Electronic structure calculations

Electronic structure calculations

Richting	Fysica
Jaar	MFYS

Bespreking

Openboekexamen. Tijdens het jaar moet je een werkje maken met ABINIT om de bandstructuur van een kristal te bepalen.

Puntenverdeling

Komt nog.

Examenvragen

Academiejaar 2019-2020 1ste zit

1. Consider an element with one valence electron in a pxpx-orbital. These elements form a two-dimensional square lattice in the x-y plane with lattice constant a.
   - Draw the Brillouin zone
   - Make a sketch of the crystal wavefunction at the high symmetry points in this two-dimensional Brillouin zone (4 points in total)
   - Also make a sketch of the band structure and indicate the Fermi energy
   - Sketch the band structure for the same crystal but with a unit cell with lattice constant 2a in the x-direction and a in the y-direction (thus with two orbitals in the unit cell)
2. We have discussed the article
   Comparison of a Hartree, Hartree-Fock, and an exact treatment of quantum-dot heliumComparison of a Hartree, Hartree-Fock, and an exact treatment of quantum-dot helium
   - Fig. 3 shows the magnetic field dependence of the ground-state energy for the state with total angular momentum M=0, both obtained in the Hartree and Hartree-Fock approximation. What is the origin of the difference of approximately 6 meV between both results?
   - What is the origin of the energy difference between the Hartree-Fock result and the exact ground-state energy for this M=0 state?
   - Explain the physical origin of the observed singlet-triplet transitions?

3. A few questions with a brief answer:
   - Correlation effects dominate in small or large quantum dots? Explain.
   - How is it possible to realize a crystal structure relaxation based on the ground-state density alone (thus without knowing derivatives of the wavefunction) in the Born-Oppenheimer approximation?
   - Does the Kohn-Sham approach suffer from self-interaction?
   - Does the Kohn-Sham approach lead to an upper bound of the total energy?
   - What is the use of a k-point shift?
   - What is the effective mass approximation?
   - The Kohn-Sham equation is given by (vergelijking gegeven). Derive an expression, for the total energy in terms of $\sum_{i=1}^{N} \epsilon_i$ with N the total numbers of electrons.
4. A few questions o k.p theory:
   - Consider the 8x8 Kane Hamiltonian on slide 83. Why is this Hamiltonian not diagonal at Gamma?
   - Is it possible to realize a diagonal k.p Hamiltonian at Gamma?
   - We have defined the Luttinger parameters γ_1, γ_2 and γ_3 in the 6 band Luttinger-Kohn Hamiltonian (leading to H_6). Suppose we would now also include the two lowest conduction bands. This would lead to an 8 band k.p Hamiltonian H_8. Which contains the 6 band Luttinger-Kohn Hamiltonian as a sub-block, but with slightly different Luttinger-like parameters γ'_1, γ'_2 and γ'_3
     - Why do the Luttinger parameters differ from the Luttinger-like parameters?
     - What is the relation between the Luttinger and the Luttinger-like parameters?

Academiejaar 2014-2015 2^e zit

1. We have discussed the article Comparison of a Hartree, Hartree-Fock, and an exact treatment of quantum-dot helium, ...
   - Show that the Hartree approach suffers from self-interaction.
   - Propose a simple approach to exclude this self-interaction for this two electron problem (without including the exchange interaction).
   - Explain the physical origin of the observed singlet-triplet transitions.
   - Show that only electrons with parallel spins feel the exchange interaction.
   - Why the exchange interaction lowers the total energy?
2. The Kohn-Sham equation is given by
$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r}) + e^2\int d\vec{r}\,'\frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|} + \frac{\delta E_{XC}[\rho]}{\delta\rho(\vec{r})}\right)\varphi_i(\vec{r}) = \epsilon_i\varphi_i(\vec{r})$$
.
   - Derive the expression for the total energy in terms of the ϵ_i's.
   - Do the Kohn-Shams equations suffer from self-interaction?
   - Does the Kohn-Sham approach lead to an upper bound for the total energy?
3. Consider the band structure of polyacetylene obtained within the tight-binding approach (with only the p_z orbitals included).
   - Make a sketch of the crystal wavefunction. Explain with it the degeneracy at the edge of the Brillouin zone.
   - Sketch the bandstructure for the case that one of the two carbon atoms in the unit cell is replaced by a Si atom (without changing the structure).
   - Sketch the bandstructure for the case that both atoms in the unit cell are replaced by Si atoms (without changing the structure).

4. Calculate the matrix element $\frac{1}{2}\langle -X-iY\uparrow|H|-X-iY\uparrow\rangle$ with $H=H_0+\frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p}+\frac{\hbar}{4m^2c^2}\nabla V_L\times\mathbf{p}\cdot\sigma$, $\frac{1}{\sqrt{2}}|-X-iY\uparrow\rangle$ an eigenfunction of H_0, $\mathbf{k}=k\vec{e}_z$ and σ determined by the Pauli matrices.

5.
   - Consider the 8×8 Kane Hamiltonian on slide 83. Why this Hamiltonian is not diagonal at Γ?
   - Is it possible to realize a diagonal $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian at Γ?

6. *Bonus question.* We have defined the Kuttinger parameters γ_1, γ_2 and γ_3 in the 6 band Luttinger-Kohn Hamiltonian (leading to $H_6(\gamma_1,\gamma_2,\gamma_3)$). Suppose we would now also include the two lowest conduction bands. This would lead to an 8 band $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian H_8

$$H_8=\left(\begin{array}{c|c} H_2 & \vdots \\ \hline \cdots & H_6(\gamma'_1,\gamma'_2,\gamma'_3) \end{array}\right),$$

which contains the 6 band Luttiner-Kohn Hamiltonian as a sub-block, but with slightlu=y different Luttinger-like parameters γ'_1, γ'_2 and γ'_3.
   - Why do the Luttinger parameters differ from the Luttinger-like parameters?
   - What is the relation between the Luttunger and the Luttinger-like parameters?

Academiejaar 2014-2015 1^e zit

1. Consider an element with one valence electron in a p_x orbital. These elements form a two-dimensional square lattice in the $x-y$ plane.
   - Make a sketch of the crystal wavefunctions at high symmetry points in the two-dimensional Brillouin zone.
   - Sketch the band structure along the paths between these high-symmetry points.
   - Do the same for an electron in a p_x orbital.

2. Consider the following two different structures of polyacetylene:
   Make a sketch of the band structure for both cases. Only take into account the p_z orbital of the carbon atoms.

3. We have discussed the article Comparison of a *Hartree, Hartree-Fock, and an exact treatment of quantum-dot helium*, Phys. Rev. B 47, 2244 (1993) from D. Pfannkuche, V. Gudmundsson, and P. Maksym.
   - Fig. 3 shows the magnetic field dependence of the ground-state energy for the state with total angular momentum $M=0$, both obtained in the Hartree and the Hartree-Fock approximation. What is the origin of the difference of approximately 6 meV between both results?
   - What is the origin of the energy difference between the Hartree-Fock result and the exact ground-state energy for this $M=0$ state?
   - Explain the physical origin of the observed singlet-triplet transitions.

4. A few questions with a brief answer:
    - Correlation effects dominate in small or large quantum dots? Explain.
    - How is it possible to realize a crystal structure relaxation based on the groundstate density alone (in the Born-Oppenheimer approximation)?
    - What is the 'exchange hole' or 'Fermi hole'?
    - Does the Kohn-Sham approach suffer from self-interaction?
    - Does the Kohn-Sham approach lead to an upper bound of the total energy?
    - What is the use of a k-point shift?
    - What are pseudopotentials and why are they useful?
    - What is the effective mass approximation?
    - The Kohn-Sham equation is given by
      $$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\vec{r}) + e^2\int d\vec{r}\,'\frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|} + \frac{\delta E_{XC}[\rho]}{\delta\rho(\vec{r})}\right)\varphi_i(\vec{r}) = \epsilon_i\varphi_i(\vec{r}).$$

      Is the total energy given by $\sum_{i=1}^{N}\epsilon_i$ with N the total number of electrons?
    - Consider the 8×8 Kane Hamiltonian on slide 83. Why this Hamiltonian is not diagonal at Γ?
    - Is it possible to realize a diagonal $k\cdot p$ Hamiltonian at Γ?
5. We have discussed the article *Energy levels of one and two holes in parabolic quantum dots*, Phys. Rev. B 53, 1507 (1996) from F. Pedersen and Y.-C. Chang. In this article, also the hole levels within a GaAs/AlGaAs quantum well are studied.
    - Are the states in figure 1 for $k_{100}=0$ pure *heavy-hole* or *light-hole* states, or mixed *heavy-hole - light-hole* states?
    - SUppose now that instead of this 4×4 model, Kane's six band Hamiltonian was used to study the hole states in this quantum well (thus including coupling with the split-off band). Would the same states at $k_{100}=0$ be pure *heavy-hole* or *light-hole* states, or mixed states?

Academiejaar 2013-2014

1. Consider an element with one valence electron in a p_z orbital. These elements form a two-dimensional square lattice in the $x-y$ plane.
    a. Make a sketch of the crystal wavefunctions at high symmetry points in the two-dimensional Brillouin zone.
    b. Sketch the band structure along the paths between these high-symmetry points.
    c. Do the same (a and b) for an electron in a NN orbital.
2. We have discussed the article Comparison of a *Hartree, Hartree-Fock, and an exact treatment of quantum-dot helium*, Phys. Rev. B 47, 2244 (1993) from D. Pfannkuche, V. Gudmundsson, and P. Maksym.
    a. Fig. 3 shows the magnetic field dependence of the ground-state energy for the state with total angular momentum $M=0$, both obtained in the Hartree and the Hartree-Fock approximation. What is the origin of the difference of approximately 6 meV between both results?
    b. What is the origin of the energy difference between the Hartree-Fock result and the exact ground-state energy for this $M=0$ state?
    c. Explain the physical origin of the observed singlet-triplet transitions.

3. A few questions with a brief answer.
    a. What is the *configuration interaction method*?
    b. Correlation effects dominate in small or large quantum dots? Explain.
    c. How is it possible to realize a crystal structure relaxation based on the groundstate density alone (in the Born-Oppenheimer approximation)?
4. The Kohn-Sham equation is given by

$$\left(-\frac{\hbar^2}{2m}\nabla^2+V_{ext}(\vec{r})+e^2\int d\vec{r}\,'\frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}+\frac{\delta E_{XC}[\rho]}{\delta\rho(\vec{r})}\right)\varphi_i(\vec{r})=\epsilon_i\varphi_i(\vec{r}).$$

    a. Derive the expression for the total energy in terms of the ϵ_i's.
    b. Do the Kohn-Shams equations suffer from self-interaction?
    c. Does the Kohn-Sham approach lead to an upper bound for the total energy?
5. Calculate the following matrix element on slide 83 explicitly

$$\langle X-iY2\downarrow|H|X-iY2\downarrow\rangle$$

    with

$$H=H_0+\frac{\hbar}{m}k\cdot p+\frac{\hbar}{4m^2c^2}\nabla V_L\times p\cdot\vec{\sigma},$$

    $|X-iY2\downarrow\rangle$ an eigenfunction of H_0, $k=k\vec{e}_z$ and

$$\sigma_x=\begin{pmatrix}0&1\\1&0\end{pmatrix},\sigma_y=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\sigma_z=\begin{pmatrix}1&0\\0&-1\end{pmatrix}.$$

6. We have discussed the article *Energy levels of one and two holes in parabolic quantum dots*, Phys. Rev. B 53, 1507 (1996) from F. Pedersen and Y.-C. Chang. In this article, also the hole levels within a GaAs/AlGaAs quantum well are studied.
    a. Are the states in figure 1 for $k_{100}=0$ pure *heavy-hole* or *light-hole* states, or mixed *heavy-hole - light-hole* states?
    b. If the same Hamiltonian is used to describe hole states in a quantum wire, are the states at the Γ point in the Brillouin none *heavy-hole* or *light-hole* states, or mixed *heavy-hole - light-hole* states?

Academiejaar 2012-2013 1$^{\text{ste}}$ zit

1. We have discussed the article Comparison of a Hartree, Hartree-Fock, and an exact treatment of quantum-dot helium, ...
    ○ Show that the Hartree approach suffers from self-interaction.
    ○ Propose a simple approach to exclude this self-interaction for this two electron problem (without including the exchange interaction).
    ○ Explain the physical origin of the observed singlet-triplet transitions.
2.
    ○ Show that only electrons with parallel spins feel the exchange interaction.
    ○ Why the exchange interaction lowers the total energy?
3. The Kohn-Sham equation is given by

$$\left(-\frac{\hbar^2}{2m}\nabla^2+V_{ext}(\vec{r})+e^2\int d\vec{r}\,'\frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}+\frac{\delta E_{XC}[\rho]}{\delta\rho(\vec{r})}\right)\varphi_i(\vec{r})=\epsilon_i\varphi_i(\vec{r})$$

    .
    ○ Derive the expression for the total energy in terms of the ϵ_i's.
    ○ Do the Kohn-Shams equations suffer from self-interaction?
    ○ Does the Kohn-Sham approach lead to an upper bound for the total energy?

4. Consider the band structure of polyacetylene obtained within the tight-binding approach (with only the pzpz orbitals included).
   - Make a sketch of the crystal wavefunction. Explain with it the degeneracy at the edge of the Brillouin zone.
   - Sketch the bandstructure for the case that one of the two carbon atoms in the unit cell is replaced by a Si atom (without changing the structure).
   - Sketch the bandstructure for the case that both atoms in the unit cell are replaced by Si atoms (without changing the structure).
5. Calculate the matrix element $1/2-\sqrt{\langle X-iY\uparrow|H|X-iY\uparrow\rangle}$ $1/2\langle X-iY\uparrow|H|X-iY\uparrow\rangle$ with $H=H_0+\frac{\hbar}{m}k\cdot p+\frac{\hbar}{4m^2c^2}\nabla V L\times p\cdot\sigma$ $H=H_0+\frac{\hbar}{m}k\cdot p+\frac{\hbar}{4m^2c^2}\nabla V L\times p\cdot\sigma$, $1/2-\sqrt{|-X-iY\uparrow\rangle}$ $1/2|-X-iY\uparrow\rangle$ an eigenfunction of $H_0 H_0$, $k=k\vec{e}_z$ $k=k\vec{e}\to z$ and $\sigma\sigma$ determined by the Pauli matrices.
6. We have discussed the article Energy levels of one and two holes in parabolic quantum dots.... In this article, also the hole levels with a GaAs/AlGaAs quantum well are studied.
   - How would you study the hole levels in a GaAs/AlGaAs quantum wire? Write down the equations.
   - For this wire, are the hole levels at the $\Gamma\Gamma$ point pure heavy or light hole states?

Academiejaar 2011-2012 1$^{\text{ste}}$ zit

1. Beschouw een atoomsoort met een valentie-elektron in een s-orbitaal. Deze atomen vormen een tweedimensionaal vierkant rooster. Bepaal de bandenstructuur via een tight-bindingmodel. Maak een schtes van de bandenstructuur. Duid hieropp ook het Fermi-niveau aan.
2. Een aantal vragen met een beknopt antwoord.
   - Wat is de configuration interaction methode?
   - Wat is correlatie-energie? Is deze energiebijdrage positief of negatief?
   - Wat is de universele functionaal, en waarom wordt die universeel genoemd?
   - Welke methode heeft last van zelf-interactie, en waarom?
3. De Kohn-Sham vergelijking wordt gegeven door
   $(-\frac{\hbar^2}{2m}\nabla^2+V_{ext}(\vec{r})+e^2\int d\vec{r}\,'\frac{\rho(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|}+\frac{\delta E_{XC}[\rho]}{\delta\rho(\vec{r})})\varphi_i(\vec{r})$
   $(-\frac{\hbar^2}{2m}\nabla^2+V_{ext}(r\to)+e^2\int dr\to'\frac{\rho(r\to')}{|r\to-r\to'|}+\frac{\delta E_{XC}[\rho]}{\delta\rho(r\to)})\varphi_i(r\to)=\epsilon_i\varphi_i(\vec{r})=\epsilon_i\varphi_i(r\to)$, Leid de uitdrukking af voor de totale energie in functie van de $\epsilon_i\epsilon_i$'s
4. We hebben het artikel Comparison of a Hartree, Hartree-Fock, and an exact treatment of quantum-dot helium, ... Besproken. Leg uit waarom er lege vakken optreden in tabel I
5. Bereken het matrixelement $1/2-\sqrt{\langle X-iY\uparrow|H|X-iY\uparrow\rangle}$ $1/2\langle X-iY\uparrow|H|X-iY\uparrow\rangle$ met $H=H_0+\frac{\hbar}{m}kp+\frac{\hbar}{4m^2c^2}\nabla V L\times p\sigma$ $H=H_0+\frac{\hbar}{m}kp+\frac{\hbar}{4m^2c^2}\nabla V L\times p\sigma$, $1/2-\sqrt{|X-iY\uparrow\rangle}$ $1/2|X-iY\uparrow\rangle$ is een eigenfunctie van $H_0 H_0$
6. We hebben het artikel energy levels of one ant two holes in parabolic quan.... besproken. Zijn de toestanden in figuur 1 voor $k_{100}=0$ pure heavy-hole of light-hole toestanden, of gemengde heavy-hole-light-hole toestanden?

Categorieën:
- Fysica
- MFYS