Green's functions

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Outline

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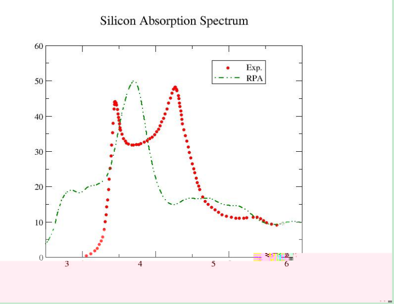
Why do we have to study more than DFT?

We have detected two problems with DFT:



1) Kohn-Sham bandgaps are much too small

2) Fermi's golden rule in the independent particle picture is not reliable to calculate absorption spectra

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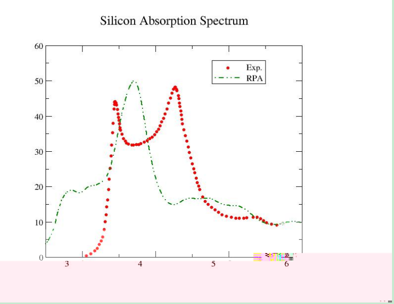

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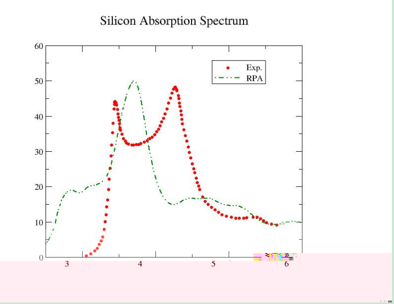

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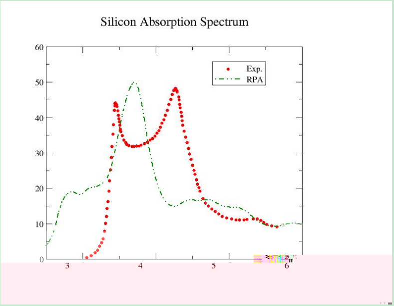

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Beyond the ground state

Ground state calculations:

$$\rho^{(1)}(\mathbf{r}) \rightarrow \rho^{(2)}(\mathbf{r})$$

$$\Longrightarrow \Delta E^{tot} = E_N^{tot,(2)} - E_N^{tot,(1)}$$

These differences are described in ground state DFT.

Spectroscopy?

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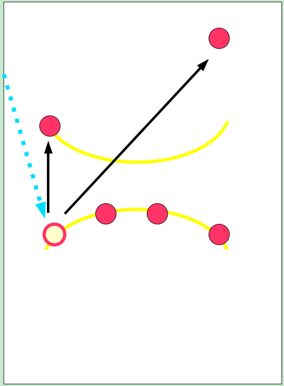

Spectroscopy is exciting!!!

Spectroscopy

Excitation: $E_N^{tot} \Longrightarrow (E_N^{tot})$

or $E_N^{tot} \Longrightarrow (E_{N\ 1}^{tot})$.

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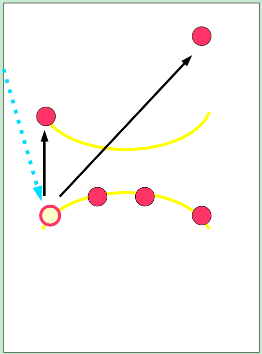

$V_{xc}(\mathbf{r}) \longrightarrow$
Non-locality $\Sigma(\mathbf{r}, \mathbf{r}\ )$ for exchange
Time $\Sigma(\mathbf{r}, \mathbf{r}\ , t - t\ )$ for response
between $\rho(\mathbf{r})$ and the full many-body wavefunction: $\rho(\mathbf{r}, \mathbf{r}\ , t - t\ )$

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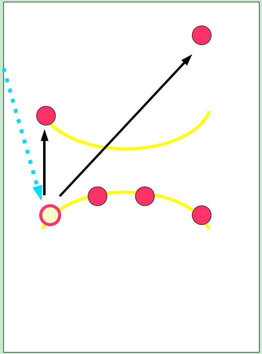

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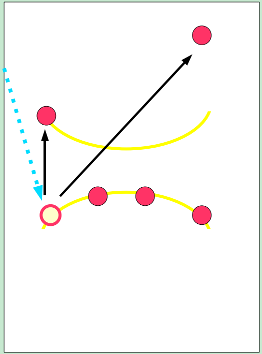

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Outline

You can make it!

Who invented Green's functions?

George Green, "An Essay on the Application of Mathematical Analysis to the Theory of Electricity and Magnetism"
Printed for the author by T. Wheelhouse, London. Sold by Hamilton, Adams & Co., Nottingham (1828)

The basis.....

....after 1 year of school (from age 8 to 9) and 26 years of hard work!

Outline

Green's functions in mathematics

Where we met G for the first time....

Suppose we want to solve

$$\hat{D}_x f(x) = F(x).$$

$\hat{D}_x$ is a differential operator (for example, $\hat{D}_x = d^2/dx^2 + c$). $F(x)$ is a function, for example, a force. The solution of

$$\hat{D}_x G(x, y) = \delta(x - y)$$

allows us to calculate

$$f(x) = \int dy G(x, y) F(y).$$

Outline

Harmonic oscillator in viscous medium

One oscillator......

$$\frac{d^2x}{dt^2} + \omega_0^2 x = F(t)$$

Green's function

$$\frac{d^2 G_0(t-t_0)}{dt^2} + \omega_0^2 G_0(t-t_0) = \delta(t-t_0)$$

and solution

$$G_0(t-t_0) = \frac{sin\omega_0(t-t_0)}{\omega_0}\Theta(t-t_0)$$

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Harmonic oscillator in viscous medium

Fourier Transform

use

$$\Theta(t) = \frac{i}{2\pi} lim_{\eta\to 0^+} \int_{\infty}^{\infty} d\omega \frac{e^{-i\omega t}}{\omega + i\eta}.$$

and obtain

$$G_0^+(\omega) = lim_{\eta\to 0^+} \left[\frac{1}{\omega_0 - i\eta - \omega} + \frac{1}{\omega_0 + i\eta + \omega}\right] \frac{1}{2\omega_0}$$

"Spectral Function" $A(\omega) = -lim_{\eta\to 0} \frac{1}{2\pi i}\left[G^-(\omega) - G^+(\omega)\right]$:

$$A(\omega) = \frac{1}{2\omega_0}\left[\delta(\omega - \omega_0) - \delta(\omega + \omega_0)\right]$$

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One oscillator...in medium

The problem:

$$\frac{d^2x}{dt^2} + 2\gamma\frac{dx}{dt} + \omega_0^2 x = F(t).$$

Fourier Transform of Green's function equation:

$$\left[-\omega^2 - 2i\gamma\omega + \omega_0^2\right] G(\omega) = 1$$

Poles at ω

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Harmonic oscillator in viscous medium

Self-energy and Dyson equation

Unperturbed oscillator:

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...in medium:

$$\left[-\omega^2 - 2i\gamma\omega + \omega_0^2\right] G(\omega) = 1$$

$$G^{-1}(\omega) = G_0^{-1}(\omega) - 2i\gamma\omega$$

Dyson equation:

$$G(\omega) = G_0(\omega) + G_0(\omega)\Sigma(\omega)G(\omega)$$

with $\Sigma(\omega) = 2i\omega\gamma$: "Self-energy".

Harmonic oscillator in viscous medium

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One-particle Green's function in Quantum mechanics

We want to arrive at the following problem:

$$\left[i\frac{\partial}{\partial t} - \hat{H}\right] G(t - t_0) = \delta(t - t_0)\mathbb{1}.$$

or

$$\left[\omega - \hat{H}(\omega)\right] G(\omega) = \mathbb{1}.$$

hence

$$G(\omega) = (\omega - \hat{H}(\omega))^{-1}.$$

and with $\hat{H} = \int \sum_\alpha E_\alpha |\alpha >< \alpha|$ (if hermitian)

$$G(\omega) = \int \sum_\alpha \frac{|\alpha >< \alpha|}{\omega - E_\alpha}.$$

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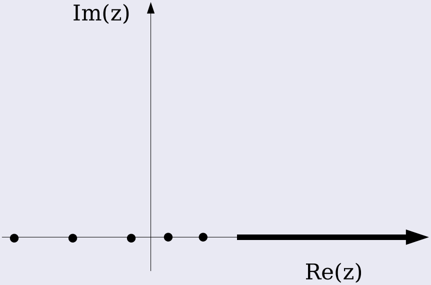
Complex plane



Complex plane. $G(z)$ has discrete poles and a branchcut on the real axis, and it is analytic elsewhere.

One-particle Green's function in Quantum mechanics

Dyson equation

$$G(z) = (z - \hat{H}(z))^{-1}.$$

If we know

$$G_0(z) = (z - \hat{H}_0(z))^{-1}$$

with $H(z) = H_0(z) + \Sigma(z)$:

$$G(z) = G_0(z) + G_0(z)\Sigma(z)G(z).$$

This can be a good starting point:

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Outline

The one-particle Green's function in detail

What is G and what is Σ?

Definition and meaning of G (at 0 K, ground state):

$$G(\mathbf{x},t;\mathbf{x}',t') = -i < \Psi_0 | T\left[\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')\right] |\Psi_0 >$$

Insert a complete set of $N+1$ or $N-1$-particle states. This yields

$$\begin{aligned} G(\mathbf{x},t;\mathbf{x}',t') &= -i\sum_j f_j(\mathbf{x}) f_j(\mathbf{x}') e^{-i\varepsilon_j(t-t')} \times \\ &\times \quad [\Theta(t-t')\Theta(\varepsilon_j-\mu) - \Theta(t'-t)\Theta(\mu-\varepsilon_j)]; \end{aligned}$$

$\varepsilon_j = E(N+1,j) - E(N,0)$ or $E(N,0) - E(N-1,j)$ for $\varepsilon_j > \mu (< \mu)$, and

$$f_j(\mathbf{x}) = \begin{cases} \langle N,0 | \psi(\mathbf{x}) | N+1,j \rangle, & \varepsilon_j > \mu \\ \langle N-1,j | \psi(\mathbf{x}) | N,0 \rangle, & \varepsilon_j < \mu \end{cases}$$

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$\varepsilon_j = E(N+1, j) - E(N, 0)$ or $E(N,0) - E(N-1, j)$ for $\varepsilon_j > \mu (< \mu)$, and

$$f_j(\mathbf{x}) = \begin{cases} \langle N, 0 | \psi(\mathbf{x}) | N+1, j \rangle, & \varepsilon_j > \mu \\ \langle N-1, j | \psi(\mathbf{x}) | N, 0 \rangle, & \varepsilon_j < \mu \end{cases}$$

The one-particle Green's function in detail

What is G? - Fourier tansform

Fourier Transform as before:

$$G(\mathbf{x}, \mathbf{x}\ , \omega) = \sum_j \frac{f_j(\mathbf{x}) f_j\ (\mathbf{x}\ )}{\omega - \varepsilon_j + i\eta sgn(\varepsilon_j - \mu)}.$$

Spectral function:

$$A(\mathbf{x}, \mathbf{x}\ ; \omega) = \sum_j f_j(\mathbf{x}) f_j\ (\mathbf{x}\ ) \delta(\omega - \varepsilon_j).$$

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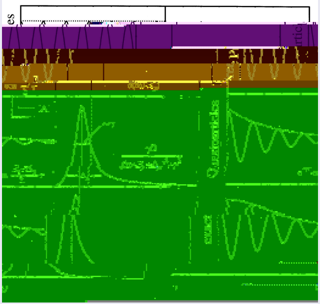
The one-particle Green's function in detail

The spectral function



Spectral function. Effects of interaction and the QP approximation. Picture copied from M. Bonitz, Quantum Kinetic Theory.

Other quantities

Also: Charge density, density matrix, total energy,.......

Outline

Only one things is missing......

We know (in principle) G, but what is Σ?

G is all we want..... ...(although we might want $G^{(2)}$ etc....)

.......but we need Σ!

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