Advanced solid state physics exam

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1 Static and dynamic screening in metals

Consider an external field. From linear response the material responds at the same frequency, giving an induced density

$$n_{ind}(r) = -qu_{tot} = -q(A_{tot}e^{iqr} + C.C) \tag{1}$$

The internal field is the total minus the induced, giving a dielectric function given by

$$\varepsilon = \frac{q^2}{q^2 + \rho(E_F)} \tag{2}$$

Inserting this in the point charge potential in Fourier space $1/r = \int 1/q^2 \exp(i\mathbf{q}\cdot\mathbf{r})\mathrm{d}\mathbf{q}$ gives screened potential

$$U = \frac{1}{r}\exp(-k_{TF}r) \tag{3}$$

$k_{TF} \approx 0.5\mathring{A}$. This model has problems. Induced charge diverges at zero, and no Friedel oscillations. Instead turn to quantum mechanical expression.

$$\varepsilon = 1 + \frac{8\pi}{q^2V}\sum_{\alpha\beta}\frac{\left|\langle\alpha|e^{i\mathbf{q}\cdot\mathbf{r}}|\beta\rangle\right|^2}{E_\beta - E_\alpha - \omega - i\eta}(f_\alpha - f_\beta) \tag{4}$$

Assume jellium/free electron gas and plug in plane waves. In the static limit this leads to Lindhart

$$\varepsilon(\omega = 0, q) = 1 + \frac{k_{TF}}{q^2}F(q/2k_{TF}) \tag{5}$$

The induced charge can in general be found as

$$\rho_{ind}(\mathbf{r}) = Ze\frac{1}{(2\pi)^3}\int\left[\frac{1}{\varepsilon(q)} - 1\right]e^{i\mathbf{q}\cdot\mathbf{r}}\mathrm{d}\mathbf{q} \tag{6}$$

This leads to two finite induced charge and Friedel.

2 Plasmons

2.1 Plasmon relation to dielectric function

Plasmons are clearly seen to exist when the dielectric function (of ω) goes to zero $\rightarrow$ induces a finite total field regardless of the size of the external.

$$v_{tot}(r,\omega) = \int \epsilon^{-1}(r,r',\omega)v_{ext}(r',\omega)\mathrm{d}r' \tag{7}$$

Single e-h excitations vs. collective excitation (Sketch tangent function)
Equation of motion technique:

$$[\hat{S}_i, \hat{H}] = (E_i - E_0)\hat{S}_i \quad , \; \hat{S}(q) = \frac{1}{\sqrt{N}}\sum_k \phi_k(q)\hat{S}_k(q) \tag{8}$$

RPA $\rightarrow$ a maximum of one excitation per excited state.
Landau damping, sketch for simple metals.

2.2 Plasmon energy dispersion

Starting from the Lindhart dielectric function. Upon solving and Taylor expanding, it is obtained

$$\varepsilon(q \rightarrow 0, \omega) = 1 - \frac{\omega_p^2}{(\omega + i\eta)^2} - \frac{3}{5}\frac{\omega_p^2}{(\omega + i\eta)^2}v_F^2 q^2 \tag{9}$$

$$\omega_{pl}(q) = \omega_p\left(1 + \frac{3v_f^2 q^2}{10\omega_p^2} + \dots\right) \tag{10}$$

2.3 Surface plasmon-polaritons

Qualitative features: couples with light. Is not self-sustained. Requires momentum transfer from e.g. umklapp.
Thin films: Plasmon-polaritons at both surfaces.

3 Linear Reponse

3.1 Kubo formula

Small perturbation $\Rightarrow$ linear response Interaction picture, where time evolution of operators is in Heisenberg

$$\hat{A}_{H_0}(t) = e^{i\hat{H}_0 t}\hat{A}(t)e^{-i\hat{H}_0 t} \tag{11}$$

While the time dependence of due to the perturbation is carried in the wave functions in the Scrödinger picture

$$|\psi(t)\rangle = U_I\,|\psi(t_0)\rangle\,, \quad U_I(t,t_0) = e^{i\hat{H}_0 t}Ue^{-i\hat{H}_0 t_0} \tag{12}$$

Inserting in Schrödinger one can obtain, after taylor expanding to first order, and moving to non interacting picture $\hat{U} \approx \hat{T}(1 - i\int_{t_0}^{0}\hat{V}_{\hat{H}_0}(t')\mathrm{d}t')e^{i\hat{H}_0 t_0}$.
A change in the expectation value of any time independent (assumption) observable to first order is

$$\delta\hat{A} = \langle 0|\hat{A}|0\rangle - \langle 0|U^{\dagger}(0)\hat{A}U(0)|0\rangle \tag{13}$$

Leading to Kubo formula

$$\delta A(t=0) = -i\int_{t_0}^{\infty}\theta(-t')\,\langle 0|\left[\hat{A}_{\hat{H}_0}(0), \hat{V}_{\hat{H}_0}(t')\right]|0\rangle\,\mathrm{d}t' \tag{14}$$

3.2 time varying pertubation

Assuming $\hat{V}(t) = e^{-i(\omega+i\eta)t}\hat{V}$, one can obtain

$$\delta A(\omega + i\eta) = \sum_s \frac{\langle 0|\hat{A}|s\rangle\ \langle s|\hat{V}|0\rangle}{\omega - \omega_{s0} + \imath\eta} - \frac{\langle 0|\hat{V}|s\rangle\ \langle s|\hat{A}|0\rangle}{\omega + \omega_{s0} + \imath\eta} \tag{15}$$

3.3 Non interacting Density-density response

Important case, related to the dielectric function. The observable is now the density $\hat{A} = \hat{n}(r)$, and the perturbation is still adiabatic and time varying, and given additionally given by $\hat{V} = \int V(r)\hat{n}(r)\mathrm{d}r$.

$$\delta n(r,\omega) = \int \chi(r,r',\omega)V(r')\mathrm{d}r' \tag{16}$$

Where

$$\chi(r,r',\omega) = \sum_s \frac{\langle 0|\hat{n}(r)|s\rangle\ \langle s|\hat{n}(r')|0\rangle}{\omega - \omega_{s0} + \imath\eta} - \frac{\langle 0|\hat{n}(r)|s\rangle\ \langle s|\hat{n}(r')|0\rangle}{\omega + \omega_{s0} + \imath\eta} \tag{17}$$

Non-interacting means we can introduce the density operator $\hat{n}(r) = \sum_i \phi_i^* \phi_i \hat{c}_i^{\dagger}\hat{c}_i$
Arrive at:

$$\chi(r,r',\omega) = \sum_{ik}(f_i - f_j)\frac{\psi_i(r)^*\psi_j(r)\psi_i(r')\psi_j(r')^*}{\omega - (\varepsilon_j - \varepsilon_i) + i\eta} \tag{18}$$

4 Density response function

The change in the total potential can be given in two ways

$$\delta v_{tot}(r,\omega) = v_{ext}(r,\omega) + \int \frac{\delta n(r_1,\omega)}{|r-r_1|}\mathrm{d}r_1 = \int \varepsilon^{-1} v_{ext}(r_1,\omega)\mathrm{d}r_1 \tag{19}$$

This defines the dielectric function. Take the functional derivative with $v_{ext}(r',\omega)$. The definition of the density-density response function is

$$\chi(r_1,r',\omega) = \frac{\delta n(r_1,\omega)}{\delta v_{ext}(r',\omega)} \tag{20}$$

Providing

$$\varepsilon^{-1}(r,r',\omega) = \delta(r-r') + \int \frac{1}{|r-r_1|}\chi(r_1,r',\omega)\mathrm{d}r_1 \tag{21}$$

4.1 Dielectric function within RPA

Again, start from (19) take functional derivative with respect to v_{ext}
Use

$$\delta v_{tot} = \delta v_{ext} + \int \frac{n(r',\omega)}{|r-r'|}\mathrm{d}r \;\Rightarrow\; \frac{\delta v_{ext}}{\delta v_{tot}} = \delta(r-r') - \int \frac{\delta n(r_1,\omega)}{\delta v_{tot}(r)}\frac{1}{|r-r_1|}\mathrm{d}r_1 \tag{22}$$

This is equal to $\epsilon(r,r',\omega)$. Identify $\chi^0(r_1,r',\omega)$.

4.2 Local Field effects

Go from

$$\epsilon(r,r',\omega) \quad \text{(FT)} \Rightarrow \quad \epsilon_{G,G'}(q,\omega) \tag{23}$$

Talk about macroscopic dielectric constant: **Think of discrete dielectric function (Matrix)**

$$\text{RIGHT}: \epsilon_M(\omega) = \lim_{q\to 0}\frac{1}{\epsilon_{00}^{-1}(q,\omega)} \quad , \text{Wrong}: \epsilon_M = \lim_{q\to 0}\epsilon_{00}(q,\omega) \tag{24}$$

5 Excitons

5.1 Joint density of states and interband transitions

- Difference from plasmons (Plasmon at higher energies, Exciton lowers energy).
- Semiconductors and insulators, interband transitions, BSE not RPA. exchange (requires overlap) vs. Coulomb (”requires” not too much screening).
- Difference from trivial excitations (Bound state).
- Joint density of states and critical points

$$\text{Critical Points at: } \nabla_k(E_{ck} - E_{vk}) = 0 \tag{25}$$

5.2 Two models: Simple two band and screened hydrogen model

Simple two band model, tight binding, localised orbitals.

$$States : |\Phi_{n,q=0}\rangle = \frac{1}{\sqrt{N}} \sum_{m=0}^{N-1} b^{\dagger}_{n+m,c} b^{\dagger}_{m,v} |\Psi_0\rangle \tag{26}$$

$$H_0 = E_0 - \left(\sum \varepsilon_v b^{\dagger}_{nv} b_{nv} + t(b^{\dagger}_{nv} b_{n+1,v} + b^{\dagger}_{nv} b_{n-1,v}) - electron \right) \tag{27}$$

$$H_{int} = - \sum_{m,m}^{N-1} \frac{U}{1 + |n - m|} b^{\dagger}_{nv} b_{nv} b^{\dagger}_{mv} b_{mv} \tag{28}$$

Solve: $\mathbf{H}\mathbf{F}_i = E_i \mathbf{F}_i$.
The screened hydrogen model takes its offset in an expansion of single particle excitation functions.

$$\Psi_{ex} = \sum_k A(k) \Phi_{c\mathbf{k}+\mathbf{k}_{ex},vk} \tag{29}$$

Using the vanishing momentum of light at optical frequencies, and assuming a two band parabolic model. One can obtain a hydrogen like equation for the envelope function

$$F(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} A(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} \tag{30}$$

Where $\mathbf{r}$ describes the distance between electron and hole. The hydrogen like equation:

$$\left[-\frac{\hbar^2 \nabla^2}{2\mu_{ex}} - \frac{e^2}{\varepsilon r} \right] F(\mathbf{r}) = (E - E_G) F(\mathbf{r}) \tag{31}$$

where $F(r)$ denotes the envelope function which physical meaning represents the position of the electron, given the hole is at the origin ($r = 0$). Typical exciton binding energies are meV for typical semiconductors, and eV for strong insulators.

5.3 Role of the effective exciton mass:

Flat bands result in a high exciton mass and a localised exciton whereas **dispersive bands** result in small exciton mass and a delocalised exciton. The exciton mass is given as $\mu_{\text{ex}}^{-1} = m_{\text{e}}^{-1} + m_{\text{h}}^{-1}$. Recall that the inverse of the effective electron and hole masses can be calculated as the curvature of the bands at $k = 0$ for the conduction and valence band (electrons and holes respectively).

6 Green functions and quasiparticles

- What is a quasiparticles?
- What is a Green function?

$$G(x,x') = -\theta(t-t')\left\langle N\middle|\left\{\Psi(x),\Psi^\dagger(x')\right\}\middle|N\right\rangle, \quad \Psi(x) = e^{-iHt}\Psi(r)e^{iHt} \tag{32}$$

- Fourier transforming the Greens function leads to

$$G(r,r';\omega) = \sum_i \frac{\Psi_{i+}^{QP}(r)\Psi_{i+}^{QP}(r')^*}{\omega - \varepsilon_{i+}^{QP} + i\eta} + \sum_i \frac{\Psi_{i-}^{QP}(r)\Psi_{i-}^{QP}(r')^*}{\omega - \varepsilon_{i-}^{QP} + i\eta} \tag{33}$$

  $\Psi_{i+}^{QP}(r)$ are quasiparticle wavefunctions.

- Spectral properties: spectral function imaginary part of Green's functions
- Projected Green's function $G_{aa}(\omega) = G_{aa}^0(\omega) + G_{aa}^0(\omega)\sum_k V_{ak}G_{ak}(\omega)$

$$[(\omega+i\eta)I - H_0]G^0(\omega) = I \quad ,[(\omega+i\eta)I - H]G(\omega) = I \tag{34}$$

- The Self-Energy: From Newns-Anderson set or from the Green's function note using the EOM technique.
- Quasi-particle eigenvalue equation. At $\omega = \varepsilon_i^{QP}$ the LHS of (35) diverges and hence the nominator must vanish.

$$\sum_i \frac{\left[(\omega+i\eta)I - H^0 - \Sigma(t)\right]\left|\Psi_i^{QP}\right\rangle\left\langle\Psi_i^{QP}\right|}{\omega - \varepsilon_i^{QP} + i\eta} = I \tag{35}$$

- Self energy and approximations: **Wideband, Narrowband, (Elliptic)**.
- Self energy changes from screening: Image charge.

7 Berry phase

- Parametric Hamiltonian
- Adiabatic limit
- Eigenstates (of any Hamiltonian) defined down to a gauge transformation.
- Finding the phase difference going from R to $R + \mathrm{d}l$ is after linearisation

$$\mathrm{d}\phi = i \left\langle \psi_m(R) \middle| \frac{\partial}{\partial R} \psi_m(R) \right\rangle \cdot \mathrm{d}l \tag{36}$$

- This is the Berry connection.
- Berry phase

$$\gamma_n(C) = i \oint_C \langle n(\mathbf{R}) | \nabla_{\mathbf{R}} n(\mathbf{R}) \rangle \cdot \mathrm{d}\mathbf{R} \tag{37}$$

- Berry curvature

$$\gamma_n = -\int\int_C \mathrm{d}\mathbf{S} \cdot \mathbf{B}_n(\mathbf{R}) \tag{38}$$

$$\mathbf{B}_n(\mathbf{R}) = -\operatorname{Im} \sum_{m \neq m} \frac{\langle n(\mathbf{R}) | \nabla_{\mathbf{R}} \hat{H}(\mathbf{R}) | m(\mathbf{R}) \rangle \times \langle m(\mathbf{R}) | \nabla_{\mathbf{R}} H(\mathbf{R}) | n(\mathbf{R}) \rangle}{\left(E_m(\mathbf{R}) - E_n(\mathbf{R})\right)^2} \tag{39}$$

- Connection to Aharanov-Bohm. Make drawing
- Barry Phase in solids: Chern number, Gauge patching.
- Other topics: