Summary: School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows

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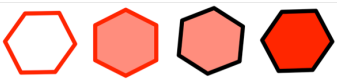
July 23, 2024

THEOS, EPFL



Overview

Overview of the School

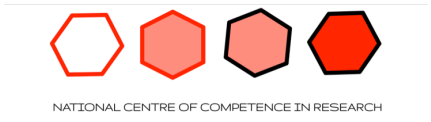
- Date: June 10-16, 2024
- Location: Austin, TX
- Focus: Electron-phonon interactions, many-body perturbation theory, and computational workflows
- Structure: Lectures, hands-on tutorials, workshops

Lecture Topics

- Electron-Phonon Interactions
- Density Functional Perturbation Theory (DFPT)
- Many-Body Perturbation Theory (GW and BSE)
- Wannier Functions and Their Applications
- Electron Transport and Superconductivity
- High-Performance Computing and Special Methods

Hands-on Tutorials

- Quantum ESPRESSO: Setup and execution
- Wannier90 for Wannier function generation
- EPW: Band structure interpolation, electron-phonon matrix elements
- Mobility and Superconductivity Calculations
- GW and BSE: Practical applications
- Automated Workflows: EPWpy, Wannierizations



Wannier function

Definition and Construction

- Wannier functions provide a localized representation of electronic states in crystalline solids. (Gregory Wannier 1937)
- Wannier functions $|\mathbf{R}j\rangle$ are constructed from Bloch functions $|\psi_{n\mathbf{k}}(\mathbf{r})\rangle$:

$$|\mathbf{R}j\rangle = \frac{V_{\text{cell}}}{(2\pi)^3} \int_{BZ} d\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{R}} \sum_{n=1}^{J} U_{\mathbf{k},nj} \, |\psi_{n\mathbf{k}}\rangle \tag{1}$$

  where V_{cell} is the volume of the unit cell and the integral is over the Brillouin zone (BZ).
- Useful for understanding electronic structure, polarization, and electron localization.

Properties of Wannier Functions

- Localization: Wannier functions are exponentially localized in insulators.
- Orthogonality: Wannier functions are orthogonal:

$$\langle \mathbf{R}_m i | \mathbf{R}_n j \rangle = \delta_{ij} \delta_{\mathbf{R}_m \mathbf{R}_n} \tag{2}$$

- Completeness: They form a complete basis set for the Hilbert space of electronic states.

Maximally Localized Wannier Functions (MLWFs)

- The most popular way to the gauge: Maximally-localized Wannier functions (MLWF).
- We minimize the quadratic spread of the position operator of a manifold

$$\Omega = \sum_{j=1}^{J} \left[\langle \mathbf{0}j \left| r^2 \right| \mathbf{0}j \rangle - |\langle \mathbf{0}j | \mathbf{r} | \mathbf{0}j \rangle|^2 \right] \tag{3}$$

  through the optimization of the unitary matrices $U_{\mathbf{k},nj}$
- This minimization ensures that Wannier functions are as localized as possible.
- Optimal smoothness in reciprocal space: good localization in real space
  N. Marzari and D. Vanderbilt, PRB 56, 12847 (1997)

Computational Echo-system for Wannier Functions

- Wannier90: A widely used software package for computing MLWFs.

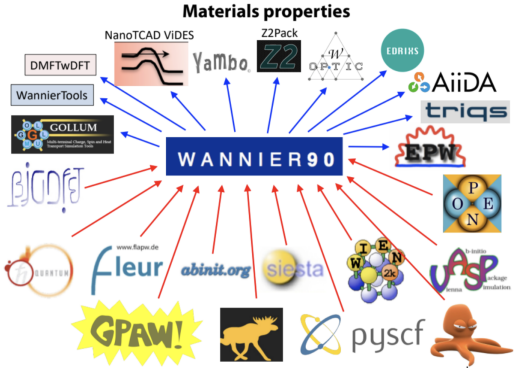


Figure: Ab initio engines using Wannier90.

Computer Physics Communications, 178(9), 685-699 (2009).
Wannier90:`http://www.wannier.org/`

Applications of Wannier Functions

- Electronic Structure:
  - Provides insight into the bonding and electronic properties of materials.
  - Used for band structure interpolation and analysis.
- Polarization and Berryology:
  - Electronic polarization, Berry phases, Berry curvature, optical and anomalous Hall conductivity, orbital magnetization
- Topological Insulators:
  - Used to study topological invariants, properties and edge states.
- Electron-Phonon Interactions:
  - Facilitate the calculation of electron-phonon coupling matrices.
- Ballistic transport and nanostructures:
  - Landauer conductance, embedding self-energies, large-scale tight binding
- Beyond DFT with localized orbitals:
  - Koopmans-Wannier spectral functionals, strongly correlated systems with DMFT.

Example: Band Structure Interpolation

- Wannier functions allow for efficient interpolation of band structures.
- Essential for calculating accurate electronic properties over the Brillouin zone.
- Example: Interpolated band structure of silicon using MLWFs.

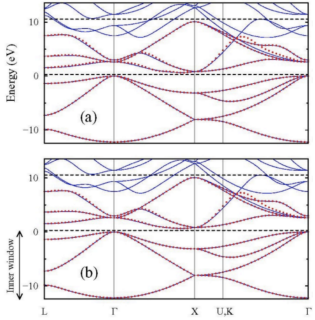
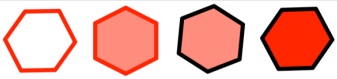


Figure: Interpolated band structure of silicon using Wannier functions.

Summary

- Wannier functions provide a localized representation of electronic states in solids.
- They are essential for various applications, including electronic structure, polarization, and topological properties.
- Computational tools like Wannier90 facilitate the practical use of Wannier functions.



GW and BSE

Introduction to GW Approximation

- GW is a many-body perturbation theory method used to calculate the electronic structure of materials.
- Theoretical framework: the many-body perturbation theory. The Green's function (G) and the screened Coulomb interaction (W).
- Beyond DFT method: Provides more accurate quasiparticle energies compared to Density Functional Theory (DFT).

Introduction to GW Approximation

- Moderately correlated systems may be solved numerically from first principles using many-body perturbation theory (e.g., GW and GW-BSE approaches, and beyond)
- Theoretical framework: the many-body perturbation theory. The Green's function (G) and the screened Coulomb interaction (W).
- Beyond DFT method: Provides more accurate quasiparticle energies compared to Density Functional Theory (DFT).

- The quasiparticle energy E_n is given by:

$$E_n = \epsilon_n + \langle \psi_n | \Sigma(E_n) - V_{xc} | \psi_n \rangle \tag{4}$$

where ϵ_n are the Kohn-Sham energies, Σ is the self-energy, and V_{xc} is the exchange-correlation potential.

- The self-energy Σ in the GW approximation is:

$$\Sigma(\mathbf{r}, \mathbf{r}'; \omega) = i \int \frac{d\omega'}{2\pi} G(\mathbf{r}, \mathbf{r}'; \omega + \omega') W(\mathbf{r}, \mathbf{r}'; \omega') \tag{5}$$

where G is the Green's function and W is the screened Coulomb interaction.

Computational Steps in GW

- Start with a DFT calculation to obtain Kohn-Sham eigenvalues and eigenfunctions.
- Compute the dielectric function $\epsilon(\mathbf{q}, \omega)$ and the screened Coulomb interaction $W(\mathbf{q}, \omega)$.
- Construct the Green's function $G(\mathbf{r}, \mathbf{r}'; \omega)$.
- Calculate the self-energy $\Sigma(\mathbf{r}, \mathbf{r}'; \omega)$.
- Solve for the quasiparticle energies E_n.

Introduction to Bethe-Salpeter Equation (BSE)

- BSE is used to calculate the optical properties of materials by including electron-hole interactions.
- Derived from the two-particle Green's function.
- Provides accurate excitonic effects and optical spectra.

Basic Principles of BSE

- The BSE describes the correlated motion of an electron-hole pair:

$$(\epsilon_c - \epsilon_v)A_{vc} + \sum_{v'c'} K_{vc,v'c'}A_{v'c'} = \Omega A_{vc} \tag{6}$$

  where ϵ_c and ϵ_v are the energies of conduction and valence bands, A_{vc} are the exciton amplitudes, K is the electron-hole interaction kernel, and Ω are the exciton energies.
- The kernel K includes the direct Coulomb interaction and the exchange interaction.

Computational Steps in BSE

- Perform a GW calculation to obtain quasiparticle energies and wavefunctions.
- Construct the electron-hole interaction kernel K.
- Solve the BSE to obtain exciton energies Ω and amplitudes A_{vc}.
- Calculate the optical absorption spectrum using the exciton amplitudes.

Applications of GW and BSE

- Electronic Structure:
  - Provides accurate band gaps and quasiparticle energies.
  - Essential for studying semiconductors and insulators.
- Optical Properties:
  - BSE captures excitonic effects in optical spectra.
  - Important for understanding light absorption and emission in materials.
- Materials Design:
  - GW and BSE are used to predict and design new materials with desired electronic and optical properties.

Example: Band Gap of Silicon

- GW calculation corrects the underestimated band gap from DFT.
- Results show excellent agreement with experimental values.

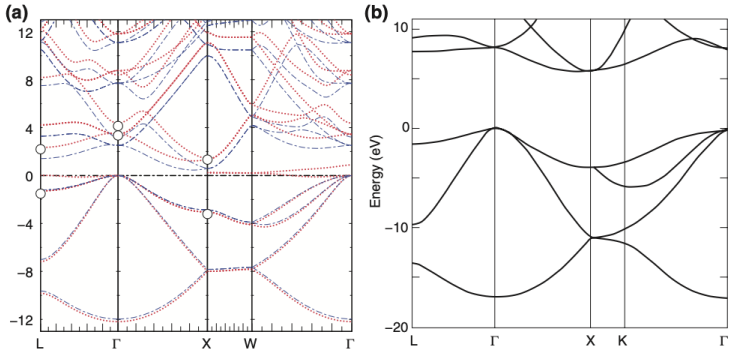


Figure: Comparison of GW (left) and DFT (right) band gaps for silicon.

Example: Optical Spectrum of MoS_2

- BSE captures excitonic peaks in the optical absorption spectrum of monolayer MoS_2.
- Matches experimental spectra and reveals excitonic binding energies.

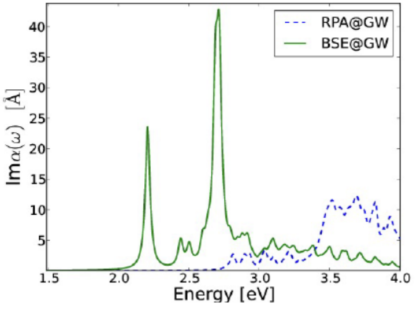


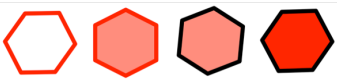
Figure: Absorption spectrum of MoS_2 calculated with the RPA and BSE using the G_0W_0 quasiparticle band structure.

Computational Tools for GW and BSE

- BerkeleyGW:
  - `http://www.berkeleygw.org/`
  - A software package for GW and BSE calculations.
  - Interfaces with DFT codes like Quantum ESPRESSO and VASP.
- Yambo:
  - `http://www.yambo-code.org/`
  - Another package for many-body calculations including GW and BSE.
  - Capable of handling large systems and complex materials.

Summary

- GW provides accurate quasiparticle energies, improving upon DFT results.
- BSE includes electron-hole interactions, essential for accurate optical spectra.
- These methods are critical for studying electronic and optical properties of materials.



DFPT

Introduction to DFPT

- DFPT is an extension of Density Functional Theory (DFT) for studying the response of a system to small perturbations.
- It allows for the calculation of phonons, dielectric properties, and electron-phonon interactions.
- Developed to overcome the limitations of finite-difference methods in calculating response functions.

Basic Principles

- DFT provides the ground-state properties of a many-electron system using the electron density $\rho(\mathbf{r})$.
- DFPT extends DFT to linear response theory, allowing the calculation of changes in $\rho(\mathbf{r})$ due to a perturbation.
- The perturbation can be an external electric field, atomic displacement, etc.

Linear Response Theory

- The response of the electron density $\rho(\mathbf{r})$ to a perturbation $V_{\text{ext}}(\mathbf{r})$ can be expressed as:

$$\delta\rho(\mathbf{r}) = \int \chi(\mathbf{r}, \mathbf{r}')\delta V_{\text{ext}}(\mathbf{r}')d\mathbf{r}' \tag{7}$$

  where $\chi(\mathbf{r}, \mathbf{r}')$ is the density-density response function.
- DFPT calculates $\chi(\mathbf{r}, \mathbf{r}')$ using perturbation theory within the DFT framework.

Key Equations in DFPT

- The self-consistent field (SCF) equations in DFT are modified to include the perturbation:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{eff}}[\rho_0](\mathbf{r}) + \delta V_{\text{eff}}[\delta\rho](\mathbf{r})\right)\psi_i(\mathbf{r}) = \epsilon_i\psi_i(\mathbf{r}) \tag{8}$$

- Here, V_{eff} is the effective potential, and δV_{eff} is its variation due to the perturbation.

Applications of DFPT

- Phonon Calculations:
  - Determines the vibrational modes and frequencies of a crystal.
  - Used to study thermal properties and stability of materials.
- Dielectric Properties:
  - Calculates the dielectric constant and piezoelectric tensors.
  - Important for understanding material responses to electric fields.
- Electron-Phonon Interactions:
  - Computes electron-phonon coupling constants.
  - Essential for studying superconductivity and electrical conductivity.

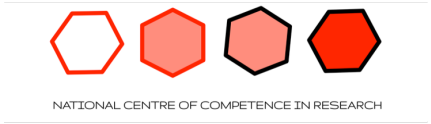
Baroni, S., de Gironcoli, S., Dal Corso, A., & Giannozzi, P. (2001). Phonons and related crystal properties from density-functional perturbation theory. *Reviews of Modern Physics*, 73(2), 515.

Summary

- DFPT extends DFT to study the response of systems to small perturbations.
- It is crucial for calculating phonons, dielectric properties, and electron-phonon interactions.
- Widely used in material science to predict and understand physical properties.

Conclusion

- Comprehensive coverage of electron-phonon physics and computational methods
- Balance of theoretical lectures and practical tutorials
- Importance of hands-on experience with state-of-the-art tools
- Networking and collaborative opportunities



Supplimentary and Misc.

- Frontiers in many-body excited-state dynamics from first principles

Certificate of Attendance

cecam
Centre Européen de Calcul Atomique et Moléculaire

This is to certify that

LIU Binbin

attended in-person the following workshop:

Frontiers in many-body excited-state dynamics from first principles

Location: CECAM-HQ-EPFL, Lausanne, Switzerland

Date: July 15 – 17, 2024

Organized by:
Marina Filip, University of Oxford, United Kingdom
Alejandro Molina Sanchez, University of Valencia, Spain
Diana Qiu, Yale University, United States
Sivan Refaely-Abramson, Weizmann Institute of Science, Israel

Prof. Andrea CAVALLI
CECAM Director

Wannierize Exitonic Bands (from the CECAM workshop)

- Maximally-Localized Exciton Wannier Functions (Haber, Qiu, da Jornada, Neaton, Phys. Rev. B 108, 125118 (2023)).
- A new representation of excitons enabling tight-binding models, geometric phases, interpolation, and physical interpretation
- Interface with Wannier90 different workflows. (Special treatment to the non-analytic term.)
- $\rightarrow$ MLXWFs can be a good localized basis for exciton-polaron physics. (Dai, Lian, Lafuente-Bartolome, Giustino, Phys. Rev. B 109, 045202 (2024))

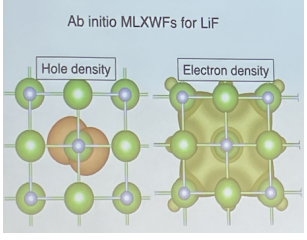


Figure: Ab initio MLXWFs for LiF(From: Neaton's group at Berkeley.)

Properties of Weyl semimetal (may be interesting)

- Thermoelectric: Practical efforts to achieve low-temperature thermoelectrics using NLSs may therefore find it fruitful to identify materials with a nearly flat nodal line. (PRXEnergy.3.023007)
- Exitonic effects in Weyl semimetals.
- Exiton in Weyl phonons: no research paper on this so far!

Applications of Direct Band Gap semiconductor

Optoelectronic devices: Direct band gap materials, with their high radiative recombination rates and strong absorption of light, are widely used in the development of lasers, LEDs, and photodetectors. These devices rely on efficient light emission and absorption for their operation. Solar cells: Direct band gap materials are also utilized in solar cells, where their high absorption coefficient enables efficient conversion of sunlight into electricity.

Figure: Solar city (Tesla)

Literature Reviews on GW and BSE

- The GW method, F Aryasetiawan and O Gunnarsson, 1998 Rep. Prog. Phys. 61 237
- Electronic excitations: density-functional versus many-body Green's-function approaches, REVIEWS OF MODERN PHYSICS, VOLUME 74, APRIL 2002
- Calculating excitons, plasmons, and quasiparticles in 2D materials and van der Waals heterostructures, Kristian Sommer Thygesen
- The GW approximation: content, successes and limitations, Lucia Reining
- The GW Compendium: A Practical Guide to Theoretical Photoemission Spectroscopy Dorothea Golze* Marc Dvorak and Patrick Rinke