

i Information

Department of Physics

Examination paper for TFY4210/FY8916 Quantum theory of many-particle systems

Academic contact during examination: Øyvind Sande Borck

Phone: 408 59 107

Examination date: 22.05.2019

Examination time (from-to): 15 - 19

Permitted examination support material: Support material code C:

Approved calculator

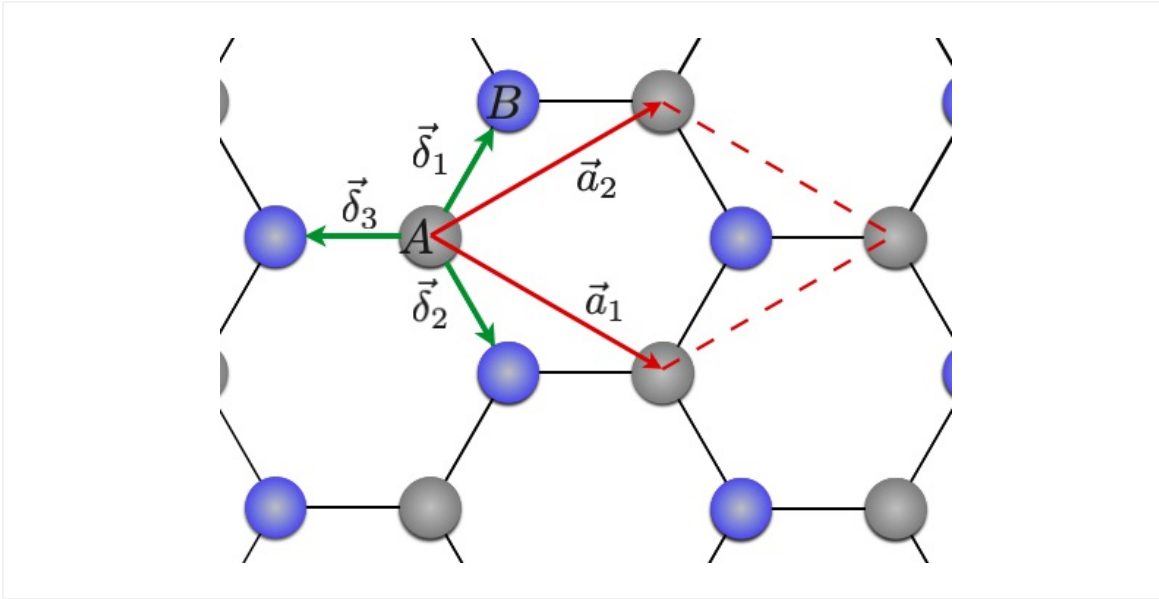
Rottman: Matematisk formelsamling

Barnett & Cronin: Mathematical Formulae

Other information:

Students will find the examination results in Studentweb. Please contact the department if you have questions about your results. The Examinations Office will not be able to answer this.

1 Problem 1-1



In the lectures we discussed a tight-binding approximation (TBA) for graphene (see figure above) with a Hamiltonian given by

$$H = t \sum_j \sum_{l=1}^3 (a_j^\dagger b_{j+l} + b_{j+l}^\dagger a_j)$$

Questions:

Give **short** answers to each of the questions below:

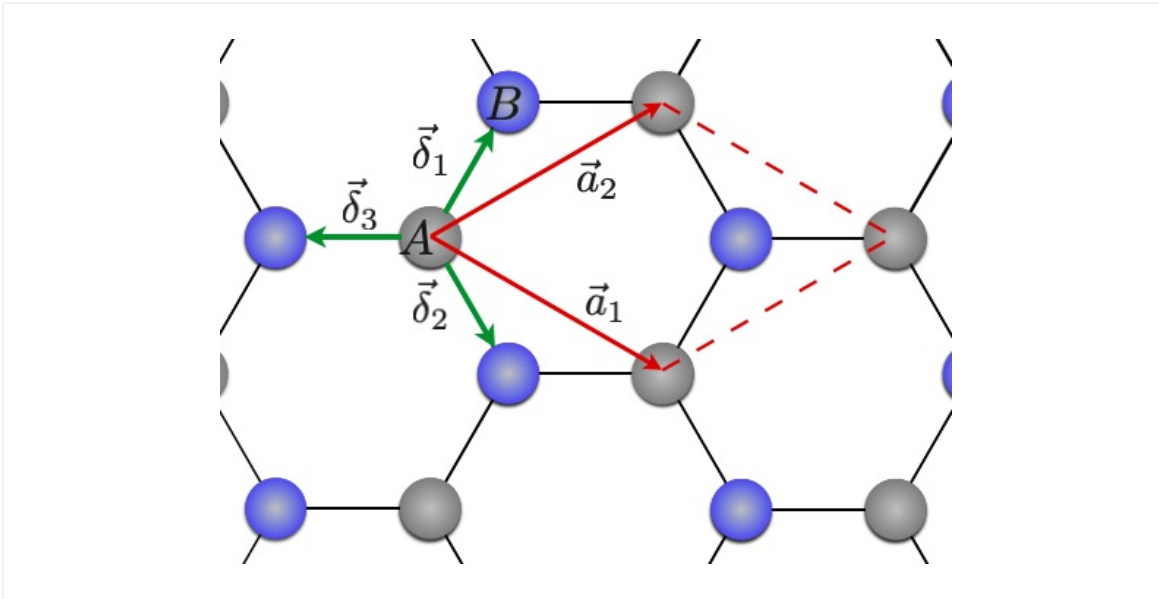
- Which assumptions are made in this approximation?
- Define/explain the symbols t , a_j^\dagger , a_j , b_{j+l} and b_{j+l}^\dagger that goes into this Hamiltonian.

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We continue our study of the Hamiltonian:

$$H = t \sum_j \sum_{l=1}^3 \left(a_j^\dagger b_{j+l} + b_{j+l}^\dagger a_j \right)$$

Assume periodic boundary conditions, introduce new operators $a_{\mathbf{k}}, b_{\mathbf{k}}$ via a Fourier transform

$$a_j = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_j} a_{\mathbf{k}}$$

$$b_j = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_j} b_{\mathbf{k}}$$

where N is the number of unit cells, and show that the Hamiltonian can be written in the form

$$H = \sum_{\mathbf{k}} \begin{pmatrix} a_{\mathbf{k}}^\dagger & b_{\mathbf{k}}^\dagger \end{pmatrix} \begin{pmatrix} 0 & tS(\mathbf{k}) \\ tS^*(\mathbf{k}) & 0 \end{pmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ b_{\mathbf{k}} \end{pmatrix}$$

Here $S(\mathbf{k}) = \sum_{l=1}^3 e^{i\mathbf{k}\cdot\boldsymbol{\delta}_l}$, where $\boldsymbol{\delta}_l$ are nearest neighbour vectors (see figure above).

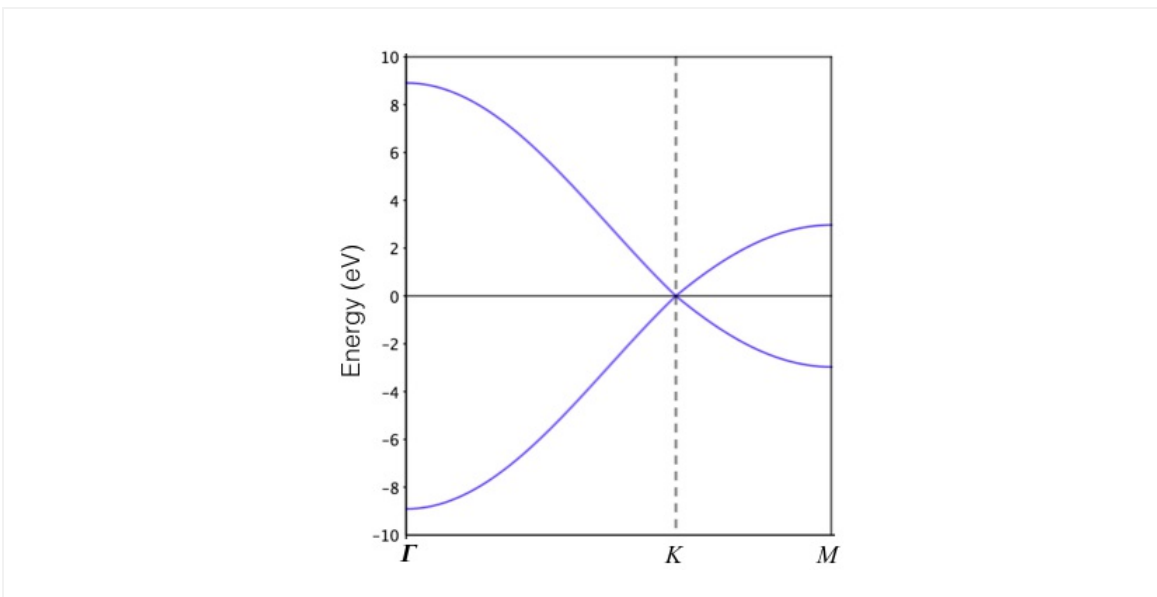
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3 Problem 1-3



The figure above shows a plot of the band structure of graphene calculated within this TBA. We shall consider the electronic states near the K-point. In the 'first-quantized' formalism, the tight-binding Hamiltonian for graphene is

$$h(\mathbf{k}) = \begin{pmatrix} 0 & tS(\mathbf{k}) \\ tS^*(\mathbf{k}) & 0 \end{pmatrix}$$

In the lectures it was shown that close to the K-point

$$S(\mathbf{q}) \approx \frac{3a}{2}(q_x - iq_y)$$

where \mathbf{q} is a small wave-vector near \mathbf{K} , that is $\mathbf{k} = \mathbf{K} + \mathbf{q}$ and $|\mathbf{q}| \ll |\mathbf{K}|$.











Problem:

Show that the effective Hamiltonian for states near \mathbf{K} takes the form

$$h(\mathbf{q}) = \hbar v_F (\sigma_x q_x + \sigma_y q_y)$$

where σ_x and σ_y are the Pauli matrices $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. Give the expression for v_F .

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Maximum marks: 6

4 **Problem 2-1**

Consider the Dirac equation for a free spin- $\frac{1}{2}$ particle in three spatial dimensions

$$(i\hbar\gamma^\mu\partial_\mu - mc)\Psi = 0$$

where γ^μ are the four Dirac γ -matrices, $\partial_\mu = \left(\frac{1}{c}\frac{\partial}{\partial t}, \nabla\right)$ is the covariant four-derivative and Ψ is a four-component spinor.

Problem:

Express Ψ in terms of two two-component spinors φ_A and φ_B , and show that for a massless particle ($m = 0$), the Dirac equation can be decoupled into the two *Weyl equations*

$$i\hbar\frac{\partial\varphi_\pm}{\partial t} = \pm c\boldsymbol{\sigma} \cdot \mathbf{p}\varphi_\pm$$

where $\varphi_\pm \equiv \varphi_A \pm \varphi_B$, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices, and $\mathbf{p} = -i\hbar\nabla$.

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5 **Problem 2-2**

In two spatial dimension the Weyl-equation for φ_+ can be expressed in terms of only two of the Pauli matrices, for example:

$$i\hbar \frac{\partial \varphi_+}{\partial t} = c(\sigma_x p_x + \sigma_y p_y) \varphi_+$$

Problems:

- Show that the energy eigenvalues for this equation are $E_{\pm} = \pm c|\mathbf{p}|$
- Compare the Hamiltonian in this equation with the effective hamiltonian for graphene near the K-point in problem 1-3 and comment.

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Problem 2-2 (Correction)

In two spatial dimension the Weyl-equation for φ_+ can be expressed in terms of only two of the Pauli matrices, for example:

$$i\hbar \frac{\partial \varphi_+}{\partial t} = c(\sigma_x p_x + \sigma_y p_y) \varphi_+$$

Problems:

- Show that the energy eigenvalues for this equation are $E_{\pm} = \pm c|\mathbf{p}|$

for a free particle with plane-wave solutions of the form

$$\varphi_+ = N e^{-\frac{i}{\hbar}(Et - \mathbf{p} \cdot \mathbf{r})}$$

6 **Problem 3-1**

Consider a system of noninteracting electrons. In the 'second-quantized' formalism the Hamiltonian is given by

$$H_0 = \sum_{\nu} \xi_{\nu} c_{\nu}^{\dagger} c_{\nu}$$

where ν is a set of quantum numbers, $\xi_{\nu} = \epsilon_{\nu} - \mu$, and μ is the chemical potential.

The Matsubara single-particle Green function is defined as

$$\mathcal{G}(\nu, \tau) = -\langle T_{\tau}(c_{\nu}(\tau)c_{\nu}^{\dagger}(0)) \rangle$$

Here $\tau \in \langle -\beta, \beta \rangle$, (where $\beta = 1/(k_B T)$ is the inverse temperature), and T_{τ} is a time-ordering operator which orders operators with earliest (imaginary) time τ to the right, introducing a minus sign when reordering is needed. The time-dependence of the operators is given by

$$c_{\nu}(\tau) = e^{-H_0 \tau} c_{\nu} e^{H_0 \tau} = e^{-\xi_{\nu} \tau} c_{\nu}$$

The Fourier transform of $\mathcal{G}(\nu, \tau)$ is given by

$$\mathcal{G}(\nu, ip_n) = \int_0^{\beta} d\tau e^{ip_n \tau} \mathcal{G}(\nu, \tau)$$

where $p_n = (2n + 1)\pi/\beta$ is a fermionic Matsubara frequency ($n \in \mathbb{Z}$).

Problem:

Calculate the Matsubara Green function for noninteracting electrons, $\mathcal{G}^{(0)}(\nu, ip_n)$, and use the result to obtain the retarded Green function $G_0^R(\nu, \omega)$.

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7 Problem 3-2

Consider electrons scattering with (randomly distributed) impurities in a metal. Neglect the electron spin. In the lectures we developed a perturbative expansion for the single-particle Matsubara Green function $\mathcal{G}(\mathbf{k}, \mathbf{k}'; ip_m)$ for such a system. By averaging over the position of the impurities, we obtained a Green function which was diagonal in \mathbf{k} : $\overline{\mathcal{G}}(\mathbf{k}, \mathbf{k}'; ip_m) = \overline{\mathcal{G}}(\mathbf{k})\delta_{\mathbf{k}\mathbf{k}'}$.

Question:

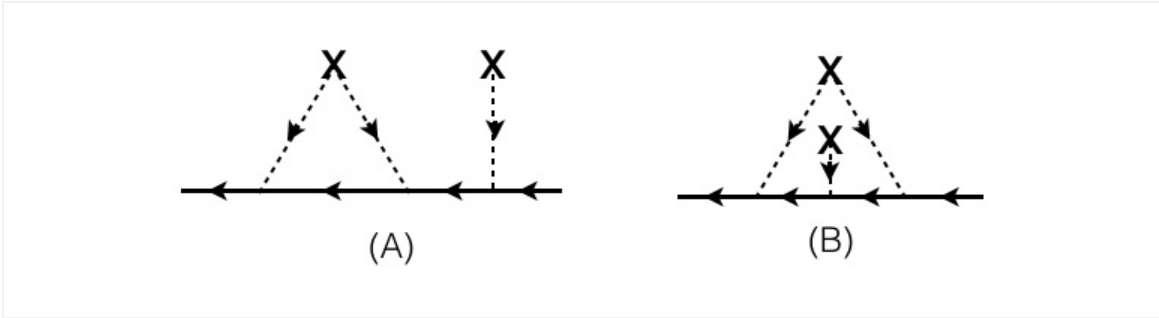
Explain why we should expect, on physical grounds, that such an averaging will make the Green function diagonal in \mathbf{k} .

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8 **Problem 3-3**

The figure above shows two of the Feynman diagrams in the perturbation expansion for $\bar{G}(\mathbf{k}, ip_m)$.

Questions:

- For each diagram, determine whether the diagram is reducible or irreducible. Justify your answer.
- Give the mathematical expression for diagram A (Do not evaluate the wave vector sum).

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9 Problem 3-4

The spectral function $A(\mathbf{k}, \omega)$ is defined as

$$A(\mathbf{k}, \omega) = -\frac{1}{\pi} \text{Im} G^R(\mathbf{k}, \omega)$$

where $G^R(\mathbf{k}, \omega)$ is the retarded Green function. In the lectures it was shown that in the limit of low impurity density n_{imp} and weak scattering potential u , the retarded Green function is given by

$$\overline{G^R}(\mathbf{k}, t) = -i\theta(t)e^{-i(\xi_{\mathbf{k}} + n_{\text{imp}}u)t} e^{-t/(2\tau)}$$

where $1/\tau = 2\pi n_{\text{imp}} u^2 D(0)$ (here $D(0)$ is the density of states at the Fermi level).

Problems

a) Calculate the spectral function for this Green function, and show that it is given by

$$\bar{A}(\mathbf{k}, \omega) = \frac{1}{\pi} \frac{1/(2\tau)}{(\omega - (\xi_{\mathbf{k}} + n_{\text{imp}}u))^2 + (1/(2\tau))^2}$$

b) Show that this spectral function satisfy the sum rule:

$$\int_{-\infty}^{\infty} d\omega \bar{A}(\mathbf{k}, \omega) = 1$$

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