More accurate effective operators for graphene

Louis Garrigue
Cergy's university

Quantissima-sur-Oise
September 15$^{\text{th}}$, 2025

Sommaire

Sommaire

Sommaire

Motivation

$$H(\lambda) = \sum_{j=1}^{N} (-\Delta_j + v(x_j)) + \lambda \sum_{1 \leqslant i < j \leqslant N} w(x_i - x_j) = H^0 + \lambda H^1$$

Motivation

$$H(\lambda) = \sum_{j=1}^{N}(-\Delta_j + v(x_j)) + \lambda \sum_{1\leqslant i<j\leqslant N} w(x_i - x_j) = H^0 + \lambda H^1$$

Know everything at $\lambda = 0$, nothing at $\lambda \neq 0$

Motivation

$$H(\lambda) = \sum_{j=1}^{N} (-\Delta_j + v(x_j)) + \lambda \sum_{1 \leqslant i < j \leqslant N} w(x_i - x_j) = H^0 + \lambda H^1$$

Know everything at $\lambda = 0$, nothing at $\lambda \neq 0$

$$\inf_{\psi \in \mathfrak{H}} \langle \psi, H(\lambda)\psi \rangle$$

Motivation

$$H(\lambda) = \sum_{j=1}^{N} (-\Delta_j + v(x_j)) + \lambda \sum_{1 \leqslant i < j \leqslant N} w(x_i - x_j) = H^0 + \lambda H^1$$

Know everything at $\lambda = 0$, nothing at $\lambda \neq 0$

$$\inf_{\psi \in \mathfrak{H}} \langle \psi, H(\lambda)\psi \rangle \qquad \longrightarrow \qquad \inf_{\psi \in \mathcal{P}\mathfrak{H}} \langle \psi, H(\lambda)\psi \rangle , \quad \mathcal{P} \text{ projector}$$

Motivation

$$H(\lambda) = \sum_{j=1}^{N}(-\Delta_j + v(x_j)) + \lambda \sum_{1\leqslant i<j\leqslant N} w(x_i - x_j) = H^0 + \lambda H^1$$

Know everything at $\lambda = 0$, nothing at $\lambda \neq 0$

$$\inf_{\psi\in\mathfrak{H}} \langle\psi, H(\lambda)\psi\rangle \qquad \longrightarrow \qquad \inf_{\psi\in\mathcal{P}\mathfrak{H}} \langle\psi, H(\lambda)\psi\rangle\,, \quad \mathcal{P} \text{ projector}$$

Call $(E(\lambda), \phi(\lambda))$ the non-degenerate ground eigenpair of $H(\lambda)$

Motivation

$$H(\lambda) = \sum_{j=1}^{N} (-\Delta_j + v(x_j)) + \lambda \sum_{1 \leqslant i < j \leqslant N} w(x_i - x_j) = H^0 + \lambda H^1$$

Know everything at $\lambda = 0$, nothing at $\lambda \neq 0$

$$\inf_{\psi \in \mathfrak{H}} \langle \psi, H(\lambda)\psi \rangle \qquad \longrightarrow \qquad \inf_{\psi \in \mathcal{P}\mathfrak{H}} \langle \psi, H(\lambda)\psi \rangle \,, \quad \mathcal{P} \text{ projector}$$

Call $(E(\lambda), \phi(\lambda))$ the non-degenerate ground eigenpair of $H(\lambda)$

$$\boxed{\mathrm{Span}\left(\left(\frac{\mathrm{d}^n}{\mathrm{d}\lambda^n} \phi(\lambda) \right)_{|\lambda=0}, 0 \leqslant n \leqslant \ell \right) \subset \mathcal{P}\mathfrak{H}}$$

Motivation

$$H(\lambda) = \sum_{j=1}^{N}(-\Delta_j + v(x_j)) + \lambda \sum_{1\leqslant i<j\leqslant N} w(x_i - x_j) = H^0 + \lambda H^1$$

Know everything at $\lambda = 0$, nothing at $\lambda \neq 0$

$$\inf_{\psi\in\mathfrak{H}} \langle\psi, H(\lambda)\psi\rangle \qquad \longrightarrow \qquad \inf_{\psi\in\mathcal{P}\mathfrak{H}} \langle\psi, H(\lambda)\psi\rangle\,, \quad \mathcal{P} \text{ projector}$$

Call $(E(\lambda), \phi(\lambda))$ the non-degenerate ground eigenpair of $H(\lambda)$

$$\boxed{\mathrm{Span}\left(\left(\frac{\mathrm{d}^n}{\mathrm{d}\lambda^n}\phi(\lambda)\right)_{|\lambda=0}, 0 \leqslant n \leqslant \ell\right) \subset \mathcal{P}\mathfrak{H}}$$

Motivation

$$H(\lambda) = \sum_{j=1}^{N} (-\Delta_j + v(x_j)) + \lambda \sum_{1 \leqslant i < j \leqslant N} w(x_i - x_j) = H^0 + \lambda H^1$$

Know everything at $\lambda = 0$, nothing at $\lambda \neq 0$

$$\inf_{\psi \in \mathfrak{H}} \langle \psi, H(\lambda)\psi \rangle \qquad \longrightarrow \qquad \inf_{\psi \in \mathcal{P}\mathfrak{H}} \langle \psi, H(\lambda)\psi \rangle, \quad \mathcal{P} \text{ projector}$$

Call $(E(\lambda), \phi(\lambda))$ the non-degenerate ground eigenpair of $H(\lambda)$

$$\boxed{\mathrm{Span}\left(\left(\frac{\mathrm{d}^n}{\mathrm{d}\lambda^n}\phi(\lambda)\right)_{|\lambda=0}, 0 \leqslant n \leqslant \ell \right) \subset \mathcal{P}\mathfrak{H}}$$

- Noor, Lowder, "Approximate techniques of structural reanalysis", 1974

Motivation

$$H(\lambda) = \sum_{j=1}^{N} (-\Delta_j + v(x_j)) + \lambda \sum_{1 \leqslant i < j \leqslant N} w(x_i - x_j) = H^0 + \lambda H^1$$

Know everything at $\lambda = 0$, nothing at $\lambda \neq 0$

$$\inf_{\psi \in \mathfrak{H}} \langle \psi, H(\lambda)\psi \rangle \qquad \longrightarrow \qquad \inf_{\psi \in \mathcal{P}\mathfrak{H}} \langle \psi, H(\lambda)\psi \rangle, \quad \mathcal{P} \text{ projector}$$

Call $(E(\lambda), \phi(\lambda))$ the non-degenerate ground eigenpair of $H(\lambda)$

$$\boxed{\mathrm{Span}\left(\left(\frac{\mathrm{d}^n}{\mathrm{d}\lambda^n} \phi(\lambda) \right)_{|\lambda=0}, 0 \leqslant n \leqslant \ell \right) \subset \mathcal{P}\mathfrak{H}}$$

- Noor, Lowder, "Approximate techniques of structural reanalysis", 1974

Motivation

$$H(\lambda) = \sum_{j=1}^{N}(-\Delta_j + v(x_j)) + \lambda \sum_{1\leqslant i<j\leqslant N} w(x_i - x_j) = H^0 + \lambda H^1$$

Know everything at $\lambda = 0$, nothing at $\lambda \neq 0$

$$\inf_{\psi\in\mathfrak{H}} \langle\psi, H(\lambda)\psi\rangle \qquad \longrightarrow \qquad \inf_{\psi\in\mathcal{P}\mathfrak{H}} \langle\psi, H(\lambda)\psi\rangle\,, \quad \mathcal{P} \text{ projector}$$

Call $(E(\lambda), \phi(\lambda))$ the non-degenerate ground eigenpair of $H(\lambda)$

$$\boxed{\mathrm{Span}\left(\left(\frac{\mathrm{d}^n}{\mathrm{d}\lambda^n}\phi(\lambda)\right)_{|\lambda=0}, 0 \leqslant n \leqslant \ell\right) \subset \mathcal{P}\mathfrak{H}}$$

- Noor, Lowder, "Approximate techniques of structural reanalysis", 1974
- Frame, He, Ipsen, Lee, Lee, Rrapaj, "Eigenvector Continuation with Subspace Learning", 2018

Motivation

$$H(\lambda) = \sum_{j=1}^{N} (-\Delta_j + v(x_j)) + \lambda \sum_{1 \leqslant i < j \leqslant N} w(x_i - x_j) = H^0 + \lambda H^1$$

Know everything at $\lambda = 0$, nothing at $\lambda \neq 0$

$$\inf_{\psi \in \mathfrak{H}} \langle \psi, H(\lambda)\psi \rangle \qquad \longrightarrow \qquad \inf_{\psi \in \mathcal{P}\mathfrak{H}} \langle \psi, H(\lambda)\psi \rangle \,, \quad \mathcal{P} \text{ projector}$$

Call $(E(\lambda), \phi(\lambda))$ the non-degenerate ground eigenpair of $H(\lambda)$

$$\boxed{\mathrm{Span}\left(\left(\tfrac{\mathrm{d}^n}{\mathrm{d}\lambda^n}\phi(\lambda)\right)_{|\lambda=0}, 0 \leqslant n \leqslant \ell \right) \subset \mathcal{P}\mathfrak{H}}$$

- Noor, Lowder, "Approximate techniques of structural reanalysis", 1974
- Frame, He, Ipsen, Lee, Lee, Rrapaj, "Eigenvector Continuation with Subspace Learning", 2018
- G., Stamm, "On reduced basis methods for eigenvalue problems, and on its coupling with perturbation theory", 2024

Norms

Take a reference A (for instance when $H = -\Delta + v$, $A = \sqrt{-\Delta}$) then on operators present in the Hamiltonian (electomagnatic potentials etc)

$$\|H\|_p := \left\|A^{-1}HA^{-1}\right\| = \left\|A^{-1}HA^{-1}\right\|_{\mathfrak{H}\to\mathfrak{H}}$$

on vectors of $\mathfrak{H}$,

$$\|\psi\|_e := \|A\psi\|$$

and on density matrices,

$$\|\Gamma\|_e := \|A\Gamma A\| .$$

Sommaire

Effective system

Variational approximation, reduced basis, projected space, Galerkin, Rayleigh-Ritz, eigenvector continuation, ...

$$\cancel{\mathfrak{H}} \qquad \longrightarrow \qquad \mathcal{P}\mathfrak{H}, \qquad \mathcal{P} \text{ orthogonal projector}$$

Effective system

Variational approximation, reduced basis, projected space, Galerkin, Rayleigh-Ritz, eigenvector continuation, ...

$$\cancel{\mathfrak{H}} \qquad \longrightarrow \qquad \mathcal{P}\mathfrak{H}, \qquad \mathcal{P} \text{ orthogonal projector}$$

The effective system for H is $\mathcal{P}H\mathcal{P}$?

Effective system

Variational approximation, reduced basis, projected space, Galerkin, Rayleigh-Ritz, eigenvector continuation, ...

$$\cancel{\mathfrak{H}} \qquad \longrightarrow \qquad \mathcal{P}\mathfrak{H}, \qquad \mathcal{P} \text{ orthogonal projector}$$

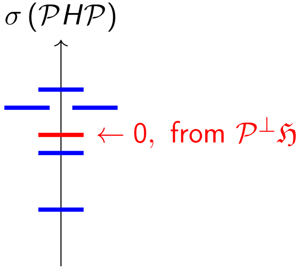
The effective system for H is $\mathcal{P}H\mathcal{P}$?

Effective system

Variational approximation, reduced basis, projected space, Galerkin, Rayleigh-Ritz, eigenvector continuation, ...

$$\cancel{\mathfrak{H}} \qquad \longrightarrow \qquad \mathcal{P}\mathfrak{H}, \qquad \mathcal{P} \text{ orthogonal projector}$$

The effective system for H is $\mathcal{P}H\mathcal{P}$?

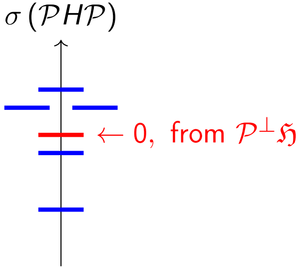


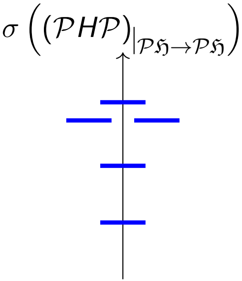
Effective system

Variational approximation, reduced basis, projected space, Galerkin, Rayleigh-Ritz, eigenvector continuation, ...

$$\cancel{\mathfrak{H}} \quad \longrightarrow \quad \mathcal{P}\mathfrak{H}, \qquad \mathcal{P} \text{ orthogonal projector}$$

The effective system for H is $\mathcal{P}H\mathcal{P}$?





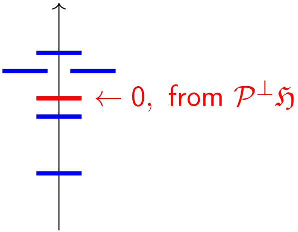
Effective system

Variational approximation, reduced basis, projected space, Galerkin, Rayleigh-Ritz, eigenvector continuation, ...

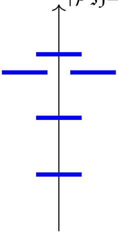
$$\cancel{\mathfrak{H}} \quad \longrightarrow \quad \mathcal{P}\mathfrak{H}, \qquad \mathcal{P} \text{ orthogonal projector}$$

The effective system for H is $\mathcal{P}H\mathcal{P}$?

$\sigma\left(\mathcal{P}H\mathcal{P}\right)$



$\sigma\left(\left(\mathcal{P}H\mathcal{P}\right)\big|_{\mathcal{P}\mathfrak{H}\to\mathcal{P}\mathfrak{H}}\right)$



The effective system for H is $\left(\mathcal{P}H\mathcal{P}\right)\big|_{\mathcal{P}\mathfrak{H}\to\mathcal{P}\mathfrak{H}}$

Error, non-degenerate case

$$\begin{array}{lll} (E,\phi) & \text{an eigenmode of} & H \\ (\mathcal{E},\psi) & \text{an eigenmode of} & (\mathcal{P}H\mathcal{P})\big|_{\mathcal{P}\mathfrak{H}\to\mathcal{P}\mathfrak{H}} \end{array}$$

Error, non-degenerate case

$$\begin{array}{lll} (E,\phi) & \text{an eigenmode of} & H \\ (\mathcal{E},\psi) & \text{an eigenmode of} & (\mathcal{P}H\mathcal{P})|_{\mathcal{P}\mathfrak{H}\to\mathcal{P}\mathfrak{H}} \end{array}$$

R the pseudo-inverse for the effective system at $\mathcal{E}$

Error, non-degenerate case

$$\begin{array}{lll} (E,\phi) & \text{an eigenmode of} & H \\ (\mathcal{E},\psi) & \text{an eigenmode of} & (\mathcal{P}H\mathcal{P})|_{\mathcal{P}\mathfrak{H}\to\mathcal{P}\mathfrak{H}} \end{array}$$

R the pseudo-inverse for the effective system at $\mathcal{E}$

Proposition (G., Stamm 2024)

In a gauge where $\langle\psi,\phi\rangle\in\mathbb{R}$,

$$\begin{aligned}\phi-\psi &= (1+RH)\mathcal{P}^\perp\phi-\frac{1}{2}\left\|\phi-\psi\right\|^2\psi+(\mathcal{E}-E)\,R\,(\phi-\psi)\\ &= (1+RH)\mathcal{P}^\perp\phi+O\left(\left\|\phi-\psi\right\|^2\right)\end{aligned}$$

Error, non-degenerate case

$$\begin{array}{lll} (E,\phi) & \text{an eigenmode of} & H \\ (\mathcal{E},\psi) & \text{an eigenmode of} & (\mathcal{P}H\mathcal{P})|_{\mathcal{P}\mathfrak{H}\to\mathcal{P}\mathfrak{H}} \end{array}$$

R the pseudo-inverse for the effective system at $\mathcal{E}$

Proposition (G., Stamm 2024)

In a gauge where $\langle\psi,\phi\rangle \in \mathbb{R}$,

$$\begin{aligned} \phi-\psi &= (1+RH)\mathcal{P}^{\perp}\phi - \tfrac{1}{2}\|\phi-\psi\|^2\,\psi + (\mathcal{E}-E)\,R\,(\phi-\psi) \\ &= (1+RH)\mathcal{P}^{\perp}\phi + O\left(\|\phi-\psi\|^2\right) \end{aligned}$$

Error, non-degenerate case

$$\begin{array}{lll} (E, \phi) & \text{an eigenmode of} & H \\ (\mathcal{E}, \psi) & \text{an eigenmode of} & (\mathcal{P} H \mathcal{P})|_{\mathcal{P}\mathfrak{H} \to \mathcal{P}\mathfrak{H}} \end{array}$$

R the pseudo-inverse for the effective system at $\mathcal{E}$

Proposition (G., Stamm 2024)

In a gauge where $\langle \psi, \phi \rangle \in \mathbb{R}$,

$$\begin{aligned} \phi - \psi &= (1 + RH)\mathcal{P}^{\perp}\phi - \frac{1}{2} \|\phi - \psi\|^2 \psi + (\mathcal{E} - E) R (\phi - \psi) \\ &= (1 + RH)\mathcal{P}^{\perp}\phi + O\left(\|\phi - \psi\|^2\right) \end{aligned}$$

- Babuška, Osborn, 1991

Error, non-degenerate case

$$\begin{array}{lll} (E,\phi) & \text{an eigenmode of} & H \\ (\mathcal{E},\psi) & \text{an eigenmode of} & (\mathcal{P}H\mathcal{P})|_{\mathcal{P}\mathfrak{H}\to\mathcal{P}\mathfrak{H}} \end{array}$$

R the pseudo-inverse for the effective system at $\mathcal{E}$

Proposition (G., Stamm 2024)

In a gauge where $\langle\psi,\phi\rangle \in \mathbb{R}$*,*

$$\begin{aligned} \phi - \psi &= (1+RH)\mathcal{P}^{\perp}\phi - \tfrac{1}{2}\left\|\phi-\psi\right\|^2\psi + (\mathcal{E}-E)\,R\,(\phi-\psi) \\ &= (1+RH)\mathcal{P}^{\perp}\phi + O\left(\left\|\phi-\psi\right\|^2\right) \end{aligned}$$

- Babuška, Osborn, 1991
- Machiels, Maday, Oliveira, Patera, Rovas, 2000

Error, non-degenerate case

$$\begin{array}{lll} (E,\phi) & \text{an eigenmode of} & H \\ (\mathcal{E},\psi) & \text{an eigenmode of} & (\mathcal{P}H\mathcal{P})|_{\mathcal{P}\mathfrak{H}\to\mathcal{P}\mathfrak{H}} \end{array}$$

R the pseudo-inverse for the effective system at $\mathcal{E}$

Proposition (G., Stamm 2024)

In a gauge where $\langle\psi,\phi\rangle \in \mathbb{R}$,

$$\begin{aligned} \phi - \psi &= (1 + RH)\mathcal{P}^\perp\phi - \frac{1}{2}\|\phi-\psi\|^2\psi + (\mathcal{E}-E)\,R\,(\phi-\psi) \\ &= (1+RH)\mathcal{P}^\perp\phi + O\left(\|\phi-\psi\|^2\right) \end{aligned}$$

- Babuška, Osborn, 1991
- Machiels, Maday, Oliveira, Patera, Rovas, 2000
- Fumagalli, Manzoni, Parolini, Verani, 2016

Error, non-degenerate case

$$
\begin{array}{lll}
(E,\phi) & \text{an eigenmode of} & H \\
(\mathcal{E},\psi) & \text{an eigenmode of} & (\mathcal{P}H\mathcal{P})|_{\mathcal{P}\mathfrak{H}\to\mathcal{P}\mathfrak{H}}
\end{array}
$$

R the pseudo-inverse for the effective system at $\mathcal{E}$

Proposition (G., Stamm 2024)

In a gauge where $\langle\psi,\phi\rangle \in \mathbb{R}$,

$$
\begin{aligned}
\phi - \psi &= (1 + RH)\mathcal{P}^\perp\phi - \frac{1}{2}\|\phi-\psi\|^2\psi + (\mathcal{E}-E)R(\phi-\psi) \\
&= (1 + RH)\mathcal{P}^\perp\phi + O\left(\|\phi-\psi\|^2\right)
\end{aligned}
$$

- Babuška, Osborn, 1991
- Machiels, Maday, Oliveira, Patera, Rovas, 2000
- Fumagalli, Manzoni, Parolini, Verani, 2016
- Taumhas, Dusson, Ehrlacher, Lelièvre, Madiot, 2023

Error, degenerate case

$$\begin{array}{llll} (E_\mu, \phi_\mu)_{\mu=1}^{\nu} & \text{eigs} & H & \Gamma := \sum_{\mu=1}^{\nu} \left|\phi_\mu\right\rangle \left\langle\phi_\mu\right| \\ (\mathcal{E}_\mu, \psi_\mu)_{\mu=1}^{\nu} & \text{eigs} & (\mathcal{P} H \mathcal{P})\big|_{\mathcal{P}\mathfrak{H} \to \mathcal{P}\mathfrak{H}} & \Lambda := \sum_{\mu=1}^{\nu} \left|\psi_\mu\right\rangle \left\langle\psi_\mu\right| \end{array}$$

Error, degenerate case

$$
\begin{array}{llll}
(E_\mu, \phi_\mu)_{\mu=1}^{\nu} & \text{eigs} & H & \Gamma := \sum_{\mu=1}^{\nu} |\phi_\mu\rangle \langle\phi_\mu| \\
(\mathcal{E}_\mu, \psi_\mu)_{\mu=1}^{\nu} & \text{eigs} & (\mathcal{P} H \mathcal{P})\big|_{\mathcal{P}\mathfrak{H} \to \mathcal{P}\mathfrak{H}} & \Lambda := \sum_{\mu=1}^{\nu} |\psi_\mu\rangle \langle\psi_\mu|
\end{array}
$$

Error, degenerate case

$$\begin{array}{llll} (E_\mu, \phi_\mu)_{\mu=1}^{\nu} & \text{eigs} & H & \Gamma := \sum_{\mu=1}^{\nu} |\phi_\mu\rangle \langle\phi_\mu| \\ (\mathcal{E}_\mu, \psi_\mu)_{\mu=1}^{\nu} & \text{eigs} & (\mathcal{P} H \mathcal{P})_{|\mathcal{P}\mathfrak{H} \to \mathcal{P}\mathfrak{H}} & \Lambda := \sum_{\mu=1}^{\nu} |\psi_\mu\rangle \langle\psi_\mu| \end{array}$$

Proposition (G., Stamm 2024)

Similarly,

$$\Gamma - \Lambda = \sum_{\mu=1}^{\nu} \Big((1 + H R_\mu) \mathcal{P}^\perp \Gamma P_{\psi_\mu} + \text{s.a} \Big) + \Omega, \quad \textit{where}\, \|\Omega\| \leqslant c \, \|\Gamma - \Lambda\|^2 .$$

Error, degenerate case

$$\begin{array}{llll} (E_\mu, \phi_\mu)_{\mu=1}^{\nu} & \text{eigs} & H & \Gamma := \sum_{\mu=1}^{\nu} |\phi_\mu\rangle \langle \phi_\mu| \\ (\mathcal{E}_\mu, \psi_\mu)_{\mu=1}^{\nu} & \text{eigs} & (\mathcal{P} H \mathcal{P})|_{\mathcal{P}\mathfrak{H} \to \mathcal{P}\mathfrak{H}} & \Lambda := \sum_{\mu=1}^{\nu} |\psi_\mu\rangle \langle \psi_\mu| \end{array}$$

Proposition (G., Stamm 2024)

Similarly,

$$\Gamma - \Lambda = \sum_{\mu=1}^{\nu} \Big((1 + H R_\mu) \mathcal{P}^\perp \Gamma P_{\psi_\mu} + \text{s.a} \Big) + \Omega, \quad \textit{where } \|\Omega\| \leqslant c \, \|\Gamma - \Lambda\|^2 .$$

- Horger, Wohlmuth, Dickopf, 2017

Error, degenerate case

$$\begin{array}{llll} (E_\mu, \phi_\mu)_{\mu=1}^{\nu} & \text{eigs} & H & \Gamma := \sum_{\mu=1}^{\nu} |\phi_\mu\rangle \langle\phi_\mu| \\ (\mathcal{E}_\mu, \psi_\mu)_{\mu=1}^{\nu} & \text{eigs} & (\mathcal{P}H\mathcal{P})|_{\mathcal{P}\mathfrak{H}\to\mathcal{P}\mathfrak{H}} & \Lambda := \sum_{\mu=1}^{\nu} |\psi_\mu\rangle \langle\psi_\mu| \end{array}$$

Proposition (G., Stamm 2024)

Similarly,

$$\Gamma - \Lambda = \sum_{\mu=1}^{\nu} \Big((1 + HR_\mu)\mathcal{P}^\perp \Gamma P_{\psi_\mu} + \text{s.a} \Big) + \Omega, \quad \textit{where } \|\Omega\| \leqslant c\, \|\Gamma - \Lambda\|^2 .$$

- Horger, Wohlmuth, Dickopf, 2017
- Cancès, Dusson, Maday, Stamm, Vohralík, 2020

Error, degenerate case

$$\begin{array}{llll} (E_\mu, \phi_\mu)_{\mu=1}^{\nu} & \text{eigs} & H & \Gamma := \sum_{\mu=1}^{\nu} |\phi_\mu\rangle \langle\phi_\mu| \\ (\mathcal{E}_\mu, \psi_\mu)_{\mu=1}^{\nu} & \text{eigs} & (\mathcal{P} H \mathcal{P})|_{\mathcal{P}\mathfrak{H} \to \mathcal{P}\mathfrak{H}} & \Lambda := \sum_{\mu=1}^{\nu} |\psi_\mu\rangle \langle\psi_\mu| \end{array}$$

Proposition (G., Stamm 2024)

Similarly,

$$\Gamma - \Lambda = \sum_{\mu=1}^{\nu} \Big((1 + H R_\mu) \mathcal{P}^\perp \Gamma P_{\psi_\mu} + \text{s.a} \Big) + \Omega, \quad \textit{where} \, \|\Omega\| \leqslant c \, \|\Gamma - \Lambda\|^2 .$$

- Horger, Wohlmuth, Dickopf, 2017
- Cancès, Dusson, Maday, Stamm, Vohralík, 2020
- Boffi, Halim, Priyadarshi, 2023

Sommaire

Perturbation theory for vectors

$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n,$$

Perturbation theory for vectors

$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad H(\lambda)\phi(\lambda) = E(\lambda)\phi(\lambda)$$

Perturbation theory for vectors

$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad H(\lambda)\phi(\lambda) = E(\lambda)\phi(\lambda)$$

$$E(\lambda) = \sum_{n=0}^{+\infty} \lambda^n E^n, \qquad \phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \phi^n$$

Perturbation theory for vectors

$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad H(\lambda)\phi(\lambda) = E(\lambda)\phi(\lambda)$$

$$E(\lambda) = \sum_{n=0}^{+\infty} \lambda^n E^n, \qquad \phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \phi^n$$

Define the partial inverse

Perturbation theory for vectors

$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad H(\lambda)\phi(\lambda) = E(\lambda)\phi(\lambda)$$

$$E(\lambda) = \sum_{n=0}^{+\infty} \lambda^n E^n, \qquad \phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \phi^n$$

Define the partial inverse $\quad K := \left((E(0) - H(0))\big|_{P^{\perp}_{\phi(0)}\mathfrak{H} \to P^{\perp}_{\phi(0)}\mathfrak{H}} \right)^{-1}$

Perturbation theory for vectors

$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad H(\lambda)\phi(\lambda) = E(\lambda)\phi(\lambda)$$
$$E(\lambda) = \sum_{n=0}^{+\infty} \lambda^n E^n, \qquad \phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \phi^n$$

Define the partial inverse $\quad K := \left((E(0) - H(0))\big|_{P^\perp_{\phi(0)}\mathfrak{H} \to P^\perp_{\phi(0)}\mathfrak{H}} \right)^{-1}$
$\Phi(\lambda) := \frac{\phi(\lambda)}{\langle \phi(0), \phi(\lambda) \rangle}$, $\Phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \Phi^n$, $\Phi^n \perp \Phi^0$

Perturbation theory for vectors

$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad H(\lambda)\phi(\lambda) = E(\lambda)\phi(\lambda)$$

$$E(\lambda) = \sum_{n=0}^{+\infty} \lambda^n E^n, \qquad \phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \phi^n$$

Define the partial inverse $\quad K := \left((E(0) - H(0))\Big|_{P^\perp_{\phi(0)}\mathfrak{H} \to P^\perp_{\phi(0)}\mathfrak{H}} \right)^{-1}$

$\Phi(\lambda) := \frac{\phi(\lambda)}{\langle \phi(0), \phi(\lambda) \rangle}$, $\Phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \Phi^n$, $\Phi^n \perp \Phi^0$

$$Q^n := (H^n - E^n) + \sum_{s=1}^{n-1} (H^{n-s} - E^{n-s}) K Q^s,$$

Perturbation theory for vectors

$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad H(\lambda)\phi(\lambda) = E(\lambda)\phi(\lambda)$$

$$E(\lambda) = \sum_{n=0}^{+\infty} \lambda^n E^n, \qquad \phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \phi^n$$

Define the partial inverse $\quad K := \left((E(0) - H(0))\big|_{P^\perp_{\phi(0)}\mathfrak{H} \to P^\perp_{\phi(0)}\mathfrak{H}} \right)^{-1}$

$\Phi(\lambda) := \frac{\phi(\lambda)}{\langle \phi(0), \phi(\lambda)\rangle}$, $\Phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \Phi^n$, $\Phi^n \perp \Phi^0$

$$Q^n := (H^n - E^n) + \sum_{s=1}^{n-1} (H^{n-s} - E^{n-s}) K Q^s, \qquad \Phi^n = K Q^n \Phi^0$$

Perturbation theory for vectors

$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad H(\lambda)\phi(\lambda) = E(\lambda)\phi(\lambda)$$

$$E(\lambda) = \sum_{n=0}^{+\infty} \lambda^n E^n, \qquad \phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \phi^n$$

Define the partial inverse $K := \left((E(0) - H(0))\big|_{P^\perp_{\phi(0)}\mathfrak{H} \to P^\perp_{\phi(0)}\mathfrak{H}} \right)^{-1}$

$\Phi(\lambda) := \frac{\phi(\lambda)}{\langle \phi(0), \phi(\lambda) \rangle}$, $\Phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \Phi^n$, $\Phi^n \perp \Phi^0$

$$Q^n := (H^n - E^n) + \sum_{s=1}^{n-1} (H^{n-s} - E^{n-s}) K Q^s, \qquad \Phi^n = K Q^n \Phi^0$$

Need bound on Φ^n

A lemma on Cauchy square series

Lemme (Cauchy square series)

Take $\beta > 0$, $x_1 := 1$ *and*

$$x_n := \beta \sum_{s=1}^{n-1} x_{n-s} x_s .$$

A lemma on Cauchy square series

Lemme (Cauchy square series)

Take $\beta > 0$, $x_1 := 1$ *and*

$$x_n := \beta \sum_{s=1}^{n-1} x_{n-s} x_s. \qquad \textit{Then} \qquad x_n \leqslant \frac{\left(2\zeta\left(\frac{3}{2}\right)\beta\right)^{n-1}}{n^{\frac{3}{2}}}.$$

A lemma on Cauchy square series

Lemme (Cauchy square series)

Take $\beta > 0$, $x_1 := 1$ *and*

$$x_n := \beta \sum_{s=1}^{n-1} x_{n-s} x_s. \qquad \textit{Then} \qquad x_n \leqslant \frac{\left(2\zeta\left(\frac{3}{2}\right)\beta\right)^{n-1}}{n^{\frac{3}{2}}}.$$

Conjecture

$$\frac{x_n}{\pi^{-\frac{1}{2}}(4\beta)^{n-1} n^{-\frac{3}{2}}} \underset{n \to +\infty}{\longrightarrow} 1.$$

A lemma on Cauchy square series

Lemme (Cauchy square series)

Take $\beta > 0$, $x_1 := 1$ *and*

$$x_n := \beta \sum_{s=1}^{n-1} x_{n-s} x_s. \qquad \textit{Then} \qquad x_n \leqslant \frac{\left(2\zeta\left(\frac{3}{2}\right)\beta\right)^{n-1}}{n^{\frac{3}{2}}}.$$

Conjecture

$$\frac{x_n}{\pi^{-\frac{1}{2}}(4\beta)^{n-1} n^{-\frac{3}{2}}} \underset{n\to+\infty}{\longrightarrow} 1.$$

Lemme

Assume $\sup_{n\in\mathbb{N}} \|H^n\|_p < +\infty$. *There exists* $a, b > 0$ *such that* $\forall n \in \mathbb{N}$

$$|E^n| + \|\phi^n\| \leqslant ab^n$$

Perturbation theory for density matrices

$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad \Gamma(\lambda) := \sum_{\mu=1}^{\nu} \left|\phi_\mu(\lambda)\right\rangle\left\langle\phi_\mu(\lambda)\right| = \sum_{n=0}^{+\infty} \lambda^n \Gamma^n$$

Perturbation theory for density matrices

$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad \Gamma(\lambda) := \sum_{\mu=1}^{\nu} \left|\phi_\mu(\lambda)\right\rangle\left\langle\phi_\mu(\lambda)\right| = \sum_{n=0}^{+\infty} \lambda^n \Gamma^n$$

Defining $K_\mu := \left((E_\mu(0) - H(0))\big|_{P^\perp_{\phi_\mu(0)}\mathfrak{H} \to P^\perp_{\phi_\mu(0)}\mathfrak{H}} \right)^{-1}$, we have

Perturbation theory for density matrices

$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad \Gamma(\lambda) := \sum_{\mu=1}^{\nu} \left|\phi_\mu(\lambda)\right\rangle\left\langle\phi_\mu(\lambda)\right| = \sum_{n=0}^{+\infty} \lambda^n \Gamma^n$$

Defining $K_\mu := \left((E_\mu(0) - H(0))\big|_{P^\perp_{\phi_\mu(0)}\mathfrak{H} \to P^\perp_{\phi_\mu(0)}\mathfrak{H}} \right)^{-1}$, we have

$$\Gamma^n = \sum_{k=1}^{n-1} \left(\left(\Gamma^0\right)^\perp \Gamma^{n-k}\Gamma^k \left(\Gamma^0\right)^\perp - \Gamma^0\Gamma^{n-k}\Gamma^k\Gamma^0 \right) + \left(\sum_{\mu=1}^{\nu} K_\mu \left(\Gamma^0\right)^\perp \sum_{k=0}^{n-1} [H^{n-k}, \Gamma^k]\Gamma^0 P_{\phi_\mu} + \text{s.a} \right)$$

- McWeeny, "Perturbation theory for the Fock-Dirac density matrix", 1962

Perturbation theory for density matrices

$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad \Gamma(\lambda) := \sum_{\mu=1}^{\nu} \left|\phi_\mu(\lambda)\right\rangle\left\langle\phi_\mu(\lambda)\right| = \sum_{n=0}^{+\infty} \lambda^n \Gamma^n$$

Defining $K_\mu := \left((E_\mu(0) - H(0))\big|_{P^\perp_{\phi_\mu(0)}\mathfrak{H} \to P^\perp_{\phi_\mu(0)}\mathfrak{H}} \right)^{-1}$, we have

$$\Gamma^n = \sum_{k=1}^{n-1} \left(\left(\Gamma^0\right)^\perp \Gamma^{n-k}\Gamma^k \left(\Gamma^0\right)^\perp - \Gamma^0\Gamma^{n-k}\Gamma^k\Gamma^0 \right) + \left(\sum_{\mu=1}^{\nu} K_\mu \left(\Gamma^0\right)^\perp \sum_{k=0}^{n-1} [H^{n-k}, \Gamma^k]\Gamma^0 P_{\phi_\mu} + \text{s.a} \right)$$

- McWeeny, "Perturbation theory for the Fock-Dirac density matrix", 1962

Lemme

There exists $a, b > 0$ such that $\|\Gamma^n\| \leqslant ab^n$

Building the reduced space

Lemme

Take $(\varphi_1, \dots, \varphi_\nu) \in \mathcal{H}$ *to be a basis of the unperturbed space* $\bigoplus_{\mu=1}^{\nu} \operatorname{Ker}(H(0) - E_\mu(0))$. *Then*

$$\sum_{n=0}^{\ell} \operatorname{Im} \Gamma^n = \operatorname{Span}\left((\phi_\mu^n)_{1 \leqslant \mu \leqslant \nu}^{0 \leqslant n \leqslant \ell} \right) = \operatorname{Span}\left((\Gamma^n \varphi_\mu)_{1 \leqslant \mu \leqslant \nu}^{0 \leqslant n \leqslant \ell} \right).$$

Quantifying the perturbation approximation

$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n$$

Exact eigenvector : $$\phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \phi^n,$$

Perturbative approximation : $$\varphi(\lambda) := \sum_{n=0}^{\ell} \lambda^n \phi^n$$

Quantifying the perturbation approximation

$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n$$

Exact eigenvector : $$\phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \phi^n,$$

Perturbative approximation : $$\varphi(\lambda) := \sum_{n=0}^{\ell} \lambda^n \phi^n$$

$$\|\phi(\lambda) - \varphi(\lambda)\| = \left\| \sum_{n=\ell+1}^{+\infty} \lambda^n \phi^n \right\| = |\lambda|^{\ell+1} \left\| \phi^{\ell+1} \right\| + O(\lambda^{\ell+2})$$

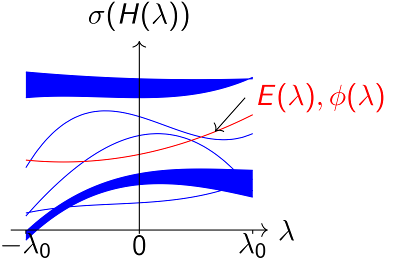
Sommaire

Global intuition

Exact eigenvector : $\phi(\lambda) = \phi^0 + \lambda\phi^1 + \lambda^2\phi^2 + O(\lambda^3)$

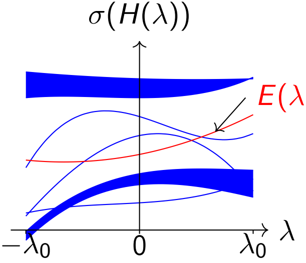
Global intuition

$$\text{Exact eigenvector : } \phi(\lambda) = \phi^0 + \lambda\phi^1 + \lambda^2\phi^2 + O(\lambda^3)$$



Global intuition

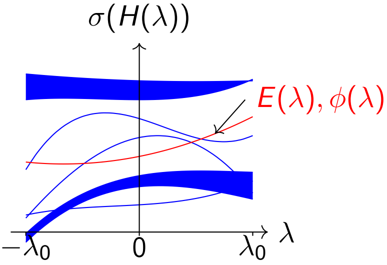
$$\text{Exact eigenvector : } \phi(\lambda) = \phi^0 + \lambda\phi^1 + \lambda^2\phi^2 + O(\lambda^3)$$

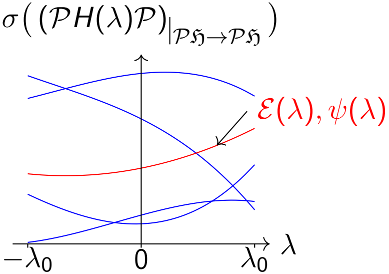


$$\boxed{\forall n \in [\![0, \ell]\!], \quad \phi^n \in \mathcal{P}\mathfrak{H}}$$

Global intuition

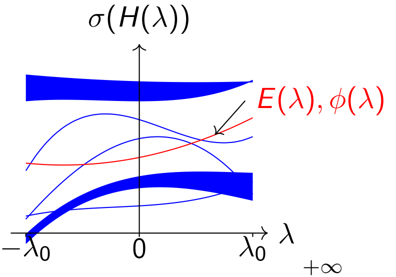
$$\text{Exact eigenvector : } \phi(\lambda) = \phi^0 + \lambda\phi^1 + \lambda^2\phi^2 + O(\lambda^3)$$

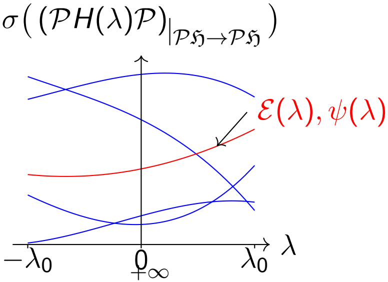




$$\boxed{\forall n \in [\![0, \ell]\!], \quad \phi^n \in \mathcal{P}\mathfrak{H}}$$

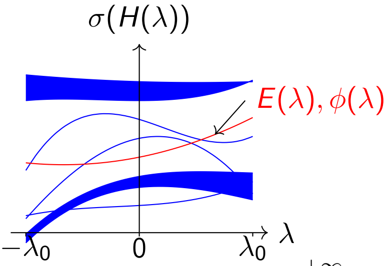
Kato-Rellich's theorem

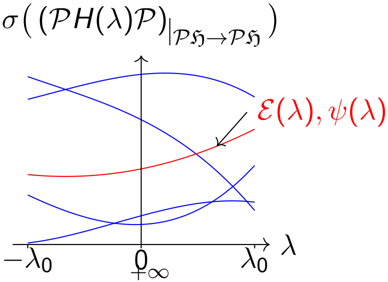




$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad \phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \phi^n$$

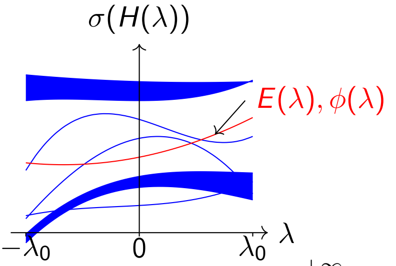
Kato-Rellich's theorem

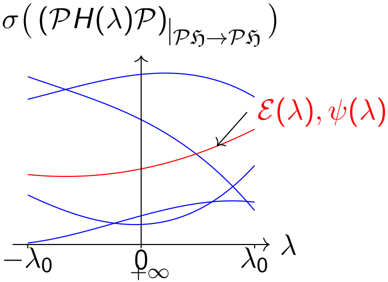




$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad \phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \phi^n$$

Kato-Rellich's theorem

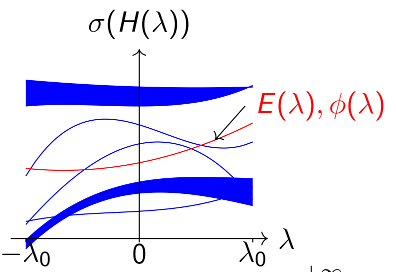


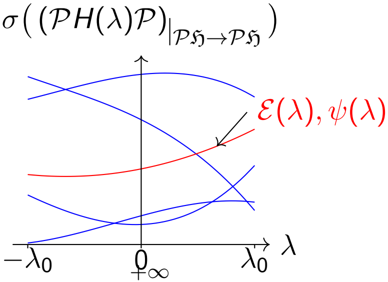


$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad \phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \phi^n$$

$$\text{VA+PT} : \boxed{\phi^n \in \mathcal{P}\mathfrak{H}} \text{ for all } n \in \{0, \dots, \ell\}$$

Kato-Rellich's theorem



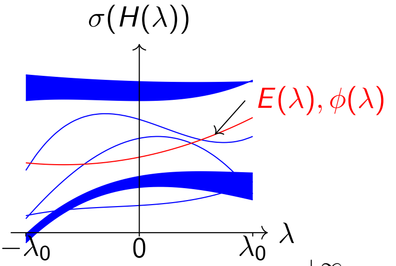


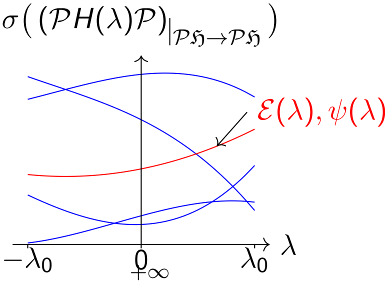
$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad \phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \phi^n$$

$$\text{VA+PT} : \boxed{\phi^n \in \mathcal{P}\mathfrak{H}} \text{ for all } n \in \{0, \dots, \ell\}$$

$\phi(0) \in \mathcal{P}\mathfrak{H}$

Kato-Rellich's theorem



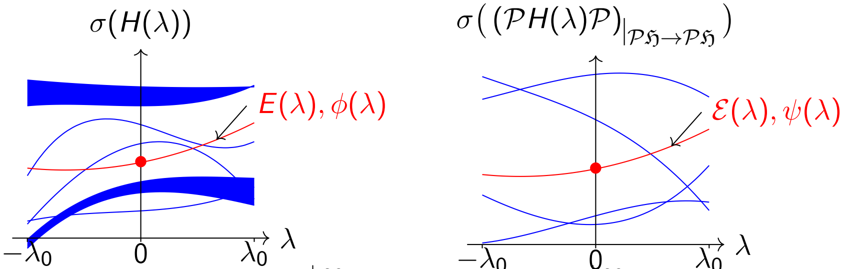


$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad \phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \phi^n$$

$$\text{VA+PT} : \boxed{\phi^n \in \mathcal{P}\mathfrak{H}} \text{ for all } n \in \{0, \dots, \ell\}$$

$$\phi(0) \in \mathcal{P}\mathfrak{H} \implies \mathcal{P}H(0)\mathcal{P}\phi(0) = E(0)\phi(0)$$

Kato-Rellich's theorem

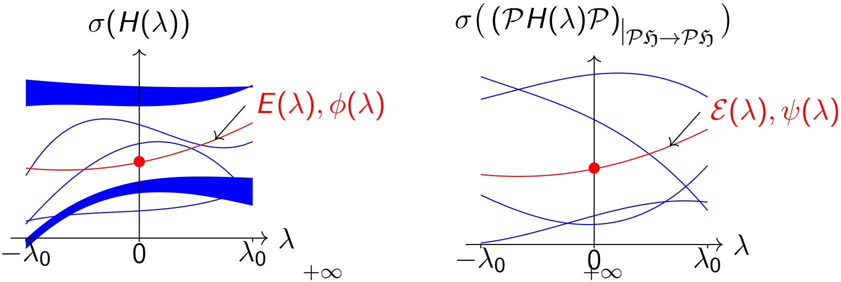


$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad \phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \phi^n$$

$$\text{VA+PT} : \boxed{\phi^n \in \mathcal{P}\mathfrak{H}} \text{ for all } n \in \{0, \dots, \ell\}$$

$\phi(0) \in \mathcal{P}\mathfrak{H} \implies \mathcal{P}H(0)\mathcal{P}\phi(0) = E(0)\phi(0)$
$\implies (E(0), \phi(0))$ is an eigenmode of $(\mathcal{P}H(0)\mathcal{P})|_{\mathcal{P}\mathfrak{H}\to\mathcal{P}\mathfrak{H}}$

Kato-Rellich's theorem



$$H(\lambda) = \sum_{n=0}^{+\infty} \lambda^n H^n, \qquad \phi(\lambda) = \sum_{n=0}^{+\infty} \lambda^n \phi^n$$

$$\text{VA+PT} : \boxed{\phi^n \in \mathcal{P}\mathfrak{H}} \text{ for all } n \in \{0, \dots, \ell\}$$

$\phi(0) \in \mathcal{P}\mathfrak{H} \quad \Longrightarrow \quad \mathcal{P}H(0)\mathcal{P}\phi(0) = E(0)\phi(0)$

$\Longrightarrow$ $(E(0), \phi(0))$ is an eigenmode of $(\mathcal{P}H(0)\mathcal{P})\big|_{\mathcal{P}\mathfrak{H}\to\mathcal{P}\mathfrak{H}}$

$\Longrightarrow$ there exists $(\mathcal{E}(\lambda), \psi(\lambda))$ eigenmode of $(\mathcal{P}H(\lambda)\mathcal{P})\big|_{\mathcal{P}\mathfrak{H}\to\mathcal{P}\mathfrak{H}}$ such that $(\mathcal{E}(0), \psi(0)) = (E(0), \phi(0))$

Main computation to quantify the error

General VA error : $$\phi(\lambda) - \psi(\lambda) = (1 + R(\lambda)H(\lambda))\,\mathcal{P}^{\perp}\phi(\lambda) + \dots$$

Main computation to quantify the error

General VA error : $\phi(\lambda) - \psi(\lambda) = (1 + R(\lambda)H(\lambda))\,\mathcal{P}^\perp\phi(\lambda) + \dots$

$$\mathcal{P}^\perp\phi(\lambda) = \mathcal{P}^\perp \sum_{n=0}^{+\infty} \lambda^n \phi^n \underset{\substack{\phi^n \in \mathcal{P}\mathfrak{H} \\ \forall 0 \leqslant n \leqslant \ell}}{=} \sum_{n=\ell+1}^{+\infty} \lambda^n \mathcal{P}^\perp \phi^n = \lambda^{\ell+1} \sum_{n=\ell+1}^{+\infty} \lambda^{n-(\ell+1)} \mathcal{P}^\perp \phi^n$$

Main computation to quantify the error

General VA error : $\phi(\lambda) - \psi(\lambda) = (1 + R(\lambda)H(\lambda))\,\mathcal{P}^\perp\phi(\lambda) + \dots$

$$\mathcal{P}^\perp\phi(\lambda) = \mathcal{P}^\perp \sum_{n=0}^{+\infty} \lambda^n \phi^n \underset{\substack{\phi^n \in \mathcal{P}\mathfrak{H} \\ \forall 0 \leqslant n \leqslant \ell}}{=} \sum_{n=\ell+1}^{+\infty} \lambda^n \mathcal{P}^\perp \phi^n = \lambda^{\ell+1} \sum_{n=\ell+1}^{+\infty} \lambda^{n-(\ell+1)} \mathcal{P}^\perp \phi^n$$

Main computation to quantify the error

General VA error : $$\phi(\lambda) - \psi(\lambda) = (1 + R(\lambda)H(\lambda))\, \mathcal{P}^\perp \phi(\lambda) + \dots$$

$$\mathcal{P}^\perp \phi(\lambda) = \mathcal{P}^\perp \sum_{n=0}^{+\infty} \lambda^n \phi^n \underset{\substack{\phi^n \in \mathcal{P}\mathfrak{H} \\ \forall 0 \leqslant n \leqslant \ell}}{=} \sum_{n=\ell+1}^{+\infty} \lambda^n \mathcal{P}^\perp \phi^n = \lambda^{\ell+1} \sum_{n=\ell+1}^{+\infty} \lambda^{n-(\ell+1)} \mathcal{P}^\perp \phi^n$$

$$\phi(\lambda) - \psi(\lambda) = (1 + R(\lambda)H(\lambda))\, \mathcal{P}^\perp \phi(\lambda) + \dots$$

Main computation to quantify the error

General VA error : $\phi(\lambda) - \psi(\lambda) = (1 + R(\lambda)H(\lambda))\, \mathcal{P}^\perp \phi(\lambda) + \dots$

$$\mathcal{P}^\perp \phi(\lambda) = \mathcal{P}^\perp \sum_{n=0}^{+\infty} \lambda^n \phi^n \underset{\substack{\phi^n \in \mathcal{P}\mathfrak{H} \\ \forall 0 \leqslant n \leqslant \ell}}{=} \sum_{n=\ell+1}^{+\infty} \lambda^n \mathcal{P}^\perp \phi^n = \lambda^{\ell+1} \sum_{n=\ell+1}^{+\infty} \lambda^{n-(\ell+1)} \mathcal{P}^\perp \phi^n$$

$$\begin{aligned} \phi(\lambda) - \psi(\lambda) &= (1 + R(\lambda)H(\lambda))\, \mathcal{P}^\perp \phi(\lambda) + \dots \\ &= \lambda^{\ell+1} (1 + R(0)H(0))\, \mathcal{P}^\perp \phi^{\ell+1} + O(\lambda^{\ell+2}) \end{aligned}$$

Statement and comparision to perturbation theory

Corollaire (VA+PT bound for vectors, (G., Stamm 2024))

If $\phi^n \in \mathcal{P}\mathfrak{H}$ *for all* $n \in \{0, \ldots, \ell\}$,

$$\|\phi(\lambda) - \psi(\lambda)\| = |\lambda|^{\ell+1} \left\| (1 + R(0)H(0))\, \mathcal{P}^{\perp} \phi^{\ell+1} \right\| + O\left((|\lambda|\, b)^{\ell+2} \right)$$

Statement and comparision to perturbation theory

Corollaire (VA+PT bound for vectors, (G., Stamm 2024))

If $\phi^n \in \mathcal{P}\mathfrak{H}$ *for all* $n \in \{0, \ldots, \ell\}$,

$$\|\phi(\lambda) - \psi(\lambda)\| = |\lambda|^{\ell+1} \left\|(1 + R(0)H(0))\, \mathcal{P}^\perp \phi^{\ell+1}\right\| + O\left((|\lambda|\, b)^{\ell+2}\right)$$

$$\phi^n = \psi^n \text{ for all } n \in \{0, \ldots, \ell\},\ \psi^{\ell+1} = \left(\mathcal{P} - R(0)H(0)\mathcal{P}^\perp\right) \phi^{\ell+1}$$

Statement and comparision to perturbation theory

Corollaire (VA+PT bound for vectors, (G., Stamm 2024))

If $\phi^n \in \mathcal{P}\mathfrak{H}$ for all $n \in \{0, \dots, \ell\}$,

$$\|\phi(\lambda) - \psi(\lambda)\| = |\lambda|^{\ell+1} \left\| (1 + R(0)H(0))\, \mathcal{P}^\perp \phi^{\ell+1} \right\| + O\left((|\lambda|\, b)^{\ell+2} \right)$$

$$\phi^n = \psi^n \text{ for all } n \in \{0, \dots, \ell\},\ \psi^{\ell+1} = \left(\mathcal{P} - R(0)H(0)\mathcal{P}^\perp\right) \phi^{\ell+1}$$

Corollaire (VA+PT bound for clusters, (G., Stamm 2024))

If $\operatorname{Im}\Gamma^n \subset \mathcal{P}\mathfrak{H}$ for all $n \in \{0, \dots, \ell\}$,

$$\|\Gamma(\lambda) - \Lambda(\lambda)\| = |\lambda|^{\ell+1} \left\| \sum_{\mu=1}^{\nu} (1 + R_\mu(0)H(0))\, \mathcal{P}^\perp \Gamma^{\ell+1} P_{\phi_\mu(0)} + s.a \right\| + O\left((|\lambda|\, b)^{\ell+2} \right)$$

Comparison to perturbation theory

VA+PT :

$$\|\phi(\lambda)-\psi(\lambda)\| = |\lambda|^{\ell+1}\left\|\left(1+R(0)H(0)\right)\mathcal{P}^{\perp}\phi^{\ell+1}\right\| + O\left(\left(|\lambda|\,b\right)^{\ell+2}\right)$$

Comparison to perturbation theory

VA+PT :

$$\|\phi(\lambda)-\psi(\lambda)\| = |\lambda|^{\ell+1}\left\|\left(1+R(0)H(0)\right)\mathcal{P}^{\perp}\phi^{\ell+1}\right\| + O\left(\left(|\lambda|\, b\right)^{\ell+2}\right)$$

Perturbation theory (PT) :

$$\|\phi(\lambda)-\varphi(\lambda)\| = |\lambda|^{\ell+1}\left\|\phi^{\ell+1}\right\| + O\left(\left(|\lambda|\, b\right)^{\ell+2}\right)$$

Comparison to perturbation theory

VA+PT :

$$\|\phi(\lambda) - \psi(\lambda)\| = |\lambda|^{\ell+1} \left\| \left(1 + R(0)H(0)\right) \mathcal{P}^{\perp} \phi^{\ell+1} \right\| + O\left(\left(|\lambda|\, b \right)^{\ell+2} \right)$$

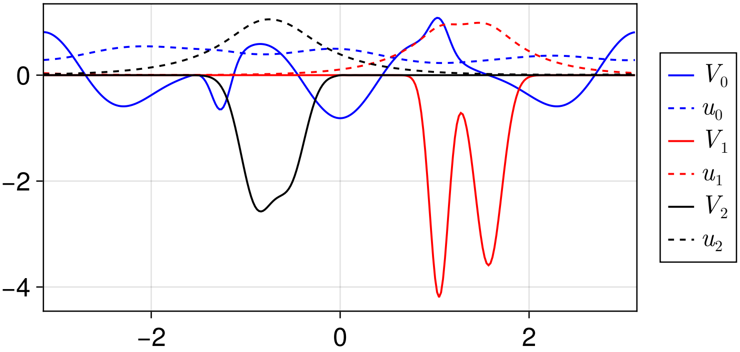
Perturbation theory (PT) :

$$\|\phi(\lambda) - \varphi(\lambda)\| = |\lambda|^{\ell+1} \left\| \phi^{\ell+1} \right\| + O\left(\left(|\lambda|\, b \right)^{\ell+2} \right)$$

Asymptotic comparison :

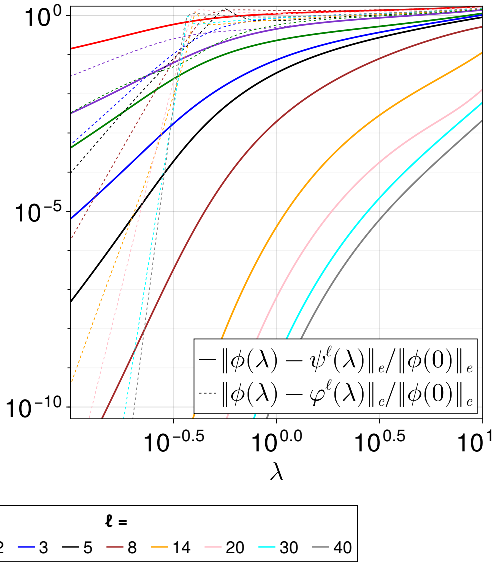
$$\xi_\ell := \lim_{\lambda \to 0} \frac{\|\phi(\lambda) - \varphi(\lambda)\|}{\|\phi(\lambda) - \psi(\lambda)\|} = \frac{\left\| \phi^{\ell+1} \right\|}{\left\| \left(1 + R(0)H(0)\right) \mathcal{P}^{\perp} \phi^{\ell+1} \right\|} \simeq \frac{\left\| \phi^{\ell+1} \right\|}{\left\| \mathcal{P}^{\perp} \phi^{\ell+1} \right\|}$$

Simulations

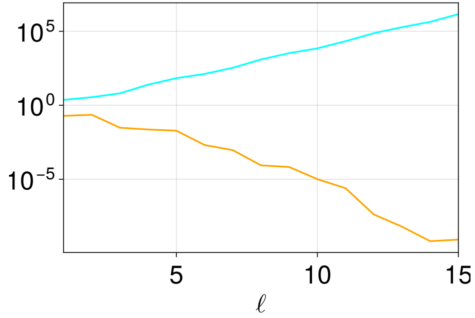


$$H^0 = -\Delta + V_0, \qquad H^1 = V_1, \qquad H^2 = V_2$$

$$H(\lambda) = \sum_{n=0}^{2} \lambda^n H^n, \qquad \mathcal{P}\mathfrak{H} = \mathrm{Span}\left(\phi^n, 0 \leqslant n \leqslant \ell\right)$$



10^0
10^{-5}
10^{-10}
$10^{-0.5}$
$10^{0.0}$
$10^{0.5}$
10^1
λ
$\|\phi(\lambda) - \psi^\ell(\lambda)\|_e / \|\phi(0)\|_e$
$\|\phi(\lambda) - \varphi^\ell(\lambda)\|_e / \|\phi(0)\|_e$
ℓ =
0 1 2 3 5 8 14 20 30 40



$\left\| \mathcal{P}^{\perp} \phi^{\ell+1} \right\|$ and $\left\| \phi^{\ell+1} \right\|$

VA+PT vs VA+excited states

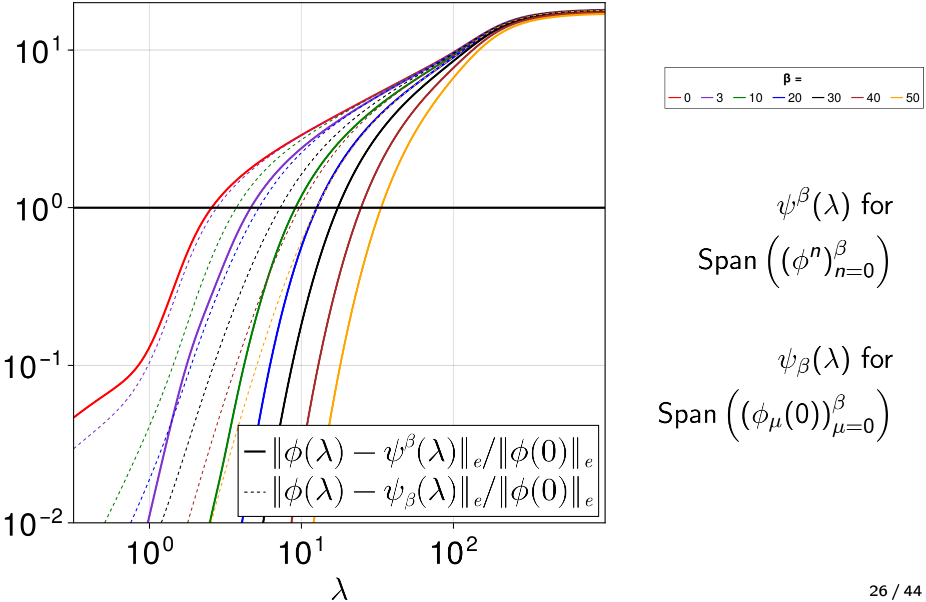
$\psi^{\beta}(\lambda)$ for

$$\mathrm{Span}\left((\phi^{n})_{n=0}^{\beta}\right)$$

$\psi_{\beta}(\lambda)$ for

$$\mathrm{Span}\left((\phi_{\mu}(0))_{\mu=0}^{\beta}\right)$$

VA+PT vs VA+excited states



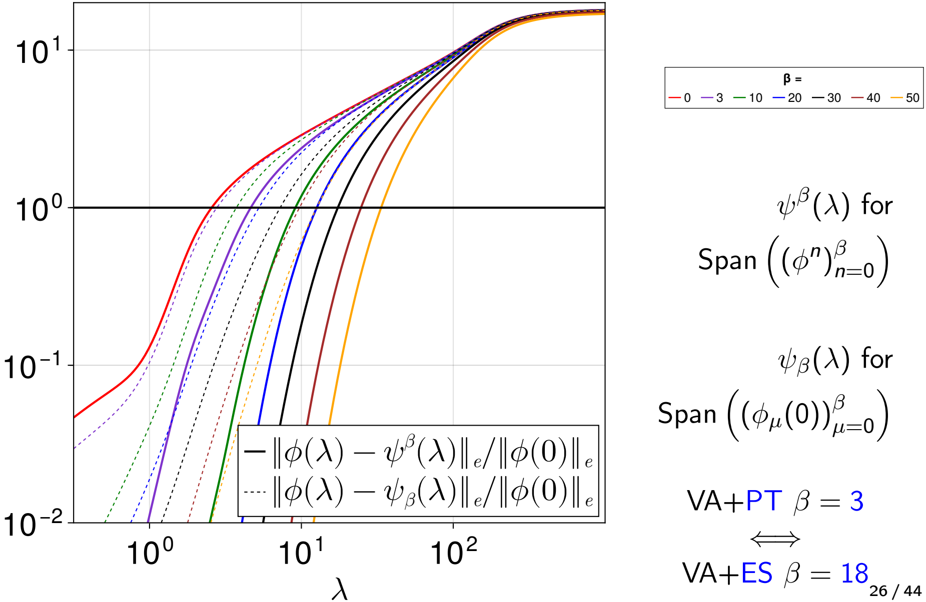
$\psi^\beta(\lambda)$ for

Span $\left((\phi^n)_{n=0}^\beta\right)$

$\psi_\beta(\lambda)$ for

Span $\left((\phi_\mu(0))_{\mu=0}^\beta\right)$

VA+PT vs VA+excited states



$\psi^\beta(\lambda)$ for

Span $\left((\phi^n)_{n=0}^\beta\right)$

$\psi_\beta(\lambda)$ for

Span $\left((\phi_\mu(0))_{\mu=0}^\beta\right)$

VA+PT $\beta = 3$

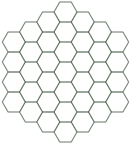
$\Longleftrightarrow$

VA+ES $\beta = 18$

Sommaire

Graphene variants

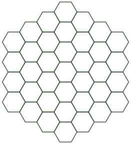
Monolayer



$$-\Delta + v(x)$$

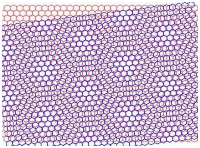
Graphene variants

Monolayer



$$-\Delta + v(x)$$

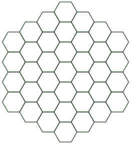
Bilayer



$$-\Delta + \mathcal{R}_{\theta}\tau_d v(x) + \mathcal{R}_{-\theta}\tau_{-d} v(x)$$

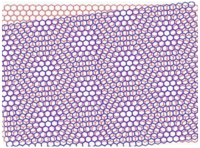
Graphene variants

Monolayer



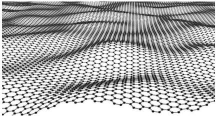
$$-\Delta + v(x)$$

Bilayer



$$-\Delta + \mathcal{R}_\theta \tau_d v(x) + \mathcal{R}_{-\theta} \tau_{-d} v(x)$$

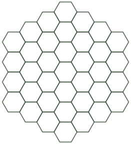
Deformed



$$-\Delta + v\left(x - \xi(\varepsilon x)\right)$$

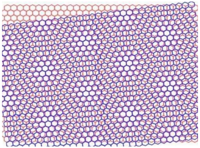
Graphene variants

Monolayer



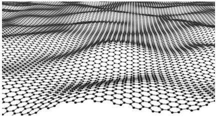
$$-\Delta + v(x)$$

Bilayer



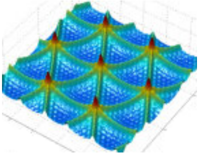
$$-\Delta + \mathcal{R}_{\theta}\tau_{d} v(x) + \mathcal{R}_{-\theta}\tau_{-d} v(x)$$

Deformed



$$-\Delta + v\left(x - \xi(\varepsilon x)\right)$$

Multi-periodic



$$-\Delta + v(x) + V(\varepsilon x)$$

Scaling in physics

v being Ω-periodic

$$-\Delta + v(x) + V(\varepsilon x), \qquad \varepsilon^{-1}\Omega - \text{periodic}$$

with $X = \varepsilon x$, physicists derive

$$v_F \sigma \cdot (-i\nabla_X) + \frac{1}{\varepsilon} V(X), \qquad v_F \in \mathbb{R}_+, v_F \sim 11 \text{ eV} \tag{1}$$

Scaling in physics

v being Ω-periodic

$$-\Delta + v(x) + V(\varepsilon x), \qquad\qquad \varepsilon^{-1}\Omega - \text{periodic}$$

with $X = \varepsilon x$, physicists derive

$$v_{\mathrm{F}}\sigma \cdot (-i\nabla_X) + \tfrac{1}{\varepsilon} V(X), \qquad v_{\mathrm{F}} \in \mathbb{R}_+, v_{\mathrm{F}} \sim 11 \text{ eV} \tag{1}$$

Rigorous way : start from

$$-\Delta + v(x) + \varepsilon V(\varepsilon x)$$

derive

$$v_{\mathrm{F}}\sigma \cdot (-i\nabla_X) + V(X).$$

A posteriori one can do $V \leftarrow \varepsilon^{-1} V$ to get (1).

Literature

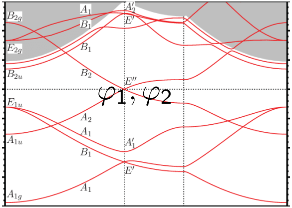
- Wallace (1946), from tight-binding, massless Dirac around K, $v_F \sigma \cdot (-i\nabla) = v_F\,(\sigma_1\partial_1 + \sigma_2\partial_2)$, $\sigma_1 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_2 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

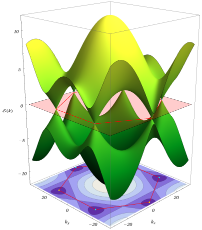
Literature

- Wallace (1946), from tight-binding, massless Dirac around K,
  $v_F \sigma \cdot (-i\nabla) = v_F (\sigma_1 \partial_1 + \sigma_2 \partial_2)$, $\sigma_1 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_2 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
- Fefferman-Weinstein (2012) studied $-\Delta + v(x)$
  where v is periodic, $\mathcal{R}_{\frac{2\pi}{3}} v = v$, $v(-x) = v(x)$

Literature

- Wallace (1946), from tight-binding, massless Dirac around K,
  $v_{\mathrm{F}}\sigma\cdot(-i\nabla) = v_{\mathrm{F}}\left(\sigma_1\partial_1+\sigma_2\partial_2\right),\ \sigma_1 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_2 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
- Fefferman-Weinstein (2012) studied $-\Delta + v(x)$
  where v is periodic, $\mathcal{R}_{\frac{2\pi}{3}} v = v$, $v(-x) = v(x)$





- $E(K+k) - E_{\mathrm{F}} = \pm v_{\mathrm{F}}\,|k| + O(k^2)$
- $\mathrm{Ker}\left(\left(-\Delta+v\right)\big|_{L^2_K(\mathbb{R}^2)} - E_{\mathrm{F}}\right) = \mathrm{Span}\{\varphi_1,\varphi_2\}$
  where $\mathcal{R}_{\frac{2\pi}{3}}\varphi_j = e^{i\frac{2\pi j}{3}}\varphi_j$, $\mathcal{PC}\varphi_1 = \varphi_2$

Fefferman-Weinstein (2014)

Take

- $i\partial_t \phi = (-\Delta + v)\,\phi$
- $i\partial_T \alpha = v_{\mathrm{F}}\sigma \cdot (-i\nabla)\alpha$
- $\psi(t,x) := e^{-itE_{\mathrm{F}}} \sum_{j=1}^{2} \varepsilon \alpha_j(\varepsilon t, \varepsilon x)\varphi_j(x)$

Assume $\phi(0,x) = \psi(0,x)$.

Théorème (Fefferman & Weinstein (2014))

Then for any $\mu > 0$, there exists $\tau > 0$ such that

$$\left\| \left(1 + |\nabla_x|\right)(\phi - \psi) \right\|_{L^2_x(\mathbb{R}^2)} = o_{\varepsilon \to 0}\left(\varepsilon^{\tau}\right)$$

uniformly in $t \in [0, \varepsilon^{-2+\mu}]$.

Fefferman & Weinstein, Wave packets in honeycomb structures and two-dimensional Dirac equations (2014)

Fefferman-Weinstein (2014)

Take

- $i\partial_t \phi = (-\Delta + v)\,\phi + \varepsilon V(\varepsilon x)\phi$
- $i\partial_T \alpha = v_{\mathrm{F}} \sigma \cdot (-i\nabla)\alpha + V\alpha$
- $\psi(t,x) := e^{-itE_{\mathrm{F}}} \sum_{j=1}^{2} \varepsilon \alpha_j(\varepsilon t, \varepsilon x)\varphi_j(x)$

Assume $\phi(0,x) = \psi(0,x)$.

Théorème (Fefferman & Weinstein (2014))

Then for any $\mu > 0$, there exists $\tau > 0$ such that

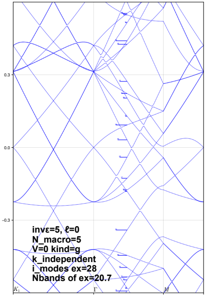
$$\left\| \left(1 + |\nabla_x|\right)(\phi - \psi) \right\|_{L^2_x(\mathbb{R}^2)} = o_{\varepsilon \to 0}\left(\varepsilon^{\tau}\right)$$

uniformly in $t \in [0, \varepsilon^{-2+\mu}]$.

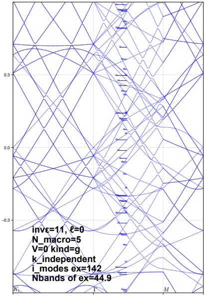
Fefferman & Weinstein, Wave packets in honeycomb structures and two-dimensional Dirac equations (2014)

Increasing ε

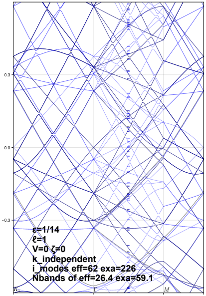
Exact operator $-\Delta + v(x)$ on $\varepsilon^{-1}\Omega$ ($V = 0$)



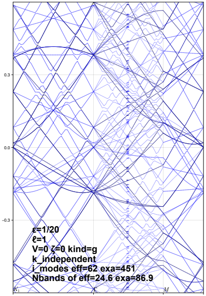
$\varepsilon = \frac{1}{5}$



$\varepsilon = \frac{1}{11}$



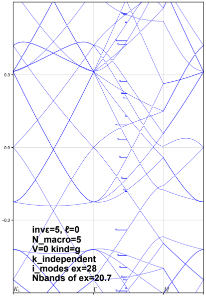
$\varepsilon = \frac{1}{14}$



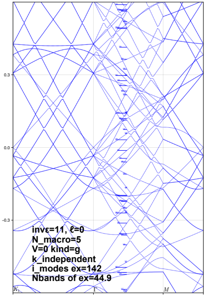
$\varepsilon = \frac{1}{20}$

Increasing ε

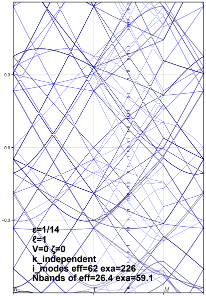
Exact operator $-\Delta + v(x)$ on $\varepsilon^{-1}\Omega$ $(V = 0)$



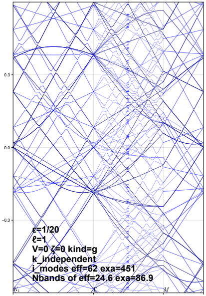
$\varepsilon = \frac{1}{5}$



$\varepsilon = \frac{1}{11}$



$\varepsilon = \frac{1}{14}$

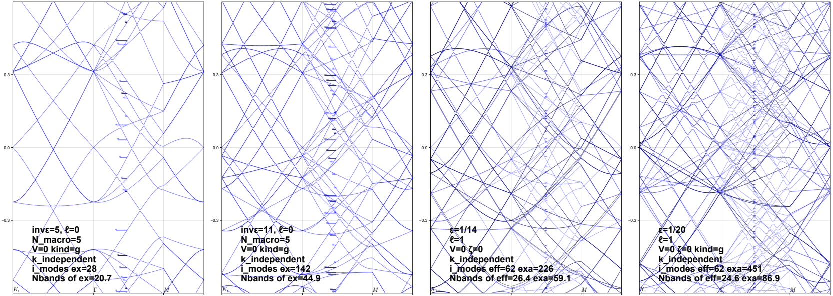


$\varepsilon = \frac{1}{20}$

$\Longrightarrow$ Isospectral result is hard

Increasing ε

Exact operator $-\Delta + v(x)$ on $\varepsilon^{-1}\Omega$ ($V = 0$)



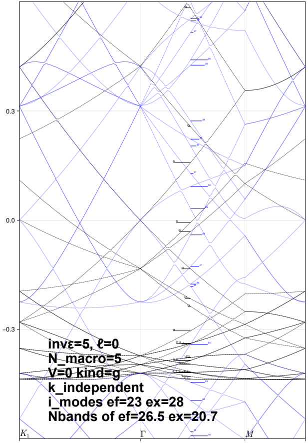
$\varepsilon = \frac{1}{5}$ $\quad$ $\varepsilon = \frac{1}{11}$ $\quad$ $\varepsilon = \frac{1}{14}$ $\quad$ $\varepsilon = \frac{1}{20}$

$\Longrightarrow$ Isospectral result is hard

$\Longrightarrow$ Dynamic results or on eigenfunctions

Existing methods are not precise

Exact operator $-\Delta + v(x)$ on $\varepsilon^{-1}\Omega$, $V = 0$, $\varepsilon = \frac{1}{5}$
Effective operator $v_{\mathrm{F}}\sigma \cdot (-i\nabla) + \varepsilon(-\Delta)$



Searching more precise effective operator

Given a familly $\mathcal{F} = \{f_1, \ldots, f_M\}$ of microscopic functions in $L^2_K(\mathbb{R}^2)$, build the variational space

$$\mathcal{V} := \left\{ \sum_{j=1}^M \varepsilon\alpha_j(\varepsilon x) f_j(x) \mid \alpha_j \in \mathcal{S}(\mathbb{R}^2) \right\} \simeq \mathcal{S}^2(\mathbb{R}^2, \mathbb{R}^M)$$

Searching more precise effective operator

Given a familly $\mathcal{F} = \{f_1, \dots, f_M\}$ of microscopic functions in $L^2_K(\mathbb{R}^2)$, build the variational space

$$\mathcal{V} := \left\{ \sum_{j=1}^M \varepsilon\alpha_j(\varepsilon x) f_j(x) \mid \alpha_j \in \mathcal{S}(\mathbb{R}^2) \right\} \simeq \mathcal{S}^2(\mathbb{R}^2, \mathbb{R}^M)$$

Define

$$H^k := (-i\nabla + K + \varepsilon k)^2 + v + \varepsilon V(\varepsilon x),$$

and $\mathcal{J}\alpha := \sum_{j=1}^M \varepsilon\alpha_j(\varepsilon x) f_j(x)$. Then

$$\left\langle \mathcal{J}\beta, H^k \mathcal{J}\alpha \right\rangle = \left\langle \beta, H^k_{\text{eff}} \alpha \right\rangle + O(\varepsilon^\infty)$$

i.e. $\mathcal{J}^* H^k \mathcal{J}$ converges weakly to H^k_{eff}.

We can expect : if

- $\left(H^k - E^k\right)\phi = 0$
- $(H^k_{\text{eff}} - E^k_{\text{eff}})\alpha = 0$
- $\psi(x) := \sum_{j=1}^{M} \varepsilon\alpha_j(\varepsilon x) f_j(x) = \mathcal{J}\alpha$

Then

$$E^k - E^0 \simeq E^k_{\text{eff}} - E^0_{\text{eff}}, \qquad\qquad \phi \simeq \psi$$

We always choose $\mathcal{F} = \{\varphi_1, \varphi_2, \dots\}$, so

We always choose $\mathcal{F} = \{\varphi_1, \varphi_2, \dots\}$, so

$$H_{\text{eff}} = \varepsilon^{-1} \begin{pmatrix} 0 & 0 \\ 0 & M \end{pmatrix} \otimes \mathbb{1} + \begin{pmatrix} v_{\mathrm{F}}\sigma & T \\ T^* & L \end{pmatrix} \cdot \otimes (-i\nabla) \\ + \begin{pmatrix} \mathbb{1} & 0 \\ 0 & S \end{pmatrix} \otimes V + \varepsilon \begin{pmatrix} \mathbb{1} & 0 \\ 0 & S \end{pmatrix} \otimes (-\Delta).$$

We always choose $\mathcal{F} = \{\varphi_1, \varphi_2, \dots\}$, so

$$H_{\text{eff}} = \varepsilon^{-1} \begin{pmatrix} 0 & 0 \\ 0 & M \end{pmatrix} \otimes \mathbb{1} + \begin{pmatrix} v_{\text{F}}\sigma & T \\ T^* & L \end{pmatrix} \cdot \otimes (-i\nabla) + \begin{pmatrix} \mathbb{1} & 0 \\ 0 & S \end{pmatrix} \otimes V + \varepsilon \begin{pmatrix} \mathbb{1} & 0 \\ 0 & S \end{pmatrix} \otimes (-\Delta).$$

- Choosing $\mathcal{F} = \{\varphi_1, \varphi_2\}$ gives $H_{\text{eff}} = v_{\text{F}}\sigma(-i\nabla) + \varepsilon(-\Delta) + V$ (Cancès, G., Gontier 2023)

We always choose $\mathcal{F} = \{\varphi_1, \varphi_2, \dots\}$, so

$$H_{\text{eff}} = \varepsilon^{-1} \begin{pmatrix} 0 & 0 \\ 0 & M \end{pmatrix} \otimes \mathbb{1} + \begin{pmatrix} v_{\text{F}}\sigma & T \\ T^* & L \end{pmatrix} \cdot \otimes (-i\nabla) + \begin{pmatrix} \mathbb{1} & 0 \\ 0 & S \end{pmatrix} \otimes V + \varepsilon \begin{pmatrix} \mathbb{1} & 0 \\ 0 & S \end{pmatrix} \otimes (-\Delta).$$

- Choosing $\mathcal{F} = \{\varphi_1, \varphi_2\}$ gives $H_{\text{eff}} = v_{\text{F}}\sigma(-i\nabla) + \varepsilon(-\Delta) + V$ (Cancès, G., Gontier 2023)
- Note $(\varphi_j)_k$ the eigenfunction such that $(-\Delta + v - E_k)_{|L^2_k(\mathbb{R}^2)} (\varphi_j)_k = 0$ for $j \in \{1, 2\}$
  Choosing $\mathcal{F} = \{\varphi_1, \varphi_2, \frac{\mathrm{d}}{\mathrm{d}k}(\varphi_1)_k(K), \frac{\mathrm{d}}{\mathrm{d}k}(\varphi_2)_k(K)\}$ gives

$$M = -\begin{pmatrix} t & re^{i2\theta_k} \\ re^{-i2\theta_k} & t \end{pmatrix}, \qquad S = \begin{pmatrix} t' & r'e^{i2\theta_k} \\ r'e^{-i2\theta_k} & t' \end{pmatrix}, \qquad \dots$$

where $e^{i\theta_k} := \frac{k_x + ik_y}{|k|}$, and

$$T = \begin{pmatrix} (r\mathbb{1} - s\sigma_2)\frac{k}{|k|} & re^{i\theta_k}\binom{1}{i} \\ re^{-i\theta_k}\binom{1}{-i} & (r\mathbb{1} + s\sigma_2)\frac{k}{|k|} \end{pmatrix}, \qquad \text{5 additional parameters}$$

- Choosing $\mathcal{F} = \{\varphi_1, \varphi_2, \partial_{k_x}(\varphi_1)_k, \partial_{k_y}(\varphi_1)_k, \partial_{k_x}(\varphi_2)_k, \partial_{k_y}(\varphi_2)_k\}$,

$$S = \begin{pmatrix} t\mathbb{1} + s'\sigma_2 & r'D \\ r'D^* & t\mathbb{1} - s'\sigma_2 \end{pmatrix}, \qquad M = -\begin{pmatrix} t\mathbb{1} + s\sigma_2 & rD \\ rD^* & t\mathbb{1} - s\sigma_2 \end{pmatrix}$$

where $D := \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix}$, and

$$T^1 = \begin{pmatrix} t & -is & r & ir \\ r & -ir & t & is \end{pmatrix}, \qquad T^2 = \begin{pmatrix} is & t & ir & -r \\ -ir & -r & -is & t \end{pmatrix}$$

- Choosing $\mathcal{F} = \{\varphi_1, \varphi_2, \partial_{k_x}(\varphi_1)_k, \partial_{k_y}(\varphi_1)_k, \partial_{k_x}(\varphi_2)_k, \partial_{k_y}(\varphi_2)_k\}$,

$$S = \begin{pmatrix} t\mathbb{1} + s'\sigma_2 & r'D \\ r'D^* & t\mathbb{1} - s'\sigma_2 \end{pmatrix}, \qquad M = -\begin{pmatrix} t\mathbb{1} + s\sigma_2 & rD \\ rD^* & t\mathbb{1} - s\sigma_2 \end{pmatrix}$$

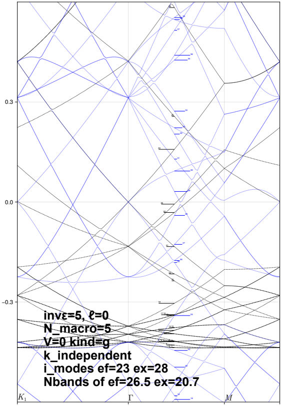
where $D := \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix}$, and

$$T^1 = \begin{pmatrix} t & -is & r & ir \\ r & -ir & t & is \end{pmatrix}, \qquad T^2 = \begin{pmatrix} is & t & ir & -r \\ -ir & -r & -is & t \end{pmatrix}$$

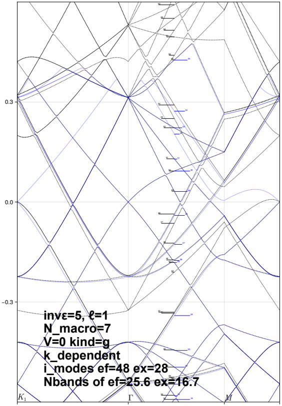
6 additional parameters

Varying ℓ

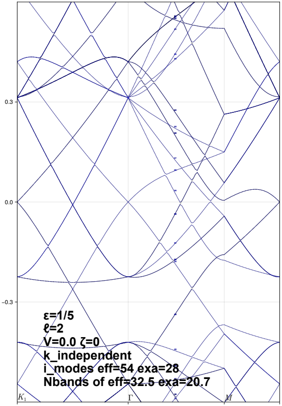
Exact operator $-\Delta + v(x)$ $(V = 0)$, $\varepsilon = \frac{1}{5}$
Effective operator



$\ell = 0$



$\ell = 1$

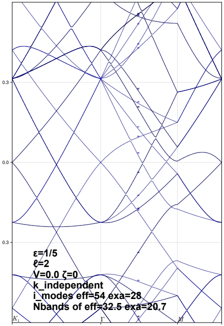


$\ell = 2$

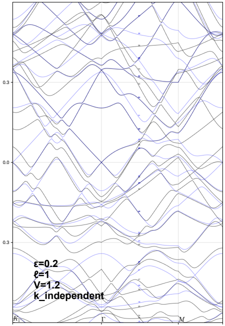
Increasing V

Exact operator $-\Delta + v(x) + \varepsilon\lambda V(\varepsilon x)$, $\varepsilon = \frac{1}{5}$

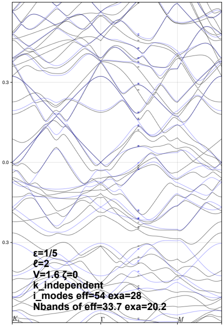
Effective operator with $\ell = 2$



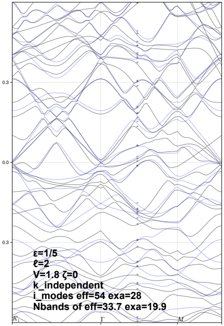
$\lambda = 0$



$\lambda = 6$



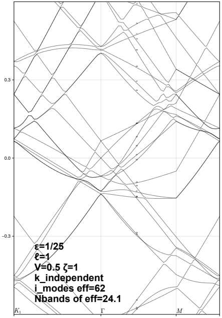
$\lambda = 8$



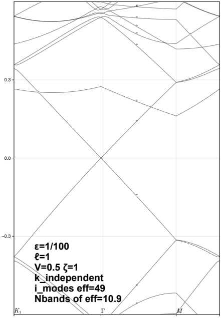
$\lambda = 10$

Decreasing ε

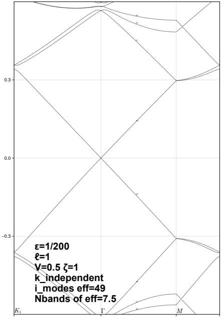
Effective operator with $\ell = 1$



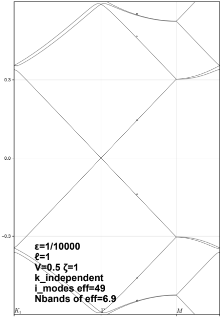
$\varepsilon = \frac{1}{25}$



$\varepsilon = \frac{1}{100}$



$\varepsilon = \frac{1}{200}$



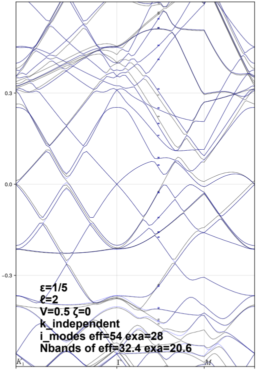
$\varepsilon = \frac{1}{10000}$

Schur the effective operator

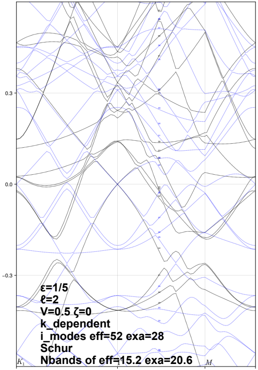
Exact operator $-\Delta + v(x) + \varepsilon V(\varepsilon x)$, $\varepsilon = \frac{1}{5}$

Schured effective operator with $\ell = 2$

$$v_F \sigma \cdot (-i\nabla) + V + +\varepsilon \left((-\Delta) + T \cdot (-i\nabla)(M^{-1} T^*) \cdot (-i\nabla)\right)$$



Not Shured

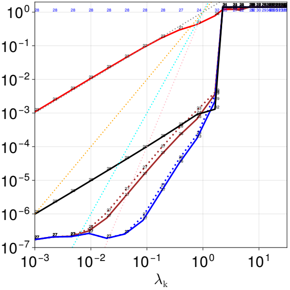


Schured

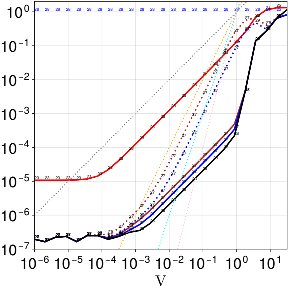
General principle for deriving effective systems

We have the exact solution when $k = 0$, $V = 0$. So there are 2 sources of error. In simulations we see

$$\|\phi - \psi\| \leqslant C\varepsilon\left(\|V\| + c\,|k|^{\ell+1}\right)$$



$|k|$ varies



$\|V\|$ varies

$\ell = 0$ · $\ell = 1, k_{\mathrm{dep}}$ · $\ell = 1, k_{\mathrm{indep}}$ · $\ell = 2, k_{\mathrm{dep}}$ · $\ell = 2, k_{\mathrm{indep}}$ · 6 eigenstates states at K

General principle for deriving effective systems

ϕ exact and ψ approximated

$$\|\phi - \psi\| \leqslant C\varepsilon^n.$$

One can work to obtain :

- large n, using perturbation theory
- small C, using variational approximation

General principle for deriving effective systems

ϕ exact and ψ approximated

$$\|\phi - \psi\| \leqslant C\varepsilon^n.$$

One can work to obtain :

- large n, using perturbation theory
- small C, using variational approximation

VA+PT can improve both of them at the same time

Conclusions

- Coupling perturbation theory and variational approximation
- Simulations on graphene :
  - effective graphene isospectral description is hard
  - Dirac operator converges slowly to exact operator
  - We don't want to go at further order in ε
  - "augmented" Dirac gives the right bands quickly in ε