

Final Exam (Fall 2016)

PHYS 530B: Quantum Mechanics II

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1. The number density of electrons in a thin film of thickness d ,

$$n_f = \frac{n_{\text{tot}}}{L_x L_y d}, \quad (1)$$

as a function of the Fermi energy E_F is conveniently expressed in terms of the parameter

$$N = \sqrt{\frac{2m^* E_F d^2}{\hbar^2 \pi^2}} = \frac{k_F d}{\pi} = \frac{2d}{\lambda_F}, \quad (2)$$

where k_F is the Fermi wave-vector and λ_F is the Fermi wavelength, by the expression

$$n_f(N) = n_f(\infty) \nu(x), \quad (3)$$

where

$$n_f(\infty) = \frac{\pi}{2d^3} \frac{2}{3} N^3 = \frac{k_F^3}{3\pi^2} \quad (4)$$

and

$$\nu(x) = \frac{3}{2} \left(x - \frac{1}{3} x^3 \right) + \frac{3}{2N} \left(1 - \frac{1}{2} x^2 \right) - \frac{1}{4N^2} x, \quad x = \frac{[N]}{N}. \quad (5)$$

Here $[N]$ is the integer part of N .

- (a) Plot $x = [N]/N$ as a function of N , for $0 < N < 10$. In particular, consider regions $0 \leq x < 1.2$.
- (b) Plot $\nu(x)$ as a function of N , for $0 < N < 10$. In particular, consider regions $0.8 \leq \nu(x) < 2.0$.
- (c) Plot $\nu(x)$ as a function of $1/N$, for $0 < 1/N < 0.5$. In particular, consider regions $0.9 \leq \nu(x) < 1.5$.
2. The electronic structure of an isolated carbon atom is $1s^2 2s^2 2p^2$. In graphene the carbon atoms arrange themselves in a single two-dimensional hexagonal pattern. The carbon atoms are 0.142 nm apart. Each carbon atom in graphene shares three electrons with three closest neighbours in sp^2 hybrid orbitals. The excitations of the remaining electron, corresponding to the remaining p-orbital oriented out of the plane (π -bond), is described by the Hamiltonian

$$H = v_F \boldsymbol{\alpha} \cdot \mathbf{p}, \quad (6)$$

where \mathbf{p} represents the momentum in two dimensions ($p_z = 0$) and $v_F/c \sim 300$. In terms of the rescaled momentum

$$\tilde{p}^\mu = \left(\frac{H}{c}, \frac{v_F}{c} \mathbf{p} \right), \quad \mu = 0, 1, 2, \quad (7)$$

and Dirac's Gamma matrices $\gamma^\mu = (\beta, \beta\alpha)$, for $\mu = 0, 1, 2$, we have the (massless) Dirac equation

$$\gamma^\mu \tilde{p}_\mu = 0. \quad (8)$$

The dielectric permittivity in this (quantum field theoretical) model is given in terms of vacuum polarization effects using the relation

$$\Pi^{ij}(0, \omega) = \delta^{ij} \omega^2 (\varepsilon - 1), \quad (9)$$

where the vacuum polarization tensor is given by

$$i\Pi^{\mu\nu}(\tilde{\mathbf{k}}, \omega) = -4\pi\alpha \operatorname{tr} \int \frac{d^3\tilde{p}}{(2\pi)^3} \gamma^\mu \frac{1}{\gamma \cdot \tilde{p}} \gamma^\nu \frac{1}{\gamma \cdot (\tilde{p} - \tilde{k})}, \quad (10)$$

$\alpha = e^2/4\pi\hbar c$ is the fine structure constant.

(a) Using the idea of rationalizing denominators show that

$$\frac{1}{\gamma \cdot \tilde{p}} = -\frac{\gamma \cdot \tilde{p}}{\tilde{p}^2}. \quad (11)$$

(b) Use Eq. (11) to move all the Gamma matrices to the numerator in the expression for vacuum polarization tensor in Eq. (10). Evaluate the trace

$$\operatorname{tr}(\gamma^\mu \gamma^\alpha \gamma^\nu \gamma^\beta) = 4(g^{\mu\alpha} g^{\nu\beta} - g^{\mu\nu} g^{\alpha\beta} + g^{\mu\beta} g^{\nu\alpha}) \quad (12)$$

and then show that

$$i\Pi^{\mu\nu}(\tilde{\mathbf{k}}, \omega) = -16\pi\alpha \int \frac{d^3\tilde{p}}{(2\pi)^3} \frac{[\tilde{p}^\mu(\tilde{p} - \tilde{k})^\nu + \tilde{p}^\nu(\tilde{p} - \tilde{k})^\mu - g^{\mu\nu} \tilde{p} \cdot (\tilde{p} - \tilde{k})]}{\tilde{p}^2(\tilde{p} - \tilde{k})^2}, \quad (13)$$

(c) Show that the inverse of an operator has the integral representation

$$\frac{1}{M} = \lim_{\delta \rightarrow 0} \frac{1}{M - i\delta} = \lim_{\delta \rightarrow 0} i \int_0^\infty ds e^{-is(M - i\delta)}, \quad (14)$$

where the parameter δ is a positive real number. Thus, show that

$$\frac{1}{\tilde{p}^2(\tilde{p} - \tilde{k})^2} = \lim_{\delta \rightarrow 0} \int_0^\infty ds_1 e^{-is_1(\tilde{p}^2 - i\delta)} \int_0^\infty ds_2 e^{-is_2[(\tilde{p} - \tilde{k})^2 - i\delta]}. \quad (15)$$

Using substitutions

$$s_1 = s(1 - u), \quad (16a)$$

$$s_2 = su, \quad (16b)$$

deduce $ds_1 ds_2 = s ds du$, where $0 \leq s < \infty$, $0 \leq u \leq 1$, and show that

$$\frac{1}{\tilde{p}^2(\tilde{p} - \tilde{k})^2} = \lim_{\delta \rightarrow 0} \int_0^\infty s ds e^{-s\delta} \int_0^1 du e^{-is(1-u)\tilde{p}^2} e^{-isu(\tilde{p}-\tilde{k})^2} \quad (17a)$$

$$= \lim_{\delta \rightarrow 0} \int_0^\infty s ds e^{-s\delta} \int_0^1 du e^{-isu(1-u)\tilde{k}^2} e^{-is(\tilde{p}-u\tilde{k})^2}. \quad (17b)$$

Thus, show that

$$\begin{aligned} i\Pi^{\mu\nu}(\tilde{\mathbf{k}}, \omega) &= \frac{2\alpha}{\pi^2} \lim_{\delta \rightarrow 0} \int_0^\infty s ds e^{-s\delta} \int_0^1 du e^{-isu(1-u)\tilde{k}^2} \\ &\times \int d^3\tilde{p} [\tilde{p}^\mu(\tilde{p} - \tilde{k})^\nu + \tilde{p}^\nu(\tilde{p} - \tilde{k})^\mu - g^{\mu\nu}\tilde{p} \cdot (\tilde{p} - \tilde{k})] e^{-is(\tilde{p}-u\tilde{k})^2}. \end{aligned} \quad (18)$$

(d) Show that, replacing $\tilde{p} - u\tilde{k} \rightarrow \tilde{p}$ leads to the integral

$$\int d^3\tilde{p} [(\tilde{p}+u\tilde{k})^\mu(\tilde{p}-(1-u)\tilde{k})^\nu + (\tilde{p}+u\tilde{k})^\nu(\tilde{p}-(1-u)\tilde{k})^\mu - g^{\mu\nu}(\tilde{p}+u\tilde{k}) \cdot (\tilde{p}-(1-u)\tilde{k})] e^{-is\tilde{p}^2}. \quad (19)$$

Evaluate this integral by computing the following integrals, (in terms of the Gaussian integral,)

$$\int d^3\tilde{p} e^{-is\tilde{p}^2} = \frac{1}{i} \left(\frac{\pi}{is} \right)^{\frac{3}{2}}, \quad (20a)$$

$$\int d^3\tilde{p} [\tilde{p}^\mu \tilde{k}^\nu] e^{-is\tilde{p}^2} = 0, \quad (20b)$$

$$\int d^3\tilde{p} [\tilde{p}^\mu \tilde{p}^\nu] e^{-is\tilde{p}^2} = -g^{\mu\nu} \frac{1}{2s} \left(\frac{\pi}{is} \right)^{\frac{3}{2}}, \quad (20c)$$

$$\int d^3\tilde{p} [\tilde{p}^2] e^{-is\tilde{p}^2} = -\frac{3}{2s} \left(\frac{\pi}{is} \right)^{\frac{3}{2}}. \quad (20d)$$

Thus, show that

$$\begin{aligned} i\Pi^{\mu\nu}(\tilde{\mathbf{k}}, \omega) &= (2\tilde{k}^\mu \tilde{k}^\nu - g^{\mu\nu} \tilde{k}^2) \frac{2\alpha}{\sqrt{i\pi}} \lim_{\delta \rightarrow 0} \int_0^1 du u(1-u) \int_0^\infty \frac{ds}{s} \sqrt{s} e^{-s[\delta+iu(1-u)\tilde{k}^2]} \\ &+ g^{\mu\nu} \frac{\alpha}{i\sqrt{i\pi}} \lim_{\delta \rightarrow 0} \int_0^1 du \int_0^\infty \frac{ds}{s} \frac{1}{\sqrt{s}} e^{-s[\delta+iu(1-u)\tilde{k}^2]} \end{aligned} \quad (21)$$

(e) Evaluate the s -integrals using the integral representation for the gamma function

$$\Gamma(z) = \int_0^\infty ds s^{z-1} e^{-s}, \quad (22)$$

and evaluate the following u -integrals using the integral representation for the beta function

$$B(x, y) = \int_0^1 du u^{x-1} (1-u)^{y-1}. \quad (23)$$

In particular, $-\frac{1}{2}\Gamma(-\frac{1}{2}) = \Gamma(\frac{1}{2}) = \sqrt{\pi}$ and $B(\frac{3}{2}, \frac{3}{2}) = \pi/8$. Thus, evaluate the vacuum polarization tensor

$$\Pi^{\mu\nu}(\tilde{\mathbf{k}}, \omega) = -\frac{\pi\alpha}{2\tilde{k}}(\tilde{k}^\mu \tilde{k}^\nu - g^{\mu\nu} \tilde{k}^2). \quad (24)$$

(f) Show that, using $\tilde{k}^2 = v_F^2 \mathbf{k} \cdot \mathbf{k} - \omega^2$,

$$\Pi^{00}(0, \omega) = 0, \quad (25a)$$

$$\Pi^{ij}(0, \omega) = -\frac{\pi\alpha}{2i\omega} \delta^{ij} \omega^2. \quad (25b)$$

Read out the dielectric permittivity of graphene, using Eq. (9), as

$$\varepsilon - 1 = -2 \times \frac{\pi\alpha}{2i\omega} = -\frac{\pi\alpha}{i\omega}, \quad (26)$$

where we multiplied by a factor of 2 for the two independent excitations (representing the Dirac points K and K').