard inner product).

Proposition 2.2.4. The Weigner-Seitz cell is a primitive cell.

Definition 2.2.3. We define the First Brillouin Zone as the Weigner-Seitz cell of \mathbb{RP}_n .

2.3 Bloch's theorem in 1 dimension.

Lemma 2.3.1. Any unitary operator \hat{U} has eigenvalues of norm 1.

Proof. Let α be the eigenvalue to the eigenstate $|\alpha\rangle$ of \hat{U} , then we have:

$$\begin{cases} \hat{T}|\alpha\rangle = \alpha|\alpha\rangle \\ \langle\alpha|\hat{T}^\dagger = \alpha^*\langle\alpha| \end{cases} \quad \text{so} \quad \langle\alpha|\hat{\text{Id}}|\alpha\rangle = \langle\alpha|\hat{T}^\dagger\hat{T}|\alpha\rangle = \alpha\alpha^*\langle\alpha|\alpha\rangle \quad \text{so} \quad |\alpha| = 1$$

Theorem 2.3.2. Bloch's theorem in 1 Dimension. Let V be a potential that is a -periodic, then the eigenstates are given by:

$$\psi_k(x) = \exp(ikx)u_k(x) \quad \text{where } u_k \text{ is } a\text{-periodic.}$$

Proof. Let $V : \mathbb{R} \rightarrow \mathbb{R}$ and $a \in \mathbb{R}$ be a function such that $V(x+a) = V(x)$. Define the translation operator: $\hat{T}\psi(x) = \psi(x+a)$. We have:

$$\psi(x+a) = \sum_{n=0}^{+\infty} \psi^{(n)}(x) \frac{a^n}{n!} = \sum_{n=0}^{+\infty} \frac{i^n a^n}{\hbar^n n!} \hat{p}^n \psi(x) = \exp\left(\frac{ia}{\hbar} \hat{p}\right) \psi(x) \quad \text{so} \quad \hat{T} = \exp\left(\frac{ia}{\hbar} \hat{p}\right)$$

Then $[\frac{\hat{p}^2}{2m}; \hat{T}] = 0$ trivially and:

$$\hat{V}(\hat{T}\psi(x)) = V(x)\psi(x+a) = V(x+a)\psi(x+a) = \hat{T}(V(x)\psi(x)) = \hat{T}(\hat{V}\psi(x)) \quad \text{so} \quad [\hat{V}, \hat{T}] = 0$$

Since \hat{T} commutes with the potential and the momentum it also commutes with the Hamiltonian and therefore the Hamiltonian and the translation operator share a common eigen-basis. Furthermore $\hat{T}^\dagger = \exp(-\frac{ia}{\hbar} \hat{p})$ so $\hat{T}^\dagger \hat{T} = \text{Id}$ so the translation operator is unitary. Applying the lemma we get that:

$$\psi(x+a) = \exp(ika)\psi(x) \quad \text{where } k \in \mathbb{R}$$

Then define $u_k = e^{-ika}\psi(x)$ and we get the desired result.

2.4 Generalization to 3 dimensions.

Theorem 2.4.1. Consider a continuous, piecewise C^1 function $U : \mathbb{R}^3 \rightarrow \mathbb{R}$. Then consider a Bravais Lattice \mathbb{B}_3 generated by $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$. Then assume that $U(\mathbf{r} + \mathbf{R}) = U(\mathbf{r})$ for any $\mathbf{R} \in \mathbb{B}_3$. Then the eigenstates of the Hamiltonian $H = -\hbar^2 \nabla^2 / 2m + U(\mathbf{r})$ can be chosen to have the form

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$$

with $u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$ for any $\mathbf{R} \in \mathbb{B}_3$. We call Bloch wave vector any such vector \mathbf{k} .

Remark 3. The index n indicates that for a given \mathbf{k} there will be more independent eigenstates.

Proposition 2.4.1. We have that $\psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k} \cdot \mathbf{R}} \psi_{n\mathbf{k}}(\mathbf{r})$ for any $\mathbf{R} \in \mathbb{B}_3$.

Proof. We have $\psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k} \cdot (\mathbf{r} + \mathbf{R})} u_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k} \cdot \mathbf{R}} \psi_{n\mathbf{k}}(\mathbf{r})$, by the periodicity of $u_{n\mathbf{k}}$.

Proposition 2.4.2. (Alternative form of Bloch's theorem) Showing the previous theorem is equivalent to proving that the eigenstates of H can be chosen such that with each eigenstates ψ there is associated a wave vector \mathbf{k} such that

$$\psi(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k} \cdot \mathbf{R}} \psi(\mathbf{r})$$

for any $\mathbf{R} \in \mathbb{B}_3$.

Proof. The first implication is true by the proposition above. Now suppose that we can choose our eigenstates as stated above. Then define the function u by $u(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{r}}\psi(\mathbf{r})$. In order to satisfy $\psi(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi(\mathbf{r})$ we must have that

$$u(\mathbf{r} + \mathbf{R}) = e^{-i\mathbf{k}\cdot(\mathbf{r}+\mathbf{R})}\psi(\mathbf{r} + \mathbf{R}) = e^{-i\mathbf{k}\cdot\mathbf{R}}\psi(\mathbf{r}) = u(\mathbf{r}).$$

Hence the conclusion follows immediately.

Proof. (of the Theorem) To prove the Theorem we can thus just prove that we can choose the eigenstates of H in such a way that for any of them, say ψ , there exists a wave vector \mathbf{k} so that $\psi(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi(\mathbf{r})$ for any $\mathbf{R} \in \mathbb{B}_3$. To do

Definition 2.4.1. (Born-von Karman Boundary Condition) Given a Bravais lattice \mathbb{B}_3 generated by $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$, given $N_1, N_2, N_3 \in \mathbb{N}$, and given U as defined above, we say that any eigenstate ψ of the Hamiltonian $H = -\hbar^2\nabla^2/2m + U(\mathbf{r})$ satisfies the Born-von Karman boundary conditions if $\psi(\mathbf{r} + N_i\mathbf{a}_i) = \psi(\mathbf{r})$, $i = 1, 2, 3$.

Proposition 2.4.3. Consider the same Bravais lattice \mathbb{B}_3 , and suppose that the eigenstates of H satisfy the Born-von Karman boundary condition, then any Bloch wave vector \mathbf{k} can be written as

$$\mathbf{k} = \sum_{i=1}^3 \frac{m_i}{N_i} \mathbf{a}_i^*, \quad m_1, m_2, m_3 \in \mathbb{Z}.$$

Proof. If we apply Bloch's theorem (in alternative form) to H then we have that we can choose eigenstates satisfying $\psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{n\mathbf{k}}(\mathbf{r})$. For each of these eigenstates to satisfy the Born-von Karman boundary condition we get, for $i = 1, 2, 3$:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = \psi_{n\mathbf{k}}(\mathbf{r} + N_i\mathbf{a}_i) = e^{i\mathbf{k}\cdot N_i\mathbf{a}_i}\psi_{n\mathbf{k}}(\mathbf{r})$$

which implies that we must have $e^{iN_i\mathbf{k}\cdot\mathbf{a}_i} = 1$, i.e. $N_i\mathbf{k} \cdot \mathbf{a}_i = 2\pi m_i$, $m_i \in \mathbb{Z}$. Since $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$ form a basis for \mathbb{R}^3 then we can write $\mathbf{k} = x_1\mathbf{a}_1^* + x_2\mathbf{a}_2^* + x_3\mathbf{a}_3^*$. From $\mathbf{a}_i^* \cdot \mathbf{a}_j = 2\pi\delta_{ij}$ it follows that we must have $N_i x_i 2\pi = 2\pi m_i$, i.e. $x_i = \frac{m_i}{N_i}$.

Definition 2.4.2. We define the vector \mathbf{k} as in the proposition above to be the quasi-momentum.

Proposition 2.4.4. We can restrict the choice of \mathbf{k} so that its tip lies in the first Brillouin zone of \mathbb{B}_3 .

Proof. Take any Bloch wave vector $\mathbf{k}' \in \mathbb{R}^3$ outside of the first Brillouin zone, then we have $\mathbf{k}' = \sum_{i=1}^3 \frac{m_i}{N_i} \mathbf{a}_i^*$ and we can write it as $\mathbf{k}' = \mathbf{k} + \mathbf{K}$ with \mathbf{K} belonging to \mathbb{RP}_3 and \mathbf{k} lying inside the first Brillouin zone. Then since $e^{i\mathbf{K}\cdot\mathbf{R}} = 1$ for any $\mathbf{R} \in \mathbb{B}_3$ the conclusion follows.

Remark 4. All the results above are valid also when we consider Bravais lattices of dimension 1 or 2.

Chapter 3

Periodic Potential problem setting and simplifications.

3.1 Impossibilities of the full problem.

3.1.1 Setting of the problem.

This problem arose from trying to model a particle in a solid that presents a periodic structure, so we shall follow the same line of reasoning.

Notation. We call N_n the number of nuclei that are in our solid and N_e the number of electrons in our solid. We call M the mass of a nucleus and m_e the mass of an electron.

Axiom. From chemistry we take the following assumptions $N_e = ZN_n$ with $N \in \mathbb{N}$.

Then the full Hamiltonian is going to be given by the following equation:

$$\hat{H} = \frac{1}{2M} \sum_{i=1}^{N_n} \hat{p}_i^2 + \frac{1}{2m_e} \sum_{i=1}^{N_e} \hat{p}_i^2 + \frac{Z^2}{2} \sum_{i \neq j}^{N_n} V_c(\mathbf{R}_i - \mathbf{R}_j) - Z \sum_{i=1}^{N_e} \sum_{j=1}^{N_n} V_c(\mathbf{r}_i - \mathbf{R}_j) + \frac{1}{2} \sum_{i \neq j}^{N_e} V_c(\mathbf{r}_i - \mathbf{r}_j)$$

3.1.2 Difficulties of the full problem.

Because of the cross terms this problem is not separable, which means that we would have to solve it in full. The idea of an analytical solution seems completely unreal since this problem is much more complicated than the problem of a single helium atom. Now looking at this problem from a numerical perspective we see that we have an amount of data points in the order of 10^{23} which is very obviously completely unmanageable, hence the need for simplifications.

3.1.3 Simplifications of the original problem.

The first obvious simplification is saying that the mass of the nuclei is much larger than the electrons we can neglect the momentum term of the nuclei and consider them as being fixed. Then since they are fixed the Coulomb interaction term between themselves is just a constant so it can be neglected as well. We then end up with the following Hamiltonian:

$$\hat{H} = \frac{1}{2m_e} \sum_{i=1}^{N_e} \hat{p}_i^2 - Z \sum_{i=1}^{N_e} \sum_{j=1}^{N_n} V_c(\mathbf{r}_i - \mathbf{R}_j) + \frac{1}{2} \sum_{i \neq j}^{N_e} V_c(\mathbf{r}_i - \mathbf{r}_j)$$

The cross term still makes this problem unsolvable. If we try to completely neglect the cross term then we get a Hamiltonian that presents an un-physical behavior. Suppose we neglected the last term and then introduce a new electron in our globally neutral system. This Hamiltonian would tell us that this new electron would be only submitted to the enormous potential of a charge $ZN_n e$ which is obviously untrue. We still need to simplify this, but we shall use a finer simplification. We say that every electron is submitted to only the potential exerted

by the nuclei plus the average potential exerted by the other electrons. Then we get:

$$\begin{aligned}
\hat{H} &= \frac{1}{2m_e} \sum_{j=1}^{N_e} \hat{p}_j^2 - Z \sum_{i=1}^{N_n} \sum_{j=1}^{N_e} V_c(\mathbf{r}_j - \mathbf{R}_i) + \frac{1}{2} \sum_{i=1}^{N_e} \langle V_c(\mathbf{r}_j - \mathbf{r}_i) \rangle_{j \in [1, N_e] \cap \mathbb{N}} \\
&= \frac{1}{2m_e} \sum_{j=1}^{N_e} \hat{p}_j^2 - \sum_{j=1}^{N_e} \left(Z \sum_{i=1}^{N_n} V_c(\mathbf{r}_j - \mathbf{R}_i) + \frac{1}{2N_n} \sum_{j=1}^{N_n} \langle V_c(\mathbf{r}_j - \mathbf{r}_i) \rangle_{j \in [1, N_e] \cap \mathbb{N}} \right) \\
&= \sum_{j=1}^{N_e} \left(\frac{\hat{p}_j^2}{2m_e} + \sum_{i=1}^{N_n} V_{\text{at}}(\mathbf{r}_j - \mathbf{R}_i) \right) = \sum_{j=1}^{N_e} \hat{H}_j
\end{aligned}$$

Where we defined V_{at} and H_j by what they replaced. So we finally managed to get a separable problem. Our major concern now is that we do not have any knowledge of V_{at} at the moment, but we can infer some information from how it was constructed. From its construction we deduce that it has to satisfy Poisson's equation and as such will need to decay exponentially at great distances. On short distances on the other hand the potential will be almost entirely dominated by the attraction of the nuclei. Furthermore, the potential should only depend on the norm of the vector, so invariant by rotations. Finally, last but certainly not least, since we are considering a crystalline solid we assume that our potential is periodic and its periodicity is dictated by the structure of the solid.

Chapter 4

Weak periodic potential model

In the setting of the model introduced in Chapter 3 we consider now a weak periodic potential, i.e. we consider energy level that are much bigger than the maximum value of the potential V .

Hypothesis 4.0.1. We will assume that our solid is a Bravais lattice (with finite size given by some positive integers N_1, N_2, N_3 and volume $\Omega = N_1 N_2 N_3$) with Born-von Karman boundary conditions and with the potential satisfying the periodicity of the lattice.

Proposition 4.0.1. For a box of volume Ω , the Hamiltonian for a free electron trapped inside is $H_0 = \frac{p^2}{2m_0}$, the eigenstates are given by $\psi_{\mathbf{k}}(\mathbf{r}) = \sqrt{\Omega} e^{i\mathbf{k} \cdot \mathbf{r}}$ and the eigenenergies are $\epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m_0}$.

Remark 5. For a 1 dimensional case the band structure reduces to a parabola.

Hypothesis 4.0.2. We assume the potential is given by $V(\mathbf{r}) = \sum_{l=1}^{N_n} V_{at}(\mathbf{r} - \mathbf{R}_l)$, as introduced in the previous chapter, being \mathbf{R}_l the position of the l -th atom.

Hypothesis 4.0.3. We will assume that V has the periodicity of the Bravais lattice and that it is continuous and piecewise C^1 .

Hypothesis 4.0.4. We will treat the potential V as a perturbation with respect to the "free electron model".

Proposition 4.0.2. Considering the non-degenerate eigenenergies of H_0 then the perturbation of these eigenenergies and relative eigenstates gives:

$$E_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \langle \mathbf{k} | V | \mathbf{k} \rangle + \sum_{\mathbf{k}' \neq \mathbf{k}} \frac{|\langle \mathbf{k} | V | \mathbf{k}' \rangle|^2}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}} + \dots$$

$$|\tilde{\mathbf{k}}\rangle = |\mathbf{k}\rangle + \sum_{\mathbf{k}' \neq \mathbf{k}} \frac{\langle \mathbf{k} | V | \mathbf{k}' \rangle}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}} |\mathbf{k}'\rangle + \dots$$

Proposition 4.0.3. We have

$$\langle \mathbf{k} | V | \mathbf{k} \rangle = \frac{1}{\Omega} \int V(\mathbf{r}) d^3\mathbf{r}$$

so that we can neglect it, being just a constant shift that doesn't change the parabolic behaviour of $E_{\mathbf{k}}$.

Proposition 4.0.4. In one dimension (i.e. for \mathbb{B}_1 generated by \mathbf{a}) we have

$$V(x) = \sum_{p=-\infty}^{\infty} V_p e^{ip(2\pi/a)x}$$

Proof. Since $V(x+a) = V(x)$ and V is continuous and piecewise C^1 , by a Theorem in Fourier Analysis we have that the Fourier Series of V converges to V .

Proposition 4.0.5. If we consider a 3 dimensional Bravais lattice \mathbb{B}_3 then we have:

$$V(\mathbf{r}) = \sum_{\mathbf{K} \in \mathbb{RP}_3} V_{\mathbf{K}} e^{i\mathbf{K} \cdot \mathbf{r}}$$

Remark 6. We have $V_{-\mathbf{K}} = V_{\mathbf{K}}^*$, being V real.

Proposition 4.0.6. We have

$$\langle \mathbf{k} | V | \mathbf{k}' \rangle = \frac{1}{\Omega} V_{\mathbf{k}-\mathbf{k}'}.$$

Proof. Indeed from the definition of the inner product we have

$$\langle \mathbf{k} | V | \mathbf{k}' \rangle = \frac{1}{\Omega} \sum_{\mathbf{K}} V_{\mathbf{K}} \int_{\Omega} e^{i(\mathbf{k}' - \mathbf{k} + \mathbf{K}) \cdot \mathbf{r}} d^3 \mathbf{r}$$

and $\int_{\Omega} e^{i(\mathbf{k}' - \mathbf{k} + \mathbf{K}) \cdot \mathbf{r}} d^3 \mathbf{r} = \delta(\mathbf{k}' - \mathbf{k} + \mathbf{K})$.

Proposition 4.0.7. We obtain

$$E_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \sum_{\mathbf{K}} \frac{|V_{\mathbf{K}}|^2}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{K}}}$$

$$|\tilde{\mathbf{k}}\rangle = |\mathbf{k}\rangle + \sum_{\mathbf{K} \neq 0} \frac{V_{\mathbf{K}}}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{K}}}$$

Remark 7. The above result works only when $|V_{\mathbf{K}}| \ll |\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{K}}|$. Notice that $\epsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}-\mathbf{K}}$ if $\mathbf{k}^2 = (\mathbf{k} - \mathbf{K})^2$, i.e. $2\mathbf{k} \cdot \mathbf{K} = \mathbf{K}^2$

Definition 4.0.1. We call Bragg vectors those vectors \mathbf{k} that satisfy the relation of the remark above.

We will now remain in the 1 dimensional case.

Proposition 4.0.8. The Bragg points in the one dimensional case are the vectors $k = \pm\pi/a$ (restricting to the First Brillouin zone).

Proof. From $K = 2m\pi/a$, $m \in \mathbb{Z}$, we must have $2k2m\pi/a = 4m^2\pi^2/a^2$, i.e. $k = m\pi/a$. Since we want to stay in the first Brillouin zone then we choose $m = \pm 1$, and we get the desired result.

Corollary. The associated energies and wavefunctions to the Bragg points are $\epsilon_0 = \hbar^2\pi^2/(2m_0a^2)$ and

$$\psi_{\pi/a} = L^{-1/2} e^{i\pi x/a}, \quad \psi_{-\pi/a} = L^{-1/2} e^{-i\pi x/a},$$

L being the length of the chain.

Proposition 4.0.9. Then we can just consider the reduced potential

$$V^{(1)}(x) = V_1(e^{i2\pi x/a} + e^{-i2\pi x/a}) = 2V_1 \cos(2\pi x/a).$$

Proof. Indeed we have that all the terms which don't have as coefficient V_1 , will give zero when computing any of the inner products $\langle \psi_{\pi/a} | H_1 \psi_{-\pi/a} \rangle$, $\langle \psi_{\pi/a} | H_1 \psi_{\pi/a} \rangle$, $\langle \psi_{-\pi/a} | H_1 \psi_{-\pi/a} \rangle$, $\langle \psi_{-\pi/a} | H_1 \psi_{\pi/a} \rangle$. For simplicity we prove it only for one of them since generalizing to the others is straightforward. Take $\langle \psi_{\pi/a} | H_1 \psi_{-\pi/a} \rangle$, then $V = \sum_{p=-\infty}^{\infty} V_p e^{ip(2\pi/a)x}$. Notice that $\langle \psi_{\pi/a} | V \psi_{-\pi/a} \rangle = \frac{1}{L} \sum_{p=-\infty}^{\infty} V_p \langle e^{i\pi x/a} | e^{i(2p-1)\pi x/a} \rangle = \frac{V_1}{L}$. Hence we see that we can keep in V only the two terms that have V_1 as a coefficient.

Corollary. We obtain that the matrix of the one-electron Hamiltonian H_1 in the basis $\psi_{\pi/a}, \psi_{-\pi/a}$ is

$$H_1 = \begin{pmatrix} \epsilon_0 & V_1 \\ V_1 & \epsilon_0 \end{pmatrix}.$$

Proof. Indeed we have

$$H_1 \psi_{\pi/a} = -\frac{\hbar^2}{2m_0} (i\pi/a)^2 \psi_{\pi/a} + V_1 (e^{i2\pi x/a} + e^{-i2\pi x/a}) L^{-1/2} e^{i\pi x/a} = \epsilon_0 \psi_{\pi/a} + V_1 \psi_{-\pi/a} + V_1 L^{-1/2} e^{i3\pi x/a}$$

then owing to the fact that $\langle e^{ik} | e^{im} \rangle = \delta_{k,m}$ we have that $\langle \psi_{\pi/a} | H_1 \psi_{\pi/a} \rangle = \epsilon_0$ and $\langle \psi_{-\pi/a} | H_1 \psi_{\pi/a} \rangle = V_1$. Similarly we do the same for $H_1 \psi_{-\pi/a}$ and we get the desired result.

Proposition 4.0.10. The eigenstates and eigenenergies of the previous hamiltonian are

$$\psi_- = \frac{1}{2}(\psi_{\pi/a} + \psi_{-\pi/a}) = \sqrt{\frac{2}{L}} \cos(\pi x/a) \quad E_- = \epsilon_0 - |V_1|$$

$$\psi_+ = \frac{1}{2}(\psi_{\pi/a} - \psi_{-\pi/a}) = i\sqrt{\frac{2}{L}} \sin(\pi x/a) \quad E_+ = \epsilon_0 + |V_1|$$

Proof. Simple computation.

Proposition 4.0.11. For $k \approx \pi/a$ we have that

$$E_k = \epsilon_k + \frac{|V_1|^2}{\epsilon_k - \epsilon_{k+2\pi/a}} + \frac{|V_1|^2}{\epsilon_k - \epsilon_{k-2\pi/a}},$$

moreover $\lim_{k \rightarrow \pi/a^\pm} E_k = E_\pm$.

Corollary. In the energy interval $\epsilon_0 - |V_1| < E < \epsilon_0 + |V_1|$ there is no stationary state of the energy. Hence we have a band gap at $k = \pm\pi/a$.

Proposition 4.0.12. As a generalization if we consider the states at $k = \pm p\pi/a$, then we have the reduced potential $V^{(p)} = 2V_p \cos(2\pi px/a)$ and the energy band gap given by any E satisfying $p^2\epsilon_0 - |V_p| < E < p^2\epsilon_0 + |V_p|$.

Chapter 5

Tight-binding model.

5.1 General resolution.

Axiom. The main assumptions that we are making with the tight-binding model is that the energies of our problem are extremely small compared to the depth of the wells that the potential creates. As consequence we assume that we can write the wavefunction of our particle as being a linear combination of the eigenstates to the highest populated eigenenergy of the wells, the valence energy. Then we write:

$$\psi_k(\mathbf{r}) = \frac{1}{\sqrt{N_n}} \sum_{l=1}^{N_n} a_{k,l} \chi_v(\mathbf{r} - \mathbf{R}_l) \quad \text{or equivalently} \quad |\psi_k\rangle = \frac{1}{\sqrt{N_n}} \sum_{l=1}^{N_n} a_{k,l} |\mathbf{R}_l\rangle$$

We also assume that the $|\mathbf{R}_l\rangle$ form an orthonormal basis of our Hilbert space.

We can now proceed with resolving our problem. With this assumption the T.I.S.E. now becomes:

$$\sum_{l=1}^{N_n} a_{k,l} \hat{H}_1 |\mathbf{R}_l\rangle = \sum_{l=1}^{N_n} a_{k,l} E_k |\mathbf{R}_l\rangle$$

And:

$$\begin{aligned} \hat{H}_1 |\mathbf{R}_l\rangle &= \left[\frac{\hat{p}_1^2}{2m_e} + \sum_{m=1}^{N_n} V_{\text{at}}(\mathbf{r}_1 - \mathbf{R}_m) \right] |\mathbf{R}_l\rangle = \left[\frac{\hat{p}_1^2}{2m_e} + V_{\text{at}}(\mathbf{r}_1 - \mathbf{R}_l) \right] |\mathbf{R}_l\rangle + \left[\sum_{m \neq l}^{N_n} V_{\text{at}}(\mathbf{r}_1 - \mathbf{R}_m) \right] |\mathbf{R}_l\rangle \\ &= E_v |\mathbf{R}_l\rangle + V_l(\mathbf{r}) |\mathbf{R}_l\rangle \end{aligned}$$

Where we defined:

$$V_l(\mathbf{r}) = \sum_{m \neq l}^{N_n} V_{\text{at}}(\mathbf{r}_1 - \mathbf{R}_m)$$

Plugging this back into the T.I.S.E. we get:

$$\sum_{l=1}^{N_n} a_{k,l} (E_v |\mathbf{R}_l\rangle + V_l(\mathbf{r}) |\mathbf{R}_l\rangle) = \sum_{l=1}^{N_n} a_{k,l} E_k |\mathbf{R}_l\rangle$$

Now multiplying on the left by $\langle \mathbf{R}_n |$ and using the fact that $\langle \mathbf{R}_n | \mathbf{R}_l \rangle = \delta_{n,l}$ we get that:

$$\begin{aligned} \sum_{l=1}^{N_n} a_{k,l} [E_v \delta_{n,l} + \langle \mathbf{R}_n | V_l | \mathbf{R}_l \rangle] &= \sum_{l=1}^{N_n} a_{k,l} E_k \delta_{n,l} \Leftrightarrow a_{k,n} E_v + \sum_{l=1}^{N_n} a_{k,l} \langle \mathbf{R}_n | V_l | \mathbf{R}_l \rangle = a_{k,n} E_k \\ \Leftrightarrow - \sum_{l=1}^{N_n} (-\langle \mathbf{R}_n | V_l | \mathbf{R}_l \rangle) a_{k,l} &= (E_k - E_v) a_{k,n} \Leftrightarrow - \sum_{l=1}^{N_n} t_{n,l} a_{k,l} = (E_k - E_v) a_{k,n} \\ \Leftrightarrow \begin{pmatrix} t_{1,1} & \cdots & t_{1,N_n} \\ \vdots & \ddots & \vdots \\ t_{N_n,1} & \cdots & t_{N_n,N_n} \end{pmatrix} \begin{pmatrix} a_{k,1} \\ \vdots \\ a_{k,N_n} \end{pmatrix} &= (E_v - E_k) \begin{pmatrix} a_{k,1} \\ \vdots \\ a_{k,N_n} \end{pmatrix} \end{aligned}$$

Where we defined $t_{n,l} = \langle \mathbf{R}_n | V_l | \mathbf{R}_l \rangle$. We see here that we have reduced our original problem to finding the eigenvalues and eigenvectors of an N_n by N_n matrix. The terms $t_{n,l}$ of the matrix are called hopping integrals, or hopping terms, these terms depend on the problem we are studying.

5.2 Linear Chain of Atoms.

We take for model a linear 1D chain of atoms spaced by a distance a . Since we are studying this in the thermodynamic limit we know that the boundary conditions will have only a small influence on the result, so we take periodic boundary conditions because they make the computations easier. By periodic boundary conditions we mean that everything has to repeat itself after N_n steps. A more graphical way to see it would be to say that we are not actually studying a linear chain of atoms. Instead we are studying a circular chain of atoms and in the thermodynamic limit we can consider as being a linear chain of atoms when we are close to it. Then the symmetry of the problem gives that $t_{n,l} = t_{|n-l|}$ and $\mathbf{R}_m \approx (ma)\mathbf{x}$. With this the general solution derived before can be rewritten as:

$$-t_0 a_{k,n} - \sum_{m=1}^{\frac{N_n}{2}-1} t_m (a_{k,n+m} + a_{k,n-m}) = (E_k - E_v) a_{k,n} \Leftrightarrow - \sum_{l=1}^{\frac{N_n}{2}-1} t_l (a_{k,n+l} - a_{k,n-l}) = (E_k - E_v + t_0) a_{k,n}$$

Furthermore since V is a -periodic we can apply Bloch's theorem, which gives us directly that:

$$a_{k,l} = a_{k,0} e^{ikla} \quad \text{and normalization forces} \quad a_{k,l} = e^{ikla}$$

Since the whole system is also N_n periodic we also get that:

$$e^{ikN_n a} = 1 \Rightarrow k = \frac{2\pi m}{N_n a}, m \in \mathbb{Z}^*$$

5.2.1 First neighbor approximation.

If we assume that the hopping integral cancel as soon as we jump from states that aren't direct neighbors the general solution then reduces to:

$$-t_1 (a_{k,n+1} + a_{k,n-1}) = (E_k - E_v + t_0) a_{k,n} \Leftrightarrow -2t_1 \cos(ka) = E_k - E_v + t_0 \Leftrightarrow E_k = E_v - t_0 - 2t_1 \cos(ka)$$

So we see that the energy is completely degenerate and we call $q = \hbar k$ the quasi-momentum.

Chapter 6

Fractals (heuristically)

Definition 6.0.1. Hausdorff dimension. Given X a set and ε take $\mathcal{U} = \{U_i\}_i$ a set of open balls of diameter smaller or equal than ε , that covers X , i.e $X \subset \bigcup_i U_i$. Then take $\delta > 0$ and define: $H_\varepsilon^\delta(X) = \inf_{\mathcal{U}} \{\sum_i \text{diam}(U_i)^\delta\}$ and set $H^\delta(X) = \lim_{\varepsilon \rightarrow 0} H_\varepsilon^\delta(X)$. Then we define the Hausdorff dimension to be:

$$\dim_H(X) = \inf\{\delta \mid H^\delta(X) = 0\}$$

Proposition 6.0.1. For any countable set X we have $\dim_H(X) = 0$.

Definition 6.0.2. Box Dimension. For $\varepsilon > 0$ let $N(\varepsilon)$ be the smallest number of ε -balls needed to cover X . Then we define the Box dimension to be:

$$\dim_B(X) = \limsup_{\varepsilon \rightarrow 0} \frac{\log(N(\varepsilon))}{\log(1/\varepsilon)}$$

Remark 8. Note that Proposition 6.0.1 does not hold for the box dimension.

Remark 9. Note that $N(\varepsilon) \sim \varepsilon^{-D_B}$ yields that:

$$\limsup_{\varepsilon \rightarrow 0} \frac{\log(N(\varepsilon))}{\log(1/\varepsilon)} = \limsup_{\varepsilon \rightarrow 0} \log_{1/\varepsilon} \left(\frac{1}{\varepsilon} \right)^{D_B} = D_B$$

Proposition 6.0.2. For any X we have that:

$$\dim_H(X) \leq \dim_B(X)$$

Definition 6.0.3. Order of an open cover \mathcal{U} of X . The order of \mathcal{U} is the smallest number n (if it exists) such that each point of X belongs to at most n sets in \mathcal{U} .

Definition 6.0.4. Refinement of \mathcal{U} . A refinement of \mathcal{U} is another set \mathcal{U}' such that $\forall U \in \mathcal{U}', \exists V \in \mathcal{U}, V \subset U$.

Definition 6.0.5. Topological dimension of X . The topological dimension of X is defined to be the minimum value of n , such that every open cover \mathcal{U} of X has a refinement with order smaller or equal to $n + 1$. If no such minimal n exists, the space is said to be of infinite covering dimension.

Definition 6.0.6. Fractal. A fractal is a set X for which the Hausdorff dimension is strictly greater than the Topological dimension.

Definition 6.0.7. Open set condition (OSC) on X . Say X is generated by the sequence of contractions ψ_i . The open set condition states that there exists a compact open set V such that

$$\bigcup_{i=1}^m \psi_i(V) \subset V$$

where the sets in union on the left are pairwise disjoint.

Proposition 6.0.3. If X satisfies the open set condition then $\dim_H(X) = \dim_B(X)$.

Chapter 7

Quasi-periodic lattice in a 1 dimensional potential well

7.1 General setting of the problem

We will consider only one dimensional systems, i.e. potential wells of width L .

Definition 7.1.1. We will call a generic eigenstate of the one-electron hamiltonian as ψ_n .

Definition 7.1.2. We define the IPR_0 (0 indicates that we are considering the ground state) for a wavefunction ψ_n as

$$IPR_0 = \frac{\int dx |\psi(x)_n|^4}{(\int dx |\psi(x)_n|^2)^2}$$

Hypothesis 7.1.1. We will use a potential $V_T(x) = \frac{V_1}{2} \cos(2k_1x) + \frac{V_2}{2} \cos(2k_2x + \phi)$ where $k_2/k_1 = (\sqrt{5} - 1)/2$ and $\phi = 4$.

Definition 7.1.3. We define a localized state as a wavefunction ψ_n such that $IPR_0(\psi_n) \sim L^0$ and extended if $IPR_0(\psi_n) \sim 1/L$. In other words the extended state has a vanishingly small IPR_0 and the localized state has a finite IPR_0 .

Definition 7.1.4. Dirichlet's boundary conditions: We will impose absorbing boundary conditions, i.e. $\psi_n(0) = \psi_n(L) = 0$.

Definition 7.1.5. For each case that we will analyse we will look for V_c , a critical value that, if overpassed by V , will determine the appearance of a Mobility Edge (ME), i.e. a value that determines the separation of the energy spectrum in localized and extended states (before V_c we have only extended states).

Remark 10. By V we mean the potential which is being varied (i.e. either both of V_1, V_2 or just one of the two).

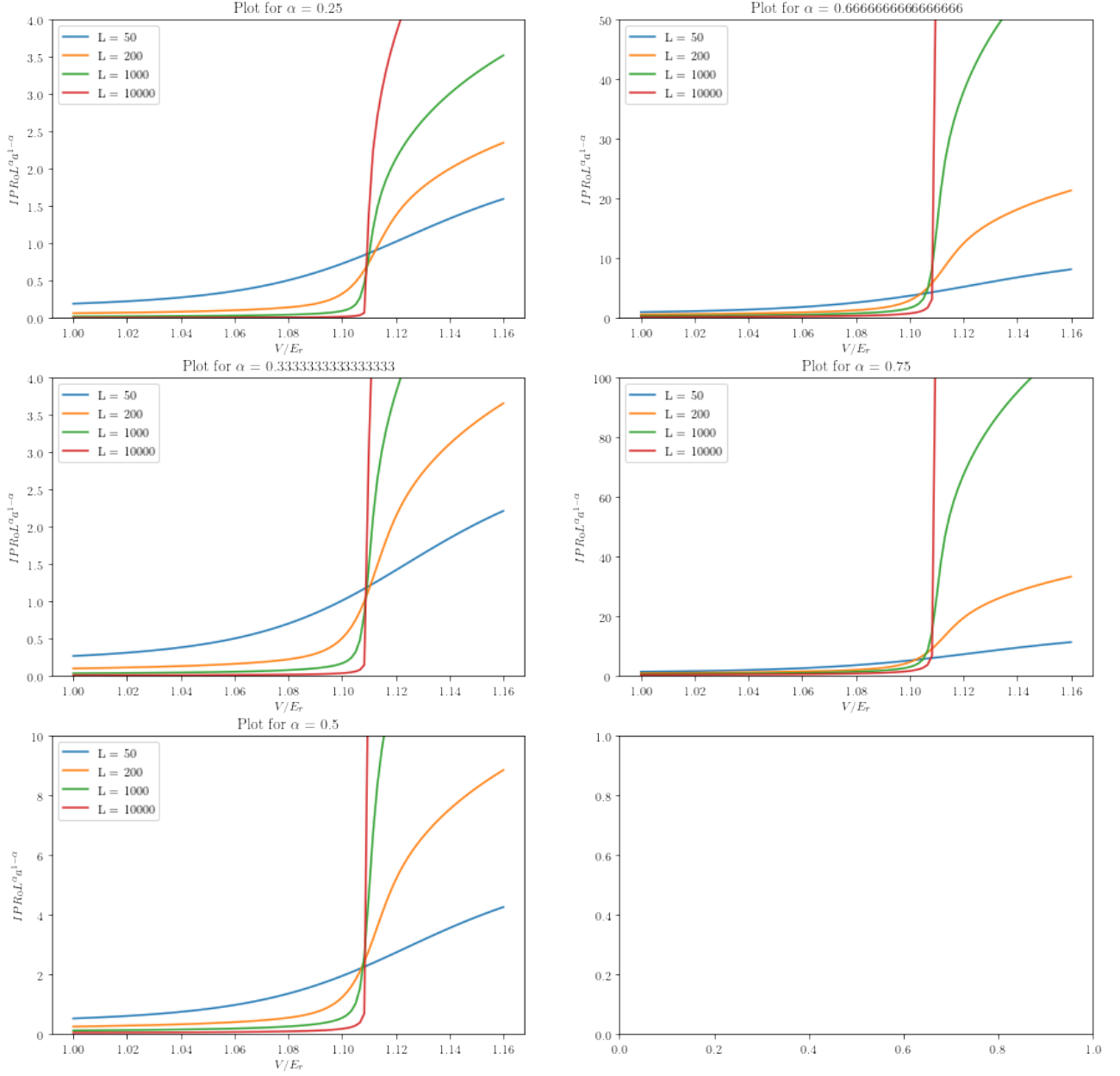
Remark 11. (For now) we propose the following subsections for each of the cases that we studied: a first subsection to represent the graph of the IPR_0 as a function of L^α , for various α , in order to determine the value of V_c , then a subsection for the determination of V_c (which is the value at which the curves of the previous section meet for different L), and then a subsection to plot IPR_0 as a function of $V - V_c$, in order to verify that for large L , $IPR_0 \sim (V - V_c)^\nu$, $\nu \approx 1/3$ for V close to the transition V_c .

7.2 Varying $V = V_1 = V_2$

When varying both potentials together we get the followings plots:

7.2.1 $IPR_0 \cdot L^\alpha$ vs. V

We will choose $\alpha \in \{1/4, 1/3, 1/2, 2/3, 3/4\}$

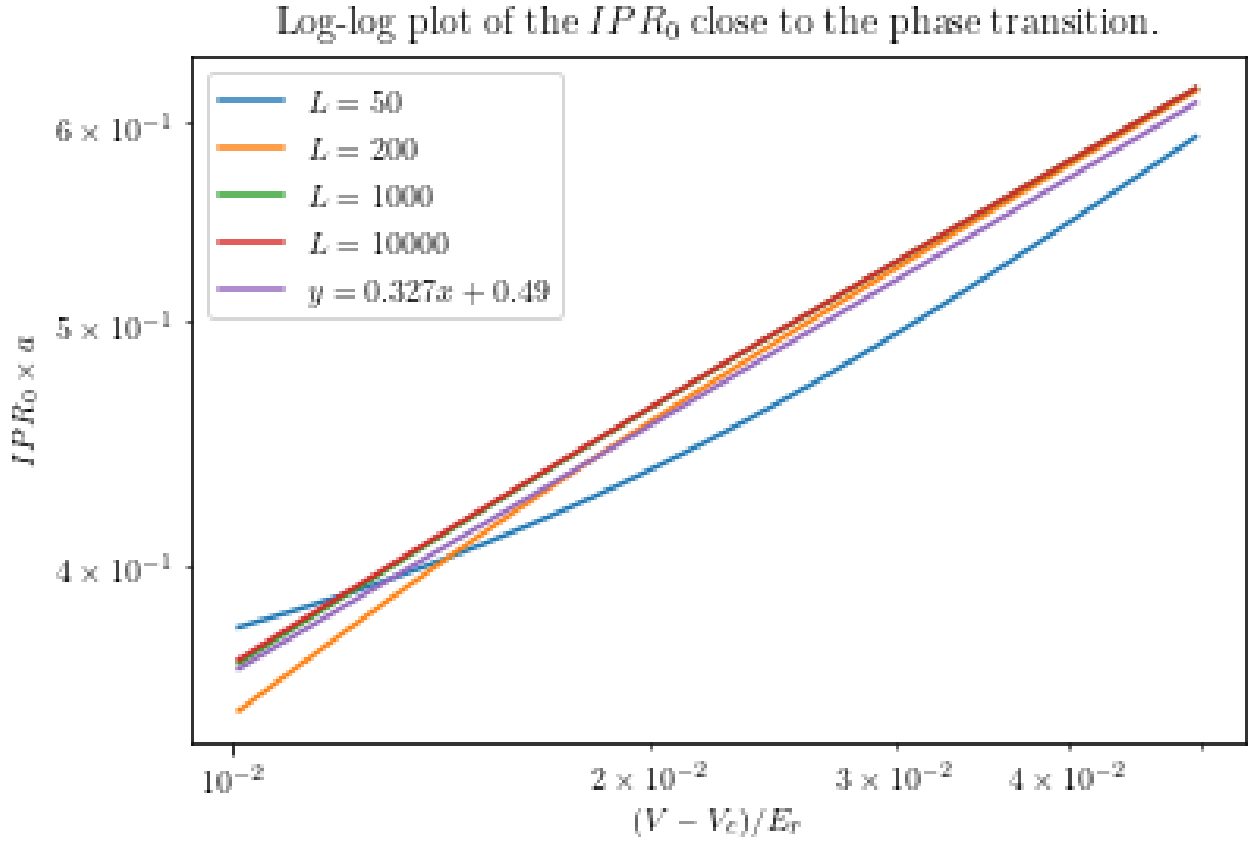


7.2.2 Computation of V_c

Now taking the case where $\alpha = 1/2$ which is clearly always the most precise one, we get that:

$$V_c = (1.1099 \pm 0.0016)E_r$$

7.2.3 IPR_0 vs. $V - V_c$

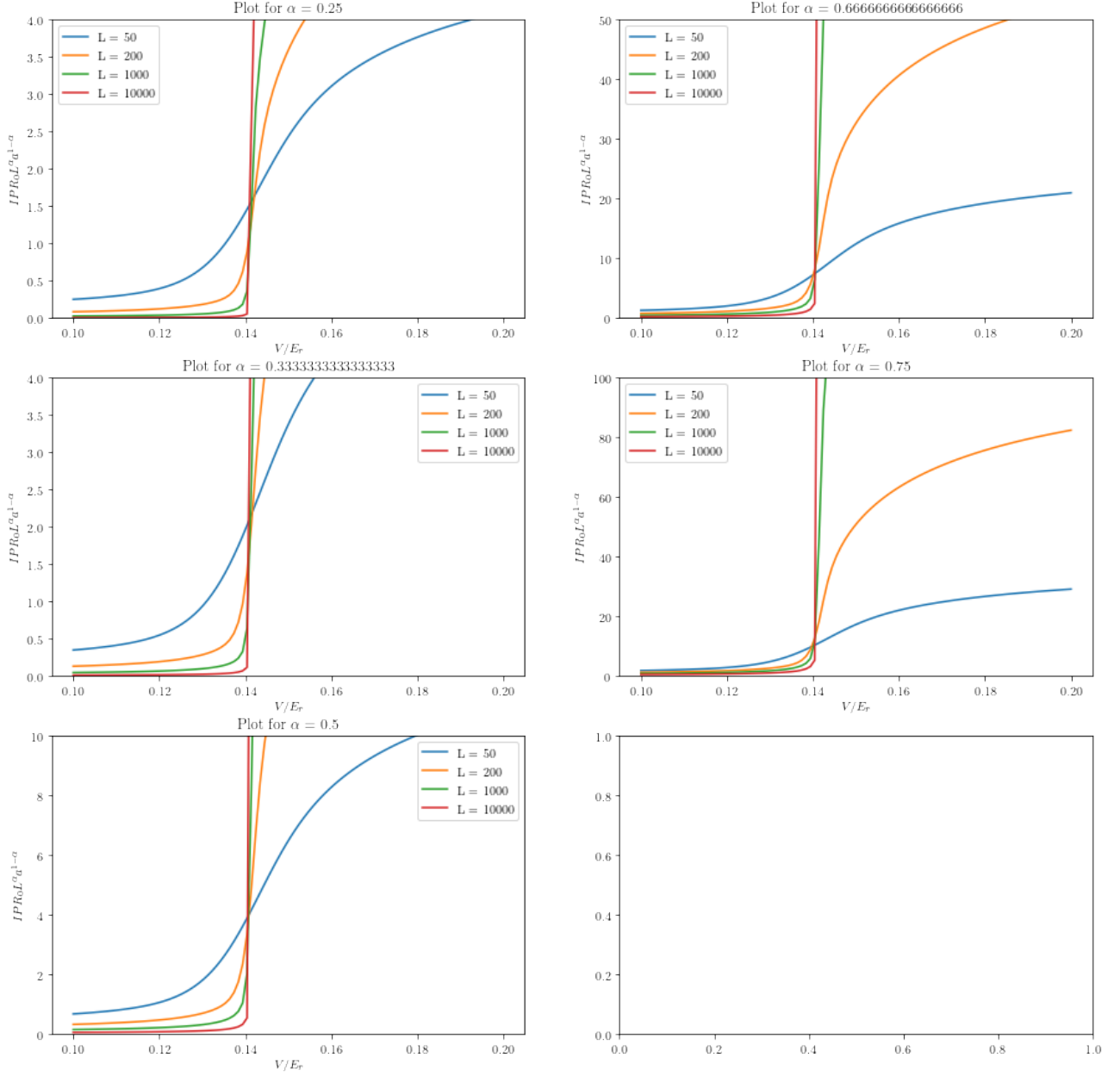


$$\nu = 0.32 \pm 0.01$$

7.3 Varying V_2 with $V_1 = 8$

7.3.1 $IPR_0 \cdot L^\alpha$ vs. V

We will choose $\alpha \in \{1/4, 1/3, 1/2, 2/3, 3/4\}$

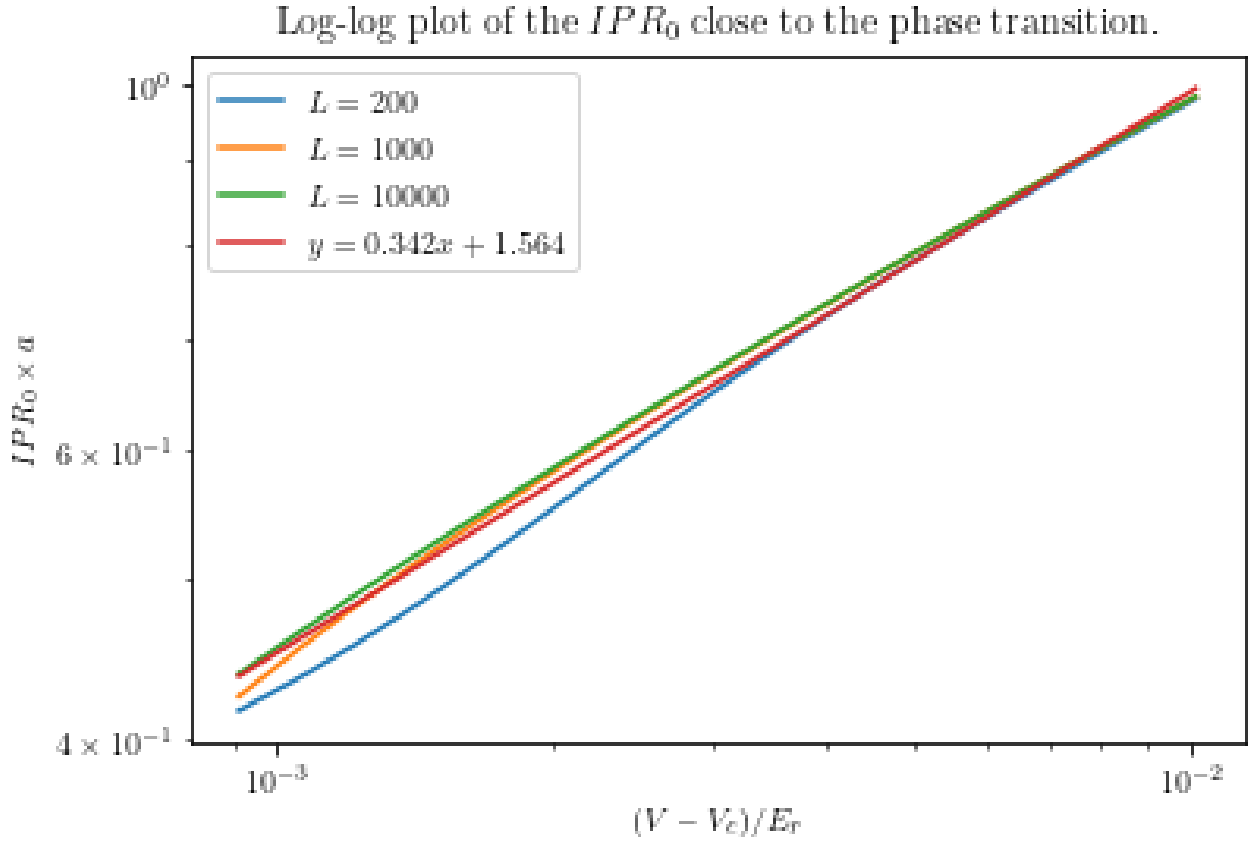


7.3.2 Computation of V_c

Now taking the case where $\alpha = 1/2$ which is clearly always the most precise one, we get that:

$$V_c = (0.1414 \pm 0.001)E_r$$

7.3.3 IPR_0 vs. $V - V_c$

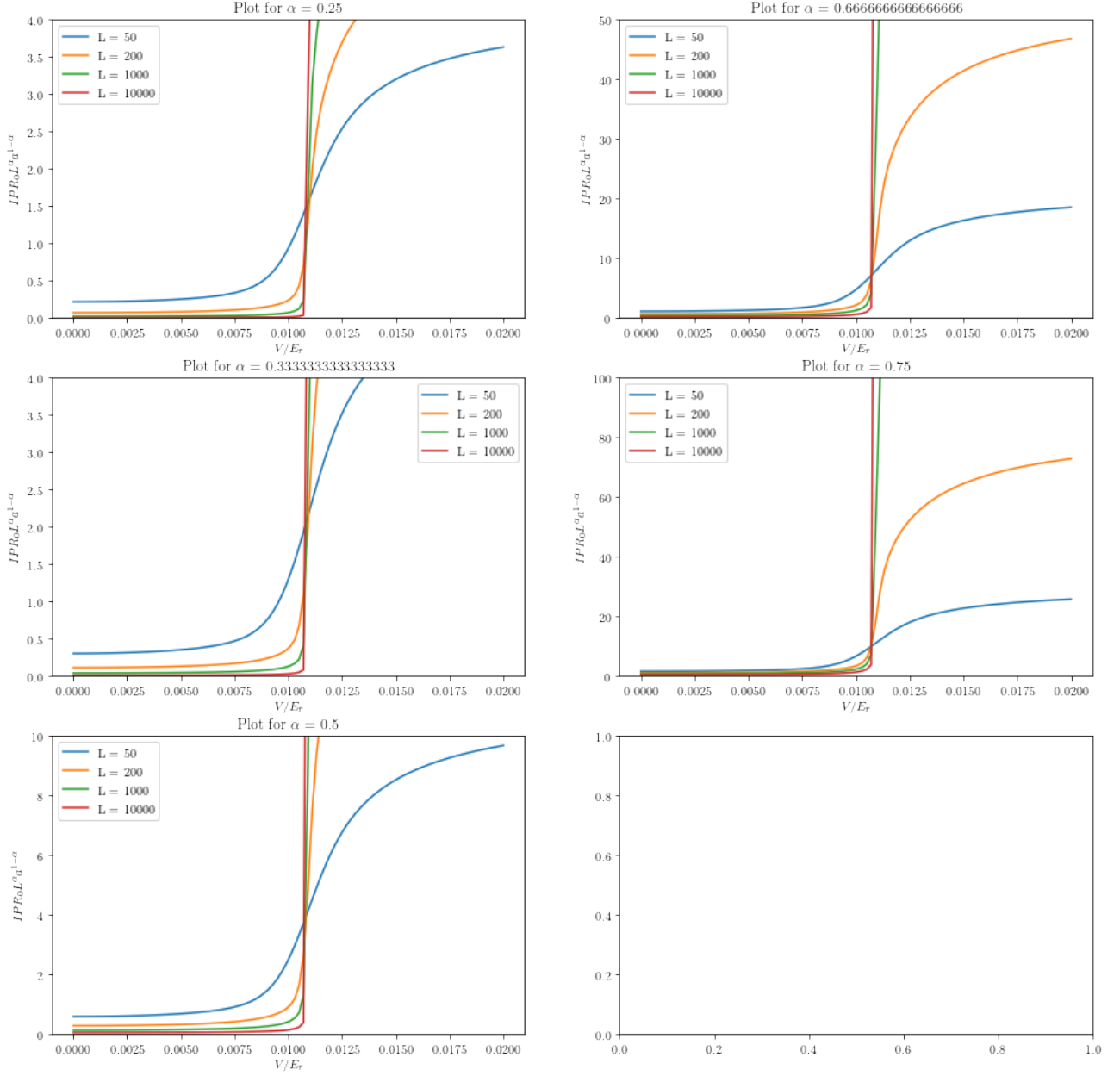


$$\nu = 0.34 \pm 0.01$$

7.4 Varying V_1 with $V_2 = 7$

7.4.1 $IPR_0 \cdot L^\alpha$ vs. V

We will choose $\alpha \in \{1/4, 1/3, 1/2, 2/3, 3/4\}$

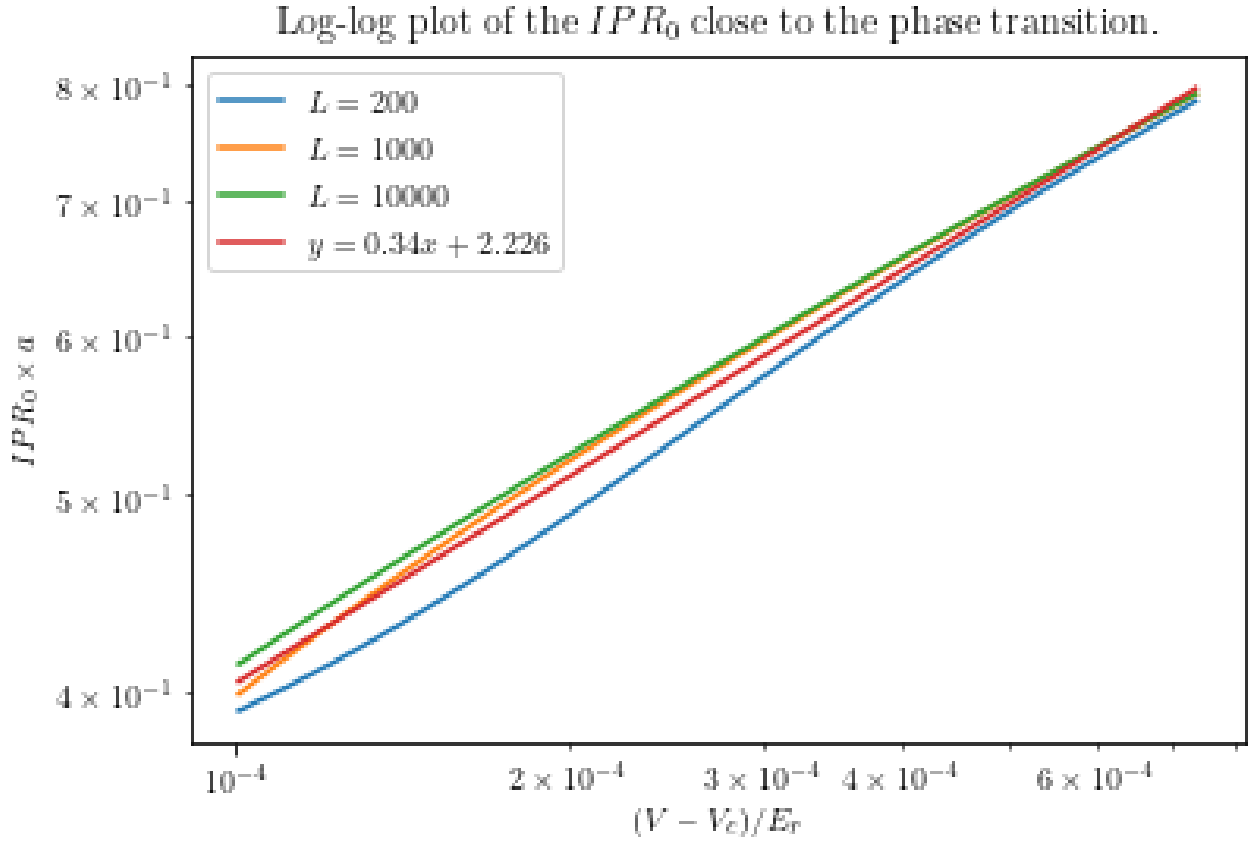


7.4.2 Computation of V_c

Now taking the case where $\alpha = 1/2$ which is clearly always the most precise one, we get that:

$$V_c = (0109 \pm 0.0002)E_r$$

7.4.3 IPR_0 vs. $V - V_c$

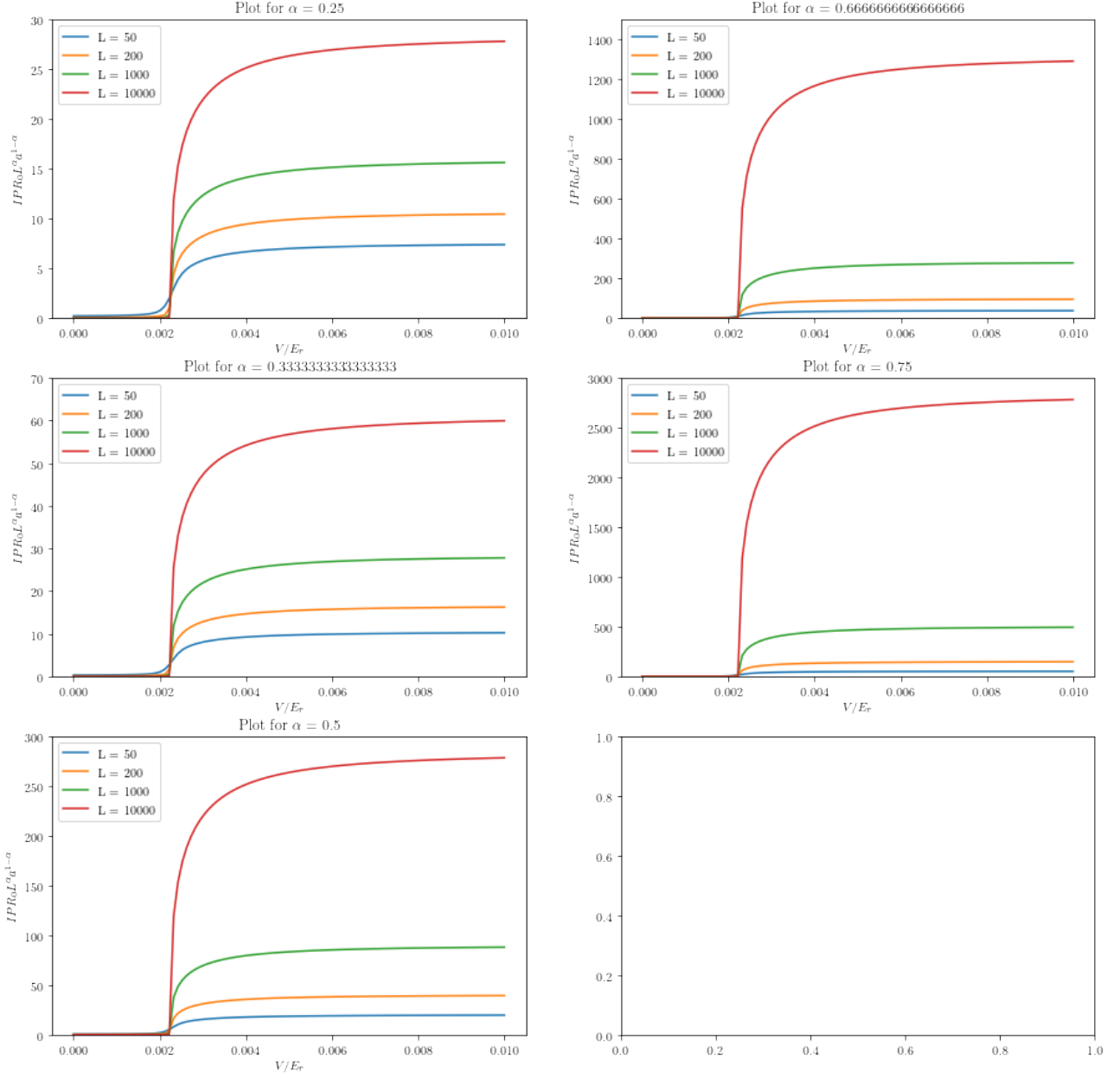


$$\nu = 0.34 \pm 0.01$$

7.5 Varying V_2 with $V_1 = 30$

7.5.1 $IPR_0 \cdot L^\alpha$ vs. V

We will choose $\alpha \in \{1/4, 1/3, 1/2, 2/3, 3/4\}$



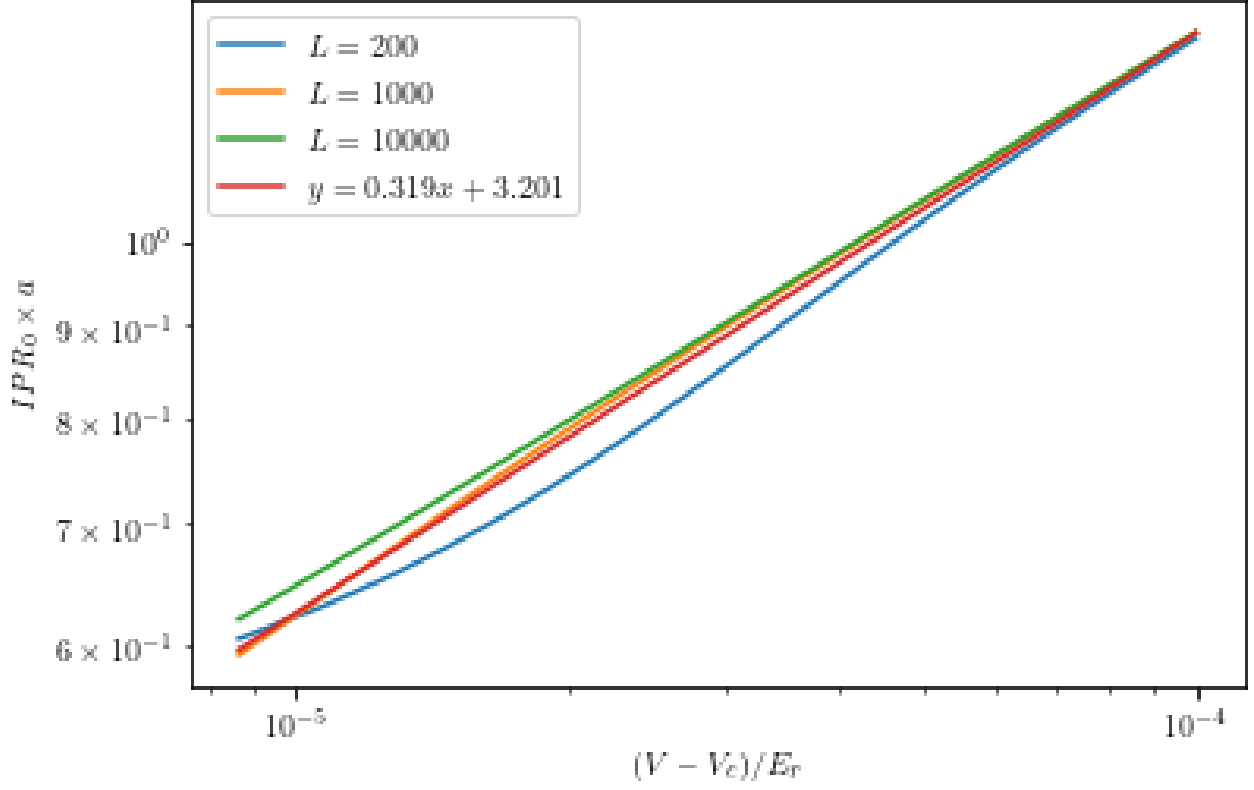
7.5.2 Computation of V_c

Now taking the case where $\alpha = 1/2$ which is clearly always the most precise one, we get that:

$$V_c = (0.0023 \pm 0.0002)E_r$$

7.5.3 IPR_0 vs. $V - V_c$

Log-log plot of the IPR_0 close to the phase transition.



$$\nu = 0.32 \pm 0.01$$

7.5.4 General table with the results

cases	V_c/E_r	Error V_c/E_r	ν	Error ν	ν'	Error ν'
Vary $V = V_1 = V_2$	1.1099	0.0016	0.32	0.01	0.26	0.01
Vary V_2 , $V_1 = 8$	0.1414	0.001	0.34	0.01	0.25	0.01
Vary V_1 , $V_2 = 7$	0.109	0.0002	0.34	0.01	0.25	0.01
Vary V_2 , $V_1 = 30$	0.0023	0.0002	0.32	0.01	0.25	0.01

Chapter 8

τ_q, IPR_q and fractality

8.1 Introduction

In this case of $V = V_1 = V_2$ we are also interested in studying the IPR_0^q for $q = 2, 3, 4$. We define

$$IPR_0^q = \frac{\int dx |\psi_n(x)|^{2q}}{(\int dx |\psi_n(x)|^2)^q}.$$

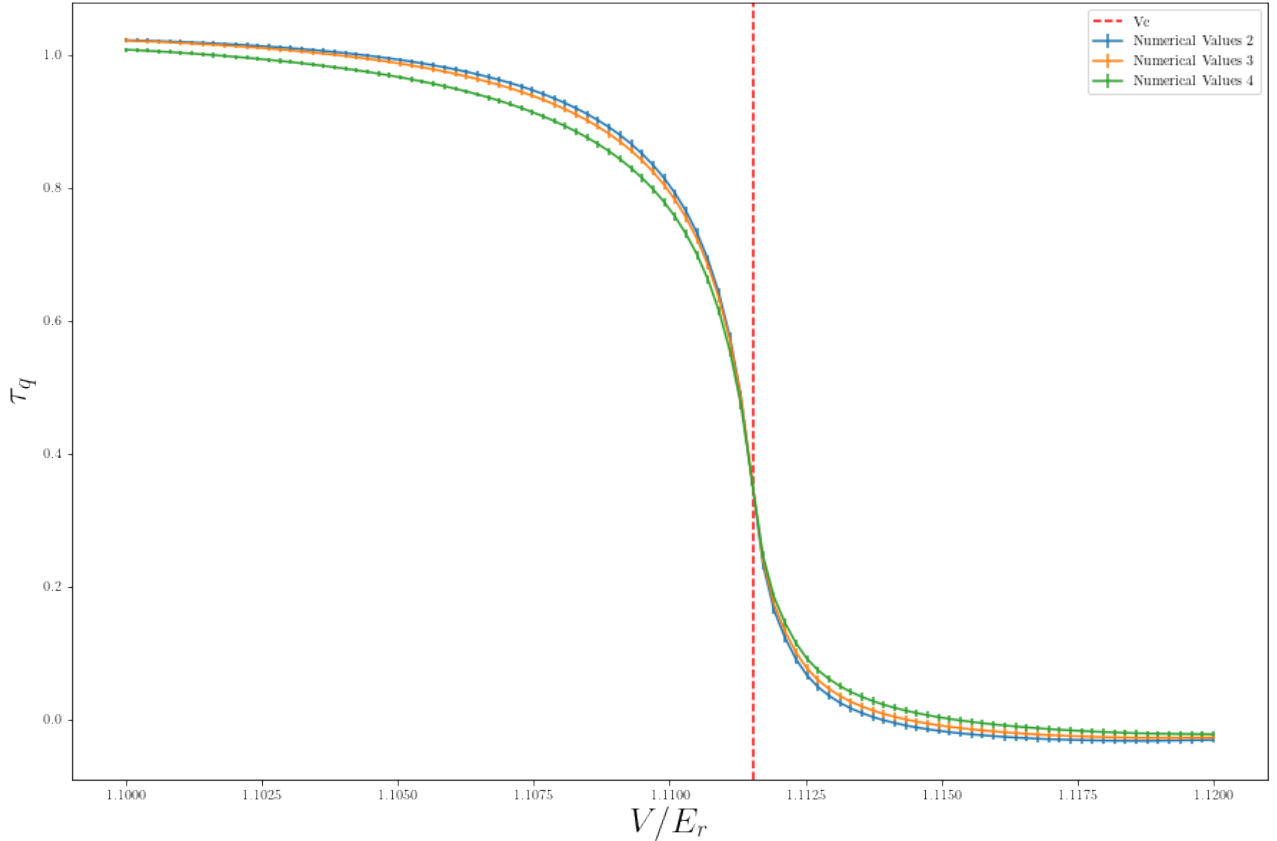
According to the research paper "RevModPhys.80.1355", we have that the IPR_0^q is important to study the fractality of the wavefunction. In particular at criticality, we have that $IPR_0^q \sim L^{-\tau_q}$.

8.2 $V = V_1 = V_2, q = 2$

8.2.1 $IPR_0^q \cdot L^{\tau_q/2}$ vs. V

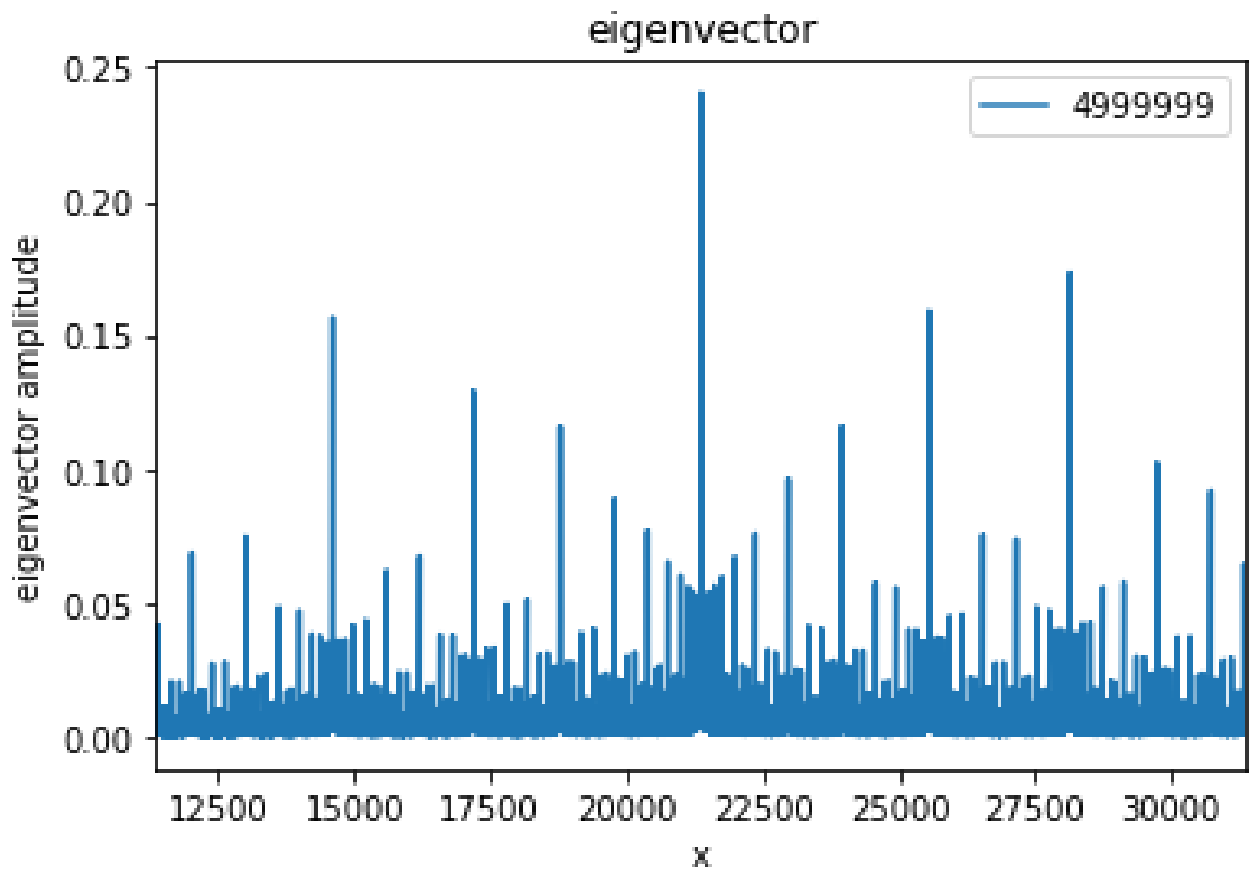
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8.2.2 τ_q vs. V at criticality for various L

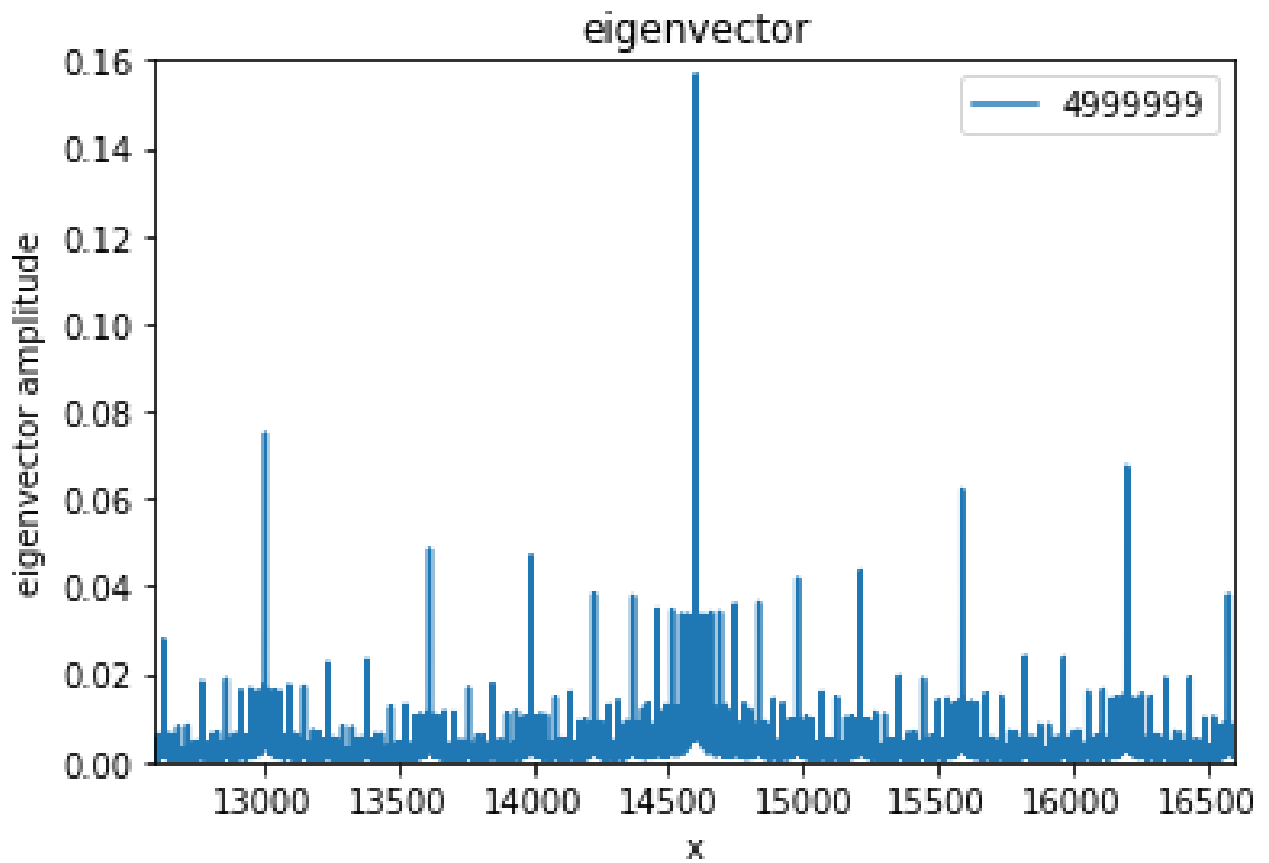


8.2.3 Wavefunction at criticality

If we plot the amplitude of the ground state, for $V = V_1 = V_2 = 1.1114E_r$ and $L = 50000a$, vs. x we get the following plot, which induces us to think of a fractal behaviour:



Then we perform a zoom to get the following self-similar structure:



Now we examine the fractality of this wavefunction.

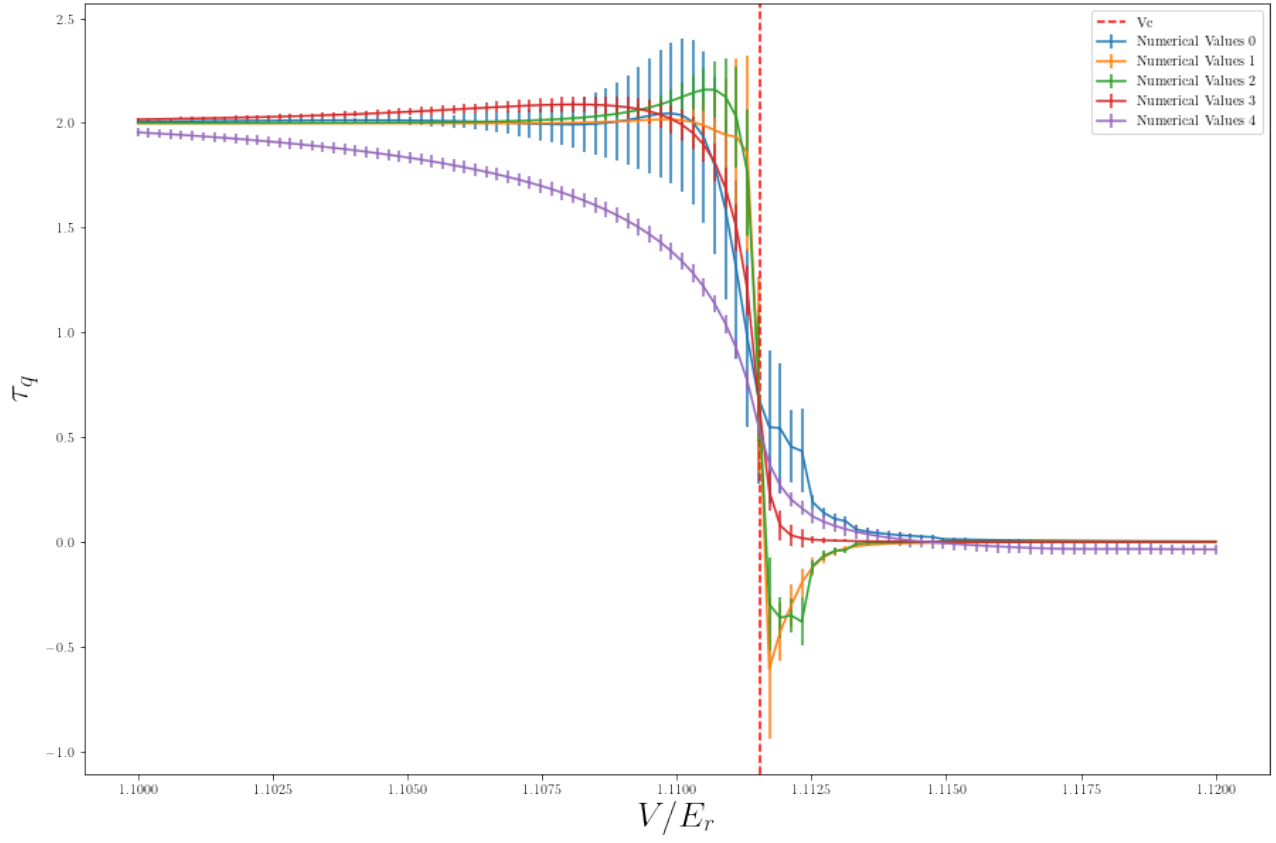
8.2.4 Extended/ localized state

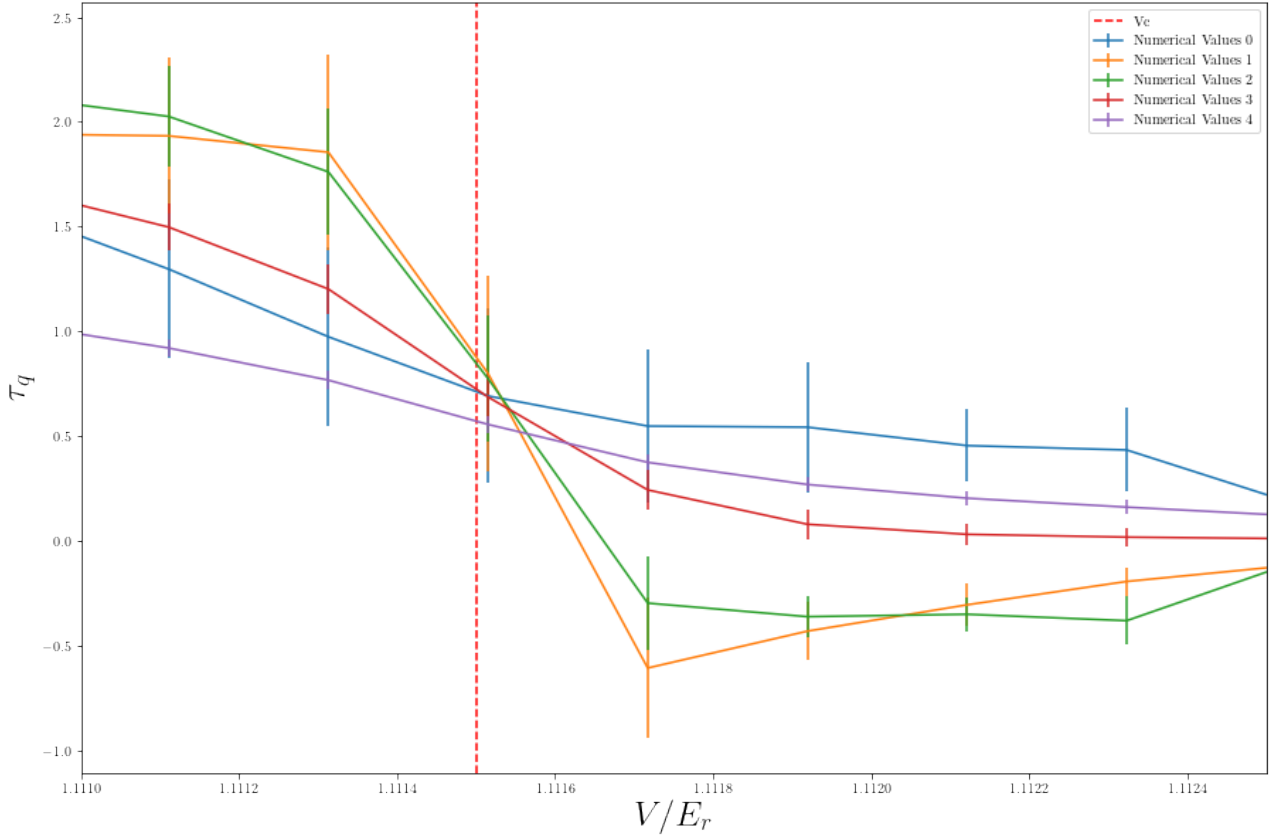
8.2.5 Fractal (Hausdorff) dimension as a function of the potential V

8.3 $V = V_1 = V_2$, $q = 3$

8.3.1 $IPR_0^q \cdot L^{\tau_q/2}$ vs. V

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8.3.2 τ_q vs. V at criticality for various L 



We can see that for various L , at criticality τ_q passes through a fast transition from the value $(q-1) = 2$ before V_c , i.e. extended state, to the value 0 after V_c , i.e. localized state.

8.3.3 Wavefunction at criticality

8.3.4 Extended/ localized state

8.3.5 Fractal (Hausdorff) dimension as a function of the potential V

8.4 $V = V_1 = V_2, q = 4$

8.4.1 $IPR_0^q \cdot L^{\tau_q/2}$

8.4.2 τ_q vs. V at criticality for various L

8.4.3 Wavefunction at criticality

8.4.4 Extended/ localized state

8.4.5 Fractal (Hausdorff) dimension as a function of the potential V

8.5 Comparison τ_2, τ_3, τ_4

Chapter 9

Mobility edge with $V_2 = 7$, varying V_1

9.1 $q=2$