Introduction to the Many-Body problem (II)

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Why so many bodies?

\[ H = \sum_i h(x_i, p_i) + \frac{1}{2} \sum_{i \neq j} \left| x_i - x_j \right|^{-1} \]
Outline

- Resume of previous lecture(s)
- Motivations to go beyond Hartree-Fock
  - Dielectric approach to correlation
  - Euristic derivation of the GW approximation
  - Second quantization and Fields
    - Green’s Functions (GF)
  - Lehmann representation and physical interpretation
  - GF: link to observables
Resume
\[ H = \sum_i h(x_i) + \frac{1}{2} \sum_{i \neq j} |x_i - x_j|^{-1} \]

\[ |\Psi\rangle \approx \prod_n |n\rangle \]

\[ H = \sum_i (h(x_i) + \delta h(x_i)) \]

\[ |\Psi\rangle \approx \prod_n |n_{qp}\rangle \]
Rossio(II)

$$H = \sum_i (h(x_i) + \delta h(x_i))$$

$$\left| \Psi \right\rangle \approx \prod_n \left| n_{qp} \right\rangle$$

$$\begin{bmatrix} h(x_1) + \sum_{j \neq i} J_j(x_1) - \sum_{j \neq i} K_j(x_1) \end{bmatrix} \chi_i(x_1) = \epsilon_i \chi_i(x_1)$$

$$K_j(x_1) \chi_i(x_1) = \left[ \int d x_2 \chi_j^*(x_2) r_{12}^{-1} \chi_i(x_2) \right] \chi_j(x_1)$$

$$J_j(x_1) = \int d x_2 |\chi_j(x_2)|^2 r_{12}^{-1}$$
Resume(IV)

= 

+
Motivations to include (properly) correlation
Semi-conductors (I)

Electronics and photonics applications

Tunable band gaps (direct/indirect) and effective masses
Do we recognize these band structures?

- $0.82 \text{ eV}$ (1.1 eV)
- $1.39 \text{ eV}$ (1.4 eV)
Motivations (I)

Theory matches Experiment within 0.3 eV

1966

Empirical pseudopotentials
ML Cohen and TK Bergstresser, Phys Rev 141, 789 (1966)

All done?
No because we want to be predictive
Motivations (II)

Disaster…
Motivations (III)

What about correlation in DFT ?!?!?

\[-\frac{1}{2} \nabla^2 \phi_i + (V_N + V_H + V_x + V_C) \phi_i = \varepsilon_i \phi_i\]

\[n = \sum_i |\phi_i|^2\]

\[\nabla^2 V_H = -4\pi n\]

\[V_{xc} = \frac{\delta E_{xc}[n]}{\delta n}\]
Disaster...

Si
0.47 vs 1.1 expt

GaAs
0.30 vs 1.4 expt

Motivations (IV)

Data from F Tran and P Blaha, Phys Rev Lett 102, 226401 (2009)
The QUASIPARTICLE concept and a dielectric approach to GW
Electron removal

Before:
- Vacuum
- Conduction
- Valence

\[ E_N \]

After:
- Au revoir...

\[ E_{N-1} \]
What is the quasiparticle band gap?

Electron addition

**Before**

- Vacuum
- Conduction
- Valence

**After**

- Electrons addition

$E_N$

$E_{N+1}$
So what?! Why is DFT correlation not enough?

Correlation is the effect of the mutual interaction of particles beyond the simple electrostatic and statistic effects.

$$V_c = V_c[\rho](\vec{r})$$

DFT$$=\phantom{0}$$

MBPT

$$V_c = \text{?}$$
The "dielectric way" to the MB problem (I)


\[ \delta \rho(\mathbf{r}) \]

\[ V_{\text{ext}}(\mathbf{r}) = \int d\mathbf{r}' |\mathbf{r} - \mathbf{r}'|^{-1} \delta \rho(\mathbf{r}) \]

\[ \delta \rho_{\text{tot}}(\mathbf{r}, t) = \int_{-\infty}^{t} dt' \int_{-\infty}^{\infty} d\mathbf{r}' \chi(\mathbf{rr}', t - t') V_{\text{ext}}(\mathbf{r}', t') = \delta \rho(\mathbf{r}) + \delta \rho_{\text{induced}}(\mathbf{r}, t) \]

\[ = \chi(\mathbf{rr}', t - t') \]
The “dielectric way” to the MB problem (II)

\[ E \equiv \langle H \rangle = E[\rho] \]

\[ \delta E[\rho, \delta \rho] = \delta E[\rho, v(\mathbf{r}, \mathbf{r}'), \chi(\mathbf{r}', \mathbf{r}')] \]

\[ E^{\text{min}} = E_1^{\text{min}} + E_2^{\text{min}} + Q_1 Q_2 W(\mathbf{r}_1, \mathbf{r}_2) \]

\[ W(\mathbf{r}_1, \mathbf{r}_2) = v(\mathbf{r}_1, \mathbf{r}_2) + \iint d\mathbf{r} \, d\mathbf{r}' v(\mathbf{r}_1, \mathbf{r}) \chi(\mathbf{r}, \mathbf{r}') v(\mathbf{r}', \mathbf{r}_2) \]

\[ W(\mathbf{r}_1, \mathbf{r}_2) = \int d\mathbf{r} \varepsilon^{-1}(\mathbf{r}_1, \mathbf{r}) v(\mathbf{r}, \mathbf{r}_2) \]
The "dielectric way" to the MB problem (III)

\[
\left[ h(\vec{x}_1) + \sum_{j \neq i} J_j(\vec{x}_1) - \sum_{j \neq i} K_j(\vec{x}_1) \right] \chi_i(\vec{x}_1) = \epsilon_i \chi_i(\vec{x}_1)
\]

Quantistic

\[
K_j(\vec{x}_1) \chi_i(\vec{x}_1) = \left[ \int d\vec{x}_2 \chi_j^*(\vec{x}_2) r_{12}^{-1} \chi_i(\vec{x}_2) \right] \chi_j(\vec{x}_1)
\]

Classical

\[
J_j(\vec{x}_1) = \int d\vec{x}_2 |\chi_j(\vec{x}_2)|^2 r_{12}^{-1}
\]

\[
\left[ h(\vec{x}) + \sum_{j \neq i} J_j(\vec{x}) - \sum_{j \neq i} K_j^{\text{screened}}(\vec{x}) \right] \chi_i(\vec{x}) = \epsilon_i \chi_i(\vec{x})
\]

\[
K_j^{\text{screened}}(\vec{x}) \chi_i(\vec{x}) = \left[ \int d\vec{x} ' \chi_j(\vec{x} ') \chi_i(\vec{x} ') W(\vec{r}, \vec{r} ') \right] \chi_j(\vec{x})
\]
Take-home messages of the "dielectric approach"

\[ H = \sum_i h(x_i) + \frac{1}{2} \sum_{i \neq j} |x_i - x_j|^{-1} \]

Exact

Many-Body Picture

\[ H \approx \sum_i \left[ h(\tilde{x}_i) + \delta h_{\text{Screened HF}}(\tilde{x}_i) \right] \]

\[ W(r, r'; \omega) \]
The "Diagrammatic" way to the many-body problem: Green's Functions
Why so many trajectories?

\[ H = \sum_i h(x_i, p_i) + \frac{1}{2} \sum_{i \neq j} |x_i - x_j|^{-1} \]

Dick Feynman told me about his "sum over histories" version of quantum mechanics. "The electron does anything it likes," he said. "It just goes in any direction at any speed, forward or backward in time, however it likes, and then you add up the amplitudes and it gives you the wave-function." I said to him, "You're crazy." But he wasn't.

Freeman Dyson
Creation/destruction operators

\[ |\Psi\rangle = \sum |x_n\rangle \langle x_n | \Psi \rangle \]

\[ \psi(x, t) = \langle x | \psi(t) \rangle \]

\[
| x_1 \rangle = \hat{\psi}^\dagger(x_1)|0\rangle \\
| x_1 x_2 \rangle = \hat{\psi}^\dagger(x_2)|x_1\rangle = \hat{\psi}^\dagger(x_2)\hat{\psi}^\dagger(x_1)|0\rangle \\
| x_1 \ldots x_N \rangle = \hat{\psi}^\dagger(x_N)|x_1 \ldots x_{N-1}\rangle = \hat{\psi}^\dagger(x_N)\ldots \hat{\psi}^\dagger(x_1)|0\rangle
\]
Second quantization and fields

\[ |\Psi\rangle = \sum |x_n\rangle \langle x_n|\Psi\rangle \]

\[ \hat{\psi}(x,t) = \sum_i \chi_i(x) \hat{c}_i(t) \]

Field operator
Complete basis
Anihilation operator

\[ H = \sum_i h(x_i) + \frac{1}{2} \sum_{i \neq j} |x_i - x_j|^{-1} \]

\[ [\hat{\psi}(x), \hat{\psi}(y)]_+ = [\hat{\psi}^+(x), \hat{\psi}^+(y)]_+ = 0 \]

\[ [\hat{\psi}(x), \hat{\psi}^+(y)]_+ = \delta(x - y) \]

\[ H = \int d\bar{x} \, \hat{\psi}(\bar{x}) h(\bar{x}) \hat{\psi}^+(\bar{x}) + \frac{1}{2} \iint d\bar{x} \, \bar{y} \, \hat{\psi}^+(\bar{x}) \hat{\psi}^+(\bar{y}) v(\bar{x} - \bar{y}) \hat{\psi}(\bar{y}) \hat{\psi}(\bar{x}) \]
Time-Dependent Perturbation Theory (II)

\[ h + \lambda H'(t) = \sum_n E_n^{(0)} |n^{(0)}\rangle \langle n^{(0)}| + \sum_{n,m} H'_{n,m}(t) |n^{(0)}\rangle \langle m^{(0)}| \]

Interaction Representation

\[ |n_I(t)\rangle = e^{iht} |n\rangle \quad O_I(t) = e^{iht} O e^{-iht} \]

\[ i \partial_t |n_I(t)\rangle = H'_I(t) |n_I(t)\rangle \]

\[ |n_I(t)\rangle = |n_I(t_0)\rangle - i \int_{t_0}^t d\tau H'_I(\tau) |n_I(\tau)\rangle \]

\[ |n_I(t)\rangle = |n_I\rangle - i |n_I\rangle \left( \int_{-\infty}^t d\tau H'_I(\tau) \right) \]
The T-product

\[ |\Psi_I(t)\rangle = |\Psi_I(t_0)\rangle - i \int_{t_0}^{t} d\tau H'_I(\tau) |\Psi_I(\tau)\rangle \]

\[ |\Psi_I(t)\rangle = |\Psi_I(t_0)\rangle - i \int_{t_0}^{t} d\tau H'_I(\tau) |\Psi_I(t_0)\rangle + i^2 \int_{t_0}^{t} d\tau \int_{t_0}^{\tau} d\tau' H'_I(\tau) H'_I(\tau') |\Psi_I(t_0)\rangle \]

\[ \hat{H} = \hat{h} + \hat{H}' \]

\[ |\Psi_I(t)\rangle = e^{i\hat{h}t} |\Psi_s(t)\rangle \]

\[ \hat{O}_I(t) = e^{i\hat{h}t} \hat{O}_s e^{-i\hat{h}t} \]

\[ \hat{U}(t,t_0) = \hat{1} - \sum_n \frac{(-1)^n}{n!} \int_{t_0}^{t} dt_1...dt_n T\{ \hat{H}'_I(t_1)...\hat{H}'_I(t_n) \} \]

Taylor expansion

T-product
The Time-ordered Product

\[ \mathcal{T} \{ A(x)B(y) \} := \begin{cases} A(x)B(y) & \text{if } x_0 > y_0, \\ \pm B(y)A(x) & \text{if } x_0 < y_0. \end{cases} \]

\[ \mathcal{T} \{ A(x)B(y) \} := \theta(x_0 - y_0)A(x)B(y) \pm \theta(y_0 - x_0)B(y)A(x), \]

More in general...

\[ \mathcal{T}\{A_1(t_1)A_2(t_2)\cdots A_n(t_n)\} = \sum_p \theta(t_{p_1} > t_{p_2} > \cdots > t_{p_n})\varepsilon(p)A_{p_1}(t_{p_1})A_{p_2}(t_{p_2})\cdots A_{p_n}(t_{p_n}) \]

\[ \varepsilon(p) \equiv \begin{cases} 1 & \text{for bosonic operators,} \\ \text{sign of the permutation} & \text{for fermionic operators.} \end{cases} \]
Green's Functions

\[ G(x_t, x'_t') \equiv (-i) \frac{\langle \Psi_0 | T[\psi(x, t) \psi^+(x, t)] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \]

Why this definition? Boh!

... but ...

Green's functions useful!

\[ \psi(x, t) = e^{iHt} \psi(x) e^{-iHt} \]

\[ \langle \hat{O} \rangle \equiv i \lim_{t' \to t^+} \int d x [O(x) G(x_t, x_t')] \]

\[ n(x_t) \equiv (-i) \lim_{t' \to t^+} G(x_t, x_t') \quad E = \frac{-i}{2} \int d x \lim_{t' \to t^+} \lim_{x' \to x} [i \partial_t - T(x)] G(x_t, x'_t') \]
Physical Meaning

\[ G(x_t, x_\prime t_\prime) \equiv (-i) \frac{\langle \Psi_0 | T[\psi(x, t)\psi^+(x, t)] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \]
Lehmann representation (I)

\[ G(x_t, x_{t'}) \equiv (-i) \frac{\langle \Psi_0 | T[\psi(x, t) \psi^+(x, t)] | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \]

\[ \psi(x, t) = e^{iHt} \psi(x) e^{-iHt} \]

\[
\langle N | \psi(x, t) | N + 1, s \rangle = \langle N | e^{iHt} \psi(x) e^{-iHt} | N + 1, s \rangle \\
= \langle N | e^{iHt} \psi(x) e^{-iE_{N+1,s}t} | N + 1, s \rangle \\
= \langle N | e^{iE_N t} \psi(x) e^{-iE_{N+1,s}t} | N + 1, s \rangle \\
= \langle N | \psi(x) | N + 1, s \rangle e^{-i(E_{N+1,s} - E_N)t} \\
= \mathcal{F}_s(x) \\
\]

\[ H | N \rangle = E_N | N \rangle \]

\[ H | N + 1, s \rangle = E_{N+1,s} | N + 1, s \rangle \]

\[ \mathcal{F}_s(x) \]

N particles system

N+1 particles system
Lehmann representation (II)

Suppose for simplicity $t > t'$

\[
G(x, x', t) = -i \langle N | \psi(x) \psi^\dagger(x, t') | N \rangle
\]

\[
= -i \langle N | e^{iHt} \psi(x) e^{-iHt} e^{iHt'} \psi^\dagger(x) e^{-iHt'} | N \rangle
\]

\[
= -i \langle N | \psi(x) e^{-i(H-E_N)(t-t')} \psi^\dagger(x) | N \rangle
\]

\[
\sum_s |N + 1, s\rangle \langle N + 1, s| = 1
\]

\[
G(x, x', \omega) = \sum_s \frac{f_s(x) f_s^*(x')}{\omega - \epsilon_s}
\]
Application of the Green's Functions Method to the Study of the Optical Properties of Semiconductors.

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1. Introduction.

The relevance of many-body effects, over and above the independent-particle approximation, on the optical properties of semiconductors has been increasingly recognized over the years. Specifically, the collective effect of screening has long been known to be essential to account for the reduction of the electron-hole attraction in an exciton and for the polarization accompanying a single-particle excitation. Only more recently however, it has been possible to give quantitative account of these phenomena by combining Green's function techniques of quantum field theory with the description of band structures in

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SOLID STATE PHYSICS
Advances in Research and Applications

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Effects of Electron-Electron and Electron-Phonon Interactions on the One-Electron States of Solids

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References (II)

The GW method

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Abstract

Calculations of ground-state and excited-state properties of materials have been one of the major goals of condensed matter physics. Ground-state properties of which have been extensively investigated for several decades within the standard density functional theory. Ultralow properties, on the other hand, were relatively ignored, in spite of considerable achievements in ab initio theoretical calculations and of the strong connection of the electronic properties of condensed matters to the Green function method. To calculate the Green functions one requires the self-energy, operator which is needed for the Green function evaluation. However, traditional methods for describing the self-energy calculations, simplified schemes, and applications in various systems are described. Self-consistency ideas and developments beyond the GW approximation are also discussed as well as the success and shortcomings of the GW approximation.

ab-initio implementations

Very useful intro to Green's function methods and spectral properties