Karlsruhe Institute of Technology
Institute for Theoretical Condensed Matter physics

Condensed Matter Theory I WS 2022/2023

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Sheet 10
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1. Hartree-Fock approximation in graphene (10 + 20 + 20 = 50 Points)

In the lecture notes, the Hartree-Fock equations have been derived for the Jellium model which assumes a homogeneous distribution of ions. However, we know that the ion cristalline structure modifies the dispersion relation. We propose in this exercise to do the same derivation for the graphene near one of the Dirac points. A special feature is that in addition to the position and spin coordinates, a sublattice coordinate $\alpha = A, B$ is needed. Then the field operator is a 2-spinor in A, B-space, $\hat{\Psi}_{\alpha,\sigma}(r)$. The Hamilton operator is

$$\begin{aligned}\hat{H} &= \sum_{\sigma,\alpha,\beta} \int d^2r \left\{ \hat{\Psi}^\dagger_{\alpha,\sigma}(r) h_{\alpha,\beta} \hat{\Psi}_{\beta,\sigma}(r) + \hat{\Psi}^\dagger_{\alpha,\sigma}(r) U^{(1)}(r) \delta_{\alpha,\beta} \hat{\Psi}_{\beta,\sigma}(r) \right\} \\ &+ \sum_{\sigma_1,\sigma_2,\alpha_1,\alpha_2} \frac{1}{2} \int\int d^2r_1 d^2r_2 \, \hat{\Psi}^\dagger_{\alpha_1,\sigma_1}(r_1) \hat{\Psi}^\dagger_{\alpha_2,\sigma_2}(r_2) \frac{e^2}{|r_1 - r_2|} \hat{\Psi}_{\alpha_2,\sigma_2}(r_2) \hat{\Psi}_{\alpha_1,\sigma_1}(r_1) \, .\end{aligned}$$

The Potential $U^{(1)}(r)$ is the homogeneous part of the Jellium potential for ions (the inhomogeneous part, i.e. crystalline structure, is already taken into account by $h_{\alpha,\beta}$).

The 2×2 matrix $h_{\alpha,\beta}$ is the Hamiltonian operator in graphene in the vicinity of a Dirac Point:

$$\hat{h} = v \begin{pmatrix} 0 & p_x + ip_y \\ p_x - ip_y & 0 \end{pmatrix}.$$

This representation is correct for momentum $|\mathbf{p}| < \Lambda$, where Λ is a cut-off. The energy spectrum is then linear $E_{\mathbf{p}} = \pm v|\mathbf{p}|$. For simplicity, we consider only one valley.

Category A

(a) Derive the Hartree-Fock equations.

(b) Show that the eigenstates of the operator $\hat{h}$ are also solutions of Hartree-Fock equations.

Use the following representation:

$$\hat{h} = vp \begin{pmatrix} 0 & e^{i\varphi_{\boldsymbol{p}}} \\ e^{-i\varphi_{\boldsymbol{p}}} & 0 \end{pmatrix},$$

where

$$\cos\varphi_{\boldsymbol{p}} = \frac{p_x}{p}, \quad \sin\varphi_{\boldsymbol{p}} = \frac{p_y}{p}, \quad p \equiv |\mathbf{p}|.$$

Category B

(c) Assume that the lower band is occupied while the upper band is empty. Using the Fock correction, derive the following results for the effective Hartree-Fock band energy:

$$\mathcal{E}_p = \pm v(p)|\mathbf{p}|, \quad v(p) = v\left(1 + \frac{e^2}{4\hbar v}\ln\frac{\Lambda}{|\mathbf{p}|}\right) \ .$$