# Green's functions in single-particle quantum mechanics

## 1 GF as Hamiltonian resolvent

- stationary Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\bar{r})\right]\psi(\bar{r}) = E\,\psi(\bar{r}) \;\rightarrow\; \hat{H}_{\bar{r}}\psi(\bar{r}) = E\,\psi(\bar{r}) \;\rightarrow\; (E-\hat{H}_{\bar{r}})\,\psi(\bar{r}) = 0$$

- introduction of GF in analogy with electrostatics

Laplace $\nabla^2\phi = 0$ Poisson $\nabla^2\phi = -\frac{1}{\varepsilon_0}\rho$ Green $\nabla^2 G = -\frac{1}{\varepsilon_0}\delta$

equation for GF $(E-\hat{H}_{\bar{r}})\,G(\bar{r},\bar{r}';E) = \delta(\bar{r}-\bar{r}')$

purpose:

1. extra Hamiltonian contributions
2. time evolution

in operator form $(E-\hat{H})\,\hat{G}(E) = \hat{1}$

$\rightarrow$ formal solution $\hat{G}(E) = \dfrac{1}{E-\hat{H}}$ (resolvent of $\hat{H}$)

connection of abstract & real-space form

$$(E-\hat{H})\,\hat{G}(E) = \hat{1}$$

coordinate representation $\quad \psi(\vec{r}) = \langle \vec{r}|\psi\rangle$

$$\sigma_{\vec{r},\vec{r}'} = \langle \vec{r}|\hat{\sigma}|\vec{r}'\rangle$$

$$\langle \vec{r}|(E-\hat{H})\int d^3\vec{r}''\,|\vec{r}''\rangle\langle \vec{r}''|\,\hat{G}(E)|\vec{r}'\rangle = \langle \vec{r}|\vec{r}'\rangle$$

definition $\quad \langle \vec{r}|\hat{G}(E)|\vec{r}'\rangle = G(\vec{r},\vec{r}';E)$

$$(E-\hat{H}_{\vec{r}})\,G(\vec{r},\vec{r}';E) = \delta(\vec{r}-\vec{r}')$$

- generalize definition to complex plane

→ full resolvent of $\hat{H}$

$$\hat{G}(z) = \frac{1}{z-\hat{H}} \qquad z\in\mathbb{C}$$

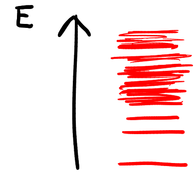
"core" GF object:

1) encodes information about $\hat{H}$ spectrum

2) captures dynamics in frequency domain

3) used to develop perturbation expansions

## ② Spectral representations & densities




- eigenspectrum of $\hat{H}$: $\hat{H}|n\rangle = E_n|n\rangle$ (discrete & continuous parts)

  orthogonality $\langle m|n\rangle = \delta_{mn}$ completeness $\sum_n |n\rangle\langle n| = \hat{1}$

- resolvent in eigenbasis

$$\hat{G}(z) = (z-\hat{H})^{-1}\,\hat{1} = (z-\hat{H})^{-1}\sum_n |n\rangle\langle n| = \sum_n \frac{|n\rangle\langle n|}{z-E_n}$$

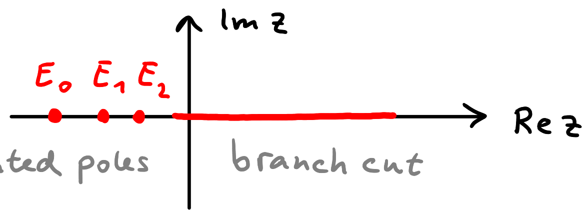
real-space representation

spatial resolution

$$G(\bar{r},\bar{r}';z) = \langle\bar{r}|\hat{G}(z)|\bar{r}'\rangle = \sum_n \frac{\langle\bar{r}|n\rangle\langle n|\bar{r}'\rangle}{z-E_n} = \sum_n \frac{\phi_n(\bar{r})\,\phi_n^*(\bar{r}')}{z-E_n}$$

energy resolution

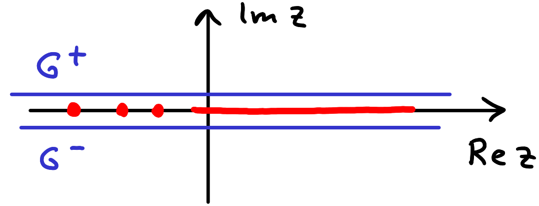
analytical structure of G



- spectral density operator / function

retarded GF: $G_{ret}(E) = G^{+}(E) = G(E + i0^{+})$

advanced GF: $G_{adv}(E) = G^{-}(E) = G(E - i0^{+})$




spectral density operator

$$\hat{A}(E) = \frac{i}{2\pi}\left[G^{+}(E) - G^{-}(E)\right] = \frac{i}{2\pi}\sum_n |n\rangle\langle n| \left(\frac{1}{E - E_n + i0^{+}} - \frac{1}{E - E_n - i0^{+}}\right)$$

$$= \sum_n \underbrace{|n\rangle\langle n|}_{\text{internal structure of states}} \underbrace{\delta(E - E_n)}_{\text{energy resolution}}$$

$$\frac{1}{x \pm i0^{+}} = \mathcal{P}\frac{1}{x} \mp i\pi\,\delta(x)$$

Sochocki - Plemelj

reconstruction of G

$$\hat{G}(z) = \int_{-\infty}^{\infty} dE\, \frac{\hat{A}(E)}{z - E}$$

spectral representation of GF

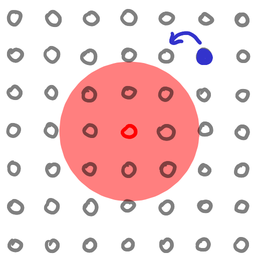
local density of states (LDOS)

$$\rho(\bar{r},E) = \langle \bar{r}|\hat{A}(E)|\bar{r}\rangle = \sum_n \underbrace{\langle \bar{r}|n\rangle}_{\phi_n(r)}\underbrace{\langle n|\bar{r}\rangle}_{\phi_n^*(\bar{r})}\,\delta(E-E_n) = \sum_n |\phi_n(\bar{r})|^2\,\delta(E-E_n)$$

density of states (DOS)

$$\mathcal{N}(E) = \int d^3\bar{r}\,\rho(\bar{r},E) = \sum_n \int d^3\bar{r}\,|\phi_n(\bar{r})|^2\,\delta(E-E_n) = \sum_n \delta(E-E_n)$$

**Ex** particle on a square lattice with extended impurity potential



tight-binding Hamiltonian + impurity

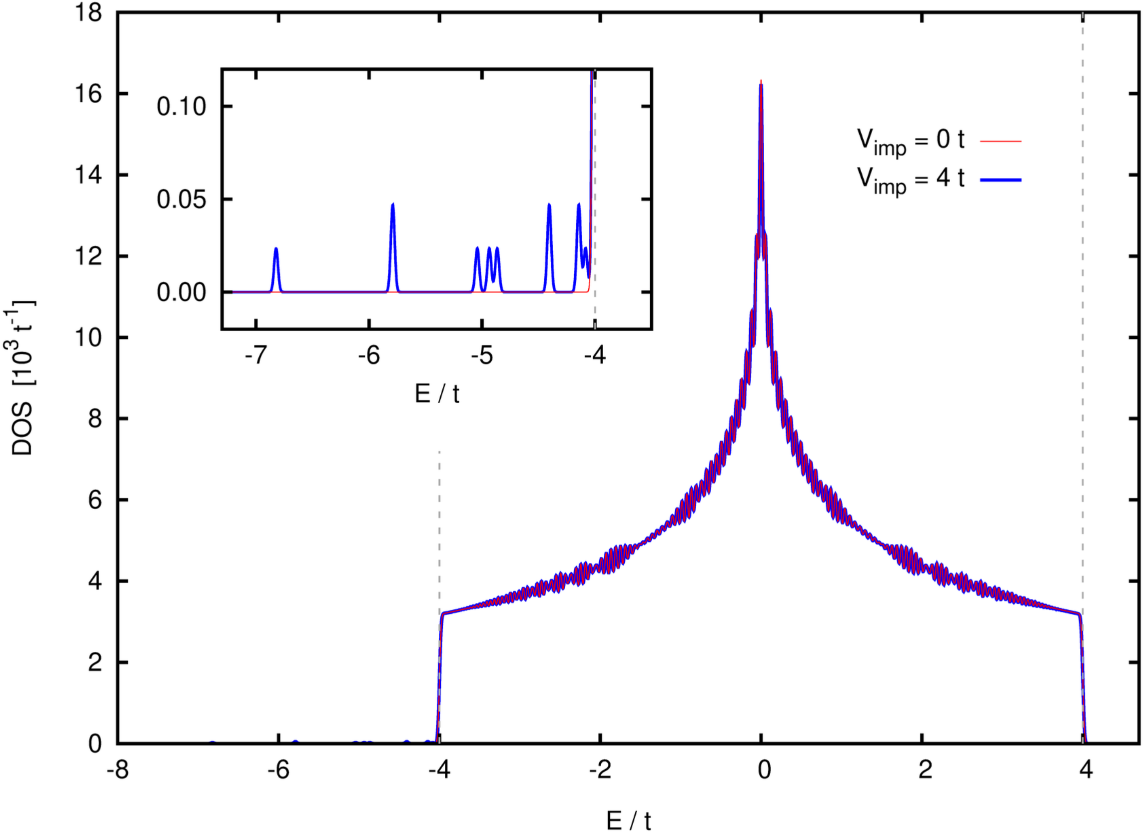
$$-V_{imp}\,e^{-(R/\lambda)^2}$$

$$\hat{H} = \sum_{\text{bonds}} -t\left(c_R^+ c_{R'} + c_{R'}^+ c_R\right) + \sum_{\text{sites}} V_R\, c_R^+ c_R$$

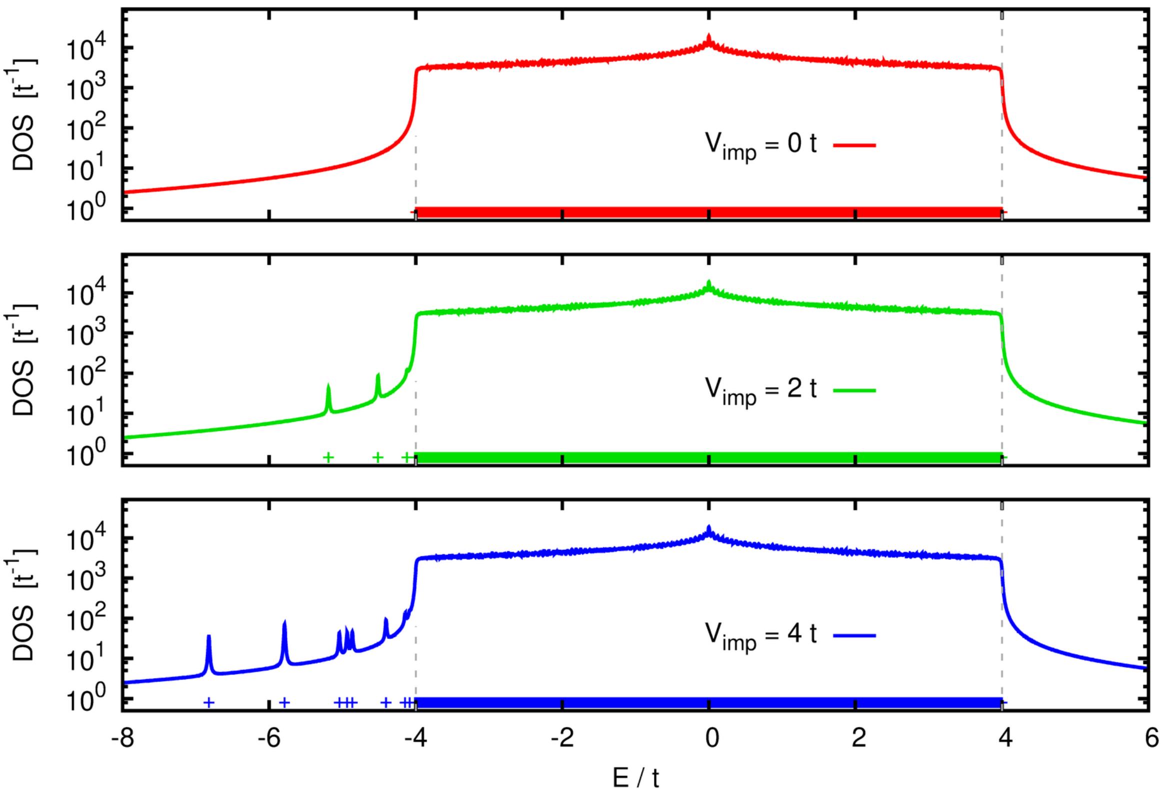
$\rightarrow$ band + localized bound states

200 x 200 sites with periodic boundary conditions $\rightarrow$ 40000 eigenstates

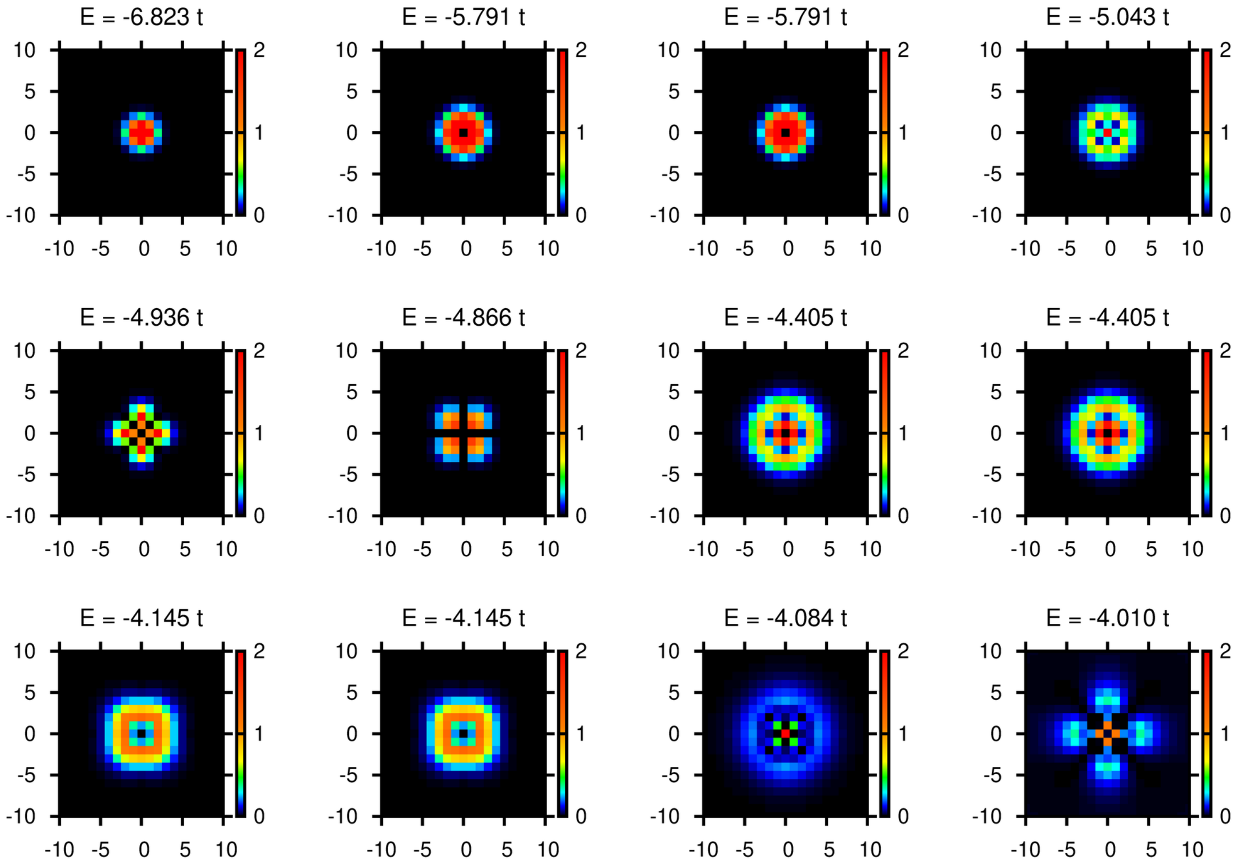
$\mathcal{N}(\varepsilon)$

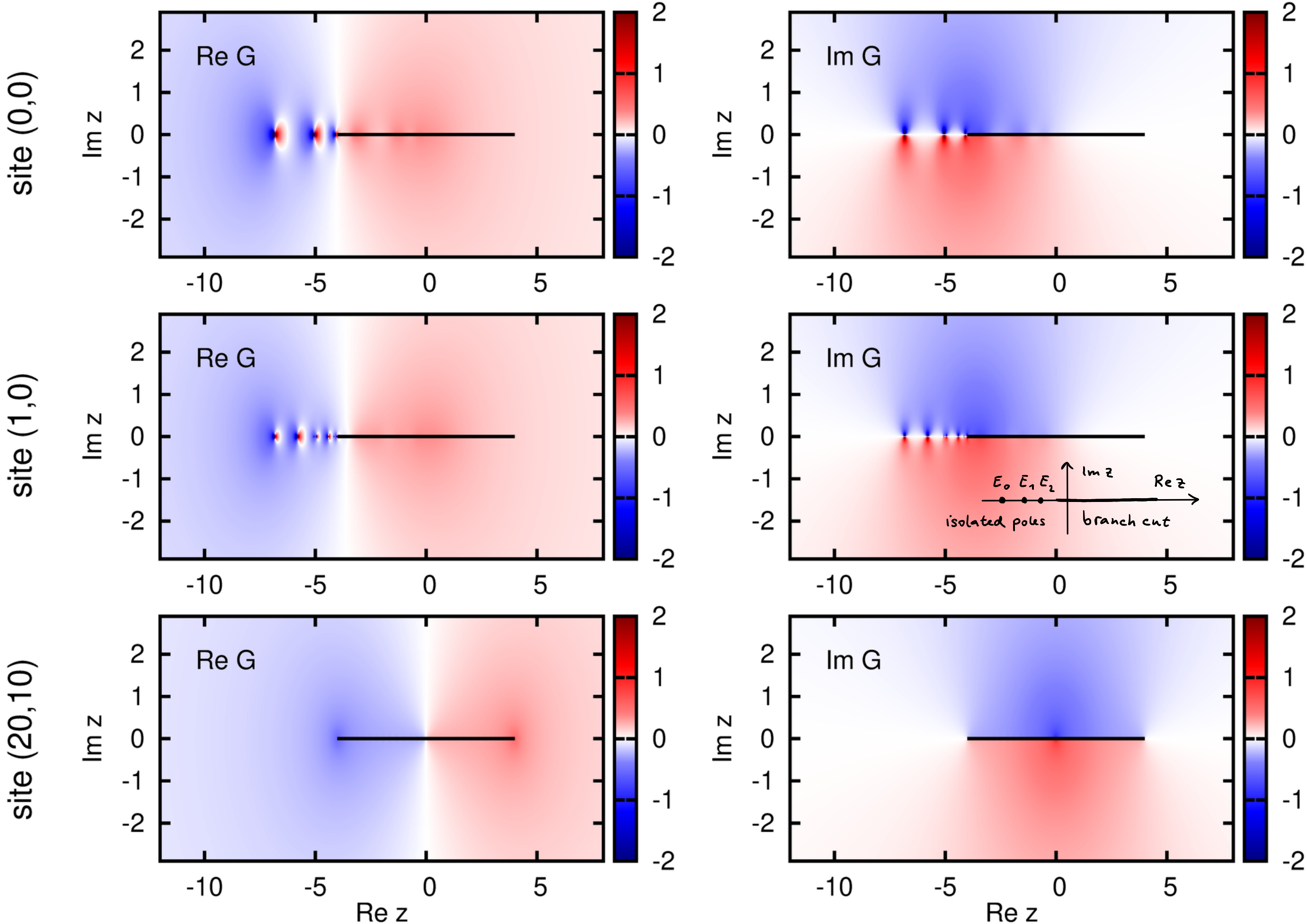


$\mathcal{N}(\varepsilon)$



LDOS at energies of localized states





site (0,0)
site (1,0)
site (20,10)
Re G
Im G
Im z
Re z
E_0 E_1 E_2
isolated poles
branch cut

## ③ Dynamics in frequency domain

- non-stationary Schrödinger equation

$$\hat{H}\,\psi(\vec{r},t) = i\hbar \frac{\partial}{\partial t}\psi(\vec{r},t) \qquad \text{Dirac:} \quad \left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right)|\psi\rangle = 0$$

time evolution for a stationary Hamiltonian

$$|\psi(t=0)\rangle = \sum_n c_n |n\rangle \quad \rightarrow \quad |\psi(t)\rangle = \sum_n c_n e^{-\frac{i}{\hbar}E_n t}|n\rangle$$

- express $\hat{G}^+(t)$ based on $\hat{G}^+(E) = \hat{G}(E+i0^+) = \sum_n \frac{|n\rangle\langle n|}{E-E_n+i0^+}$ poles at $E_n - i0^+$

$$\hat{G}^+(t) = \int_{-\infty}^{\infty}\frac{dE}{2\pi\hbar}\, e^{-\frac{i}{\hbar}Et}\sum_n \frac{|n\rangle\langle n|}{E-E_n+i0^+} = -\frac{i}{\hbar}\sum_n |n\rangle\langle n|\, e^{-\frac{i}{\hbar}E_n t}\,\vartheta(t)$$

$\rightarrow$ $G^+(E)$ captures time evolution in frequency/energy domain

## ④ Perturbation expansion

- perturbed Hamiltonian $\hat{H} = \hat{H}_0 + \hat{W}$

$\hat{H}_0 |\psi\rangle = E|\psi\rangle$ exactly solvable $\hat{G}_0(E) = (E - \hat{H}_0)^{-1}$

$\hat{H} |\psi\rangle = E|\psi\rangle$ to be solved $\hat{G}(E) = (E - \hat{H}_0 - \hat{W})^{-1}$

$$\left.\begin{array}{l} \hat{G}_0(E) = (E - \hat{H}_0)^{-1} \\ \hat{G}(E) = (E - \hat{H}_0 - \hat{W})^{-1} \end{array}\right\} \hat{G}_0^{-1} = \hat{G}^{-1} + \hat{W}$$

- expansion in powers of $\hat{W}$

$\hat{G}_0^{-1} = \hat{G}^{-1} + \hat{W} \rightarrow \hat{G}_0 \cdot (\ \ ) \cdot \hat{G} \rightarrow \hat{G} = \hat{G}_0 + \hat{G}_0 \hat{W} \hat{G}$ Dyson's equation

by repeated insertions $\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{W} \hat{G}_0 + \hat{G}_0 \hat{W} \hat{G}_0 \hat{W} \hat{G}_0 + \dots$

diagrammatically