NATURAL SCIENCES TRIPOS Part II

Friday 2 June 2017   1.30 pm to 3.30 pm

PHYSICS (7)
PHYSICAL SCIENCES: HALF SUBJECT PHYSICS (7)

QUANTUM CONDENSED MATTER PHYSICS

Candidates offering this paper should attempt a total of **three** *questions. The questions to be attempted are* **1**, **2** *and* **one** *other question.*

The approximate number of marks allocated to each question or part of a question is indicated in the right margin. This paper contains **six** *sides, including this coversheet, and is accompanied by a handbook giving values of constants and containing mathematical formulae which you may quote without proof.*

STATIONERY REQUIREMENTS
2 × 20 Page Answer Book
Rough workpad
Yellow master coversheet

SPECIAL REQUIREMENTS
Mathematical Formulae handbook
Approved calculator allowed

You may not start to read the questions printed on the subsequent pages of this question paper until instructed that you may do so by the Invigilator.

QUANTUM CONDENSED MATTER PHYSICS

1   *Attempt **all** parts of this question. Answers should be concise and relevant formulae may be assumed without proof.*

(a) In the Lorentz oscillator model, the electron cloud is described as a damped harmonic oscillator,

$$m\ddot{u} + m\gamma\dot{u} + m\omega_T^2 u = qE \, ,$$

where u is the displacement of the cloud, q is the electron charge, ω_T is the natural frequency and γ is the damping rate. Derive the resulting polarisability χ_ω and sketch the qualitative behaviour of the real and imaginary parts of the relative permittivity $\epsilon = \chi_\omega + 1$ as a function of ω.   [3]

(b) Describe single photon sources based on self-assembled InAs quantum dots, indicating the characteristic dimensions (dot diameter, height, density). Explain briefly the mechanism by which photons are emitted.

The figure below shows emission intensity as a function of current and energy. Explain the origin of the two main features labelled X and X_2.
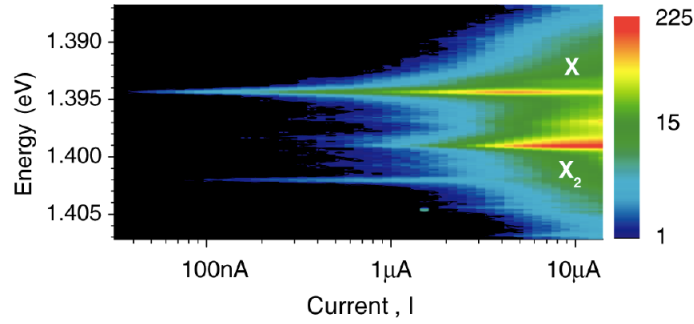
[credit: Z. Yuan et al., Science **295**, 102 (2002)]

Assuming that the emitted photon carries the full energy of an exciton (taken to be in its lowest energy state), that the energy required to create an electron-hole pair in an InAs dot is $E_g = 1.415$ eV and that the dielectric constant is $\varepsilon_r = 15$, compute the reduced effective mass of the exciton.   [5]

(c) In the Stoner-Hubbard model, at mean-field level, the energies of the two spin bands are shifted by an applied magnetic field H according to the following equations:

$$\begin{aligned}
\varepsilon_{k,\uparrow} &= \varepsilon_k + U\,\bar{n}_\downarrow - \mu_0\mu_B H \, , \\
\varepsilon_{k,\downarrow} &= \varepsilon_k + U\,\bar{n}_\uparrow + \mu_0\mu_B H \, ,
\end{aligned}$$

where U is the energy penalty of a doubly occupied site, $\bar{n}_\uparrow$ and $\bar{n}_\downarrow$ are the mean-field densities of carriers in the two spin bands, μ_B is the Bohr magneton, and all other constants have the usual meaning. Obtain the static magnetic susceptibility as a function of the density of states per atom, which may be

assumed constant at its value at the Fermi energy, $g(E_F)$. Describe briefly the Stoner criterion for ferromagnetism. [4]
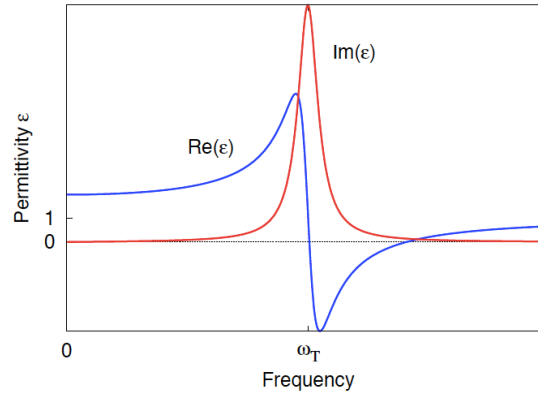

(a) In frequency space $u = u_\omega e^{-i\omega t}$, the equation of motion becomes [1]

$$-\omega^2 u_\omega - i\omega\gamma u_\omega + \omega_T^2 u_\omega = qE_\omega/m.$$

The polarisability relates the polarisation to the applied electric field $E = E_\omega e^{-i\omega t}$ via the relation $P_\omega = \epsilon_0 \chi_\omega E_\omega$, where $P_\omega = (N/V)qu_\omega$. Therefore [1]

$$\chi_\omega = \frac{N}{V}\frac{q^2}{m\epsilon_0\left(\omega_T^2 - \omega^2 - i\gamma\omega\right)}.$$

From the lecture notes: [1]

(b) InAs has lattice constant 7% greater than GaAs, and can be readily grown on a flat surface of the latter to form 3D islands. The islands are typically buried in GaAs. The characteristic dimensions are: dot diameter $10 - 15$ nm, height $4 - 8$ nm, and density $10^9 - 10^{11}$ cm^{-2}. [1]

The dots have good photoluminescence and electrical properties, and they tend to collect electrons and holes due to the narrower InAs band gap (with respect to GaAs). Photons with well defined energy are emitted upon ricombination of electrons and holes. [1]

Emission can occur from both 'excitons' (recombinations of one electron and one hole) and 'bi-excitons' (recombinations of two electrons and two holes), which correspond to the two energy peaks shown in the figure, X and X_2 respectively. [1]

The energy of an exciton is given by

$$\epsilon_n = E_g + \frac{\mu^* 13.6\text{ eV}}{m_e \varepsilon_r^2 n^2},$$

where we are told that $E_g = 1.415$ eV, $\varepsilon_r = 15$, and $n = 1$. If the emitted photon carries the full energy of an exciton, then we can read from the figure that $\epsilon_n = 1.395$ eV. Inverting the formula we obtain:

$$\mu^* = \frac{\epsilon_n - E_g}{13.6\text{ eV}} m_e \varepsilon_r^2 n^2 = 0.0221\ m_\text{e}.$$

(TURN OVER

(If $\epsilon_n = 1.39$ eV or $\epsilon_n = 1.40$ eV is chosen, somewhat erroneously, then $\mu^* = 0.0276$ m_e or $\mu^* = 0.0165$ m_e respectively.) [2]

(c) The average spin density can be obtained self-consistently [1]

$$\frac{N}{V}\left(\overline{n}_\uparrow - \overline{n}_\downarrow\right) = \left[U\left(\overline{n}_\uparrow - \overline{n}_\downarrow\right) + 2\mu_0\mu_B H\right]\frac{1}{2}\frac{N}{V}g(E_F).$$

From the magnetisation $M = \mu_B(\overline{n}_\uparrow - \overline{n}_\downarrow)$ one can then obtain the static susceptibility [2]

$$\chi = \frac{M}{H} = \mu_0 \frac{\mu_B^2 g(E_F)}{1 - \frac{Ug(E_F)}{2}}.$$

Contrary to the non-interacting case, the magnetic susceptibility can diverge, leading to the onset of ferromagnetism. This happens for $Ug(E_F) > 2$, which is known as the Stoner criterion. [1]

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2   *Attempt this question. Credit will be given for well-structured and clear explanations, including appropriate diagrams and formulae. Detailed mathematical derivations are not required.*

Write brief notes on **two** of the following: [13]

(a) screening and Thomas–Fermi theory;

(b) optical phonons in atomic chains;

(c) Fermi liquids.

(a) Inserting a test charge in a metal produces a re-distribution of carriers that will attempt to compensate the change and set the local electric field to zero. This phenomenon is knwn as screening. [1]

Screening is never perfect but occurs over a short but finite distance from the test charge. This is due for instance to the quantum nature of the electrons and the resulting competition between kinetic energy (electrons need to be localised to perfectly screen a point charge) and electrostatic potential. [2]

Thomas-Fermi theory relates to the calculation of the response of the metal to the insertion of the test charge (or more generally to an external potential). [1]

The key approximation in the theory, valid for long-wavelength perturbations, is to assume that the leading effect is a shift of the free electron energy levels (equivalently: a spatially varying Fermi energy), and momentum remains a valid quantum number. In the calculation of the response of the system, one typically assumes that the perturbing potential is small and the equations are correspondingly expanded to linear order. [2.5]

(b) Optical phonons appear in atomic chains where, for instance, the interactions between atoms alternate in strength, or the unit cell comprises two atoms with different masses. [1]

They are called 'optical' because at long wavelengths these phonons can interact (either by absorption, or scattering) with light. [1]

Bonus mark: optical phonons are prominent features in the absorption and Raman spectra of solids in the infrared spectrum.

The qualitative pattern of atomic displacements and the phonon dispersion are: [2]
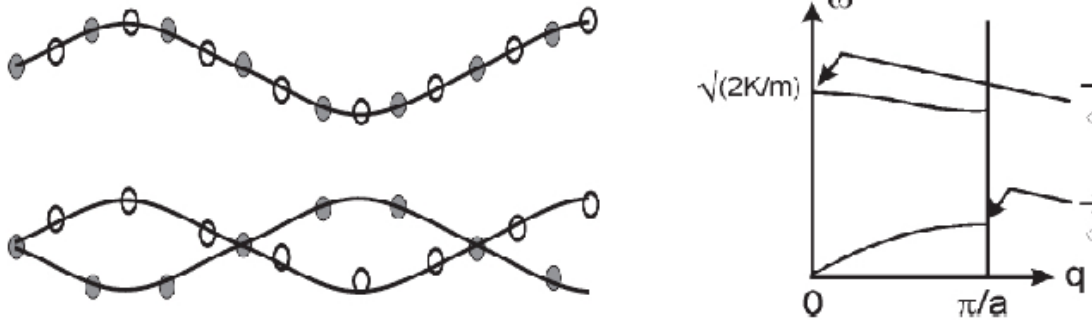
The value of $\omega(q \to 0)$ for the optical branch is given by $\sqrt{2K/m}$ for the case of alternating elastic constants $K \gg K'$, and by $\sqrt{2K(1/m_A + 1/m_B)}$ for the case of alternating masses m_A and m_B. [2.5]

Bonus mark: Given that $K \gg K'$, to a first approximation the pairs of atoms linked by K can be treated as independent molecules, each with a vibrational mode where the two atoms oscillate out of phase with frequency $\sqrt{2K/m}$.

Bonus mark: a wavelike solution with the correct phase relationship between pairs of atoms (perturbatively in K') will hardly change the restoring force and therefore the frequency of optical phonons is nearly independent of q.

(c) Remarkably, a Fermi gas of non-interacting particles survives the inclusion of (Coulomb) interactions, but with renormalised parameters (e.g., an effective mass near the Fermi surface). [2]

The electrons are replaced in the non-interacting theory by quasi-particles with the same quantum numbers, which are however collective excitations with a finite life time. Near the Fermi surface the quasi-particle lifetime is long enough to be approximated as infinite, say, for experimentally relevant purposes. [2.5]

Credit for examples: He^3, heavy-fermion metals (Bonus mark: $m_{\text{eff}} \sim 10 - 100 m_e$). [2]

3   *Attempt* **either** *this question* **or** *question 4.*

Explain the difference between direct and indirect band gap semiconductors. Sketch the dispersion near the Γ point. What is meant by 'heavy hole band', 'light hole band' and 'split-off hole band'? Why are the split-off hole bands not important in intrinsic semiconductors?   [6]

Direct band gap semiconductors refer to systems where the global minimum of the conduction band is at the Γ point, whereas in indirect band gap semiconductors the global minimum is finitely away in the Brillouin zone (and the Γ point can be a local minimum).   [2]

In complex semiconductors there can be more than one valence band that are degenerate at the Γ point. However, they can have different curvature resulting in different effective hole masses – hence labelled light hole and heavy hole bands. Moreover, spin-orbit interactions can cause a valence band to spit off and fall lower in the energy spectrum.   [3]
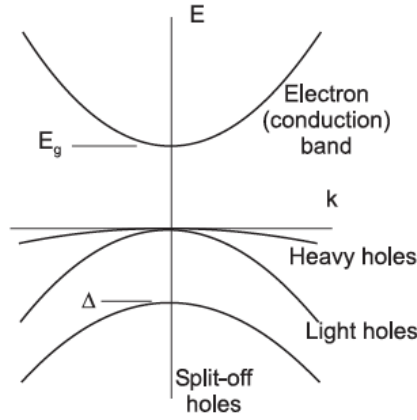
In intrinsic semiconductors, the gap is sufficiently small with respect to temperature to result in a non-negligible thermal population of the conduction band (and corresponding depletion of the valence bands). Split-off hole bands are further separated from the conduction band and their thermal depletion is exponentially suppressed with respect to the other valence bands, and can usually be neglected.   [1]

Given the densities of states for the conduction (e) and valence (h) band

$$g_e(E) = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}\sqrt{E - E_c}\,, \qquad g_h(E) = \frac{1}{2\pi^2}\left(\frac{2m_h^*}{\hbar^2}\right)^{3/2}\sqrt{E_v - E}\,,$$

derive the intrinsic carrier concentrations of electrons and holes, and from them illustrate the law of mass action. Here m_e^* and m_h^* are the effective electron and hole masses, and E_c and E_v are the energies of the conduction and valence bands at the Γ point. In your calculations, you should consider the case $|E - \mu| \gg k_B T$, where μ is the chemical potential and T is the temperature of the semiconductor.   [8]

You may find the following integral helpful in your calculations:

$$\int_0^\infty dx \ \sqrt{x} \, e^{-(x+\alpha)/\beta} = \frac{\sqrt{\pi}}{2}\beta^{3/2}e^{-\alpha/\beta} \qquad \text{for } \alpha \in \mathbb{R}, \ \beta > 0 \,.$$

The carrier density is given by

$$n = \int_{E_c}^\infty dE \ g_e(E) f(E) \qquad p = \int_{-\infty}^{E_v} dE \ g_h(E) \left[1 - f(E)\right]$$

where $f(E)$ is the Fermi function

$$f(E) = \frac{1}{1 + e^{(E-\mu)/k_B T}} \simeq \begin{cases} e^{-(E-\mu)/k_B T} & E - \mu \gg k_B T \\ 1 - e^{-(\mu-E)/k_B T} & \mu - E \gg k_B T \end{cases}$$

(non-degenerate Fermi gas). [3]

Carrying out the integral in the appropriate limit gives [3]

$$n \simeq 2\left(\frac{m_e^* k_B T}{2\pi\hbar^2}\right)^{3/2} e^{-(E_c-\mu)/k_B T} \,, \qquad p \simeq 2\left(\frac{m_h^* k_B T}{2\pi\hbar^2}\right)^{3/2} e^{-(\mu-E_v)/k_B T} \,.$$

Notice that the product

$$np = 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 \left(m_e^* m_h^*\right)^{3/2} e^{-E_g/k_B T} \,,$$

where $E_g = E_c - E_v$ is the size of the energy gap, is independend of the chemical potential. This result is called the law of mass action. [2]

Use the result to obtain an expression for the chemical potential of an intrinsic semiconductor as a function of the gap energy $E_\text{g} = E_\text{c} - E_\text{v}$, temperature and the effective electron and hole masses. [3]

For an intrinsic semiconductor, the electron and hole densities are equal. Therefore, from the law of mass action obtained above we find [1]

$$n = p = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2} \left(m_e^* m_h^*\right)^{3/4} e^{-E_g/2k_B T} \,.$$

Substituting back into, say, the expression for n derived earlier, we can work out the value of the chemical potential: [2]
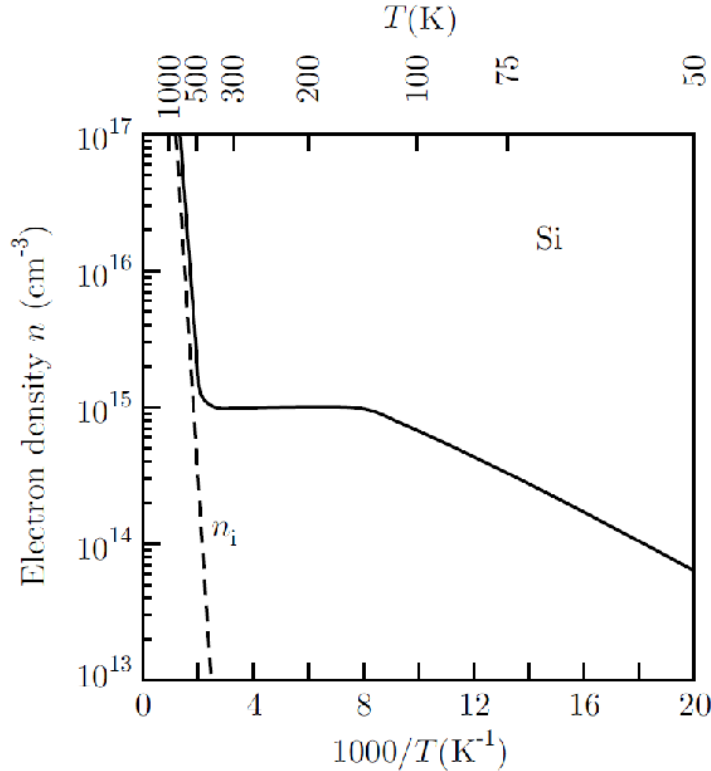
$$2\left(\frac{m_e^* k_B T}{2\pi\hbar^2}\right)^{3/2} e^{-(E_c-\mu)/k_B T} = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2} \left(m_e^* m_h^*\right)^{3/4} e^{-E_g/2k_B T}$$

$$e^{-(E_c-\mu-E_g/2)/k_B T} = \left(\frac{m_h^*}{m_e^*}\right)^{3/4} \,,$$

and

$$\mu = \frac{E_c + E_v}{2} + \frac{3k_B T}{4} \ln\left(\frac{m_h^*}{m_e^*}\right).$$

When a semiconductor is doped, the temperature dependence of its electron density changes to the typical behaviour illustrated in the figure.

Identify the three different temperature regimes and describe briefly what is happening in each regime. [3]

For $T < 100$ K, the extrinsic electrons *freeze out* onto the donors. Bonus mark: the gradient depends on the donor ionisation energy. [1]

For 150 K$< T < 300$ K, all the donors are ionised. This is called the *saturation range* and n is approximately constant. [1]

For $T > 500$ K, the intrinsic contribution to n becomes larger than the extrinsic contribution. [1]

The figure above refers to Si with a net donor density $N_D - N_A = 10^{15}$ cm^{-3}, $m_e^* = 0.98\, m_e$, and $m_h^* = 0.49\, m_e$. Explain how you can determine the gap energy E_g from the figure and estimate its value. Using these parameters or otherwise, estimate the electron and hole densities at room temperature. [5]

As long as the number of donors and acceptors is low enough so that the chemical potential lies in the bandgap, the law of mass action holds. [1]

You can obtain the gap at room temperature ($E_g = 1.11$ eV) from the figure by

extrapolating n_i to room temperature and using the earlier formula for the intrinsic density,

$$n = p = 2\left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2} \left(m_e^* m_h^*\right)^{3/4} e^{-E_g/2k_B T} .$$

A rough extrapolation gives $n_i = 2\,10^8$ cm^{-3}, from which one obtains indeed
$E_g = 1.11 - 1.12$ eV. [1]

Then we have that

$$n - p = N_D - N_A = 10^{15} \text{ cm}^{-3} \qquad np = 4\left(\frac{k_B T}{2\pi\hbar^2}\right)^3 \left(m_e^* m_h^*\right)^{3/2} e^{-E_g/k_B T} = 5.1\,10^{16} \text{ cm}^{-6} .$$

If we call the first quantity A and the second B, a few lines of algebra give $p = A/n$ and
$n^2 + Bn - A = 0$. The latter can be solved to obtain

$$n = \frac{A \pm \sqrt{A^2 + 4B}}{2} .$$

Only the positive sign is an acceptable solution for a physical $n \geq 0$. Therefore,
$n = 2.0\,10^{15}$ cm^{-3} and $p = 51.0$ cm^{-3}. [3]

Note the spectacular suppression of the density of holes due to extrinsic electron doping.

4   *Attempt* **either** *this question* **or** *question 3.*

Consider a non-interacting electron with momentum $\boldsymbol{k}$ and energy ε_k. By taking the Fourier transform of its time dependent wave function $\psi_k(t)$, derive the electron spectral function.   [3]

The time dependent wave function can be written as $\psi_k(t) = \psi_k \exp(-i\varepsilon_k t/\hbar)$. In Fourier space,   [1]

$$\psi_k(\omega) = \int_{-\infty}^{\infty} dt\, \psi_k \exp\left(-i\frac{\varepsilon_k t}{\hbar} + i\omega t\right) = 2\pi\psi_k \delta\left(\omega - \frac{\varepsilon_k}{\hbar}\right).$$

The probability amplitude of finding an electronic state with energy $\hbar\omega$ and momentum $\boldsymbol{k}$ is therefore proportional to

$$A(\boldsymbol{k}, \omega) = \delta\left(\omega - \frac{\varepsilon_k}{\hbar}\right),$$

which is usually called the electron spectral function.   [2]

Discuss how the electron spectral function is modified by interactions, commenting in particular on the dispersion relation ε_k and the (quasi)particle lifetime. Derive the corresponding quasiparticle spectral function and show that it can be written as

$$A(\boldsymbol{k}, \omega) = -\frac{1}{\pi}\Im\left[\frac{1}{\omega - \frac{\varepsilon_k}{\hbar} + i\Gamma_k}\right],$$

where $\Im$ indicates the imaginary part and Γ_k is the quasiparticle scattering rate.   [5]

In Fourier space,

$$\psi_k(\omega) = \int_{-\infty}^{\infty} dt\, \psi_k \exp\left(-i\frac{\varepsilon_k t}{\hbar} - \Gamma_k|t| + i\omega t\right) = 2\psi_k \Re\left[\frac{1}{\Gamma_k - i\left(\omega - \frac{\varepsilon_k}{\hbar}\right)}\right]$$

(either by quoting a known integral or using Cauchy integragion).   [4]

Comparing this result with the definition of the spectral function introduced earlier, we arrive at the result

$$A(\boldsymbol{k}, \omega) = -\frac{1}{\pi}\Im\left[\frac{1}{\omega - \frac{\varepsilon_k}{\hbar} + i\Gamma_k}\right],$$

which is customarily expressed in terms of the imaginary rather than real part.   [1]

Assuming that the renormalised dispersion takes the form $\varepsilon_k = \hbar^2 k^2/2m^*$ and that the quasiparticle scattering rate is real, $\Gamma_k = \gamma(\boldsymbol{k}) > 0$, show that the spectral function $A(\boldsymbol{k}, \omega)$ has a single maximum as a function of ω, and find its position and the Half Width at Half Maximum.   [5]

For the given choices of $\varepsilon_k = \hbar^2 k^2 / 2m^*$ and $\Gamma_k = \gamma(k)$ we have

$$A(k, \omega) = -\frac{1}{\pi} \Im \left[\frac{1}{\omega - \frac{\hbar k^2}{2m^*} + i\gamma(k)} \right] = \frac{\gamma(k)/\pi}{\left[\omega - \frac{\hbar k^2}{2m^*} \right]^2 + [\gamma(k)]^2} .$$

By inspection or taking derivatives with respect to ω, one can show that $A(k, \omega)$ has a maximum at $\omega = \hbar k^2 / 2m^*$, where it takes the value $A_{\max} = [\pi \gamma(k)]^{-1}$. [2]

In order to find the HWHM, we need to find the value(s) of ω where $A(k, \omega)$ drops to $1/2$ of its maximum value:

$$\frac{\gamma(k)/\pi}{\left[\omega - \frac{\hbar k^2}{2m^*} \right]^2 + [\gamma(k)]^2} = \frac{1}{2\pi\gamma(k)} ,$$

which leads to the equation $\omega^2 - (\hbar k^2 / m^*)\omega + (\hbar k^2 / 2m^*)^2 - [\gamma(k)]^2 = 0$. This admits two solutions $\omega_{\pm} = \hbar k^2 / 2m^* \pm \gamma(k)$, and the HWHM is therefore given by $\gamma(k)$. [2]

Sketch the behaviour of the electron spectral function for a Fermi gas and for a Fermi liquid. [2]

(a) (b)
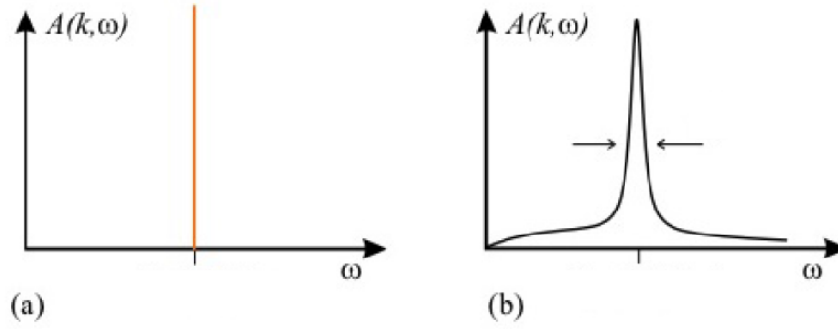
[3]

Discuss how photoemission can be used to measure directly the electron spectral function. You should include equations for the relevant conservation laws and you may use sketches to help illustrate the technique. [6]


In photoemission experiments, photons incident (nearly perpendicularly) to the surface of a solid induce a transition from occupied states to plane-wave states well above the vacuum energy. The excited electron is then collected in a detector. [1]

The photon carries little momentum and therefore the component of the momentum of the electron parallel to the surface is nearly conserved, and therefore $k_i^{\parallel} = k_f^{\parallel} = k_f \sin\theta$ where θ is the detector angle. The perpendicular component is not conserved. Energy is also conserved in the process, if we account for the work function ϕ required to extract the electron from the solid:

$$E_f = \frac{\hbar^2 k_f^2}{2m} = E_i + \hbar\omega - \phi .$$

Here f and i refer to the initial (occupied) and final (plane-wave) state of the electron. [3]

Either by verbal discussion or by drawing, the answer should include the concepts illustrated by these two figures from the lecture notes:
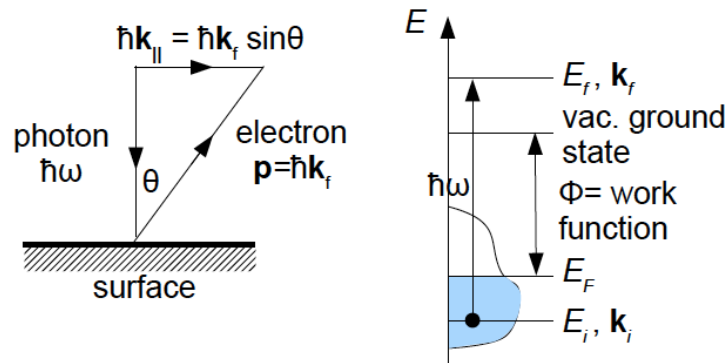
The angle of the detector is used to select the parallel component of the momentum.   [2]

Bonus mark: the data are easiest to interpret when there is little dispersion perpendicular to the surface, e.g., in anisotropic layered materials. Photoemission only gives information about occupied states.

Explain how you can use the ARPES measurements illustrated in the figure below to identify the approximate value of the Fermi energy and Fermi velocity in the material, and obtain their values.   [4]
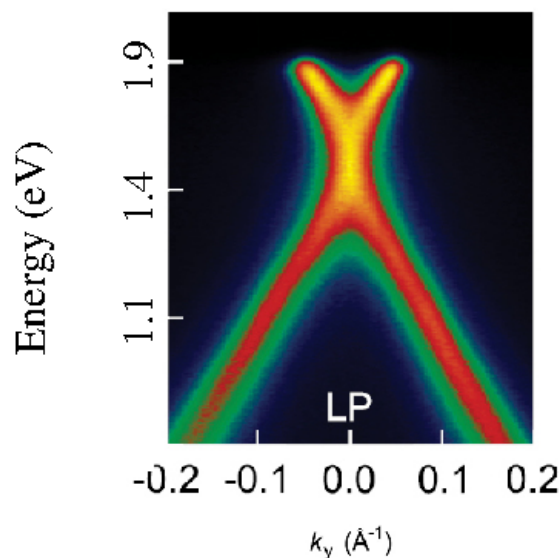
[credit: J. Phys.: Condens. Matter 26 (2014) 335501]

At temperatures much smaller than the Fermi energy, the states above E_F are not populated and the intensity of the ARPES signal vanishes correspondingly. From the figures we can see that this happens around $E_F = 1.9$ eV.   [2]

Looking a the plot, I the dispersion close to the Fermi energy is linear, and one can estimate an energy change $\Delta E \simeq 0.4$ eV over $\Delta k_y \simeq 0.08$ Å^{-1}. This gives $v_F = \Delta E/(\hbar \Delta k_y) \simeq 8 \; 10^5$ m/s. [Note not for credit: the value is indeed consistent with typical

$v_F \sim 10^6$ m/s in graphene, where the figure is from]. [2]

END OF PAPER