Numerical integration in the Brillouin zone

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First part with É Cancès, V. Ehrlacher, D. Gontier, D. Lombardi, Numerische, 2019
Second part with I. Duchemin, L. Genovese, E. Letournel, S. Ruget, preprint 2022

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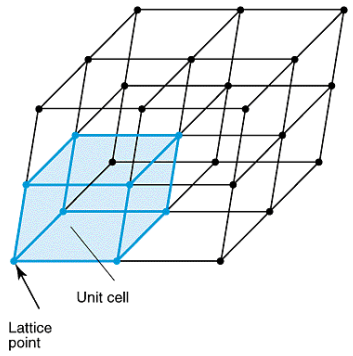
Summary

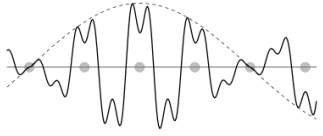
Brillouin zone sampling

Consider non-interacting electrons in a perfectly periodic Hamiltonian $H = -\frac{1}{2}\Delta + V$ with lattice $\mathcal{R}$, and a $L \times L \times L$ supercell



- Because of periodicity, eigenstates can be searched as Bloch waves

$$\psi_k(r) = e^{ik\cdot r} u_k(r)$$



where u_k is cell-periodic and k is in the discrete Brillouin zone

$$\mathcal{B}_L = \left\{ \sum_{i=1}^{3} k_i a_i^*, k_i \in \left\{ 0, \ldots, \frac{L-1}{L} \right\} \right\}$$

- Yields eigenstates

$$H\psi_{nk} = \varepsilon_{nk}\psi_{nk}$$

Electrons in a supercell

Occupied states are those for which $\varepsilon_{nk} \leq \varepsilon_F$, where

$$L^3 N_{\text{el}} = \sum_{k \in \mathcal{B}_L, n \in \mathbb{N}} \mathbb{1}(\varepsilon_{nk} \leq \varepsilon_F)$$

with total energy

$$L^3 E^L = \sum_{k \in \mathcal{B}_L, n \in \mathbb{N}} \varepsilon_{nk} \mathbb{1}(\varepsilon_{nk} \leq \varepsilon_F)$$

When $L \to \infty$:

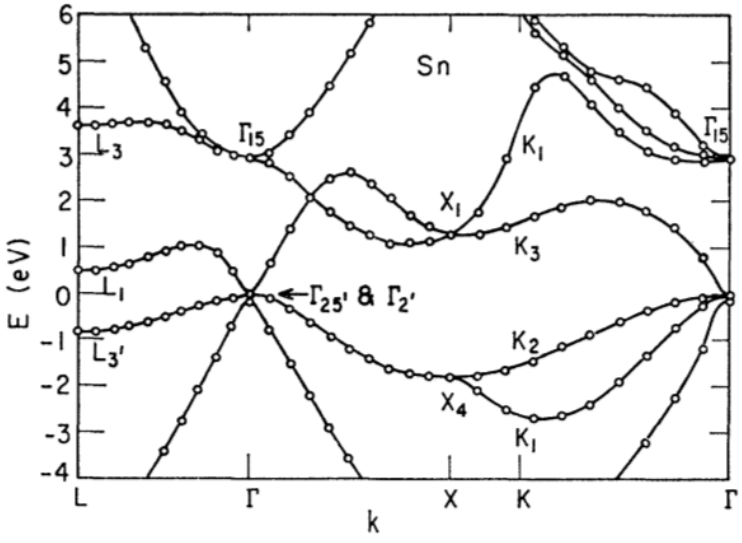
$$\lim_{L \to \infty} E^L = \fint_{\mathcal{B}} \sum_{n \in \mathbb{N}} \varepsilon_{nk} \mathbb{1}(\varepsilon_{nk} \leq \varepsilon_F) dk$$

$$\text{where } N_{\text{el}} = \fint_{\mathcal{B}} \sum_{n \in \mathbb{N}} \mathbb{1}(\varepsilon_{nk} \leq \varepsilon_F) dk$$

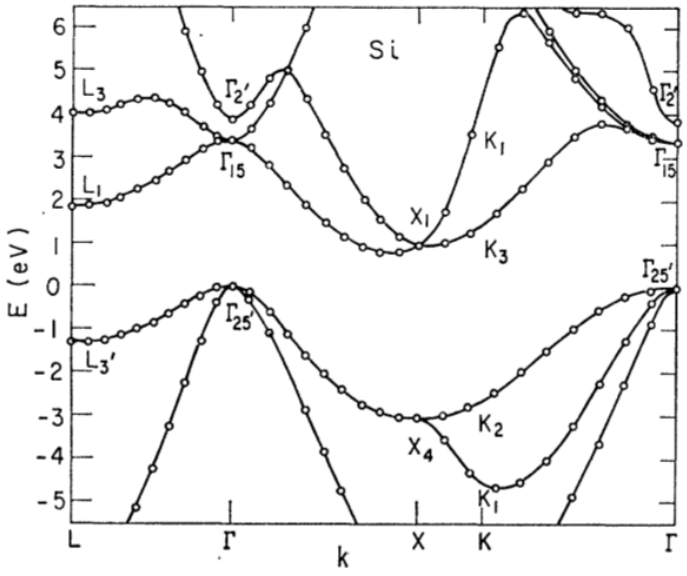
What is the speed of convergence with respect to L? Can it be improved?

Major practical issue (second source of errors after pseudopotentials)

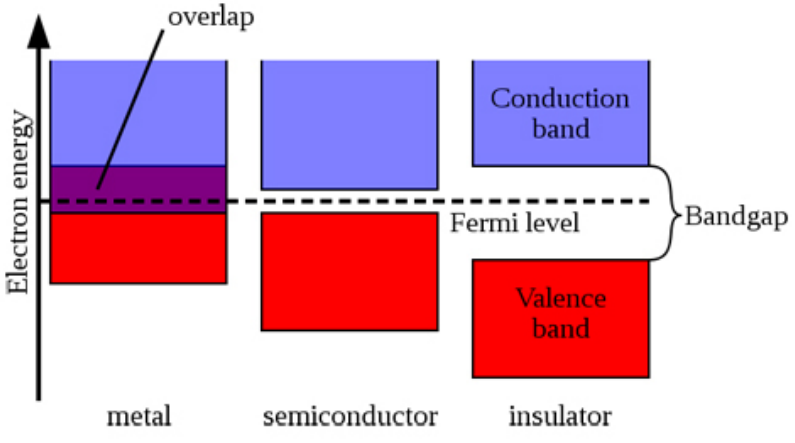
Band structure



Tin (metal)



Silicon (semiconductor)



Summary

Numerical analysis: the case of insulators

- In a gapped system (insulator, semiconductor),

$$\inf_{\mathbf{k}\in\mathcal{B}} \varepsilon_{N_{\mathrm{el}}+1,\mathbf{k}} - \sup_{\mathbf{k}\in\mathcal{B}} \varepsilon_{N_{\mathrm{el}}\mathbf{k}} \geq g > 0,$$

  and so there are exactly N_{el} bands filled at each $\mathbf{k}$:

$$E = \sum_n \fint_{\mathcal{B}} \varepsilon_{n\mathbf{k}} \mathbb{1}(\varepsilon_{n\mathbf{k}} \leq \varepsilon_F) d\mathbf{k} = \fint_{\mathcal{B}} \sum_{n=1}^{N_{\mathrm{el}}} \varepsilon_{n\mathbf{k}} d\mathbf{k}$$

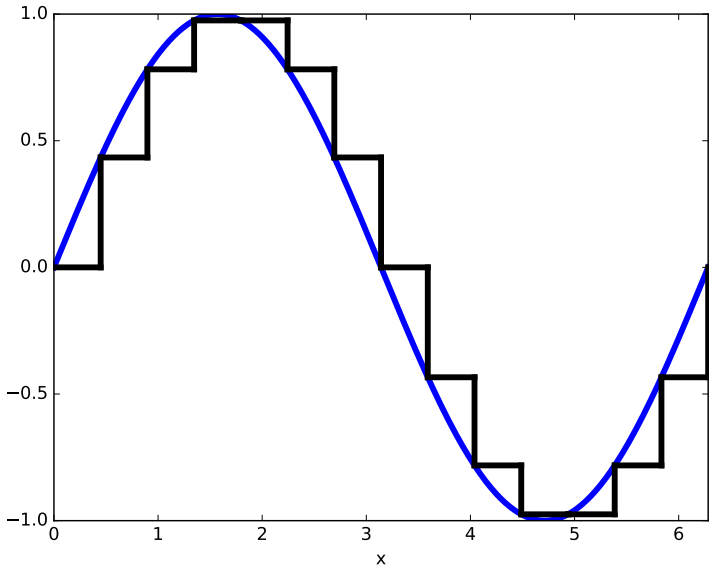
$$E^L = \frac{1}{L^3} \sum_{n=1}^{N_{\mathrm{el}}} \sum_{\mathbf{k}\in\mathcal{B}_L} \varepsilon_{n\mathbf{k}} d\mathbf{k}$$

Theorem (Gontier-Lahbabi '16)

Under suitable hypotheses on V_{per}, there is $\alpha > 0, C > 0$ such that

$$|E - E^L| \leq Ce^{-\alpha L}$$

Ideas of the proof: Riemann sums of periodic functions



- For a periodic f, what is the error made by

$$\int_0^{2\pi} f(x)dx \approx \frac{2\pi}{L} \sum_{k=0}^{L-1} f(2\pi k/L)$$

- Usual estimates (Taylor): $O(1/L)$
- But large error cancellation: quadrature exact for e^{inx}, $|n| < L$

(Ideas of the proof: exponential convergence)

Theorem (Classical: Trefethen-Weideman '14, Gontier-Lahbabi '16)

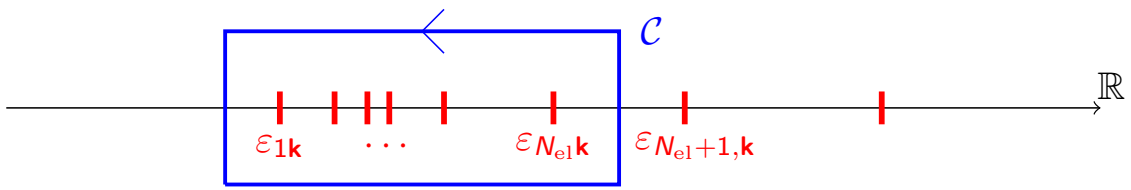
1. *If f is periodic and smooth, then the integration error is $O(L^{-p})$ for all p*
2. *If f is complex analytic on the strip $\mathbb{R} + [-A, A]i$, then the integration error is $O(e^{-\beta AL})$, β a universal constant.*

(proof: regularity $\Longleftrightarrow$ decay of Fourier coefficients)

$$E = \fint_{\mathcal{B}} \sum_{n=1}^{N_{\mathrm{el}}} \varepsilon_{n\mathbf{k}} d\mathbf{k}$$

- In general, $\varepsilon_{n\mathbf{k}}$ is smooth (and even complex analytic on a strip) outside *eigenvalue crossings* $\varepsilon_{n,\mathbf{k}} = \varepsilon_{n',\mathbf{k}}$
- But sums of eigenvalues are smooth when $\varepsilon_{N_{\mathrm{el}},\mathbf{k}} < \varepsilon_{N_{\mathrm{el}}+1,\mathbf{k}}$

$$E = \fint_{\mathcal{B}} \mathrm{Tr}(P_{N_{\mathrm{el}}}(H_{\mathbf{k}})H_{\mathbf{k}})d\mathbf{k}, \quad P_{N_{\mathrm{el}}}(H_{\mathbf{k}}) = \frac{1}{2\pi i}\oint_{\mathcal{C}}(\lambda - H_{\mathbf{k}})^{-1}d\lambda$$



□

Summary

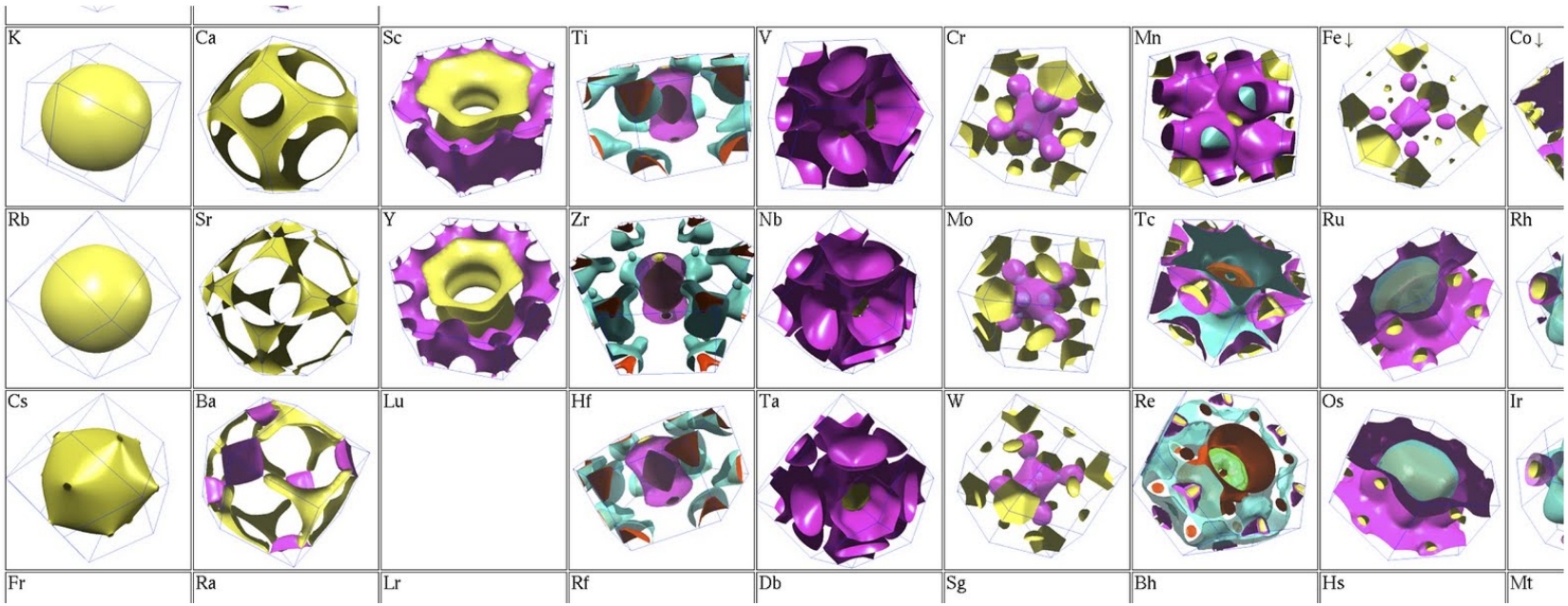
Metals and Fermi surface

In metals, there is no gap

$$E = \sum_n \fint_{\mathcal{B}} \varepsilon_{n\mathbf{k}} \mathbb{1}(\varepsilon_{n\mathbf{k}} \leq \varepsilon_F) d\mathbf{k}, \quad N_{\text{el}} = \sum_n \fint_{\mathcal{B}} \mathbb{1}(\varepsilon_{n\mathbf{k}} \leq \varepsilon_F) d\mathbf{k}$$

Key concept: Fermi surface

$$S(\varepsilon_F) = \cup_n S_n(\varepsilon_F), \quad S_n(\varepsilon_F) = \{\mathbf{k} \in \mathcal{B}, \varepsilon_{n\mathbf{k}} = \varepsilon_F\}.$$



Periodic table of Fermi surfaces

`http://www.phys.ufl.edu/fermisurface/periodic_table.html`

Assumptions

$$S(\varepsilon_F) = \cup_n S_n(\varepsilon_F), \quad S_n(\varepsilon_F) = \{\mathbf{k} \in \mathcal{B}, \varepsilon_{n\mathbf{k}} = \varepsilon_F\}.$$

Assumptions

1. $S(\varepsilon_F) \neq \emptyset$ (metal)
2. $S_n(\varepsilon_F) \cap S_{n'}(\varepsilon_F) = \emptyset$ (no crossing on Fermi surface)
3. $\nabla \varepsilon_{n,\mathbf{k}} \neq 0$ on $S_n(\varepsilon_F)$ (no flat bands)

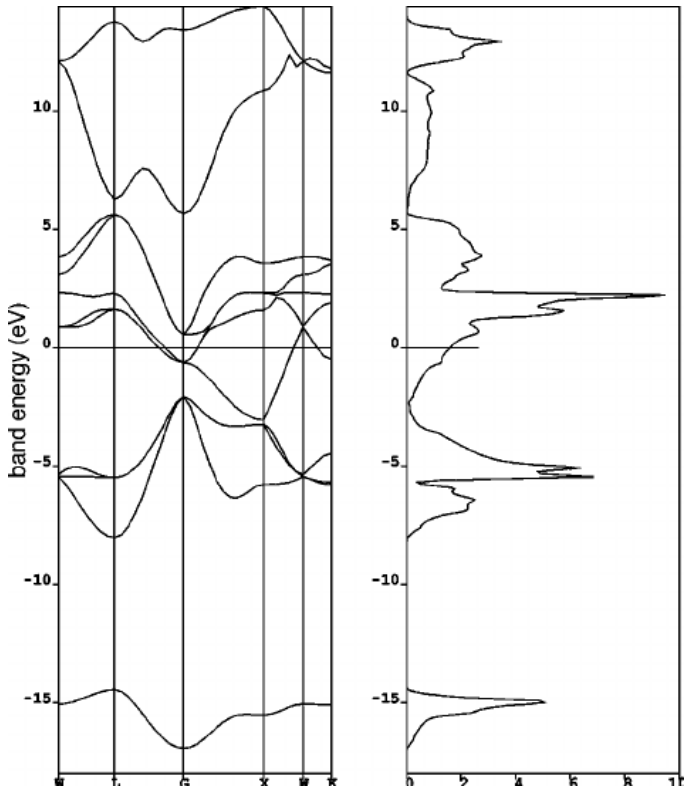
- Excludes semi-metals (graphene) and highly symmetric systems (free electron gas)
- No crossing: $\varepsilon_{n\mathbf{k}}$ is smooth on a neighborhood of $S_n(\varepsilon_F)$
- No flat bands: $S = \cup_n \varepsilon_{n\mathbf{k}}^{-1}(\{\varepsilon_F\})$ is a smooth surface

Density of states

Theorem (Co-area formula, integration over level sets)

If $\mathbf{k} \to f(\mathbf{k})/|\nabla E(\mathbf{k})|$ *is* L^1,

$$\fint_{\mathcal{B}} f(\mathbf{k}) d\mathbf{k} = \int_{\mathbb{R}} \left(\int_{E^{-1}(\{\varepsilon\})} \frac{f(\mathbf{k})}{|\nabla E(k)|} d\sigma(\mathbf{k}) \right) d\varepsilon$$



DoS of TiN

Integrated density of states

$$\mathcal{N}(\varepsilon) = \sum_n \fint_{\mathcal{B}} \mathbb{1}(\underbrace{\varepsilon_{n\mathbf{k}}}_{E(\mathbf{k})} \leq \varepsilon) d\mathbf{k}$$

$$" = " \int_{-\infty}^{\varepsilon} \underbrace{\sum_n \int_{S_n(\varepsilon')} \frac{1}{|\nabla \varepsilon_{n\mathbf{k}}|} d\sigma(\mathbf{k})}_{\mathcal{D}(\varepsilon')} d\varepsilon'$$

$\mathcal{N}$ is smooth near ε_F and

$$\mathcal{D}(\varepsilon_F) = \mathcal{N}'(\varepsilon_F) > 0$$

Error analysis for interpolation

- Approximate $\varepsilon_{n\mathbf{k}}$ by an interpolated $\varepsilon^{p}_{n\mathbf{k}}$ with order p on a $L \times L \times L$ grid and integrate

$$\begin{cases} E^L = \sum_n \fint_{\mathcal{B}} \varepsilon^{L,p}_{n\mathbf{k}} \mathbb{1}(\varepsilon^{L,q}_{n\mathbf{k}} \leq \varepsilon^L_F) d\mathbf{k} \\ N = \sum_n \fint_{\mathcal{B}} \mathbb{1}(\varepsilon^{L,q}_{n\mathbf{k}} \leq \varepsilon^L_F) d\mathbf{k} \end{cases}$$

- Interpolate integrand with order p and domain of integration with order q
- Most often used in practice: $p = 2, q = 1$ (Blochl's corrections $\approx$ higher-dimensional Euler-MacLaurin)

Theorem

There is $C > 0$ such that

$$|\varepsilon^L_F - \varepsilon_F| \leq \frac{C}{L^{q+1}}$$

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$$|\varepsilon^L_F - \varepsilon_F| \leq \frac{C}{L^{q+1}}$$

$$|E^L - E| \leq C \left(\frac{1}{L^{p+1}} + \frac{1}{L^{2q+2}} \right)$$

(Ideas of the proof: error on the Fermi level)

Approximate integrated density of states

$$\mathcal{N}^L(\varepsilon) = \sum_n \fint_{\mathcal{B}} \mathbb{1}(\varepsilon_{n\mathbf{k}}^{L,q} \leq \varepsilon) d\mathbf{k}$$

ε_F^L is defined by $\mathcal{N}^L(\varepsilon_F^L) = N_{\mathrm{el}} = \mathcal{N}(\varepsilon_F)$.
$\varepsilon_{n\mathbf{k}}$ is smooth near ε_F, so $\mathcal{N}^L$ and $\mathcal{N}$ are $O(L^{q+1})$-close near ε_F. From $\mathcal{N}'(\varepsilon_F) = \mathcal{D}(\varepsilon_F) > 0$, it follows that

$$|\varepsilon_F^L - \varepsilon_F| \leq \frac{C}{L^{q+1}} \quad \square$$

For the energy:

$$E^L - E = \underbrace{\sum_n \fint_{\mathcal{B}} (\varepsilon_{n\mathbf{k}}^{L,p} - \varepsilon_{n\mathbf{k}}) \mathbb{1}(\varepsilon_{n\mathbf{k}}^{L,q} \leq \varepsilon_F^L) d\mathbf{k}}_{\textit{bulk}, O(L^{-(p+1)})}$$

$$+ \underbrace{\sum_n \fint_{\mathcal{B}} \varepsilon_{n\mathbf{k}} (\mathbb{1}(\varepsilon_{n\mathbf{k}}^{L,q} \leq \varepsilon_F^L) - \mathbb{1}(\varepsilon_{n\mathbf{k}} \leq \varepsilon_F)) d\mathbf{k}}_{\textit{surface}, O(L^{-(q+1)})}$$

(Ideas of the proof: error on the energy)

$$\text{surface error} = \sum_n \fint_{\mathcal{B}} \varepsilon_{n\mathbf{k}} (\mathbb{1}(\varepsilon_{n\mathbf{k}}^{L,q} \leq \varepsilon_F^L) - \mathbb{1}(\varepsilon_{n\mathbf{k}} \leq \varepsilon_F)) d\mathbf{k}$$

Naively, this is controled by the size of the integration domain so $O(L^{-(q+1)})$, but

$$\begin{aligned}\text{surface error} &= \sum_n \fint_{\mathcal{B}} (\varepsilon_{n\mathbf{k}} - \varepsilon_F)(\mathbb{1}(\varepsilon_{n\mathbf{k}}^{L,q} \leq \varepsilon_F^L) - \mathbb{1}(\varepsilon_{n\mathbf{k}} \leq \varepsilon_F)) d\mathbf{k} \\ &\quad + \underbrace{\varepsilon_F(\mathcal{N}^L(\varepsilon_F^{L,q}) - \mathcal{N}(\varepsilon_F))}_{=0} \\ &= O(L^{-(2q+2)})\end{aligned}$$

□

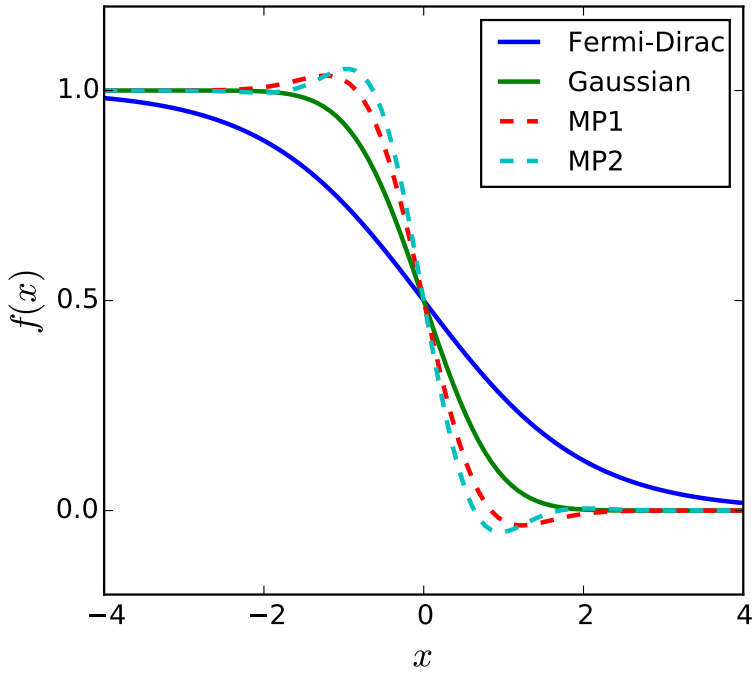
This trick is special for the energy ("the energy is variational in the Fermi surface"), only $O(L^{-(q+1)})$ for other quantities (Fermi level, density...)

Summary

Smearing

$$E^T = \sum_n \fint_{\mathcal{B}} \varepsilon_{n\mathbf{k}} f\left(\frac{\varepsilon_{n\mathbf{k}} - \varepsilon_F^T}{T}\right) d\mathbf{k}$$

$$N = \sum_n \fint_{\mathcal{B}} f\left(\frac{\varepsilon_{n\mathbf{k}} - \varepsilon_F^T}{T}\right) d\mathbf{k}$$



- $f(x)$ is an approximation of $\mathrm{Heaviside}(-x)$
- T is a regularization parameter (physically, a temperature)
- The integrand is now smooth, and therefore efficiently computed by Riemann sums: $E^{T,L}$
- Two sources of errors:

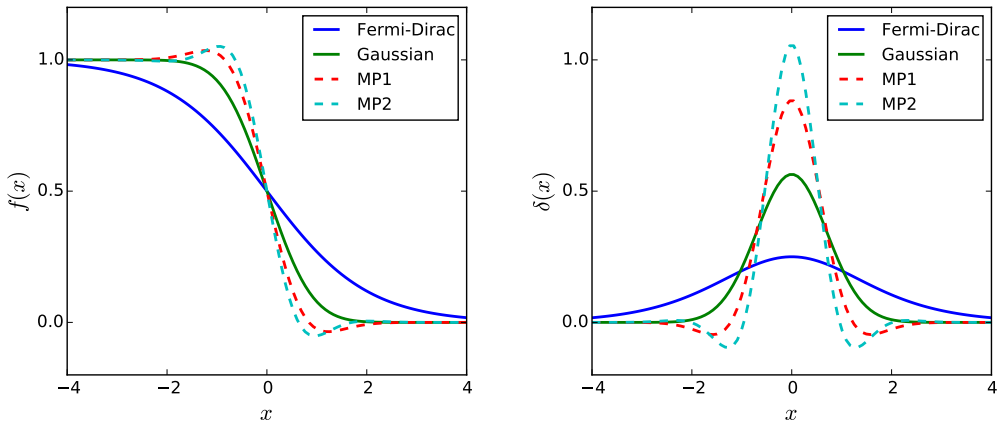
$$|E^{T,L} - E| \leq \underbrace{|E^T - E|}_{\textit{smearing error}} + \underbrace{|E^{T,L} - E^T|}_{\textit{quadrature error}}$$

Smearing error

A smearing function is of order p if

$$\int_{-\infty}^{+\infty} (f(\varepsilon) - \mathbb{1}(\varepsilon < 0))P(\varepsilon)d\varepsilon = 0$$

for any polynomial P of degree $p-1$.
Several choices in the literature: Fermi-Dirac, Gaussian smearing (order 1), Methfessel-Paxton (higher order)...



Theorem

If f has decaying tails and is of order p, there is $C > 0$ such that

$$|\varepsilon_F^T - \varepsilon_F| \leq CT^{p+1}$$
$$|E^T - E| \leq CT^{p+1}$$

(Ideas of the proof)

Formally, using the co-area formula,

$$\mathcal{N}^T(\varepsilon) = \sum_n \fint_{\mathcal{B}} f\left(\frac{\varepsilon_{n\mathbf{k}} - \varepsilon}{T}\right) d\mathbf{k} = \int_{\mathbb{R}} f\left(\frac{\varepsilon' - \varepsilon}{T}\right) \mathcal{D}(\varepsilon') d\varepsilon'$$

$$= T \int_{\mathbb{R}} f(x) \mathcal{D}(\varepsilon + Tx) dx$$

f has decaying tails, so $\mathcal{D}$ is evaluated T-close to ε, around which $\mathcal{D}$ can be expanded into Taylor series, and therefore

$$\mathcal{N}^T(\varepsilon) - \mathcal{N}(\varepsilon) = T \int_{\mathbb{R}} (f(x) - \mathbb{1}(x \leq 0)) \mathcal{D}(\varepsilon + Tx) dx$$

$$= T \sum_{n=0}^{p-1} \frac{T^n}{n!} \mathcal{D}^{(n)}(\varepsilon) \underbrace{\int_{\mathbb{R}} (f(x) - \mathbb{1}(x \leq 0)) x^n dx}_{=0} + O(T^{p+1})$$

Similarly,

$$\sum_n \fint_{\mathcal{B}} \varepsilon_{n\mathbf{k}} f\left(\frac{\varepsilon_{n\mathbf{k}} - \varepsilon}{T}\right) d\mathbf{k} = \int_{\mathbb{R}} \varepsilon' f\left(\frac{\varepsilon' - \varepsilon}{T}\right) \mathcal{D}(\varepsilon') d\varepsilon'$$

(Quadrature error)

$$E^T = \sum_n \fint_{\mathcal{B}} \varepsilon_{n\mathbf{k}} f\left(\frac{\varepsilon_{n\mathbf{k}} - \varepsilon_F^T}{T}\right) d\mathbf{k}, \quad N = \sum_n \fint_{\mathcal{B}} f\left(\frac{\varepsilon_{n\mathbf{k}} - \varepsilon_F^T}{T}\right) d\mathbf{k}$$

- Integrand smooth, approximate by Riemann sums $E^{T,L}, \varepsilon^{T,L}$

Theorem (Classical: Trefethen-Weideman '14, Gontier-Lahbabi '16)

If g is complex analytic on a strip $S_A = \mathbb{R}^3 + i[-A, A]$, then the error between its integral and Riemann sum is bounded by

$$C\left(\sup_{\mathbf{z}\in S_A} g(\mathbf{z})\right) e^{-cAL}$$

Find an analytic continuation of

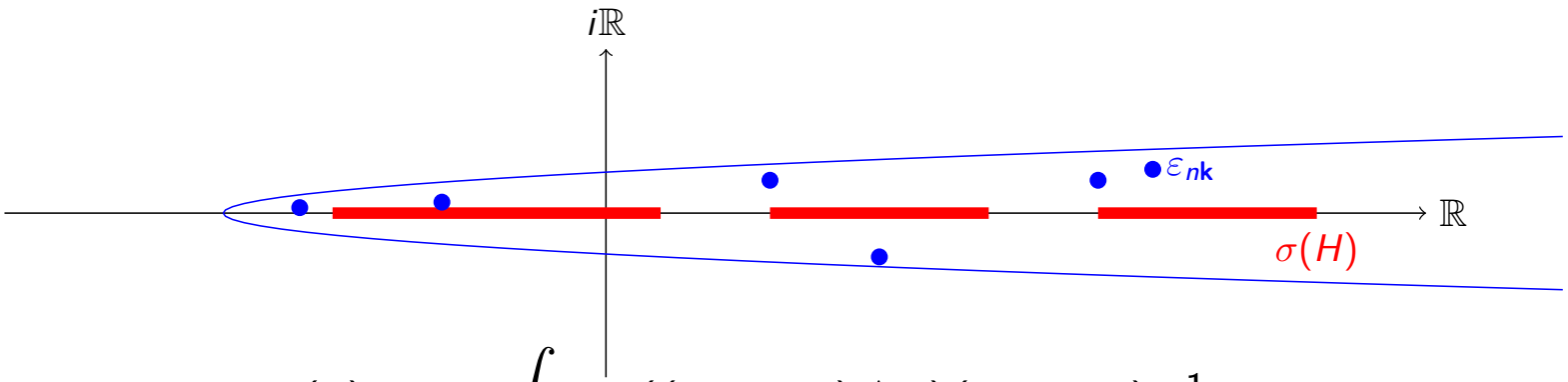
$$g(\mathbf{k}) = \sum_n \varepsilon_{n\mathbf{k}} f\left(\frac{\varepsilon_{n\mathbf{k}} - \varepsilon_F}{T}\right)$$

1. Fermi-Dirac $f(x) = (1 + e^x)^{-1}$ analytic on a strip (poles at $(2\mathbb{Z} + 1)\pi i$)
2. Gaussian $f(x) = \operatorname{erfc}(x)/2$ entire

(Analytic properties of the integrand)

$$g(\mathbf{z}) = \sum_n \varepsilon_{n\mathbf{z}} f\left(\frac{\varepsilon_{n\mathbf{z}} - \varepsilon_F}{T}\right) \qquad \text{but } \varepsilon_{n\mathbf{z}} \text{ not analytic}$$

$$= \mathrm{Tr}\left[H_{\mathbf{z}} f\left(\frac{H_{\mathbf{z}} - \varepsilon_F}{T}\right)\right] \qquad \text{but } H_{\mathbf{z}} \text{ is not self-adjoint, } f(H_{\mathbf{z}})?$$



$$g(\mathbf{z}) = \mathrm{Tr} \oint_C \lambda f((\lambda - \varepsilon_F)/T)(\lambda - H_{\mathbf{z}})^{-1} d\lambda$$

But $(\lambda - H_{\mathbf{z}})^{-1}$ is not trace-class ($\varepsilon_{n\mathbf{k}} \approx n^{2/d}$)... finally

$$g(\mathbf{z}) = \oint_C \lambda(\lambda + \Sigma) f((\lambda - \varepsilon_F)/T)\, \mathrm{Tr}\left[(\lambda - H_{\mathbf{z}})^{-1}(\Sigma + H_{\mathbf{z}})^{-1}\right] d\lambda$$

is an analytical continuation of $g(\mathbf{k}) = \sum_n \varepsilon_{n\mathbf{k}} f\left(\frac{\varepsilon_{n\mathbf{k}} - \varepsilon_F}{T}\right)$

Sampling of smeared quantities

Theorem

The integrand is complex analytic in $\mathbf{k}$*, on a strip of size* $O(T)$ *(Fermi-Dirac smearing), and on the whole complex plane (Gaussian-type smearing).*
There is $C(T), c(T)$ *such that*

$$|E^{T,L} - E^{T}| \leq C(T)e^{-c(T)L^{\beta}}$$
$$|\varepsilon_F^{T,L} - \varepsilon_F^{T}| \leq C(T)e^{-c(T)L^{\beta}}$$

with $\beta = 1$ *(Fermi-Dirac) or* $\beta = 4/3$ *(Gaussian-type)*

Total error similar in spirit to

$$|E - E^{T,L}| \leq C(\underbrace{T^{p+1}}_{E-E^{T}} + \underbrace{e^{-cTL}}_{E^{T}-E^{T,L}}).$$

For a given L, pick $T = 1/L$ to obtain error $C(L^{-(p+1)})$ (up to log factors)

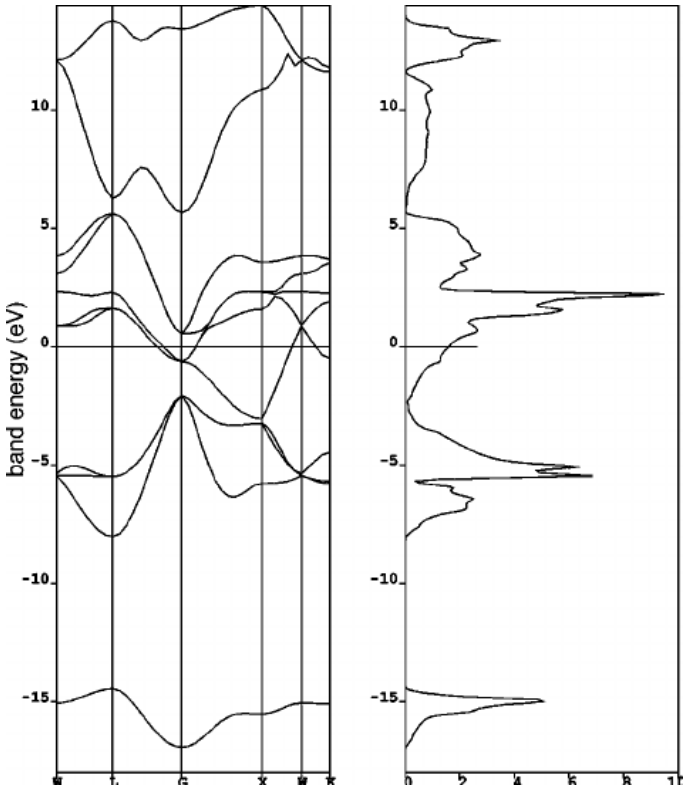
Conclusion: metals

- For interpolation, order as expected, but bonus order for the energy
- For smearing, optimization of T as a function of L
- Prove rigorously some results known heuristically in the physical literature, plus
  1. Importance of hypotheses (generically true but violated in some symmetry-protected systems like graphene)
  2. Convergence like $Ce^{-cL^{4/3}}$ for Gaussian-type smearing (!)
  3. Optimal choice of T
- Possibly better schemes: Wannier functions, reduced basis (Shirley), adaptive grids...
- Open problems: systems with symmetries, non-smooth Fermi surfaces (e.g. graphene)

Summary

DOS

Consider now the problem of computing the density of states



DoS of TiN

$$D(E) = \fint_{\mathcal{B}} \sum_{n\in\mathbb{N}} \delta(\varepsilon_{nk} - E)dk$$

$$= \lim_{\eta\to 0^+} \frac{1}{\pi}\mathrm{Im} \fint_{\mathcal{B}} \sum_{n\in\mathbb{N}} \frac{1}{\varepsilon_{nk} - E + i\eta} dk$$

and more generally of

$$G(E) = \lim_{\eta\to 0^+} \frac{1}{H - E + i\eta}$$

(useful for many electronic properties)

Solutions as before: interpolation or regularization, but gives non-analytic $D(E) \Rightarrow$ problem for resonances

A simpler problem: contour deformation to the rescue

Compute the analytic continuation of

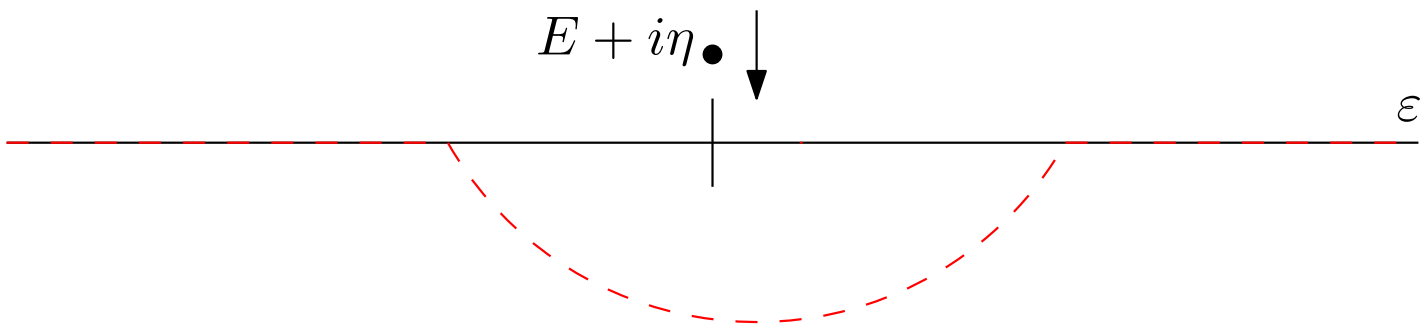
$$I_1(z) = \int_{\mathbb{R}} \frac{\phi(\varepsilon)}{z-\varepsilon} d\varepsilon \quad \text{from } \mathrm{Im(z)} > 0 \text{ to } \mathrm{Im(z)} < 0$$

- When $z = E + i\eta$, $\eta > 0$,

$$\frac{\phi(\varepsilon)}{z-\varepsilon} = \phi(\varepsilon)\frac{E-\varepsilon+i\eta}{(E-\varepsilon)^2+\eta^2}$$

  Bump of height $1/\eta$, width η around $\varepsilon = E$
- Numerical integration needs $N \gg \frac{1}{\eta}$ quadrature points
- Continuation past $\eta = 0$ impossible once discretized

Solution: contour deformation

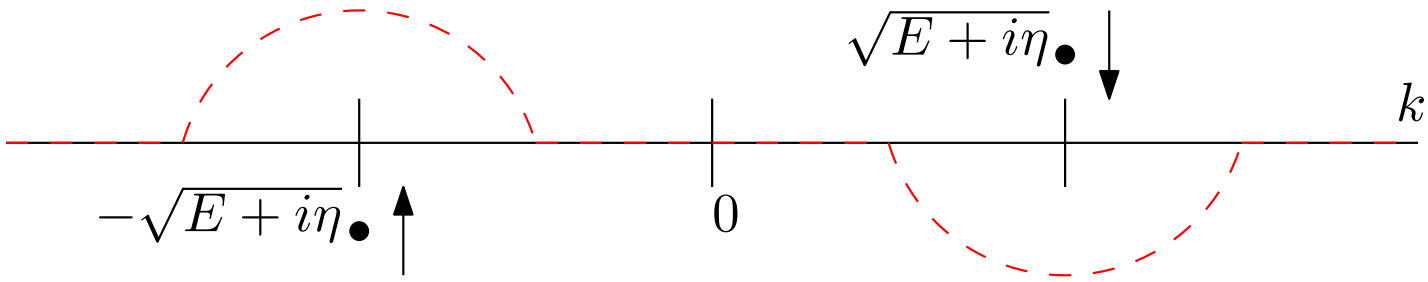


A more complicated problem

Compute the analytic continuation of

$$I_2(z) = \int_{\mathbb{R}} \frac{\phi(k)}{z - \varepsilon(k)} dk \quad \text{from } \mathrm{Im(z)} > 0 \text{ to } \mathrm{Im(z)} < 0$$

Eg if $\varepsilon(k) = k^2$, singularities near the Fermi surface $k = \pm\sqrt{E}$



- More generally, at $z = E + i\eta$, if k_0 is a point of the Fermi surface $\varepsilon(k_0) = E$, singularity at

$$k = k_0 + \frac{i\eta}{\varepsilon'(k_0)} + O(\eta^2)$$

- Need $\varepsilon' \neq 0$, no continuation possible otherwise (van Hove singularity, zero group velocity)

One band, multiple dimensions: Brillouin zone deformation

Lemma

Let $A(k)$ be a $(2\pi)^d-$ periodic function, analytic in an open set $U = \mathbb{R}^d + i[-\eta, \eta]^d$. Then, for all periodic and smooth functions $k_i(k) : \mathbb{R}^d \to [-\eta, \eta]^d$, we have

$$\int_{[-\pi,\pi]^d} A(k)dk = \int_{[-\pi,\pi]^d} A(k + ik_i(k)) \det(1 + ik_i'(k))dk$$

Proof:

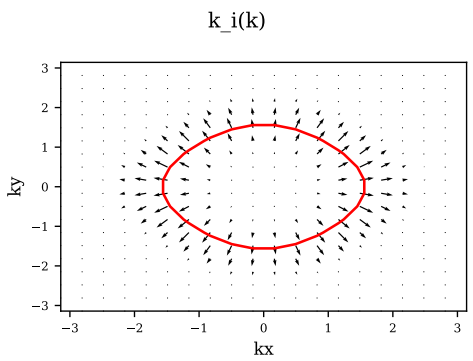
$$I(\alpha) = \int_{[0,2\pi]^d} A(k + \alpha k_i(k)) \det(1 + \alpha k_i'(k))dk,$$

is analytic and constant in $\alpha \in [-1, 1] \Rightarrow I(i) = I(0)$. □

Take k_i such that $k + ik_i(k)$ avoids the Fermi surface:

$$\boxed{k_i = -\alpha \nabla \varepsilon(k) \chi(\varepsilon(k) - E)}$$

where χ is a cutoff function and E the energy of interest.



The full problem

$$G_0(r, r'; z) = \int_{\mathrm{BZ}} \sum_{n=1}^{\infty} \frac{e^{ik(r-r')} u_{nk}(r) \overline{u_{nk}(r')}}{z - \varepsilon_{nk}} dk$$

deformed with $k \to k + ik_i(k)$ with

$$k_i(k) = -\alpha \sum_n \chi(\varepsilon_{nk} - E) \nabla \varepsilon_{nk}$$

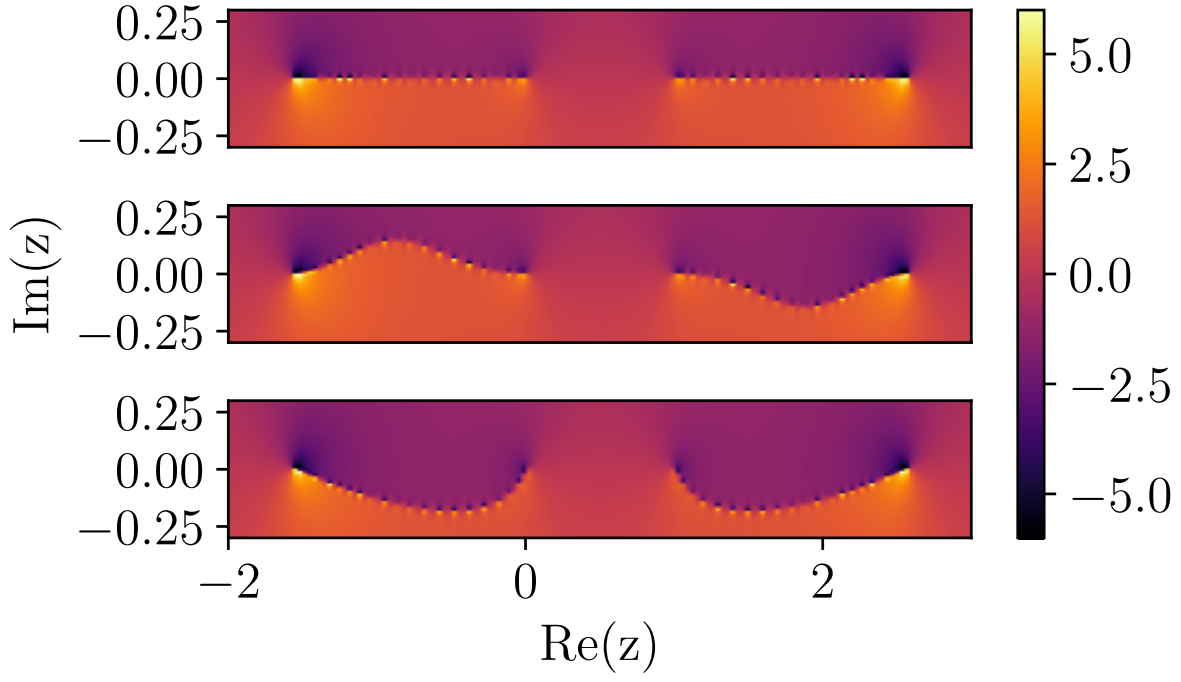
where χ is a cutoff function and E the energy of interest.

Can continue numerically near E if there are no van Hove singularities (crossing or bands with zero gradient at the "Fermi surface" $\{k, \varepsilon_{nk} = E\}$)

- **Only requires unit cell computations**
- Exponential convergence wrt Brillouin zone sampling
- Natural generalization of complex scaling to periodic systems: when $H_0 = -\frac{1}{2}\Delta$, $\nabla\varepsilon(k) = k$, compare with complex scaling $k \to e^{-i\alpha} k$

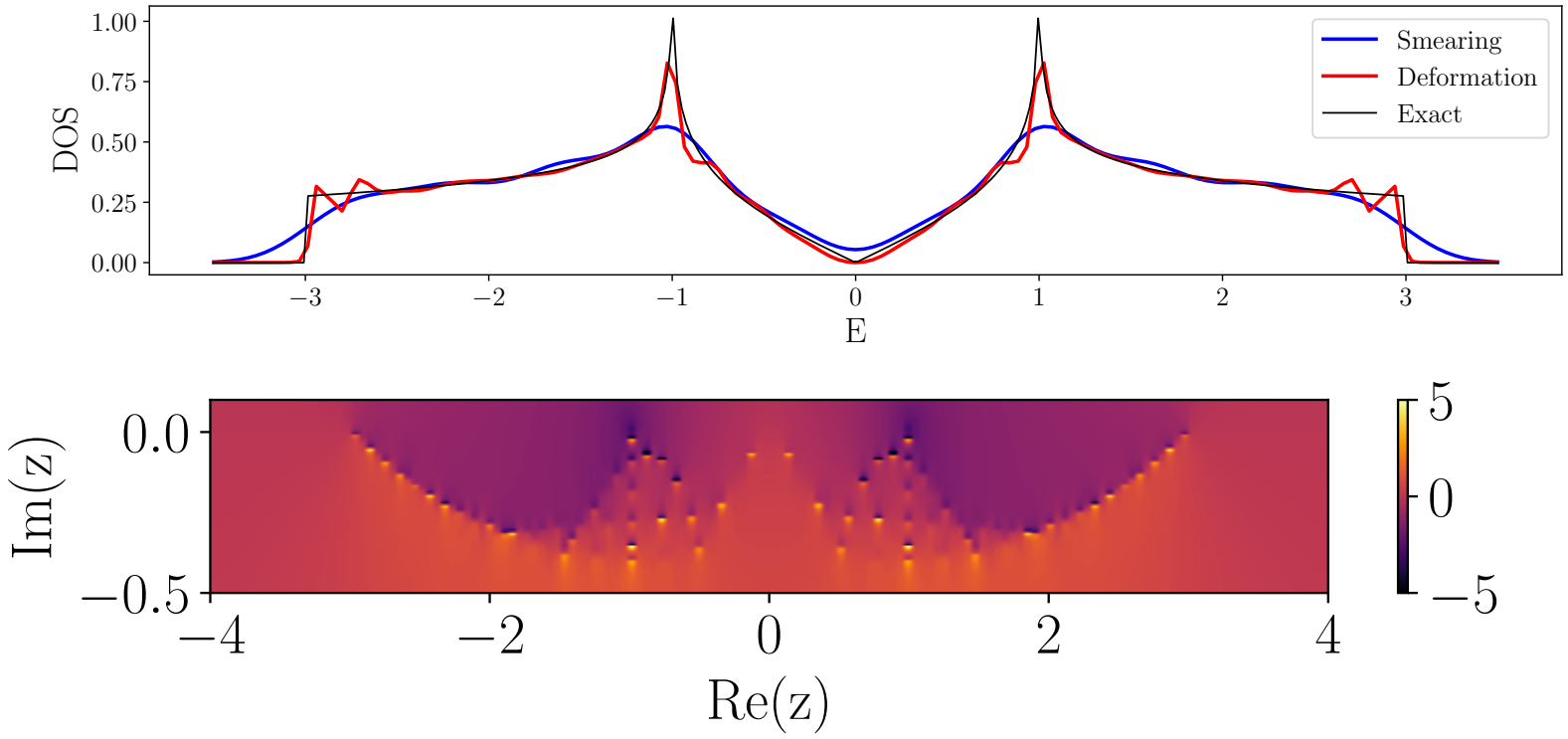
Example: 1D diatomic chain

$$H_0 = \begin{pmatrix} \ddots & \ddots & \ddots & & & & \\ & 1 & E_a & 1 & & & \\ & & 1 & E_b & 1 & & \\ & & & 1 & E_a & 1 & \\ & & & & 1 & E_b & 1 \\ & & & & & \ddots & \ddots & \ddots \end{pmatrix}$$



Top to bottom: periodic Green functions with (a) no deformation, (b) deformation at fixed $E = 2$, (c) deformation at $E = \mathrm{Re}(z)$.

Example: tight-binding model of graphene



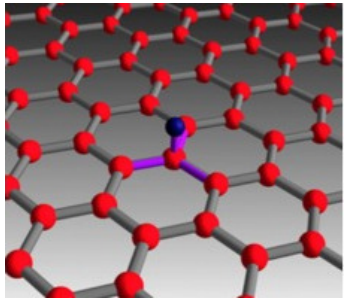
Bonus: resonances

- Consider a local impurity: $H = H_0 + V$
- Resonances are poles of the analytic continuation of matrix elements of $G(z) = 1/(z - H)$ from $\mathrm{Im}(z) > 0$ to $\mathrm{Im}(z) < 0$
- Can use resolvent/Dyson formula:

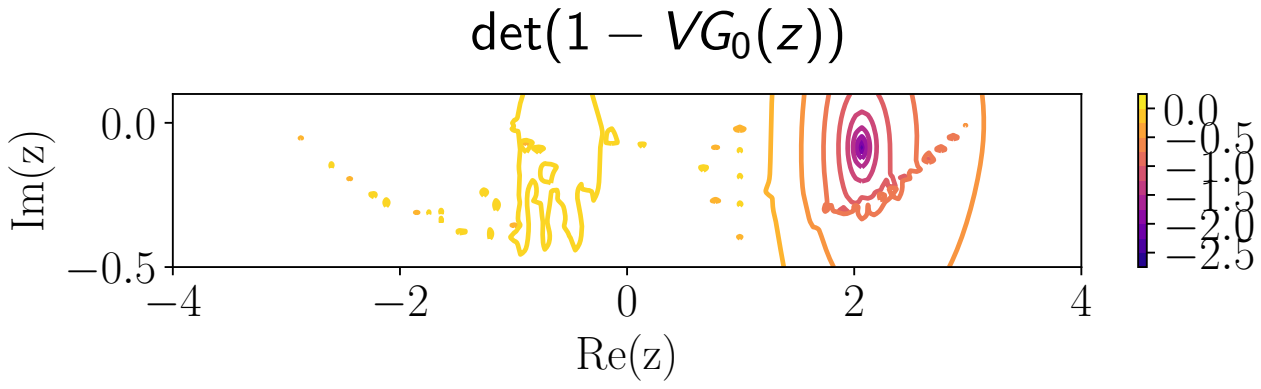
$$G(z) = G_0(z)(1 - VG_0(z))^{-1}$$

- Need to compute analytic continuation of $G_0(z) \Rightarrow$ contour deformation

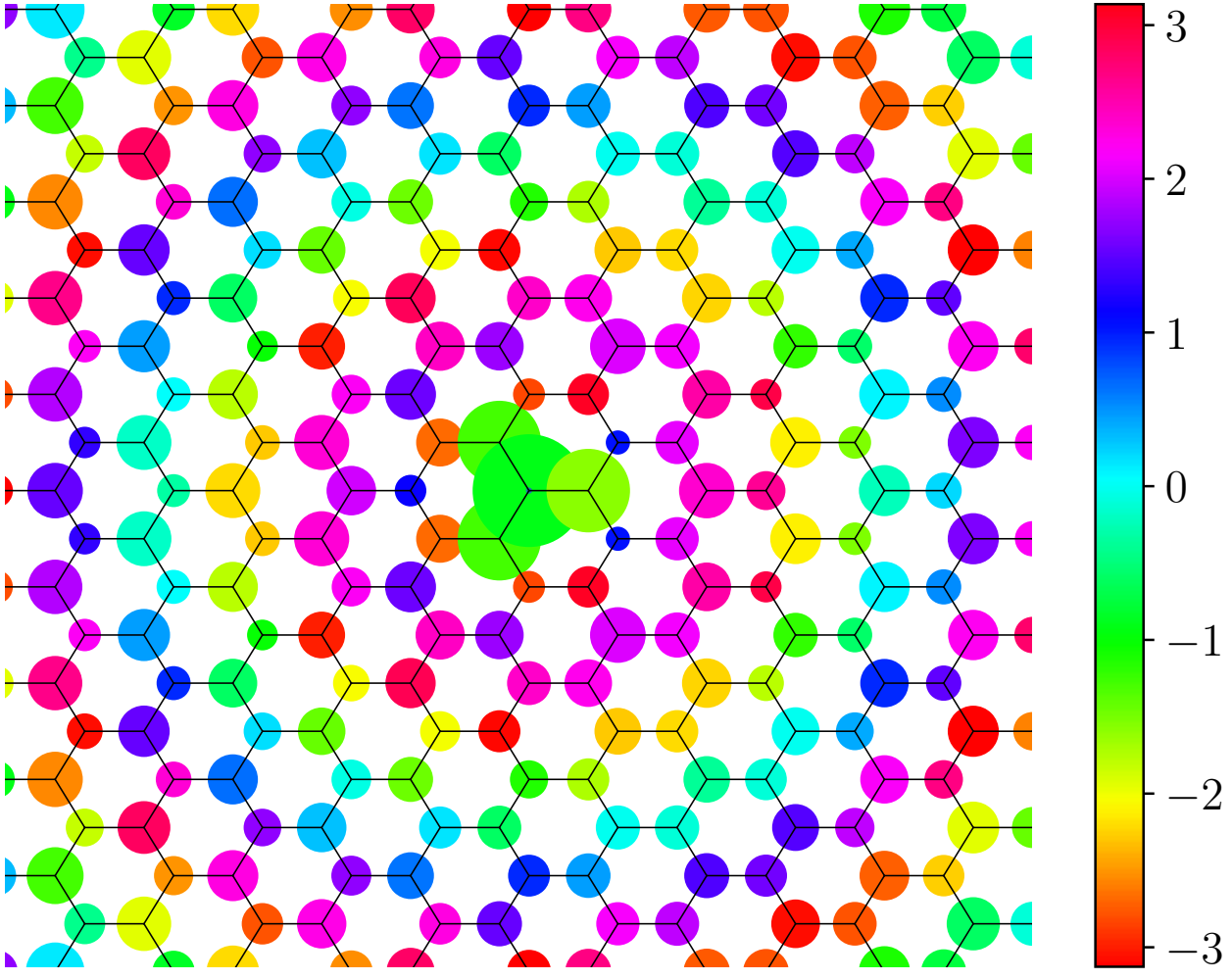
Example: adatom on 2D surface



H_0: graphene sheet + isolated adatom. V: graphene-adatom coupling



Example: adatom on 2D surface



Perspectives

Methodology

- Avoid expensive sums over eigenstates (Sternheimer formalism $\Rightarrow$ only iterative preconditioned eigen/linear problems)
- Find poles efficiently (nonlinear eigenvalue problem)
- Extend to TDDFT
- Implement in DFT codes

Applications

- Include resonant states in basis set expansions?
- Materials science: conductivity?
- General scattering problems?