TFY4210/FY8916 Quantum theory of many-particle systems
Solution sketch to the exam May 22, 2019

Problem 1-1

a) The assumptions made in the approximation are: 1) Only one electron (orbital) per site. 2) There is a small amplitude for hopping between sites (characterized by t), in this particular case only nearest-neighbour jumps are allowed.

b) t is the hopping amplitude. $a_j^\dagger$ (a_j) are creation (annihilation) operators for electrons on sublattice A, and $b_{j+\ell}^\dagger$ ($b_{j+\ell}$) creation (annihilation) operators for electrons on sublattice B.

Problem 1-2

Start with the Hamiltonian:

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

Considering only the first sum, and substituting

$$a_j^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}_j} a_{\mathbf{k}}^\dagger \tag{2}$$

$$b_{j+\ell} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r}_j+\boldsymbol{\delta}_\ell)} b_{\mathbf{k}} \tag{3}$$

we get

$$\begin{aligned}
\sum_j \sum_{\ell=1}^{3} a_j^\dagger b_{j+\ell} &= \sum_j \sum_{\ell=1}^{3} \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{r}_j} a_{\mathbf{k}}^\dagger \frac{1}{\sqrt{N}} \sum_{\mathbf{k}'} \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot(\mathbf{r}_j+\boldsymbol{\delta}_\ell)} b_{\mathbf{k}'} \\
&= \sum_{\mathbf{k},\mathbf{k}'} \sum_{\ell=1}^{3} \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\boldsymbol{\delta}_\ell} a_{\mathbf{k}}^\dagger b_{\mathbf{k}'} \frac{1}{N} \sum_j \mathrm{e}^{\mathrm{i}(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}_j} \\
&= \sum_{\mathbf{k},\mathbf{k}'} \sum_{\ell=1}^{3} \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\boldsymbol{\delta}_\ell} a_{\mathbf{k}}^\dagger b_{\mathbf{k}'} \delta_{\mathbf{k}'\mathbf{k}} \\
&= \sum_{\mathbf{k}} \sum_{\ell=1}^{3} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\boldsymbol{\delta}_\ell} a_{\mathbf{k}}^\dagger b_{\mathbf{k}}
\end{aligned} \tag{4}$$

The second sum is just the Hermitian conjugate of the first sum, so

$$\sum_j \sum_{\ell=1}^{3} b_{j+\ell}^\dagger a_j = \sum_{\mathbf{k}} \sum_{\ell=1}^{3} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\boldsymbol{\delta}_\ell} b_{\mathbf{k}}^\dagger a_{\mathbf{k}} \tag{5}$$

Defining

$$S(\mathbf{k}) = \sum_{\ell=1}^{3} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\boldsymbol{\delta}_\ell} \tag{6}$$

the Hamiltonian (1) can be written

$$\begin{aligned} H &= \sum_{\mathbf{k}} \left(tS(\mathbf{k}) a_{\mathbf{k}}^\dagger b_{\mathbf{k}} + tS^*(\mathbf{k}) b_{\mathbf{k}}^\dagger a_{\mathbf{k}} \right) \\ &= \sum_{\mathbf{k}} \left(a_{\mathbf{k}}^\dagger, b_{\mathbf{k}}^\dagger \right) \begin{pmatrix} 0 & tS(\mathbf{k}) \\ tS^*(\mathbf{k}) & 0 \end{pmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ b_{\mathbf{k}} \end{pmatrix} \end{aligned} \tag{7}$$

as was to be shown.

Problem 1-3

Substituting

$$S(\mathbf{q}) = \frac{3a}{2}(q_x - \mathrm{i}q_y)$$

in

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

we get

$$h(\mathbf{q}) = \frac{3at}{2} \begin{pmatrix} 0 & q_x - \mathrm{i}q_y \\ q_x + \mathrm{i}q_y & 0 \end{pmatrix}$$

$$= \frac{3at}{2} \left[q_x \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + q_y \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \right] \tag{8}$$

$$= \hbar v_{\mathrm{F}} \left(\sigma_x q_x + \sigma_y q_y \right) \tag{9}$$

where

$$v_{\mathrm{F}} = \frac{3at}{2\hbar}$$

Problem 2-1

Setting the mass equal to zero in the Dirac equation we get

$$i\hbar\gamma^\mu\partial_\mu\Psi = 0$$

which can be written

$$i\hbar\gamma^0\partial_0\Psi = -i\hbar\gamma^k\partial_k\Psi$$

$$i\hbar\gamma^0\partial_t\Psi = c\gamma^k p_k\Psi$$

where $\partial_t = \dfrac{\partial}{\partial t} = \dfrac{1}{c}\partial_0$ and $p_k = -i\hbar\partial_k$. Expressing Ψ in terms of two two-component spinors φ_A and φ_B

$$\Psi = \begin{pmatrix}\varphi_A\\ \varphi_B\end{pmatrix}$$

and using

$$\gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I\end{pmatrix}, \quad \gamma^k = \begin{pmatrix} 0 & \sigma_k \\ -\sigma_k & 0\end{pmatrix}$$

we get

$$\begin{pmatrix} i\hbar\partial_t & 0 \\ 0 & -i\hbar\partial_t\end{pmatrix}\begin{pmatrix}\varphi_A\\ \varphi_B\end{pmatrix} = \begin{pmatrix} 0 & \sigma_k p_k \\ -\sigma_k p_k & 0\end{pmatrix}\begin{pmatrix}\varphi_A\\ \varphi_B\end{pmatrix}$$

which is equivalent to the set of equations:

$$i\hbar\partial_t\varphi_A = \sigma_k p_k\varphi_B \tag{10}$$

$$i\hbar\partial_t\varphi_B = \sigma_k p_k\varphi_A \tag{11}$$

Adding (10) and (11), we get

$$i\hbar\partial_t(\varphi_A + \varphi_B) = \sigma_k p_k(\varphi_A + \varphi_B) \tag{12}$$

Subtracting (11) from (10), we get

$$i\hbar\partial_t(\varphi_A - \varphi_B) = -\sigma_k p_k(\varphi_A - \varphi_B) \tag{13}$$

Introducing $\varphi_\pm = \varphi_A \pm \varphi_B$ and $\boldsymbol{\sigma}\cdot\mathbf{p} = \sigma_k p_k$, Eqs. (12) and (13) can be written

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

which was to be shown.

Problem 2-2

a) Substituting the plane-wave solution $\varphi_+ = Ne^{-\frac{i}{\hbar}(Et-\mathbf{p}\cdot\mathbf{r})}u$, where u is a two-component spinor into the Weyl-equation, we get

$$c(\sigma_x p_x + \sigma_y p_y)u = Eu$$

The eigenvalues can be found from solving the secular equation

$$\begin{vmatrix} -E & c(p_x + \mathrm{i}p_y) \\ c(p_x - \mathrm{i}p_y) & -E \end{vmatrix} = 0$$

That is

$$E^2 - c^2(p_x + \mathrm{i}p_y)(p_x - \mathrm{i}p_y) = 0$$
$$E^2 = c^2(p_x^2 + p_y^2) \tag{14}$$

That is,

$$E_\pm = \pm c|\mathbf{p}|$$

which was to be shown.

b) Close to the K-point of graphene, the electrons behave as effectively massless relativistic particles, with a velocity v_F (which is approximately $1/300c$).

Problem 3-1 The Matsubara Green function for noninteracting electron is

$$\begin{aligned}
\mathcal{G}^{(0)}(\nu,\tau) &= -\langle T_\tau(c_\nu(\tau)c_\nu^\dagger(0))\rangle \\
&= -\theta(\tau)\langle c_\nu(\tau)c_\nu^\dagger(0)\rangle + \theta(-\tau)\langle T_\tau(c_\nu^\dagger(0)c_\nu^\dagger(\tau))\rangle \\
&= -e^{-\xi_\nu\tau}\left[\tau(\theta)\langle c_\nu c_\nu^\dagger\rangle - \theta(-\tau)\langle c_\nu^\dagger c_\nu\rangle\right] \\
&= -e^{-\xi_\nu\tau}\left[\tau(\theta)\langle 1 - c_\nu^\dagger c_\nu\rangle - \theta(-\tau)\langle c_\nu^\dagger c_\nu\rangle\right] \\
&= -e^{-\xi_\nu\tau}\left[\tau(\theta)(1 - n_F(\xi_\nu)) - \theta(-\tau)n_F(\xi_\nu)\right]
\end{aligned} \tag{15}$$

where

$$n_F(\xi_F) = \langle c_\nu^\dagger c_\nu\rangle = \frac{1}{e^{\beta\xi_F} + 1}$$

is the Fermi-Dirac-distribiution. Fourier-transfoming $\mathcal{G}^{(0)}(\nu,\tau)$, we get

$$\mathcal{G}^{(0)}(\nu,\mathrm{i}p_n) = \int_0^\beta \mathrm{d}\tau e^{\mathrm{i}p_n\tau}\mathcal{G}^{(0)}(\nu,\tau)$$

$$= -(1 - n_F(\xi_\nu)) \int_0^\beta \mathrm{d}\tau e^{(\mathrm{i}p_n - \xi_\nu)\tau}$$

$$= -(1 - n_F(\xi_\nu)) \left[\frac{1}{\mathrm{i}p_n - \xi_\nu} e^{(\mathrm{i}p_n - \xi_\nu)\tau} \right]_0^\beta$$

$$= \frac{1}{\mathrm{i}p_n - \xi_\nu} (-1)(1 - n_F(\xi_\nu)) \left[e^{(\mathrm{i}p_n - \xi_\nu)\beta} - 1 \right] \tag{16}$$

Now, using

$$e^{\mathrm{i}p_n\beta} = e^{(2n+1)\pi} = -1$$

and

$$1 - n_F(\xi_\nu) = \frac{e^{\beta\xi_\nu}}{e^{\beta\xi_\nu + 1}}$$

we get

$$\mathcal{G}^{(0)}(\nu, \mathrm{i}p_n) = \frac{1}{\mathrm{i}p_n - \xi_\nu} \frac{e^{\beta\xi_\nu}}{e^{\beta\xi_\nu + 1}} \left[e^{-\beta\xi_\nu} + 1 \right]$$

$$= \frac{1}{\mathrm{i}p_n - \xi_\nu} \tag{17}$$

Finally, we get the retarded Green function for noninteracting electrons by substituting $\mathrm{i}p_n \to \omega + \mathrm{i}\eta$ in the Matsubara Green function:

$$G_0^R(\nu, \omega) = \frac{1}{\omega - \xi_\nu + \mathrm{i}\eta}$$

Problem 3-2

After averaging the position of the impurities, the electrons will 'see' the same environment everywhere in the system, thus the system is made translationally invariant, and the Green functions will be diagonal in $\mathbf{k}$.

Problem 3-3

a) A reducible diagram is a diagram which may be divided into two parts by cutting an internal line. Following this definition, diagram (A) is reducible, and (B) is irreducible.

b) Mathematical expression:

$$\sum_{\mathbf{k}_1} \mathcal{G}^{(0)}(\mathbf{k}) N U(\mathbf{k} - \mathbf{k_1}) \mathcal{G}^{(0)}(\mathbf{k}_1) U(\mathbf{k}_1 - \mathbf{k}) \mathcal{G}^{(0)}(\mathbf{k}) N U(0) \mathcal{G}^{(0)}(\mathbf{k})$$

Problem 3-4

a) The spectral function of the retarded Green function is

$$\begin{aligned}\overline{A}(\mathbf{k},\omega) &= -\frac{1}{\pi}\mathrm{Im}\overline{G}^{R}(\mathbf{k},\omega)\\ &= -\frac{1}{\pi}\mathrm{Im}\int_{-\infty}^{\infty}\mathrm{d}te^{\mathrm{i}\omega t}\overline{G^{R}}(\mathbf{k},t)\\ &= \frac{1}{\pi}\mathrm{Im}\int_{0}^{\infty}\mathrm{d}t\mathrm{i}e^{-(\frac{1}{2\tau}-\mathrm{i}(\omega-(\xi_{\mathbf{k}}+n_{\mathrm{imp}}u))t}\\ &= \frac{1}{\pi}\mathrm{Im}\left[\frac{\mathrm{i}e^{-(\frac{1}{2\tau}-\mathrm{i}(\omega-(\xi_{\mathbf{k}}+n_{\mathrm{imp}}u))t}}{-1/(2\tau)+\mathrm{i}(\omega-(\xi_{\mathbf{k}}+n_{\mathrm{imp}}u))}\right]_{0}^{\infty}\\ &= \frac{1}{\pi}\mathrm{Im}\frac{\mathrm{i}}{1/(2\tau)-\mathrm{i}(\omega-(\xi_{\mathbf{k}}+n_{\mathrm{imp}}u))}\\ &= \frac{1}{\pi}\mathrm{Im}\frac{\mathrm{i}/(2\tau)-(\omega-(\xi_{\mathbf{k}}+n_{\mathrm{imp}}u))}{(\omega-(\xi_{\mathbf{k}}+n_{\mathrm{imp}}u))^{2}+(1/2\tau)^{2}}\\ &= \frac{1}{\pi}\frac{1/(2\tau)}{(\omega-(\xi_{\mathbf{k}}+n_{\mathrm{imp}}u))^{2}+(1/2\tau)^{2}} \qquad (18)\end{aligned}$$

which was to be shown.

b) We shall show that the spectral function satisfy the sum rule

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

$$\begin{aligned}\int_{-\infty}^{\infty}\mathrm{d}\omega\overline{A}(\mathbf{k},\omega) &= \frac{1}{2\pi\tau}\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{1}{(\omega-(\xi_{\mathbf{k}}+n_{\mathrm{imp}}u))^{2}+(1/2\tau)^{2}}\\ &= \frac{2\tau}{\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{1}{(2\tau(\omega-(\xi_{\mathbf{k}}+n_{\mathrm{imp}}u))^{2}+1)} \qquad (19)\end{aligned}$$

Now, changing variable

$$x=2\tau(\omega-(\xi_{\mathbf{k}}+n_{\mathrm{imp}}u)),\quad \mathrm{d}x=2\tau\mathrm{d}\omega$$

we get

$$\int_{-\infty}^{\infty}\mathrm{d}\omega\overline{A}(\mathbf{k},\omega)=\frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{d}x\frac{1}{x^{2}+1}$$

$$
\begin{aligned}
&= \frac{1}{\pi} \left[\arctan x\right]_{-\infty}^{\infty} \\
&= \frac{1}{\pi}\pi \\
&= 1 \quad \square
\end{aligned}
\tag{20}
$$