2. Lecture – Contents

- Strong (resonant) scattering, (generalized) T-Matrix

  wave functions, scattering phase shifts

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- Strong (resonant) scattering, (generalized) T-Matrix

  wave functions, scattering phase shifts
- δ-function scatterers and finite band width; graphene
- Comments on real space calculations on a lattice

T-Matrix

Schrödinger equation in integral form:

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \varphi_{\boldsymbol{k}}(\boldsymbol{r}) + \int d^D\rho\, G^0(\boldsymbol{r}-\boldsymbol{\rho}, \varepsilon(\boldsymbol{k}))\, V(\boldsymbol{\rho})\, \psi_{\boldsymbol{k}}(\boldsymbol{\rho})$$

Defining the T-Matrix: $T(\boldsymbol{p},\boldsymbol{k}) = \int d^D\rho\, \varphi^*_{\boldsymbol{p}}(\boldsymbol{\rho})\, V(\boldsymbol{\rho})\; \psi_{\boldsymbol{k}}(\boldsymbol{\rho})$

leads to $\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \varphi_{\boldsymbol{k}}(\boldsymbol{r}) + \int \frac{d^D p}{(2\pi)^D}\, \varphi_{\boldsymbol{p}}(\boldsymbol{r})\; \hat{G}^0(\boldsymbol{p}, \varepsilon(\boldsymbol{k}))\; T(\boldsymbol{p},\boldsymbol{k})$

from which

$$T(\boldsymbol{k},\boldsymbol{k'}) = V(\boldsymbol{k}-\boldsymbol{k'}) + \int \frac{d^D p}{(2\pi)^D} V(\boldsymbol{k}-\boldsymbol{p})\; G^0\left(\boldsymbol{p}, \varepsilon(\boldsymbol{k'})\right)\; T(\boldsymbol{p},\boldsymbol{k'})$$

follows!

From the wave function $\psi_{\boldsymbol{k}}(\boldsymbol{r})$ we can construct the Green Function

$$G_E(\boldsymbol{r},\boldsymbol{r'}) = \int \frac{d^D k}{(2\pi)^D} \frac{\psi_{\boldsymbol{k}}(\boldsymbol{r})\,\psi_{\boldsymbol{k}}(\boldsymbol{r'})}{E + i\delta - \varepsilon(\boldsymbol{k})}$$

$-\frac{1}{\pi}\,\mathcal{I}m\,G_E(\boldsymbol{r},\boldsymbol{r}) = \mathcal{N}(\boldsymbol{r},E)$ is the Local Density of States (LDOS)

T-Matrix

single rotationally invariant defect in a 2D free electron gas

Fourier series expansion with respect to the scattering angle

$$T(k', k, \cos\phi) = T_0(k', k) + 2\sum_{m=1}^{\infty} T_m(k', k)\, \cos m\phi$$

for an isotropic system leads to a set of decoupled 1D integral equations

$$T_m(k', k) = v_m(k', k) + \int_0^{\infty} \frac{dp\, p}{2\pi}\, v_m(k', p)\, G_k^0(p)\, T_m(p, k)\,.$$

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$$T_m(k, k) = \frac{2}{\mu}\, \frac{1}{\cot\delta_m + i}$$

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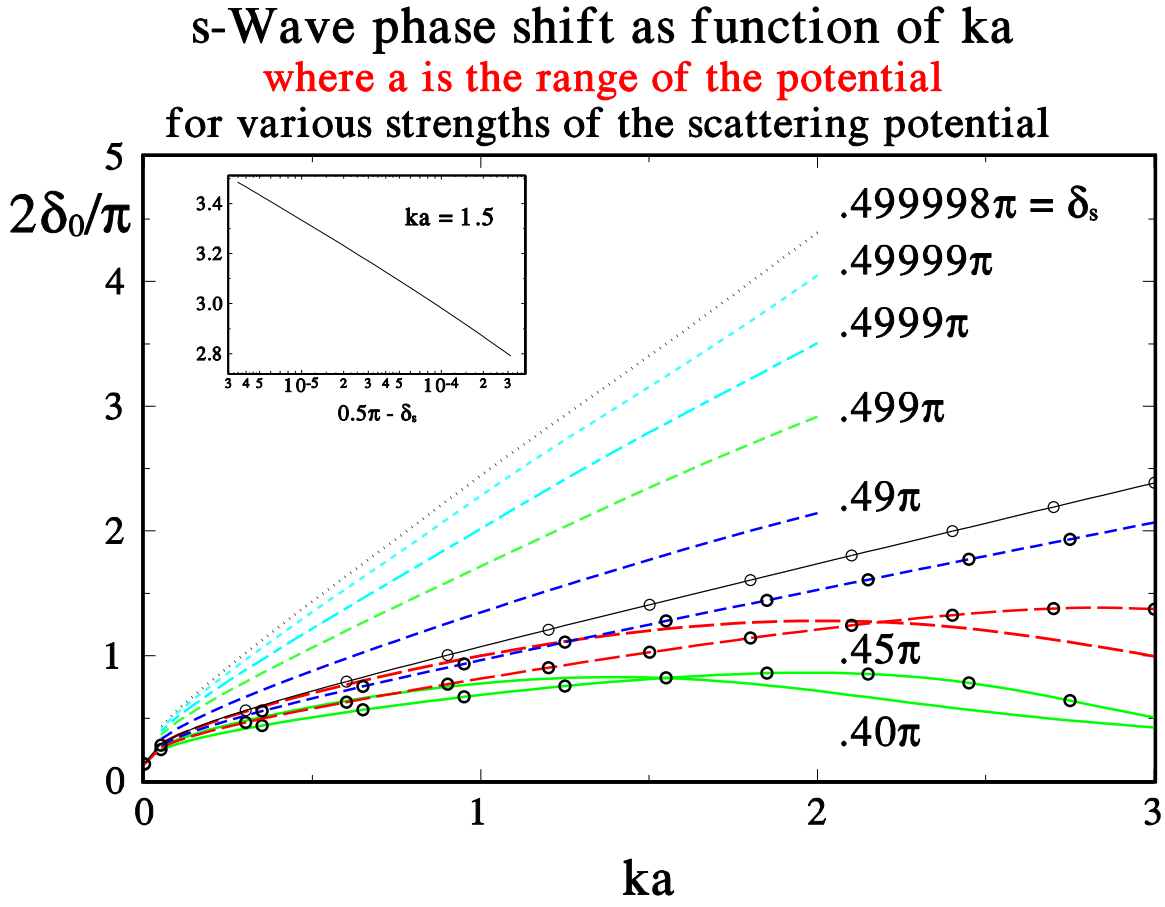
These relations do not hold for the generalized T-matrix

Results: Scattering Phase Shifts



Curves marked with a circle are the results for a disk, the unmarked ones are for a Gaussian potential. The numbers are the phase shifts $\tan \delta_s = \pi \mathcal{N} \bar{v}$ characterizing the strength of the scattering potential.

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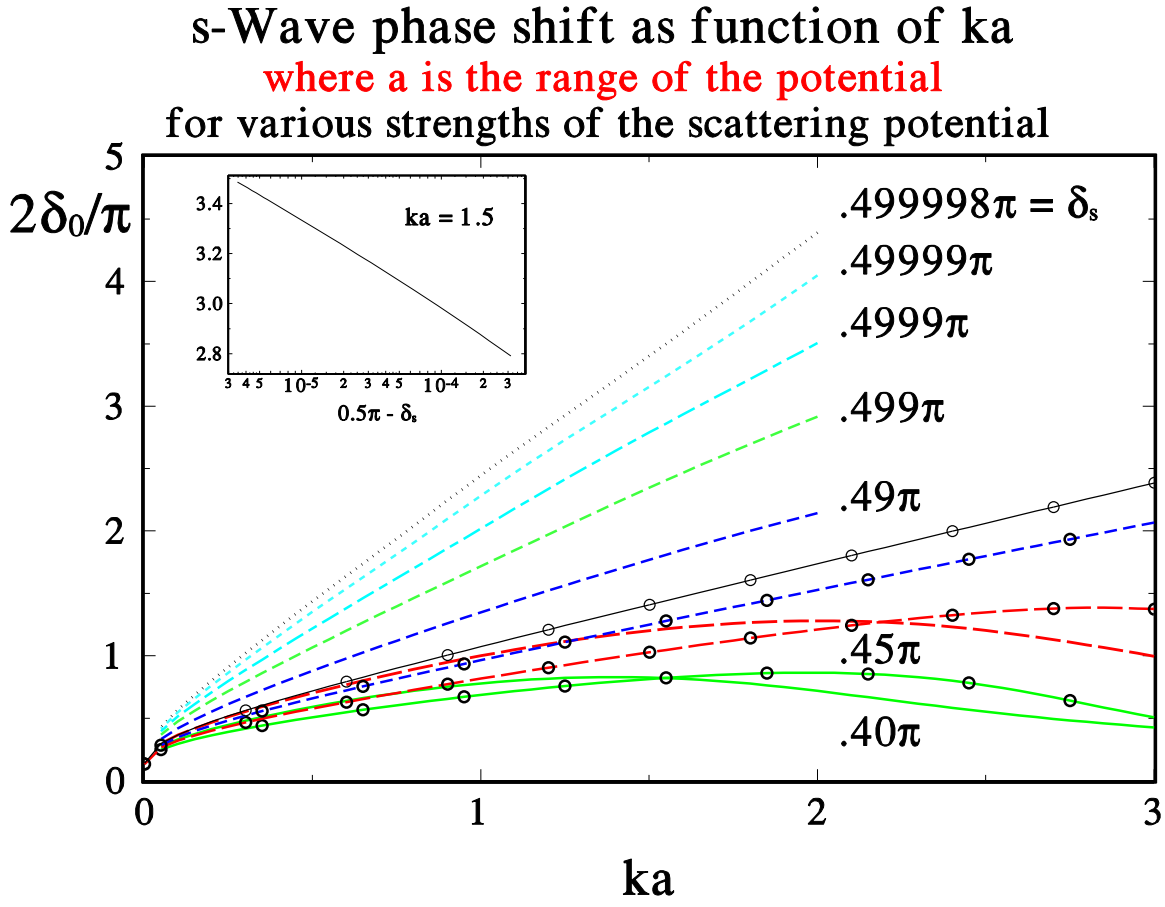

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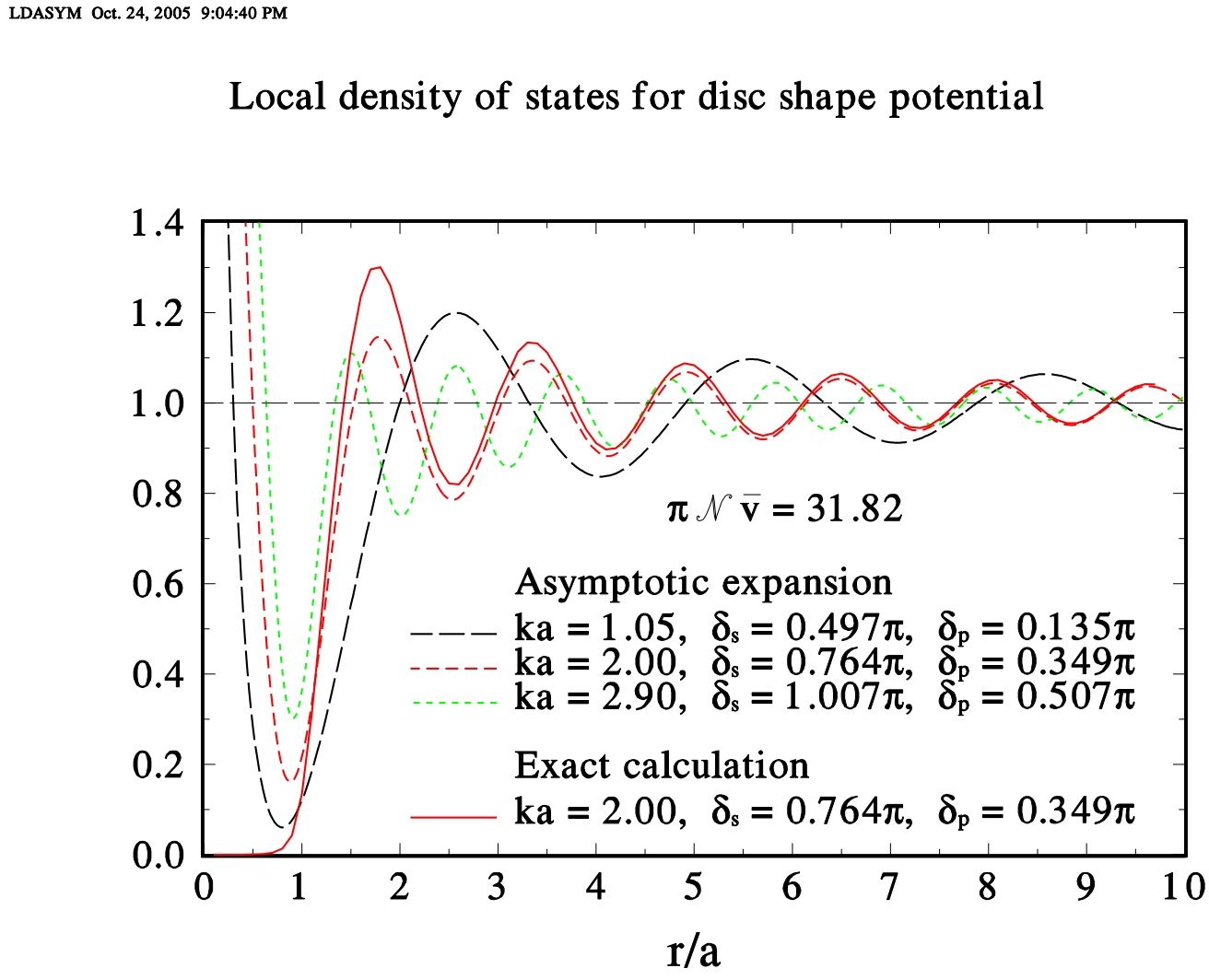
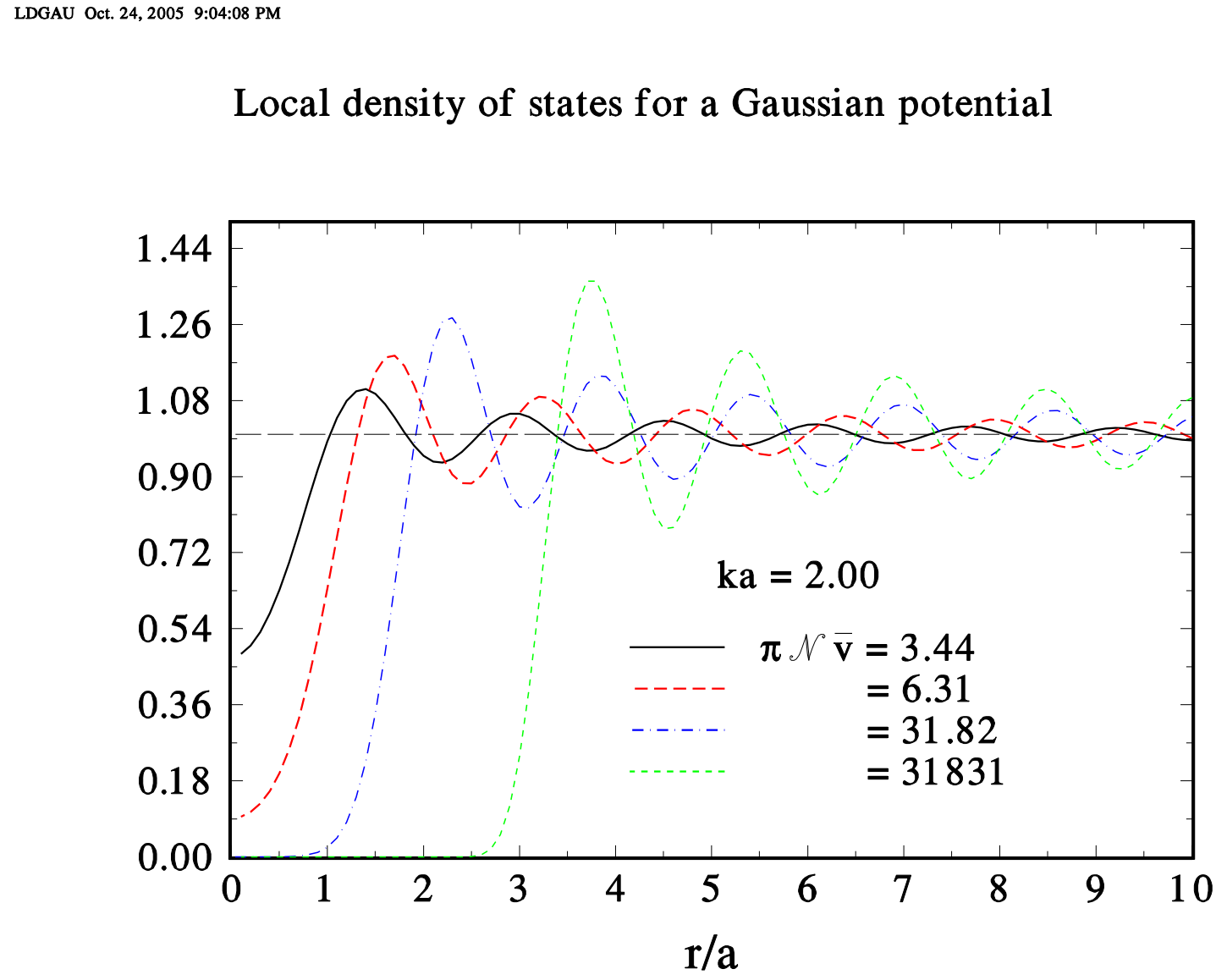
For $a \longrightarrow 0$, the T-matrix vanishes logarithmically!

Local Density of States: Disk



Note the difference between the exact and the asymptotic calculation for $r/a < 1$ and the large Friedel oscillations in 2D

Local Density of States: Gaussian



The LDOS for a fixed energy $ka = 2.00$ and different potential strength

GRAPHENE

Equation of motion for the Green functions in integral form:

$$\hat{G}(\mathbf{r},\mathbf{r}';\omega) = \hat{G}^0(\boldsymbol{r}-\boldsymbol{r'};\omega) + \int d^2\rho\, \hat{G}^0(\boldsymbol{r}-\boldsymbol{\rho};\omega)\, V(\boldsymbol{\rho})\hat{\sigma}_3\, \hat{G}(\boldsymbol{\rho},\boldsymbol{r'};\omega)$$

Given $\hat{G}^0(\mathbf{r}-\mathbf{r}';\omega)$ and $V(\boldsymbol{\rho})$, this could be solved directly.
For $V(\boldsymbol{\rho}) = V\,\delta(\boldsymbol{\rho})$, the solution is trivial:

$$\begin{aligned}\hat{G}(\boldsymbol{r},\boldsymbol{r'};\omega) \;\; &= \;\; \hat{G}^0(\boldsymbol{r}-\boldsymbol{r'};\omega) + \\ &+V\,\hat{G}^0(\boldsymbol{r};\omega)\,\hat{\sigma}_3\left(\hat{\sigma}_0 - V\,\hat{G}^0(0;\omega)\,\hat{\sigma}_3\right)^{-1}\hat{G}^0(-\mathbf{r}';\omega)\end{aligned}$$

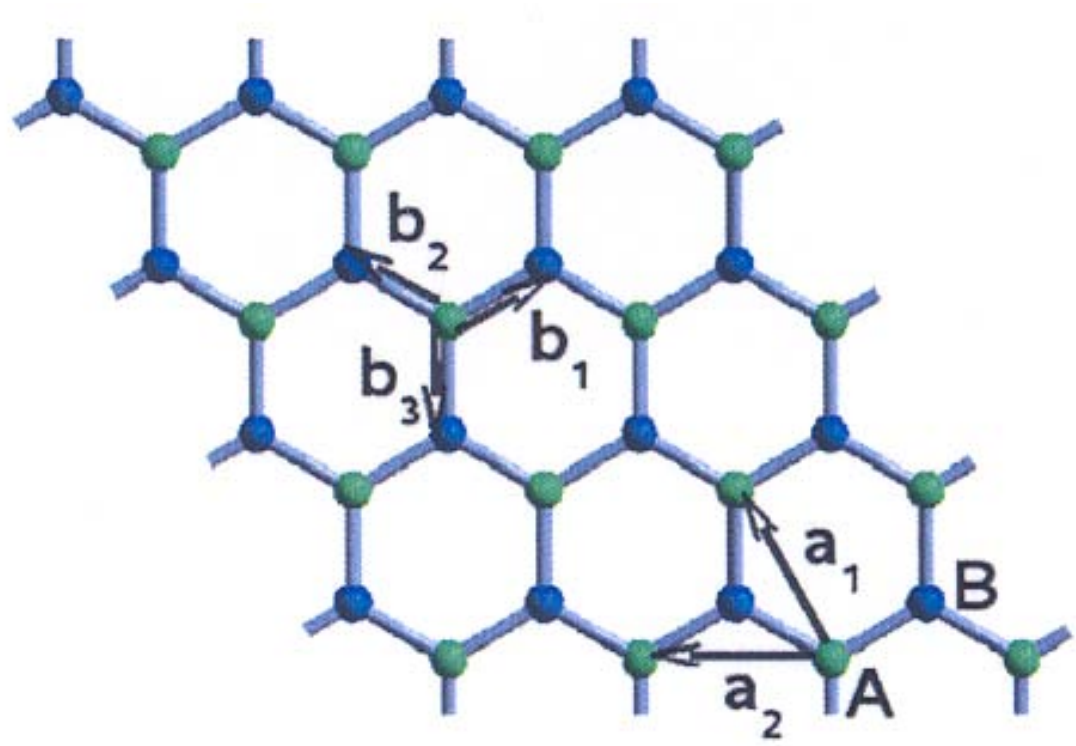
This equation was used to calculate the LDOS of graphene.

Hardest task: Calculation of $\hat{G}^0(-\mathbf{r};\omega)$ for a realistic band of finite width.

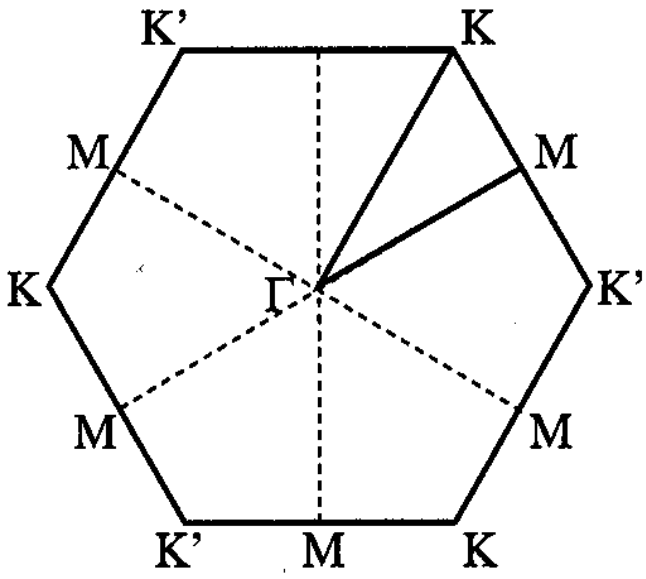
$\hat{G}^0$ is a 2×2 matrix because Graphene has a lattice with a basis.
Two impurities on neighboring inequivalent lattice sites are studied.

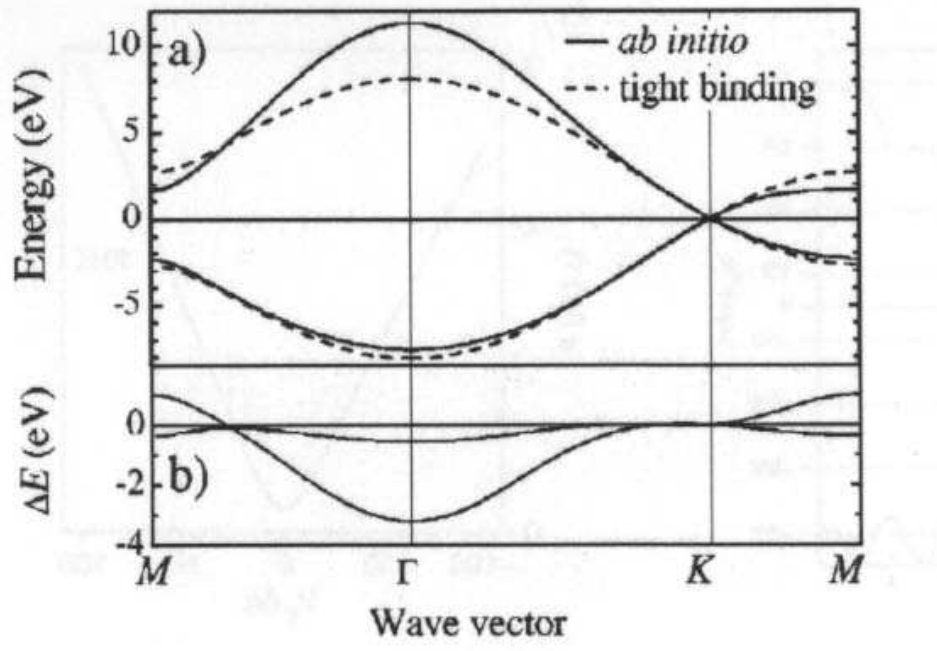
Graphene - Crystal Structure

Honeycomb crystal structure of graphene. There are two atoms per primitive unit cell or, alternatively, two degenerate sublattices A and B.



Graphene - Band Structure





The band formed from p_z orbitals intersects the Fermi energy at the K-point. $\rightarrow$ The dispersion near K is linear! $\rightarrow$ massless fermions!

There is some similarity here with nodal quasiparticles in high-T_c superconductors.

Graphene - Green Function

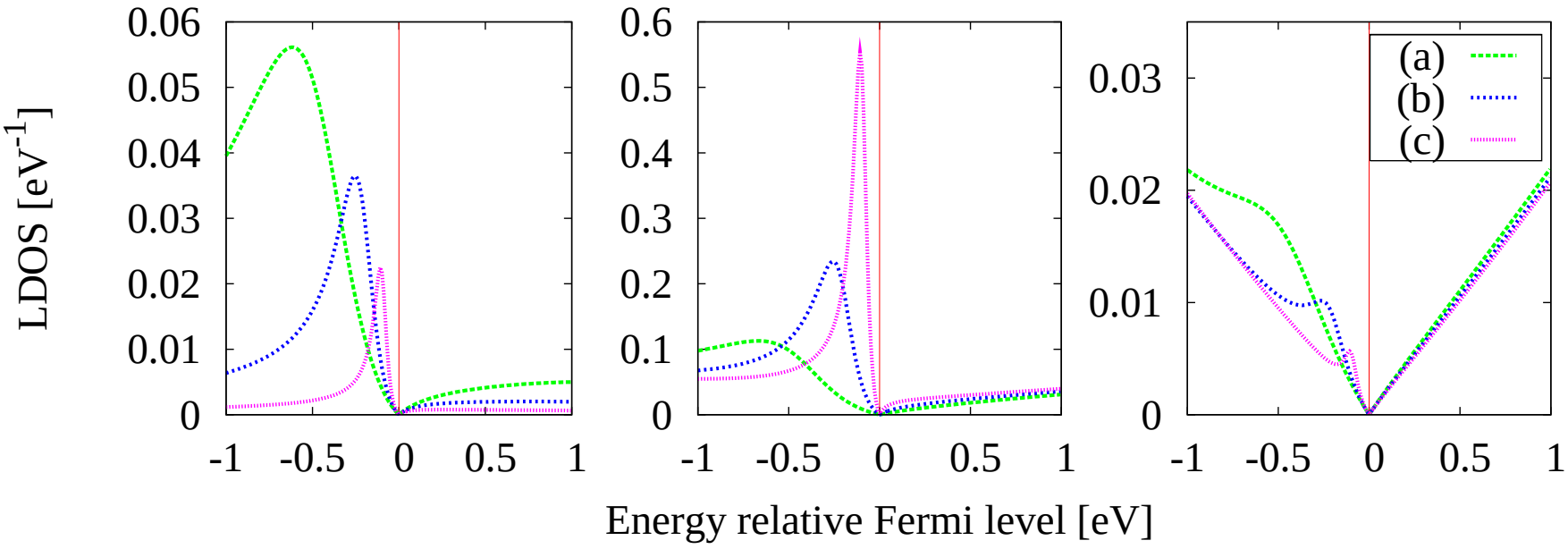
$$\hat{G}^0(\mathbf{k},\omega) = \frac{1}{\omega_+^2 - |\xi(\mathbf{k})|^2} \begin{pmatrix} \omega & \xi(\mathbf{k}) \\ \xi^*(\mathbf{k}) & \omega \end{pmatrix}$$

$$\xi(\mathbf{k}) \approx t\left(1 + e^{i\mathbf{k}\cdot(\mathbf{b}_2-\mathbf{b}_1)} + e^{i\mathbf{k}\cdot(\mathbf{b}_2-\mathbf{b}_1)}\right)$$

within a tight binding approximation

A double integral over this singular integrand has to be performed to obtain the desired Green function in position space.

Results: Single Impurity



on-site

nearest neighbour

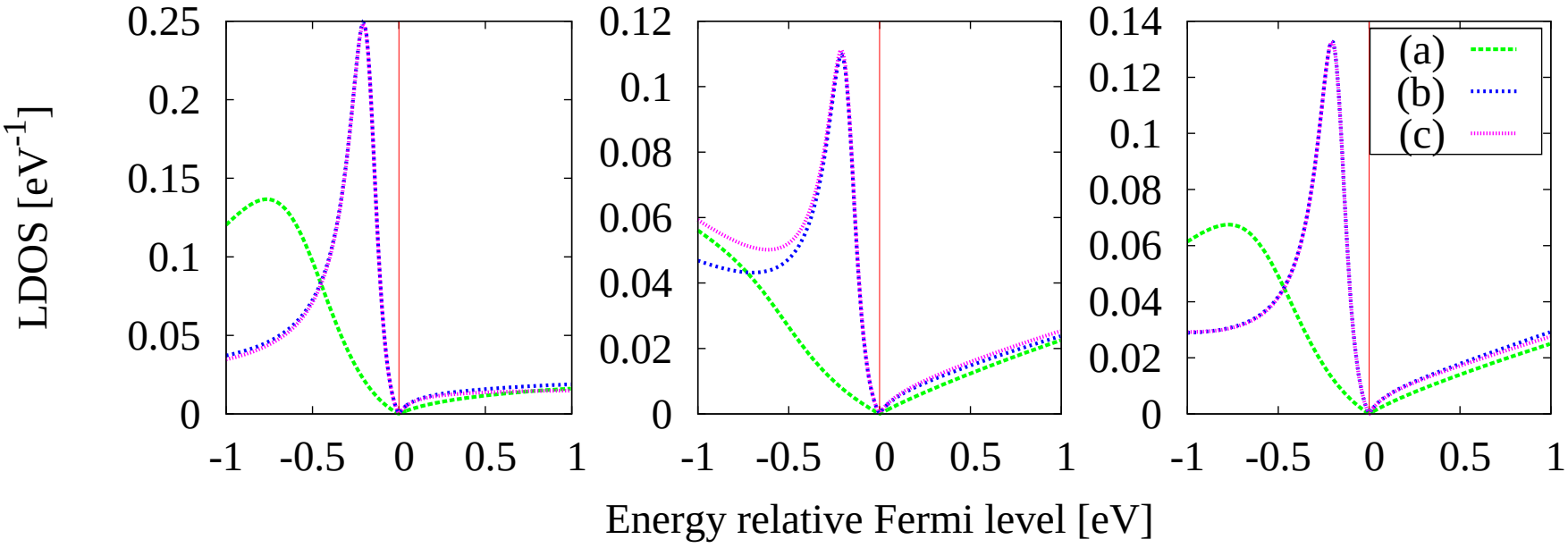
next nearest neighbour

(a) $V = 10$ eV,

(b) $V = 20$ eV,

(c) $V = 40$ eV,

Results: Double Impurity

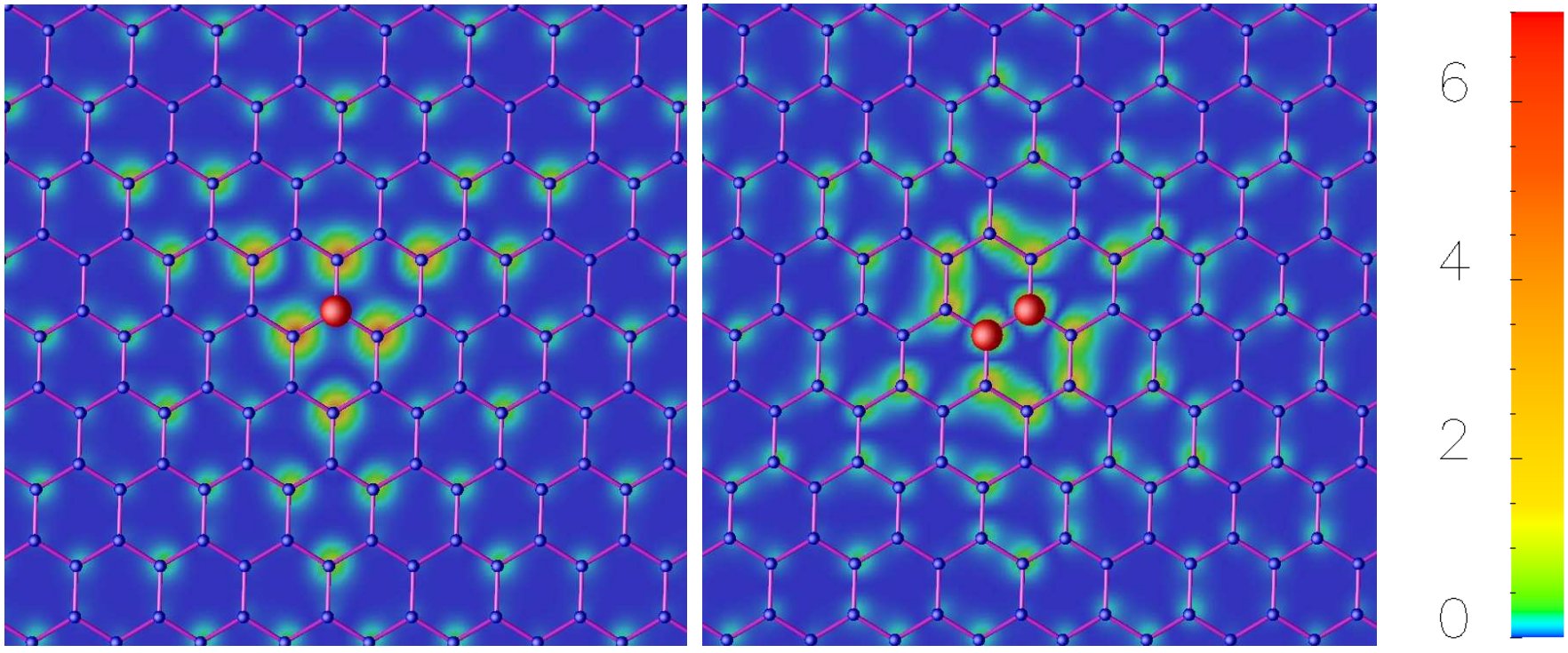


on-site | nearest neighbour | next nearest neighbour

(a) $V = 4$ eV, (b) $V = 4$ eV, $V_1 = -2$ eV (c) $V = 6$ eV,

V_1 is the change in the hopping matrix element, when two neighbouring sites are occupied by impurities.

When $V - V_1$ is kept constant, results are very similar! [(b) and (c)]


6
4
2
0

Comments on real space calculations on a lattice

Defect Hamiltonian in 2nd quantization $H_D = \int d^D r\, \psi^+(\mathbf{r})\, \mathbf{V}(\mathbf{r})\, \psi(\mathbf{r})$

Expand in terms of Bloch states : $H_D = \sum_{\mathbf{k},\mathbf{k}'} V(\mathbf{k},\mathbf{k}')\, c^+_{\mathbf{k}} c_{\mathbf{k}'}$

with $V(\mathbf{k},\mathbf{k}') = \int d^D r e^{-i(\mathbf{k}-\mathbf{k}')} u^*_{\mathbf{k}}(\mathbf{r})\, V(\mathbf{r}) u_{\mathbf{k}'(\mathbf{r})}$

Expand in terms of Wanier states: $H_D = \sum_{\ell,\ell'}\ V_{\ell,\ell'}\, c^+_{\ell} c_{\ell'}$

with $V_{\ell,\ell'} = \int d^D r\, w^*(\mathbf{r}-\mathbf{R}_\ell)\, V(\mathbf{r})\, w(\mathbf{r}-\mathbf{R}_{\ell'})$

This is a three-center integral, containing a lot of physics (finite range potential, modification of the hopping matrix element), which is in most cases reduced to a one-center integral, however!