SPECTRAL ANALYSIS FOR THE BI-LAYER TWO-DIMENSIONAL GRAPHENE OPERATOR

MCQM

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Presentation's route:

1. Tight binding model for the graphene Hamiltonian.
2. Spectral bounds for the non self-adjoint case.
3. Conclusion and remarks.

1.1 Tight-binding model

Lattice structure with $\{R_m \mid \textit{Sites Position}\} \longrightarrow$ Bloch's Theorem

$$\text{Hydrogen like}: \qquad \phi_j \qquad \textit{'Basis function'}$$

$$\text{Generalized Orbiltals}: \quad \Phi_j(k, r) = \frac{1}{\sqrt{N}} \sum_{m=1}^{N} e^{i\,k \cdot R_m} \phi_j(r - R_m)$$

The index $j-$ distinguishes among different types of orbital shapes.

Energy of the j-th band:

$$E_j(k) = \frac{\langle \Phi_j | H | \Phi_j \rangle}{\langle \Phi_j | \Phi_j \rangle} \quad \longrightarrow \quad \det(H - E_j S) = 0.$$

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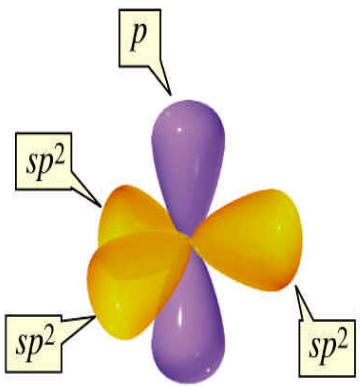
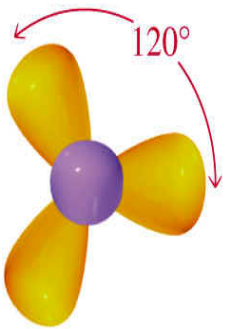
1.2 A bit of fancy...

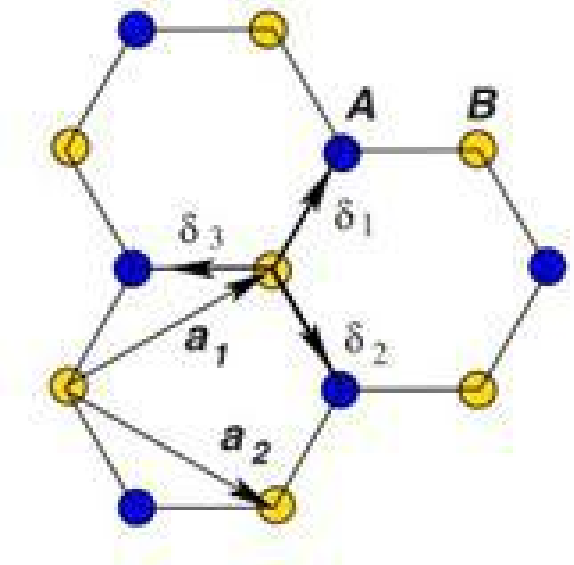
In graphene, each site of the lattice corresponds to a carbon atom which has 4 valence electrons: only one turns out to be free to conduct.



side view



top view



1.3 The Hamiltonian

The index of the independent orbitals runs among $j = A, B$:

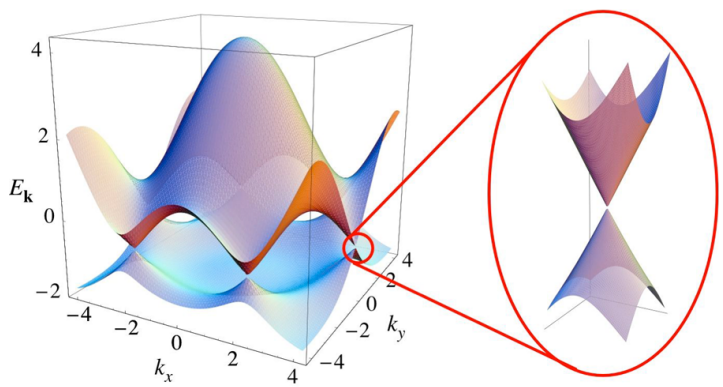
$$H = \begin{pmatrix} \epsilon_{2p_z} & -\gamma_0 f(k) \\ -\gamma_0 f^*(k) & \epsilon_{2p_z} \end{pmatrix}$$

where:

ϵ_{2p_z} is the *onsite energy* $\gamma_0 f(k)$ is the *hopping energy*,

$$f(k) = e^{ik_y \frac{a}{\sqrt{3}}} + 2e^{-ik_y \frac{a}{2\sqrt{3}}} \cos\left(k_x \frac{a}{2}\right) \approx -\frac{\sqrt{3}a}{2\hbar}(\pm p_x - ip_y).$$

$$E_\pm = \frac{\epsilon_{2p_z} \pm \gamma_0 |f(k)|}{1 \pm S_0 |f(k)|}$$



2D Single-layer graphene:

$$H_{0,1} = v \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix} \qquad \texttt{(2D-Dirac)}$$

2D Bi-layer graphene : (*tight binding model*)

$$H = \begin{pmatrix} \epsilon_{2p} & -\gamma_0 f(k) & 0 & 0 \\ -\gamma_0 f^*(k) & \epsilon_{2p} & \gamma_1 & 0 \\ 0 & \gamma_1 & \epsilon_{2p} & -\gamma_0 f(k) \\ 0 & 0 & -\gamma_0 f^*(k) & \epsilon_{2p} \end{pmatrix}$$

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1.5 In summary

2D Single-layer graphene:

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2D Bi-layer graphene:

$$H_{0,2} = -\frac{1}{2m} \begin{pmatrix} 0 & (p_x - ip_y)^2 \\ (p_x + ip_y)^2 & 0 \end{pmatrix} \qquad \texttt{(2D Dirac-like)}$$

Both the models share a *pseudo-spin* interpretation of charge distribution.

2.1 2D Bilayer operator

We want to study the spectral properties of $D = D_\tau + V$ in $L^2(\mathbb{R}^2) \otimes \mathbb{C}^2$ where:

$$D_\tau = \begin{pmatrix} \tau & 4\partial_{\bar{z}}^2 \\ 4\partial_z^2 & -\tau \end{pmatrix}$$

endowed with an external non-Hermitian potential $V = (V_{ij})$.

We recall:

$$\partial_{\bar{z}} = \frac{1}{2}\Big(\frac{\partial}{\partial x_1} + i\frac{\partial}{\partial x_2}\Big), \qquad \partial_z = \frac{1}{2}\Big(\frac{\partial}{\partial x_1} - i\frac{\partial}{\partial x_2}\Big)$$

are the usual Wirtinger derivatives.

2.2 Bound for complex eigenvalues: 1D Dirac

Theorem (J-C.Cuenin, A.Laptev, C.Tretter)

Consider the operator $H = H_0 + V$ is defined on $L^2(\mathbb{R}) \otimes \mathbb{C}^2$ where:

$$H_0 = -i\frac{d}{dx}\sigma_1 + mc^2\sigma_3, \quad \sigma_1 := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \sigma_3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$V = (V_{ij})^2$ with $V_{ij} \in L^1(\mathbb{R})$ for $i, j = 1, 2$ s.t.

$$\|V\|_1 = \int_{\mathbb{R}} |V(x)|\, dx = \int_{\mathbb{R}} \Big(\sum_{i,j=1\ldots,2} |V_{ij}(x)|^2 \Big)^{1/2} dx \; < 1$$

Then every non-embedded eigenvalue $z \in \mathbb{C} \setminus \sigma(H_0)$ of H lies in a region $\mathcal{R}$ which is the disjoint union of two disks

$$z \in \mathcal{R} := D(mx_0, |mr_0|) \cup D(-mx_0, |mr_0|).$$

2.2 Bound for complex eigenvalues: 1D Dirac

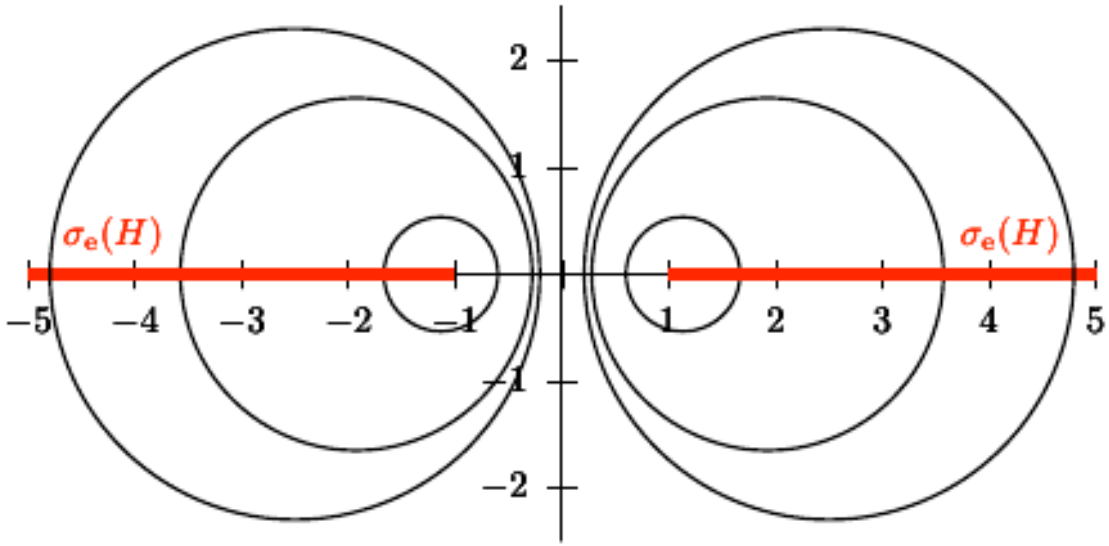


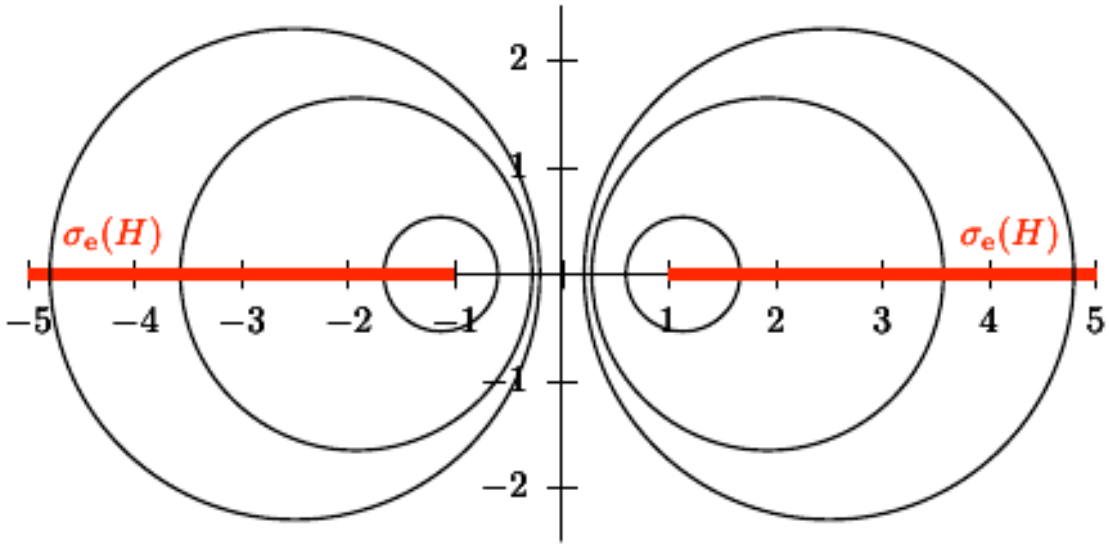
FIGURE 1. The two disks of Theorem 2.1 for three different values of $\|V\|_1 \in (0,1)$ and $m = 1$.

$$x_0 := \sqrt{\frac{\|V\|_1^4 - 2\|V\|_1^2 + 2}{4(1 - \|V\|_1^2)} + \frac{1}{2}} \qquad r_0 := \sqrt{\frac{\|V\|_1^4 - 2\|V\|_1^2 + 2}{4(1 - \|V\|_1^2)} - \frac{1}{2}}$$

Question:

Is it possible to determine a similar kind of bound for the bilayer case?

2.2 Bound for complex eigenvalues: 1D Dirac



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2.3 Bound for complex eigenvalues: 2D Bilayer

Theorem

Let $k \notin \sigma(D_\tau)$ be a complex eigenvalue of the operator $D = D_\tau + V$ and consider $1 < p < 4/3$. Then:

$$C \frac{\omega(k,\tau)^p}{|\mu|^{p-1}} \int_{\mathbb{R}^2} |V(x)|^p dx \geq 1$$

where C is independent from V and k, and where we set:

$$\mu^2 = k^2 - \tau^2, \qquad \omega(k,\tau) = \Big(\sqrt{\Big|\frac{k-\tau}{k+\tau}\Big|} + \sqrt{\Big|\frac{k+\tau}{k-\tau}\Big|} + 1 \Big).$$

In particular if $\tau = 0$, then:

$$|k|^{p-1} \leq C \int_{\mathbb{R}^2} |V(x)|^p dx.$$

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$$C\Big(|\ln|\mu||\sup_{x\in\mathbb{R}^2}\int_{|x-y|<(2|\mu|)^{-1}}|V(y)|\,dy+ \sup_{x\in\mathbb{R}^2}\int_{\mathbb{R}^2}\Big(1+|\ln|x-y||\Big)|V(y)|dy+ +\omega(k,\tau)\int_{\mathbb{R}^2}|V(x)|dx\Big)\geq 1.$$

If $\tau = 0$ then for small potential:

$$r \approx \exp\Big(-\frac{C}{\int|V|dx}\Big) \qquad \text{as} \qquad \int|V|dx \to 0.$$

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Let $k \notin \sigma(D_\tau)$ be an eigenvalue of the operator $D = D_\tau + V$ with $V = iW^2$ such that $W_{i,j} \geq 0$. Then $\mathrm{Re}(k) > 0$ and it holds:

$$\left(C\left(\left|\frac{k+\tau}{k-\tau} - 1\right| + \left|\frac{k-\tau}{k-\tau} - 1\right|\right) + 1\right)\frac{\pi}{4}\int_{\mathbb{R}^2} \mathrm{tr}|V|dx \geq 1, \qquad (1)$$

where the constant C is independent of V and k.

If $\tau = 0$ and

$$\frac{\pi}{4}\int_{\mathbb{R}^2} \mathrm{tr}|V|dx < 1, \qquad (2)$$

then the operator $D = D_0 + V$ does not have eigenvalues outside of the real line $\mathbb{R}$, i.e. the spectrum of D is real.

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First theorem proof sketch:

Consider the polar decomposition $V = U|V|$ for the potential:

$$V = BA = \left(U|V|^{1/2}\right)|V|^{1/2}$$

The proof is based on the *Birman-Schwinger's principle*:

- k is an eigenvalue of H if and only if -1 is an eigenvalue of:

$$Q(k) := A(D_\tau - k)^{-1}B \colon \mathcal{H} \to \mathcal{H}, \qquad k \in \rho(D_m).$$

where $Q(k)$ is a bounded Hilbert-Schmidt operator.

So it follows that if $k \in \rho(H_0)$:

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First theorem proof sketch:

We use the following factorization:

$$(D_\tau - k)^{-1} = (\tau\sigma_3 + k - \mu)(\Delta^2 - \mu^2)^{-1} + (D_0 + \mu)(\Delta^2 - \mu^2)^{-1}$$

where $\mu^2 = k^2 - \tau^2$.

The resolvent kernel of the bi-harmonic operator $(\Delta^2 - \mu^2)^{-1}$ is explicit:

$$g_\mu(x, y) = \frac{i}{8\mu}\Big(H_0^{(1)}(\sqrt{\mu}|x - y|) - H_0^{(1)}(i\sqrt{\mu}|x - y|)\Big).$$

So that the kernel of $(D_0 - k)^{-1}$ reads as:

$$\rho_\mu(|x - y|) = \begin{pmatrix} \mu\, g_\mu(x, y) & \partial_{\bar{z}}^2 g_\mu(x, y) \\ \partial_z^2 g_\mu(x, y) & \mu g_\mu(x, y) \end{pmatrix}$$

First theorem proof sketch:

Let's consider $\mu = e^{i\theta}$

$$|g_\theta(r)| \approx r^2 |\log(r)| \qquad r \leq 1/2$$
$$|g_\theta(r)| \approx 1/\sqrt{r} \qquad r > 1/2$$

...so that the constraint $1 < p < 4/3$ appears

$$||A(D_0 - k)^{-1} B||^p \leq C \frac{1}{|\mu|^{p-1}} \int_{\mathbb{R}^2} |V(x)|^p dx, \qquad \mu^2 = k^2 - m^2.$$

$$||A(D_0 + k)(\Delta^2 - \mu^2)^{-1} B||^p \leq C \frac{\Big(\omega(k,m) - 1\Big)^p}{|\mu|^{p-1}} \int_{\mathbb{R}^2} |V(x)|^p dx.$$

where C is actually dependent on an integral estimate for the kernel $\rho_\mu(|x - y|)$ but independent from k and V.

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3.1 Final remarks and conclusion

- ⋆ We can extend the result to all real $p > 1$, introducing the hypothesis of k lying in a sector of the complex plane which doesn't contain the real positive axis.

- ⋆ It's reasonable to expect an improvement in the kernel decay at zero:

$$|g_\theta(r)| \approx r^{2+\epsilon} |\log(r)| \qquad\qquad r \leq 1/2$$

- ⋆ The operator on bounded domains requires different boundary conditions depending on the different cut operated to the lattice.
  Ref.[*Freitas*, *Seigl*(2012)]

Thank you!

3.Oscillating random potential

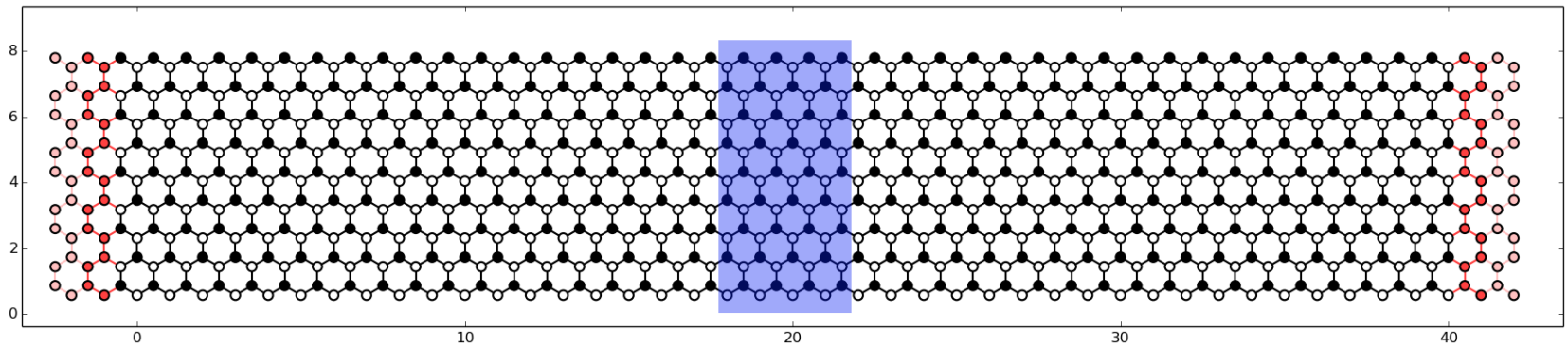

Figure : Image obtained with KWANT python package.

Two different type of potential:

- S Static: Due to imperfections of graphene.
- D Dynamic: Due to the presence of an oscillating in time potential, for example induced by water molecules.

Our meaningful property will be the *Transmission*.
In order to define it we consider the system in a general electronic state before and after the scattering:

$$\Psi_{OUT} = \mathcal{S} \cdot \Psi_{IN}$$

where $\Psi_{IN/OUT}$ are the *open channel* and

$$S = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \qquad \textit{Scattering matrix}$$

The *Transmission* is defined by:

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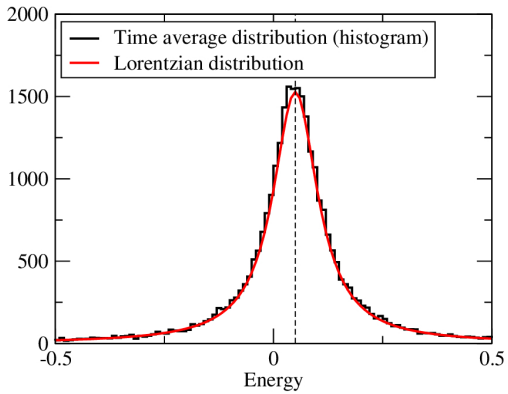
3.Oscillating random potential

Lorentzian distribution:

$$\mathcal{L}(\alpha_r, \beta_r)(x) = \frac{1}{\pi\beta_r\left(1 + (\frac{x-\alpha_r}{\beta_r})^2\right)}$$



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- D Water: $\beta_w = 0.0625, \alpha_w = 0.025$

Energy on each site:

$$E_j(t) = \mathcal{L}(\frac{\alpha_j}{2}, \beta_w)(t)$$

which is depending on time t.

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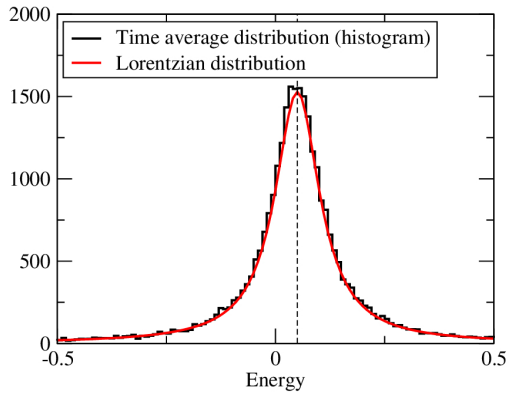

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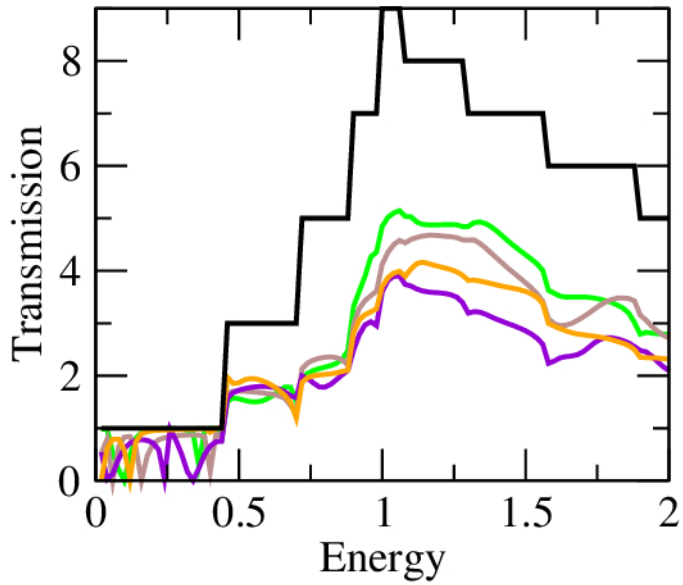

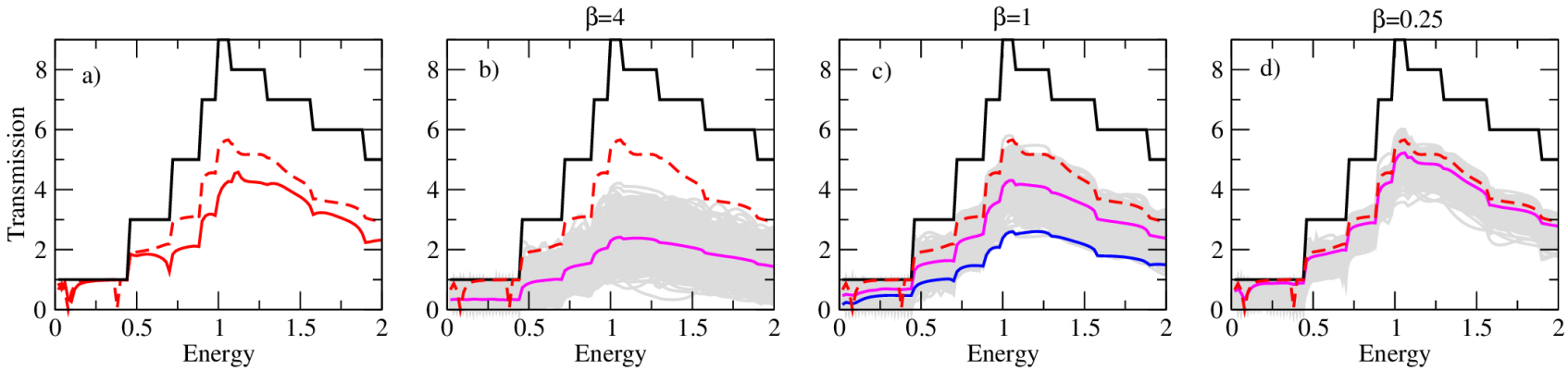

Why Lorentzian?

Are the time average of all the transmissions and the transmission of an average state comparable?

$$\langle \text{Transmission}(\Psi_t) \rangle \quad \stackrel{?}{=} \quad \text{Transmission}(\langle \Psi_t \rangle)$$

What is the average state $\langle \Psi_t \rangle$*?* It is a Lorentzian distribution!
If we consider a complex potential s.t.

$$E_j = \frac{\alpha_j}{2} + i\beta_w,$$

then

$$\text{DOS}(E_j) = \lim_{\epsilon \to 0} \left[\text{Im} \frac{1}{E_j - (\frac{\alpha_j}{2} + i\beta_w) + i\epsilon} \left(\frac{E_j + (\frac{\alpha_j}{2} + i\beta_w) + i\epsilon}{E_j + (\frac{\alpha_j}{2} + i\beta_w) + i\epsilon} \right) \right]$$

$$= \frac{1}{\pi \beta_w^2} \frac{\beta_w}{(E_j - \frac{\alpha_j}{2})^2 + \beta_w^2} = \mathcal{L}(\frac{\alpha_i}{2}, \beta_w)(E_j)$$

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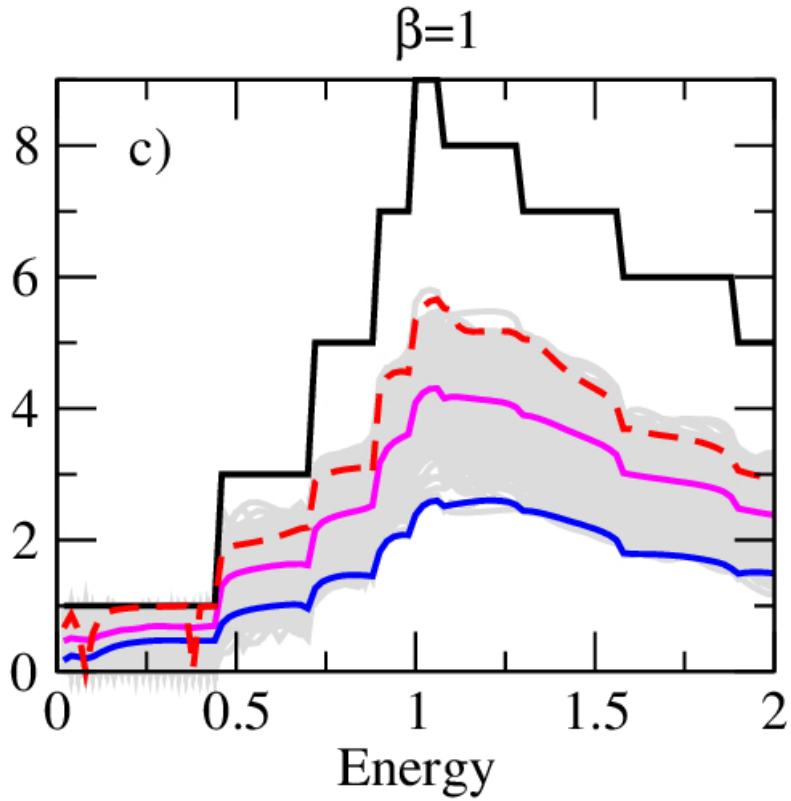

- Good qualitative response!
- Unfortunately there's a quantitative gap.