Karlsruhe Institute of Technology
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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, $\hat{\Psi}_{\alpha,\sigma}(\mathbf{r})$. The Hamilton operator is

$$\begin{aligned}\hat{H} &= \sum_{\sigma,\alpha,\beta}\int d^2r\left\{\hat{\Psi}^\dagger_{\alpha,\sigma}(\mathbf{r})h_{\alpha,\beta}\hat{\Psi}_{\beta,\sigma}(\mathbf{r}) + \hat{\Psi}^\dagger_{\alpha,\sigma}(\mathbf{r})U^{(1)}(\mathbf{r})\delta_{\alpha,\beta}\hat{\Psi}_{\beta,\sigma}(\mathbf{r})\right\}\\ &+ \sum_{\sigma_1,\sigma_2,\alpha_1,\alpha_2}\frac{1}{2}\int\int d^2\mathbf{r}_1 d^2\mathbf{r}_2\,\hat{\Psi}^\dagger_{\alpha_1,\sigma_1}(\mathbf{r}_1)\hat{\Psi}^\dagger_{\alpha_2,\sigma_2}(\mathbf{r}_2)\,\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\,\hat{\Psi}_{\alpha_2,\sigma_2}(\mathbf{r}_2)\hat{\Psi}_{\alpha_1,\sigma_1}(\mathbf{r}_1)\ .\end{aligned}$$

The Potential $U^{(1)}(\mathbf{r})$ 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.

Solution: First, we substitute the definition of $\hat{\Psi}$-operators, $\hat{\Psi}_{\alpha,\sigma}(\mathbf{r}) = \sum_\mathbf{p}\phi_{\alpha,\sigma,\mathbf{p}}(\mathbf{r})\hat{c}_\mathbf{p}$, into the Hamiltonian ($\mathbf{p}$ is the momentum that labels the unknown single-particle eigenstates $\phi_{\alpha,\sigma,\mathbf{p}}(\mathbf{r})$ of H, $\phi_{\alpha,\sigma,\mathbf{p}}(\mathbf{r})$ is a bispinor):

$$\begin{aligned}\hat{H} &= \sum_{\sigma,\alpha,\beta}\int d^2r\sum_{\mathbf{p},\mathbf{p}'}\phi^*_{\alpha,\sigma,\mathbf{p}}(\mathbf{r})\Big(h_{\alpha,\beta}+U^{(1)}(\mathbf{r})\Big)\phi_{\beta,\sigma,\mathbf{p}}(\mathbf{r})\hat{c}^\dagger_\mathbf{p}\hat{c}_{\mathbf{p}'} +\\ &+ \frac{1}{2}\sum_{\sigma_{1,2},\alpha_{1,2}}\iint d^2\mathbf{r}_1 d^2\mathbf{r}_2\sum_{\mathbf{p},k,k',p'}\phi^*_{\alpha_1,\sigma_1,\mathbf{p}}(\mathbf{r}_1)\phi^*_{\alpha_2,\sigma_2,\mathbf{k}}(\mathbf{r}_2)\,\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\,\phi_{\alpha_2,\sigma_2,\mathbf{k}'}(\mathbf{r}_2)\phi_{\alpha_1,\sigma_1,\mathbf{p}'}(\mathbf{r}_1)\times\\ &\times\hat{c}^\dagger_\mathbf{p}\hat{c}^\dagger_\mathbf{k}\hat{c}_{\mathbf{k}'}\hat{c}_{\mathbf{p}'}\ .\end{aligned}$$

The ground state, which determines the Fermi sea, is $|\Phi\rangle = \prod_{\alpha,\sigma,|\mathbf{p}|<k_F} \hat{c}^\dagger_{\alpha,\sigma,\mathbf{p}}|\text{vacuum}\rangle$. In the Jellium model, the ion potential is $U^{(1)}(\mathbf{r}) = -nU_0$, where n is the density of ions and the extensive constant U_0 is given by $U_0 = \int d^2\mathbf{r}\frac{e^2}{|\mathbf{r}|}$. Then we define the Lagrange functional $\mathcal{L}$ with the multipliers $\mathcal{E}_\mathbf{p}$:

$$\mathcal{L} = \langle\Phi|\hat{H}|\Phi\rangle - \sum_{\alpha,\sigma,\mathbf{p}} \mathcal{E}_\mathbf{p} \int d^2r |\phi_{\alpha,\sigma,\mathbf{p}}(\mathbf{r})|^2 \ .$$

For the unperturbed part we have for the average:

$$\langle\Phi|\hat{c}^\dagger_\mathbf{p}\hat{c}_{\mathbf{p}'}|\Phi\rangle = \delta_{\mathbf{p},\mathbf{p}'} \ .$$

For the interaction term we have:

$$\langle\Phi|\hat{c}^\dagger_\mathbf{p}\hat{c}^\dagger_\mathbf{k}\hat{c}_{\mathbf{k}'}\hat{c}_{\mathbf{p}'}|\Phi\rangle = \delta_{\mathbf{p},\mathbf{p}'}\delta_{\mathbf{k},\mathbf{k}'} - \delta_{\mathbf{p},\mathbf{k}'}\delta_{\mathbf{k},\mathbf{p}'} \ .$$

Now we can write for the energy stored by the state $|\Phi\rangle$ (in all sums we assume $|\mathbf{p}| < k_F$):

$$\begin{aligned}
\langle\Phi|\hat{H}|\Phi\rangle &= \sum_{\sigma,\alpha,\beta}\int d^2r \sum_p \phi^*_{\alpha,\sigma,p}(\mathbf{r})\Big(h_{\alpha,\beta} - nU_0\Big)\phi_{\beta,\sigma,p}(\mathbf{r}) + \\
&+ \frac{1}{2}\sum_{\sigma_{1,2},\alpha_{1,2}}\iint d^2\mathbf{r}_1 d^2\mathbf{r}_2 \sum_{\mathbf{p},\mathbf{k}} \phi^*_{\alpha_1,\sigma_1,\mathbf{p}}(\mathbf{r}_1)\phi^*_{\alpha_2,\sigma_2,\mathbf{k}}(\mathbf{r}_2)\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\phi_{\alpha_2,\sigma_2,\mathbf{k}}(\mathbf{r}_2)\phi_{\alpha_1,\sigma_1,\mathbf{p}}(\mathbf{r}_1) - \\
&- \frac{1}{2}\sum_{\sigma_{1,2},\alpha_{1,2}}\iint d^2\mathbf{r}_1 d^2\mathbf{r}_2 \sum_{\mathbf{p},\mathbf{k}} \phi^*_{\alpha_1,\sigma_1,\mathbf{p}}(\mathbf{r}_1)\phi^*_{\alpha_2,\sigma_2,\mathbf{k}}(\mathbf{r}_2)\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\phi_{\alpha_2,\sigma_2,\mathbf{p}}(\mathbf{r}_2)\phi_{\alpha_1,\sigma_1,\mathbf{k}}(\mathbf{r}_1)
\end{aligned}$$

The condition for the variation of the Lagrangian, $\frac{\delta\mathcal{L}}{\delta\phi^*_{\alpha,\sigma,\mathbf{p}}(\mathbf{r})} = 0$, yields

$$\mathcal{E}_p\phi_{\alpha,\sigma,\mathbf{p}}(\mathbf{r}) = \frac{\delta\langle\Phi|\hat{H}|\Phi\rangle}{\delta\phi^*_{\alpha,\sigma,\mathbf{p}}(\mathbf{r})} = \sum_\beta\Big(h_{\alpha,\beta} - nU_0\delta_{\alpha,\beta}\Big)\phi_{\beta,\sigma,\mathbf{p}}(\mathbf{r}) +$$

$$+\sum_{\sigma_1,\alpha_1}\int d^2\mathbf{r}_1 \sum_\mathbf{k}\phi^*_{\alpha_1,\sigma_1,\mathbf{k}}(\mathbf{r}_1)\frac{e^2}{|\mathbf{r}-\mathbf{r}_1|}\phi_{\alpha_1,\sigma_1,\mathbf{k}}(\mathbf{r}_1)\phi_{\alpha,\sigma,p}(\mathbf{r}) -$$

$$-\sum_{\sigma_1,\alpha_1}\int d^2\mathbf{r}_1 \sum_\mathbf{k}\phi^*_{\alpha_1,\sigma_1,\mathbf{k}}(\mathbf{r}_1)\frac{e^2}{|\mathbf{r}-\mathbf{r}_1|}\phi_{\alpha,\sigma,\mathbf{k}}(\mathbf{r})\phi_{\alpha_1,\sigma_1,\mathbf{p}}(\mathbf{r}_1) \ .$$

In the second line (Hartree term), we calculate the sum over one of momenta k and obtain an electron density at the position $\mathbf{r}_1$: $n(\mathbf{r}_1) = \sum_{\alpha_1,\sigma_1,k}\phi^*_{\alpha_1,\sigma_1,k}(\mathbf{r}_1)\phi_{\alpha_1,\sigma_1,k}(\mathbf{r}_1)$. Assuming that $n(\mathbf{r}_1)$ is homogeneous, i.e., $n(\mathbf{r}_1) = n$, the integral over $\mathbf{r}_1$ yields $\int d^2\mathbf{r}_1\frac{e^2 n(\mathbf{r}_1)}{|\mathbf{r}-\mathbf{r}_1|} = nU_0$. As a result, the Hartree term cancels the term related to ion density in the first line. Finally, the Hartree-Fock equation reads:

$$\mathcal{E}_\mathbf{p}\phi_{\alpha,\sigma,\mathbf{p}}(\mathbf{r}) = \sum_\beta h_{\alpha,\beta}\phi_{\beta,\sigma,\mathbf{p}}(\mathbf{r}) - \sum_{\sigma_1,\alpha_1}\int d^2\mathbf{r}_1 \sum_\mathbf{k}\phi^*_{\alpha_1,\sigma_1,\mathbf{k}}(\mathbf{r}_1)\frac{e^2}{|\mathbf{r}-\mathbf{r}_1|}\phi_{\alpha,\sigma,\mathbf{k}}(\mathbf{r})\phi_{\alpha_1,\sigma_1,\mathbf{p}}(\mathbf{r}_1) \ .$$

In this equation, the Fock term can be also written as a convolution,

$$\mathcal{E}_{\mathbf{p}}\phi_{\alpha,\sigma,\mathbf{p}}(\mathbf{r}) = \sum_{\beta} h_{\alpha,\beta}\phi_{\beta,\sigma,\mathbf{p}}(\mathbf{r}) - \sum_{\sigma_1,\beta}\int d^2\mathbf{r}_1 F_{\alpha,\beta,\sigma,\sigma_1}(\mathbf{r},\mathbf{r}_1)\phi_{\beta,\sigma_1,\mathbf{p}}(\mathbf{r}_1)\ .$$

Here, the effective matrix potential $F_{\alpha,\beta,\sigma,\sigma_1}$ acting on $\phi_{\alpha,\sigma,p}(\mathbf{r}_1)$ is created by other particles; it reads

$$F_{\alpha,\beta,\sigma,\sigma_1}(\mathbf{r},\mathbf{r}_1) = \sum_{\mathbf{k}} \phi_{\alpha,\sigma,\mathbf{k}}(\mathbf{r})\,\frac{e^2}{|\mathbf{r}-\mathbf{r}_1|}\,\phi^*_{\beta,\sigma_1,\mathbf{k}}(\mathbf{r}_1).$$

(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

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

Solution: We obtain below an approximate solution of the Hartree-Fock equation in graphene. The equation is non-linear and one can solve it iteratively. Let us find the solution after the first iteration, $\phi^{(1)}_{\alpha,\sigma,\mathbf{p}}$. In this case, the zero approximation for $\phi_{\alpha,\sigma,\mathbf{p}}$ is given by the known wave functions of non-interacting electrons in graphene, $\psi_{\alpha,\sigma,\mathbf{p}}$, i.e., $\phi^{(0)}_{\alpha,\sigma,\mathbf{p}} = \psi_{\alpha,\sigma,\mathbf{p}}$. Namely, $\psi_{\alpha,\sigma,\mathbf{p}}$ satisfies the Schrödinger equation with the non-interacting Hamiltonian, $\sum_{\beta} h_{\alpha,\beta}\psi_{\beta,\mathbf{p}}(\mathbf{r}) = \mathcal{E}^{(0)}_{\mathbf{p}}\psi_{\alpha,\mathbf{p}}(\mathbf{r})$. (The spin operators commute with h, hence, we omitted the σ-index here.) This solution is given by a spinor in α-space: $\psi_{\mathbf{p},b}(\mathbf{r}) = \dfrac{1}{\sqrt{2S}}\begin{pmatrix} be^{i\theta_{\mathbf{p}}} \\ 1 \end{pmatrix} e^{ipr}$ where S is the area in 2D space and $\theta_{\mathbf{p}} = \arctan\dfrac{p_y}{p_x}$. The energies corresponding to the wave vectors $\mathbf{p}$ define the Dirac spectrum $\mathcal{E}^{(0)}_p = bvp$, where $p = \sqrt{p_x^2+p_y^2}$ and $b = \pm 1$ determines the states in the upper (lower) Dirac cones. We use this solution to obtain an approximate form of the potential $F_{\alpha,\beta,\sigma,\sigma_1}(\mathbf{r},\mathbf{r}_1) \approx \delta_{\sigma,\sigma_1}F^{(0)}_{\alpha,\beta}(\mathbf{r}-\mathbf{r}_1)$ where $F^{(0)}_{\alpha,\beta}$-matrix involves $\phi^{(0)}_{\alpha,\mathbf{p}} = \psi_{\alpha,\mathbf{p}}$:

$$F^{(0)}(\mathbf{r}) = \frac{1}{2S}\sum_{\mathbf{k}}\frac{e^2 e^{i\mathbf{kr}}}{|\mathbf{r}|}\begin{bmatrix} be^{i\theta_{\mathbf{k}}} \\ 1 \end{bmatrix}\begin{bmatrix} be^{-i\theta_{\mathbf{k}}} & 1 \end{bmatrix} = \frac{e^2}{2S|\mathbf{r}|}\sum_{\mathbf{k}} e^{i\mathbf{kr}}\begin{bmatrix} 1 & be^{i\theta_{\mathbf{k}}} \\ be^{-i\theta_{\mathbf{k}}} & 1 \end{bmatrix}\ .$$

The equation for $\phi^{(1)}_{\alpha,\sigma,\mathbf{p}}$ becomes linear under the above approximation:

$$\mathcal{E}^{(1)}_{\mathbf{p}}\phi^{(1)}_{\alpha,\mathbf{p}}(\mathbf{r}) = \sum_{\beta} h_{\alpha,\beta}\phi^{(1)}_{\beta,\sigma,\mathbf{p}}(\mathbf{r}) - \sum_{\beta}\int d^2\mathbf{r}_1 F^{(0)}_{\alpha,\beta}(\mathbf{r}-\mathbf{r}_1)\phi^{(1)}_{\beta,\mathbf{p}}(\mathbf{r}_1)\ .$$

We find solutions in a basis of plane waves, $\phi^{(1)}_{\alpha,b,\mathbf{p}}(\mathbf{r}) = C_{\alpha,b,\mathbf{p}}e^{i\mathbf{pr}}$, where $C_{\alpha,\mathbf{p}}$-components are to be found. Using this substitution, we have

$$\mathcal{E}^{(1)}_{\mathbf{p},b}C_{\alpha,b,\mathbf{p}} = \sum_{\beta}\Big(h_{\alpha,\beta,\mathbf{p}} - F^{(0)}_{\alpha,\beta,\mathbf{p}}\Big)C_{\beta,b,\mathbf{p}}\ .$$

where the Fourier transformed matrix potential is $F^{(0)}_{\mathbf{p}} = \int d^2\mathbf{r} F^{(0)}(\mathbf{r}) e^{-i\mathbf{pr}}$. It reads

$$F^{(0)}_{\mathbf{p}} = \int d^2\mathbf{r} \frac{e^2}{2S|\mathbf{r}|} \sum_{\mathbf{k}} e^{-i(\mathbf{p}-\mathbf{k})\mathbf{r}} \begin{bmatrix} 1 & be^{i\theta_{\mathbf{k}}} \\ be^{-i\theta_{\mathbf{k}}} & 1 \end{bmatrix} = \Lambda \frac{e^2}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + b \sum_{\mathbf{k}} U_{\mathbf{p}-\mathbf{k}} \begin{bmatrix} 0 & e^{i\theta_{\mathbf{k}}} \\ e^{-i\theta_{\mathbf{k}}} & 0 \end{bmatrix} \tag{1}$$

where Λ is a cutoff momentum (it determines the minimal possible distance in our theory, $|\mathbf{r}| \sim 1/\Lambda$) and the Fourier transformed Coulomb potential,

$$U_{\mathbf{q}} = \int d^2\mathbf{r} \frac{e^2}{2S|\mathbf{r}|} e^{-i\mathbf{qr}} = \frac{e^2}{2S} \int_0^{\infty} r dr \int_0^{2\pi} d\varphi \frac{e^{-i|\mathbf{q}|r\cos\varphi}}{r} = \frac{e^2}{2S} \int_0^{\pi} d\varphi \int_{-\infty}^{\infty} e^{-i|\mathbf{q}|x\cos\varphi} dx =$$

$$= \frac{e^2}{2S} \int_0^{\pi} d\varphi 2\pi\delta(|\mathbf{q}|\cos\varphi) = \frac{\pi e^2}{S|\mathbf{q}|}.$$

The term $\sim \Lambda$ in (1) is not important, it shifts the background potential. The second one in (1) is most relevant:

$$b \sum_{\mathbf{k}} U_{\mathbf{p}-\mathbf{k}} \begin{bmatrix} 0 & e^{i\theta_{\mathbf{k}}} \\ e^{-i\theta_{\mathbf{k}}} & 0 \end{bmatrix} = b \int \frac{S d^2\mathbf{k}}{(2\pi)^2} \frac{\pi e^2}{S|\mathbf{p}-\mathbf{k}|} \begin{bmatrix} 0 & e^{i\theta_{\mathbf{k}}} \\ e^{-i\theta_{\mathbf{k}}} & 0 \end{bmatrix} =$$

$$= b \frac{e^2}{4\pi} \int_0^{\infty} \int_0^{2\pi} \frac{k dk d\varphi}{\sqrt{p^2 + k^2 - 2pk\cos\varphi}} \begin{bmatrix} 0 & e^{i\theta_{\mathbf{p}}+i\varphi} \\ e^{-i\theta_{\mathbf{p}}-i\varphi} & 0 \end{bmatrix}.$$

In the last line we introduced the angle φ between $\mathbf{k}$ and $\mathbf{p}$. Hence, the angle of the vector $\mathbf{k}$ is $\theta_{\mathbf{k}} = \theta_{\mathbf{p}} + \varphi$. We should leave only the even in φ part of the integrand ($\sim \cos\varphi$) because the odd one ($\sim \sin\varphi$) gives zero. As a result, we have for the Fock term:

$$b \sum_{\mathbf{k}} U_{\mathbf{p}-\mathbf{k}} \begin{bmatrix} 0 & e^{i\theta_{\mathbf{k}}} \\ e^{-i\theta_{\mathbf{k}}} & 0 \end{bmatrix} = b\hbar\mathcal{V}_{\mathbf{p}} \begin{bmatrix} 0 & p_x + ip_y \\ p_x - ip_y & 0 \end{bmatrix} \tag{2}$$

where the momentum dependent correction for the velocity v of Dirac fermions has been introduced,

$$\mathcal{V}_p = \frac{e^2}{4\pi\hbar p} \int_0^{\infty} \int_0^{2\pi} \frac{k\cos\varphi \; dk d\varphi}{\sqrt{p^2 + k^2 - 2pk\cos\varphi}}. \tag{3}$$

We note that the matrix structure in (2) is the same as for the graphene Hamiltonian $h_{\mathbf{p}} = \hbar v \begin{bmatrix} 0 & p_x + ip_y \\ p_x - ip_y & 0 \end{bmatrix}$. It means that the wave functions, which are given by the solution $C_{\mathbf{p}}$ of Hartree-Fock equation are the same as for $\psi_{\mathbf{p}}$ in the non-interacting case. However, the dispersion relation $\mathcal{E}^{(1)}_{\mathbf{p}}$ changes, i.e., the Dirac cone is deformed:

$$\mathcal{E}^{(1)}_{\pm,\mathbf{p}} = \pm\hbar(v + \mathcal{V}_p)p \; .$$

In this result we have chosen $b = -1$ in the Fock term (2) to obtain the positive energies $\mathcal{E}^{(1)}_{\mathbf{p}} > 0$ in the conduction band. The negative sign $b = -1$ compensates the minus sign in the Fock term. To obtain $\mathcal{E}^{(1)}_{\mathbf{p}} < 0$ in the valence band with we choose $b = 1$ in the Fock term.

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:

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

Solution: If the valence band is occupied and the conduction one is empty then the Fermi level crosses the Dirac point where $p = 0$. We calculate $\mathcal{V}_p$ near this point (the long wavelength limit of small p). The integral (3) is accumulated at large momenta $k \sim \Lambda$ while at small ones, $k \lesssim p$, the integrating function is regular. To obtain the asymptotic expression for $\mathcal{V}_p$ we expand the integrand in the leading order in small $1/k$ and set the lower limit as p (it plays a role of the cutoff at small momenta):

$$\mathcal{V}_p \approx \frac{e^2}{4\pi\hbar p}\int\limits_p^\Lambda dk \int\limits_0^{2\pi}\left(1 + \frac{p}{k}\cos\varphi\right)\cos\varphi\, d\varphi = \frac{e^2}{4\hbar}\int\limits_p^\Lambda \frac{dk}{k} = \frac{e^2}{4\hbar}\ln\frac{\Lambda}{p} .$$

Finally, we find for the renormalized velocity near the Dirac point:

$$v(p) = v\left(1 + \frac{e^2}{4v\hbar}\ln\frac{\Lambda}{p}\right) .$$

It diverges logarithmically at $p \to 0$.