Phys. 598SC – Fall 2015
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Lecture 4 Recap: normal metals and the electron-phonon interaction*

1. Normal metals: Sommerfeld-Bloch picture
2. Screening
3. Fermi liquid theory
4. Electron-phonon interaction.

Crucial point: (most) normal metals characterized by various frequency scales (plasma frequency, Fermi energy, band gap…: Debye θ_D). T_c is small compared to all of these, hence in discussing relevant properties of normal states can take $T \to 0$ limit. [not necessarily true in exotics]

1. Normal metals

Sommerfeld: groundstate is determinant of plane wave states with $\varepsilon(p) = p^2/2m$, filled up to Fermi momentum $p_F = \hbar k_F$, $k_F = (3\pi^2 n)^{1/3}$. Thus ε_F typically ~ a few eV. (and $k_F \sim 1 Å^{-1}$). At finite T, Fermi distribution with chemical potential $\mu(T) = \varepsilon_F + 0\,(T^2/\in_F)$
$\Rightarrow c_V = (\pi^2/3)\, k_B^2 T\, (dn/d\varepsilon)$, $dn/d\varepsilon$ = DOS of both spins at FS $= 3n/2\varepsilon_F$. $\chi = \mu_B^2 (dn/d\varepsilon)$. $\sigma = ne^2\tau/m$, τ determined by (a) impurities (b) e-phonon collisions (no e^- - e^- collision effect on σ in this model) WF: $\kappa/\sigma\, T$ = const. (if $\tau_\kappa = \tau_\sigma$).

Bloch: $\psi(\boldsymbol{r}) = u_{kn}(\boldsymbol{r}) \exp ik \cdot \boldsymbol{r}$, (where $u_{kn}(\boldsymbol{r} + \boldsymbol{R}) \equiv u_{kn}(\boldsymbol{r})$) $\varepsilon = \varepsilon_n(\underline{k})$.
$\boldsymbol{k}$ = quasimomentum of e^-. velocity $\mathbf{v(k)} = \frac{1}{\hbar} \frac{\partial \varepsilon_n(\underline{k})}{\partial \underline{k}}$, electric current = $e\mathrm{v}(k)$.

Can define Fermi surface as before, but in general not spherical: also define

$$DOS: \ \frac{dn}{d\varepsilon} = \frac{2}{(2\pi\hbar)^2} \int^{F.S.} dS/\mathrm{v}_F(\hat{\underline{n}})$$

still have c_v/T, $\chi \propto dn/d\varepsilon$ so unique ratio for $c_v/\chi T$. Note e^- - e^- processes can contribute to σ (or rather ρ) in Bloch theory, because total quasimomentum $\boldsymbol{K}$ not conserved by U-process. Still expect that to extent $\tau_\kappa = \tau_\sigma$, WF law obeyed

* Ref: AJL, Quantum Liquids, appendix 5A

2. **Screening**. [will mostly neglect band-structure effects here]

In 3D long-range part of Coulomb interaction very important: will tend to screen out localized charge impurities, and also greatly affect response to applied electric field. Simplest theory is RPA: system responds like free gas but to local field which is sum of externally applied one and that generated by the redistribution of the charge itself. Quantitatively, let $\chi_o(q\omega)$ be "bare"[†] response to external field, *i.e.* that calculated without account of long-range part of Coulomb interaction. Technically[*]

$$e^2\,\chi_o(q\omega) \;\equiv\; -\left.\frac{\delta\rho(q\omega)}{\delta\varphi(q\omega)}\right|_{no\ LRF} \qquad\qquad \varphi(q\omega) = F.T. \text{ of electrostatic potential}$$

[note defined so that χ_{stat} is positive]. Then basic assumption of RPA is

$$\delta\rho(q\omega) = -e^2\chi_o\,(q\omega)\,\varphi_{tot}(q\omega), \text{ where}$$
$$\varphi_{tot}(q\omega) \;\equiv\; \varphi_{ext}(q\omega) + \varphi_{ind}(q\omega)$$

But $\varphi_{ind}(q\omega)$ obeys Poisson's law

$$\nabla^2\varphi_{ind}\,(rt) = -\rho(rt)/\epsilon_o$$

or equivalently

$$q^2\varphi_{ind}(q\omega) = -\rho(q\omega)/\epsilon_o$$

putting these together:

$$\delta\rho(q\omega) = \left(\frac{-e^2\chi_o(q\omega)}{1+\frac{e^2}{\varepsilon_o q^2}\chi_o(q\omega)}\;.\right)\;\phi_{ext}(q\omega)$$

If then we define the "true" response $\chi(q\omega) \equiv \frac{-\delta\rho(q\omega)}{\delta\,\varphi_{ext}(q\omega)}$, we get

$$\boxed{\chi(q\omega) = \frac{\chi_o(q\omega)}{1+\frac{e^2}{\epsilon_o q^2}\,\chi_o(q\omega)}} \qquad (\S) \qquad\qquad (SI\text{: in cgs}, e^2/\varepsilon_o \Rightarrow 4\pi e^2)$$

[†] called by PN the "screened" RF. [beware sign conventions (and factors of *e* !) in this argument!]

[*] thus $\chi_o(q\omega)$ is the (particle) density response function rather than that of the charge density (ρ ≡ charge density).

3 important consequences of basic formula (§):

1. Static (TF) screening: in general χ(q0) is a complicated function, but for $q \ll k_F$ reduces to $\chi_o(q0) \cong \text{const.} = dn/d\varepsilon$. Thus, if we define $k_{FT}^2 \equiv (e^2/\varepsilon_o)\,(dn/d\varepsilon\,,)$ then

$$\chi(q0) \underset{(q \ll k_F)}{\cong} \frac{(dn/d\varepsilon)}{1 + k_{FT}^2/q^2}$$

If we apply this formula to the case of a finite impurity charge at the origin, we find the total potential induced by it plus the screening cloud falls off as $r^{-1} \exp - k_{FT} r$. Typical values of kFT are of the same order as kF or somewhat larger [quantitatively: $k_{FT}/k_F = 0.815\,(r_s/a_o)^{1/2}, r_s \equiv$ interparticle distance $(3/4\pi n)^{1/3}$, ao = Bohr radius].

2. Plasmons: if at any point $\chi(q\omega)$ has a pole, this indicates the possibility of a free oscillation in absence of external field. Now in general, by perturbation theory

$$\chi_o(q\omega) = \sum_n 2\omega_{no} \frac{\left|\langle n|\rho_q|o\rangle\right|^2}{\omega_{no}^2 - \omega^2}$$

and since† ρ_q can excite only particle-hole pairs with $\omega_{no} \sim v_F\, q$, for $\omega \gg v_F q$.

$$\chi_o(q\omega) = -\omega^{-2} \sum_n 2\omega_{no} \left|\langle n|\rho_q|0\rangle\right|^2 = -nq^2/m\omega^2$$

(TRK sum rule)

⇒in this regime,

$$\chi(q\omega) = \frac{\chi_o(q\omega)}{1 - \dfrac{ne^2}{\varepsilon_o m\omega^2}}$$

⇒pole occurs at

$$\boxed{\omega^2 = ne^2/m\varepsilon_o \equiv \omega_p^2} \qquad \omega_p \text{ typically } \sim 5 - 10eV \text{ (so} > \varepsilon_F)$$

(strictly speaking, Sommerfeld-model result (jellium). Not quantitatively valid in presence of finite band structure.)

$\delta\varphi_{ext}(qo) = Ze/\varepsilon_o q^2 \;\Rightarrow\; \delta\rho(r) = -e^2 \left(\frac{dn}{d\varepsilon}\right) \frac{Ze}{4\pi\varepsilon_o r} \exp = k_{FT}\, r$

† Argument valid only for translation-invariant case.

3. Nature of groundstate in RPA.

   A general expression for the Coulomb energy in 3D is

$$\langle V_c \rangle = \frac{1}{2}\sum_q V_q \ \langle \rho_q \rho_{-q} \rangle \ . \quad V_q = \ e^2/\varepsilon_o q^2$$

   In the free-gas GS, $<\rho_q\, \rho_{-q}>$ is given (for $q \neq 0$) by the HF expression $\sum_k n_{k-q/2}\left(1 - n_{k+q/2}\right) \sim \hbar q \mathrm{v}_F (dn/d\varepsilon)$. This would give a contribution to the Coulomb energy which is $\propto \ q^{-1}$ and thus v. large as $q \ \rightarrow 0$. The system can avoid this by creating a "cancelling" density fluctuation of wavelength q, but this costs an energy $\sim \hbar q \mathrm{v}_F$. Thus we must compromise by building in an appropriate no. of "virtual" plasmons into the free RPA GS. It turns out (not obviously, at this level!)* that the contribution of the mode q to the GSE is $\ll$ above, in fact simply $\frac{1}{2}\hbar\omega_p$. (see e.g. P+N QL § 5.3)

3. **Fermi liquid theory** (first for liquid ^{3}He, then normal metals)

The Coulomb interaction in real metals is very strong, and at shorter wavelengths RPA is almost certainly not a complete account of its effects. Why, nevertheless, do many metals behave so like the Bloch-Sommerfeld ("textbook") model?

Note: Fermi liquid approach rests on ansatz about GS (excluding superconductivity for the moment). Cannot be demonstrated a priori for any particular metal!

Landau ideas of adiabatic evolution: definition of quasiparticles, "occupation number" $\delta n(\mathbf{p}\sigma)$.

Translationally and rotationally invariant system: definition of $m^*, F_\ell, Z_\ell \left(\equiv F_\ell^{(s)}, F_\ell^{(a)}\right)$. Generalization to system with crystal-lattice effects.

Molecular fields (generalization of RPA).

Note molecular fields only come into play in presence of "macroscopic polarization" $\Rightarrow$ no effect on eg specific heat, nor on transport props provided we work in terms of "conductivities" rather than "diffusivities".

Modern theory of normal metals combining Landau, Bloch and screening (RPA) considerations. In general, $\chi_o(q\omega)$ is effected by Landau molecular fields, eg. $\chi_o(q0)_{q \ll q_F} \sim (dn/d\varepsilon)\left(1 + F_o^{(s)}\right)^{-1}$, so k_{FT} is quantitatively modified. However, for the translation-invariant ("jellium") case, ω_p is not affected, since the result $\chi_o(q\omega) \cong \ -n\, q^2/m\omega^2$ turns out still to be valid.

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* If we write $\Psi_o \sim \left(1 + \ \alpha Q_p^+\right)|0\rangle$ where $|0\rangle$ is free-gas GS and Q_p^+ creates plasmon, then $\langle V_c \rangle \sim (1-\alpha)$.const. /q and the extra KE $\propto \ \alpha^2$. Hence there is an optimum value of α.

[Another demonstration: Consider the sum rules for the true $\chi(q\omega)$:

$$\pi^{-1}\int_o^\infty \omega^{-1}\ \chi(q\omega)\,d\omega \overset{(KK)}{=} \chi(qo) \rightarrow \frac{q^2\varepsilon_o}{e^2}\ (q\rightarrow 0)\left(+o(q^4)\right)$$

$$\pi^{-1}\int_o^\infty \omega\,\chi(q\omega)\,d\omega = nq^2/m \qquad (TRK)$$

$$\pi^{-1}\int_o^\infty \omega^3\ \chi(q\omega) = \langle\left[j_q,\left[j_{-q},H\right]\right]\rangle \quad \text{(translation invariant system only!)}$$

$$= \frac{n^2e^2q^2}{m^2\varepsilon_o} + o(q^4) \qquad \text{Mihara Puff}$$

Together these imply that for $q\rightarrow 0$ $\chi(q\omega)$ is exhausted by a single pole at $\omega_p \equiv (ne^2/m\varepsilon_o)^{1/2}$.]

4. Electron-phonon interaction

Simplest theory is generalization of RPA. Define the "bare" responses $\chi_{el}^{(o)}(q\omega), \chi_{ion}^{(o)}(q\omega)$

of the electron and ion particle densities to the local field, and the "true" responses $\chi_{el}(q\omega),\chi_{ion}(q\omega)$ similarly, (*i.e.* in calculating $\chi^{(o)}$'s can ignore all *LR* Coulomb forces, whether el-el, el-ion or ion-ion). Only problem is to keep signs straight! Define the χ's as particle density responses and the $\delta\rho$'s as charge densities, then

$$\delta\rho_{el}(q\omega) = -e^2\chi_{el}^{(o)}(q\omega)\varphi_{tot}(q\omega)$$

$$\delta\rho_{ion}(q\omega) = -Z^2e^2\chi_{ion}^{(o)}(q\omega)\varphi_{tot}(q\omega) \qquad \text{[(charge on ion = } Ze\text{)}$$

$$\varphi_{tot}(q\omega) \equiv \varphi_{ext}(q\omega) + \varphi_{ind}(q\omega)$$

where $\varphi_{ind}(q\omega)$ satisfies (Poisson)

$$\nabla^2\varphi_{ind} = \frac{1}{\epsilon_o}(\delta\rho_{el} + \delta\rho_{ion})$$

Solving these:

$$\delta\rho_{el}(q\omega)/\delta\varphi_{ext} \equiv -e^2\chi_{el}(q\omega)$$

$$= \frac{-e^2\chi_{el}^{(o)}}{1+\frac{e^2}{\epsilon_o q^2}\left(\chi_{el}^{(o)} + Z^2\chi_{ion}^{(o)}\right)}$$

and similarly for $\delta\rho_{ion}(q\omega)$. Thus,

$$\chi_{el}(q\omega) = \frac{\chi_{el}^{(o)}}{1 + \frac{e^2}{\epsilon_o q^2}\left(\chi_{el}^{(o)} + Z^2\chi_{ion}^{(o)}\right)}$$

$$\chi_{ion}(q\omega) = \frac{\chi_{ion}^{(o)}}{1 + \frac{e^2}{\epsilon_o q^2}\left(\chi_{el}^{(o)} + Z^2\chi_{ion}^{(o)}\right)} \qquad (\dagger)$$

These formulas are general but rather messy. To see the essence of the results, it is convenient to consider limit $\omega \ll q v_F \ll k_F v_F$ (thus neglecting plasmons) and moreover neglect all short-range interactions of ions: thus equation of motion is taken to be

$$\frac{\partial \rho_{ion}}{\partial t} = -\boldsymbol{\nabla}\cdot\boldsymbol{J}_{ion}, \quad \frac{\partial J_{ion}}{\partial t} = \frac{n_{ion}}{m}\boldsymbol{F}$$

and thus from definition of $\chi_{ion}^{(o)}$, $\quad \chi_{ion}^{(o)}(q\omega) = -n_{ion}q^2/M\omega^2$.

If we define the "bare" ion plasma frequency by

$$\Omega_p^2 \equiv Z^2 n_{ion} e^2/M\epsilon_o$$

and the electron TF wave vector by

$$k_{TF}^2 \equiv (e^2/\epsilon_o)\left(\chi(q,0)_{q\ll k_F}\right) \equiv \kappa\left(\cong (e^2/\epsilon_o)(dn/d\epsilon)\right)$$

we can write the results in the form

$$\chi_{el} = \frac{\kappa}{1 + k_{TF}^2/q^2 - \Omega_p^2/\omega^2}$$

$$\chi_{ion} = \frac{-n_{ion}q^2/M\omega^2}{1 + k_{FT}^2/q^2 - \Omega_p^2/\omega^2}$$

In the limit of infinitely massive ions, ($M\to\infty$, $\Omega_p\to 0$) we recover the previous RPA results for the electrons.

The expressions for χ_{el} and χ_{ion} have a pole, which for $q \ll k_{TF}$, $\omega \ll \Omega_p$ occurs at

$$\omega = c_s q \qquad c_s \equiv \Omega_p / k_{TF}$$

For a jellium model the quantity Ω_p/k_{TF} is equal to $\left(\frac{mZ}{3M}\right)^{1/2} v_F$ so the velocity of sound $c_s \sim (m/M)^{1/2} v_F$ (Bohm-Staver). In the more general case we have $\omega_{ph}^2(q) = \Omega_p^2/(1 + k_{TF}^2/q^2)$

Effective electron-electron potential

The above results are equivalent to the replacement of φ_{ext} by the screened potential

$$\varphi(q\omega) \equiv \frac{\varphi_{\text{ext}}\,(q\omega)}{1 + k_{TF}^2/q^2 - \Omega_p^2/\omega^2}$$

Now let us take $\varphi_{\text{ext}}(q\omega)$ to be the potential of a second electron, *i.e.* $e^2/\varepsilon_o q^2$. This gives an effective e^-–e^- interaction.

$$V_{\text{eff}}^{\text{el}-\text{el}}(q\omega) = \frac{e^2/\epsilon_o q^2}{1 + k_{TF}^2/q^2 - \Omega_p^2/\omega^2}$$

or using above relation to eliminate Ω_p in terms of $\omega_{pk}(q)$:*

$$\boxed{V_{\text{eff}}^{\text{el}-\mu}(q\omega) = \frac{e^2}{e_o} \cdot \frac{1}{q^2 + k_{TF}^2} \left\{1 + \frac{\omega_{ph}^2(q)}{\omega^2 - \omega_{ph}^2(q)}\right\}}$$

First term is e^- – e^- interaction self-consistently by e^- gas, second is interaction via exchange of virtual phonons. Note second contains ω and thus is <u>retarded in time</u> (illustrate with "polarization" picture). In this simple model V_{eff} is zero at zero frequency, then increasingly attractive for $\omega < \omega_{ph}(q)$. [↑: This would predict <u>all</u> metals superconducting.] ↑: likely quantitative inaccuracy of above for real metals with $q \sim q_F$.

* We need to use the relation $\omega_{pk}(q) = \frac{\Omega_r q}{(k_{FT}^2 + q^2)^{1/2}}$ (cf. (†) above)

The quantum picture.

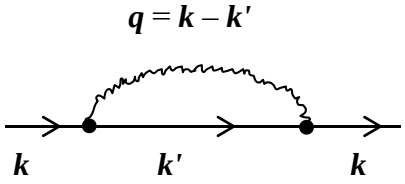
The above argts. never referred to the fact that the ionic vibrations are quantized. However, it should be possible to interpret them in terms of the emission and absorption of phonons.

Consider a given wave vector $\boldsymbol{q}$. With it is associated a classical lattice vibration (longitudinal acoustic) with frequency. $\omega_{ph}(\boldsymbol{q})$ and a phonon of energy $\hbar\omega_{ph}(\boldsymbol{q})$. Consider a process in which an electron of wave vector $\underline{k}$ emits (say) a phonon of wave vector $\boldsymbol{q}$, going thereby into a state of wave vector $\boldsymbol{k}'$. Because of the periodicity of the lattice we must satisfy the condition

$$\mathbf{k} - \mathbf{k}' = \mathbf{q} + \mathbf{G}$$

As usual, we call the process normal (N) if G = 0, Umklapp (v) if G ≠ 0. For the moment let us focus on N^- processes. If the process is a real one, we must also involve conservation of energy, but for a process leading to a virtual intermediate state energy need not be conserved.

There will be some matrix element $g_{kk'}$ for this process. To find it, we could either (1) go back to first principles, or (2) rederive the effective el – el interaction in terms of phonons and compare with our earlier result based in a classical treatment. (2) is more instructive and will now be done:



Consider the process depicted graphically above, in which an electron, initially in state $\boldsymbol{k}$, emits a phonon of wave vector $\boldsymbol{q}$, going thereby into an (empty) state $\boldsymbol{k}'$; subsequently it re-absorbs the phonon and returns to its original state. The intermediate state of the system is virtual. This changes the energy of the state |0> of the system, which contains one electron in $\boldsymbol{k}$: by straightforward 2nd-order perturbation theory.

$$\Delta E_o = \sum_i \frac{|\langle 0|\mathrm{V}|i\rangle|^2}{E_o - E_i}$$

In our case, E_o is $\in \boldsymbol{k}$), E_i is the energy of the state with electron in $\boldsymbol{k}'$ and the phonon in $\boldsymbol{q}$, *i.e.* $\in(\boldsymbol{k}') + \hbar\omega(\boldsymbol{q})$, and $<0|V|\, i>$ is the matrix element $g_{kk'}$ (which is what we essentially want to find). Hence we have, with the sum over $\boldsymbol{k}'$ going over unoccupied states only,

$$\Delta\epsilon_k = \sum_{\substack{k' \\ (unocc) \\ (\sigma'=\sigma)}} \frac{|g_{kk\prime}|^2}{\epsilon(k) - \epsilon(k') - \hbar\omega(\boldsymbol{q})} \equiv \sum_{k\prime}(1 - n_{k\prime})\frac{|g_{kk\prime}|^2}{\epsilon(k) - \epsilon(k') - \hbar\omega}$$

The total change in energy of the system due to exchange of phonons is

$$\Delta E = \sum_{k\sigma} n_{k\sigma}\Delta\epsilon_{k\sigma}$$

$$= \sum_{\substack{kk' \\ \sigma}} n_{k\sigma}(1 - n_{k\prime\sigma})\frac{(g_{kk\prime})^2}{\epsilon(k) - \epsilon(k') - \hbar\omega(\boldsymbol{q})}$$

If we add a term with $\boldsymbol{k}$ and $\boldsymbol{k}'$ interchanged and divide by ½, we get (a) a term which is linear in the n_k and can be written

$$\sum_k n_{fk}$$

. (f_k ind of $n_{k'}$) and (b) a term in $n_k n_{k'}$:

$$\Delta E = \sum_{k\sigma} n_{k\sigma} f_k - \frac{1}{2}\sum_{k\sigma} n_k n_{k\prime}|g_{kk'}|^2 \left\{\frac{1}{\epsilon(k) - \epsilon(k') - \hbar\omega_{ph}(\boldsymbol{q})} + \frac{1}{\epsilon(k') - \epsilon(k) - \hbar_{\omega ph}(\boldsymbol{q})}\right.$$

$$= \sum_{k\sigma} n_{k\sigma} f_k - \frac{1}{2}\sum_{\substack{kk' \\ \sigma}} n_k n_{k\prime} \cdot \frac{2\hbar\omega_{ph}|g_{kk'}|^2}{[\epsilon(k) - \epsilon(k')]^2 - \hbar^2\omega^2{}_{pk}(\boldsymbol{q})}$$

The effective interaction $V_{eff}^{el-el}(\boldsymbol{k}, \boldsymbol{k}')$ which leads to the second term as a Hartree-Fock term is given by the second derivative -- $\partial^2 E/\partial n_k \partial n_{k'}$,

$$i.e. \Delta E \equiv -\frac{1}{2}\sum_{kk\prime} V_{eff}(kk')n_k n_{k\prime}$$

$$V_{k,k\prime}^{\text{eff}} = +\frac{2\hbar\omega_{ph}|g_{kk\prime}|^2}{[\epsilon(k) - \epsilon(k')]^2 - \hbar^2\omega_{ph}^2(q)}, \qquad \boldsymbol{q} \equiv \boldsymbol{k} - \boldsymbol{k}'$$

This result is quite general and independent of the detailed form of the matrix element $g_{\boldsymbol{kk}'}$.

Let us now ask: What is the matrix element in the simple ("jellium") model we used above? We compare the expression just derived with the classical result

$$V_{\text{eff}}(q,\omega) = \frac{e^2}{\epsilon_o}\frac{1}{q^2+k_{FT}^2}\left\{1+\frac{\omega_{ph}^2(q)}{\omega^2-\omega_{ph}^2(q)}\right\}$$

and put $\boldsymbol{q} = \boldsymbol{k}-\boldsymbol{k}'$, $\omega=(\in(k)-\in(k')/\hbar$. The first term above is irrelevant, since it gives the effect of the screened electron-electron interaction, and does not refer to phonons. If we demand agreement for the second, the matrix element must be given by

$$\boxed{|g_{kk'}|^2 = \frac{1}{2}\frac{e^2/\epsilon_o}{q^2+k_{FT}^2}\hbar\omega_{ph}(q)} \qquad (\boldsymbol{q}\equiv\boldsymbol{k}-\boldsymbol{k}')$$

This formula should not be taken quantitatively when q is too large ~ (k_F, k_{TF} or k_D). But for reasonably small q it should give at least the qualitatively correct behavior. The crucial point to notice is that for $q\to 0$, the matrix element to emit (or absorb) an acoustic phonon of wave vector q is proportional to $q^{1/2}$. (since $\omega_{ph}(q)\sim q$). This result is actually not model-dependent. Note that in view of the definition of k_{FT}^2, the long-wavelength matrix element can be written simply

$$|g_{kk'}|^2_{q\to 0} = \frac{1}{2}\cdot\frac{\hbar\omega_{ph}(q)}{g(\epsilon_F)}$$

i.e. inversely proportional to $g(\epsilon_F)$ (because efficiency of screening $\propto g(\epsilon_F)$)