

(Short) summary of three lectures on

P O L A R O N S

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(Short) Summary of three lectures
on POLARONS. (I.C.T.P. Trieste
July 1971)

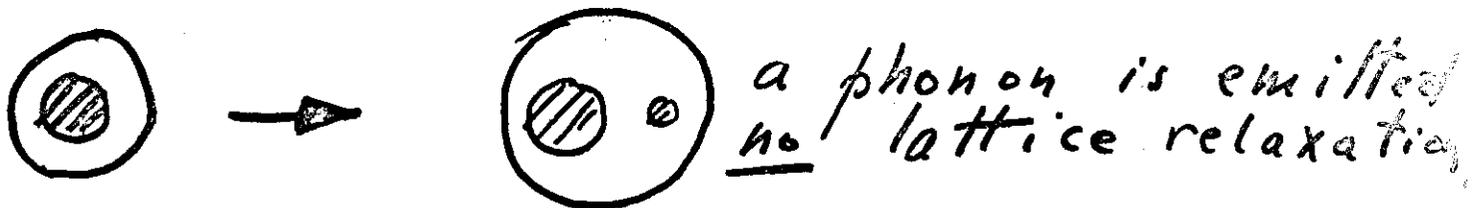
J. Devreese, Univ. Antwerp.

① Optical properties of polarons //
(WEAK \vee STRONG COUPLING).

1. Weak coupling [REF 1] [REF 2]

The optical absorption is calculated
following [ref 2].

We start from the golden rule
for the transition probability for
a polaron to go from the groundstate
to a scattering state:

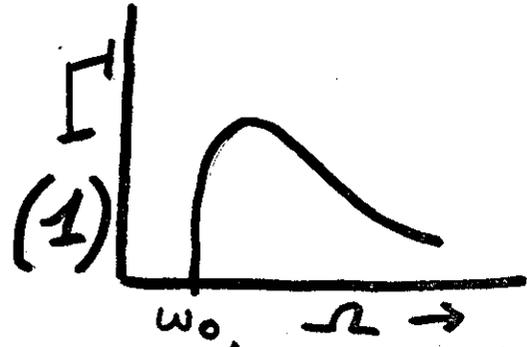


By eliminating intermediate states
one obtains the KUBO-FORMULA
but for $T=0$ and one polaron.

Subsequently the Lee Low Pines
formalism is used. This formalism
is based on two canonical

transformations. The first introduces the electron as "reference point." (One moves with the electron) The second takes the lattice deformation into account at weak coupling.

We obtain:

$$\Gamma = \frac{1}{c\epsilon_0 n} \frac{2}{3} \alpha \frac{\sqrt{\Omega - \omega_0}}{\Omega^3} \quad (1)$$


- Γ = optical absorption coefficient
- Ω = frequency of the incident light
- ω_0 = phonon wavelength optical
- α = phonon frequency coupling constant.

The derivation given in REF 2 is simple but the result (1) is a special case of results obtained in [ref 1] with highly involved techniques.

It is possible to improve eq (1) so that it is reliable for $\alpha \approx 1$. We obtain:

$$\Gamma = \frac{1}{c\epsilon_0 n} \frac{2}{3} \left(\frac{m^*}{m}\right)^{\frac{3}{2}} \alpha \frac{\sqrt{\Omega - \omega_0}}{\Omega^3} e^{-\gamma \frac{m^*}{m} |\Omega - \omega_0|} \quad (2)$$

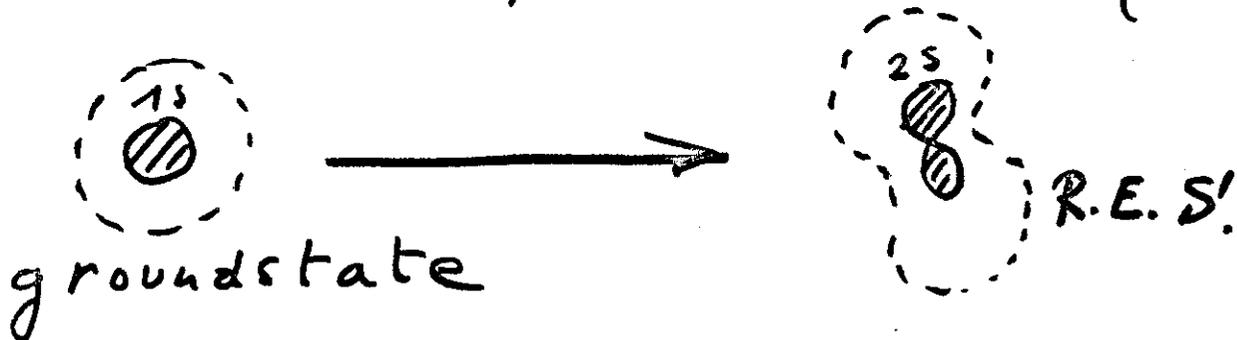
γ_α is a slowly varying function of α
($0.1 < \gamma < 1$).

(2) is a limiting case obtained from expressions discussed below
2. Strong coupling. [ref 3][ref 4]

[ref 3] is the main paper; [ref 4] contains mathematical refinements.

It is proved that internal excitations of polarons play a role at large α . LATTICE RELAXATION can occur for excited states and then one speaks of RELAXED EXCITED STATES: R.E.S.

Pictorial representation: (large α)



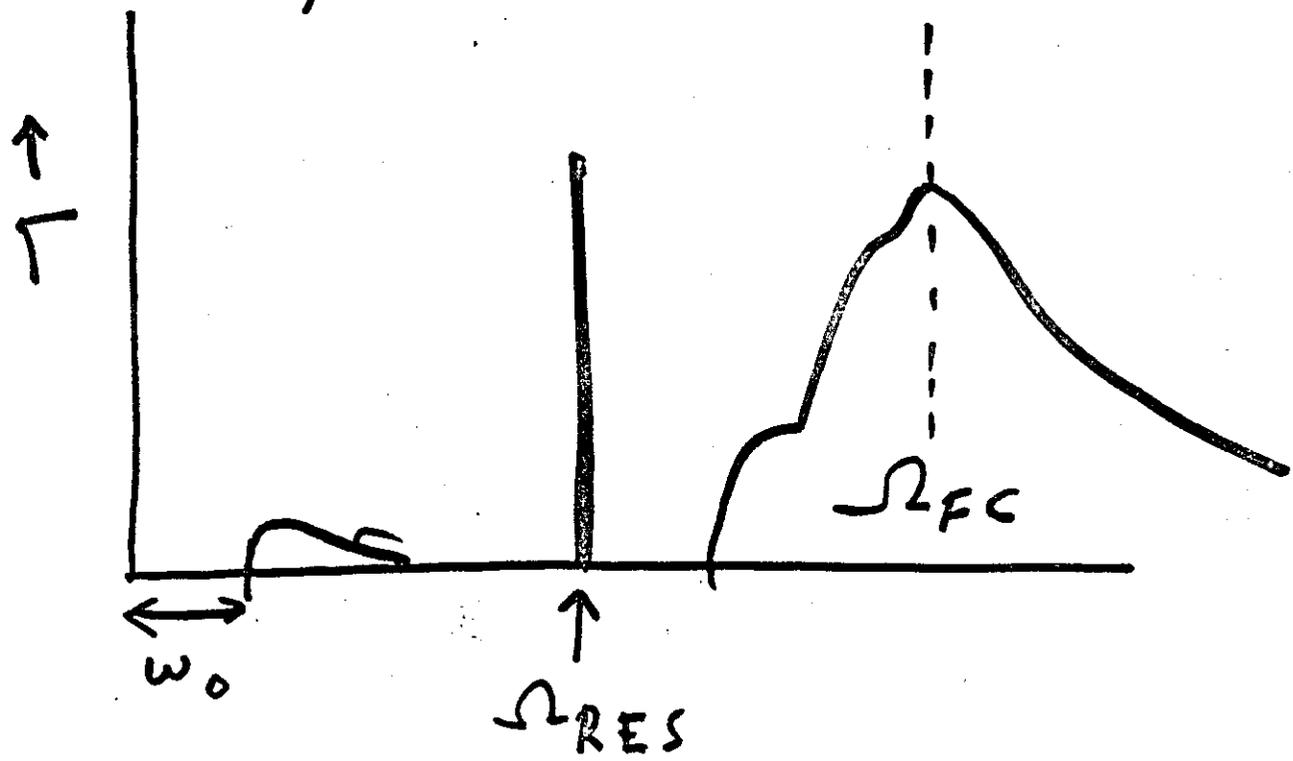
⊗ ⊗ : electron states

○ ○ ○ : symbolizes lattice polarization.

With golden rule transition probability from ground state to R.E.S. R.E.S. + n phonons should be calculated.

The lifetime of the R.E.S. is calculated using Wigner-Weiskopf theory.

This leads for $\alpha > 6$ to intense peak for ZERO-PHONON TRANSITION and complex SIDEBAND STRUCTURE with maximum at the "FRANK-CONDON" frequency (no lattice readaptation)



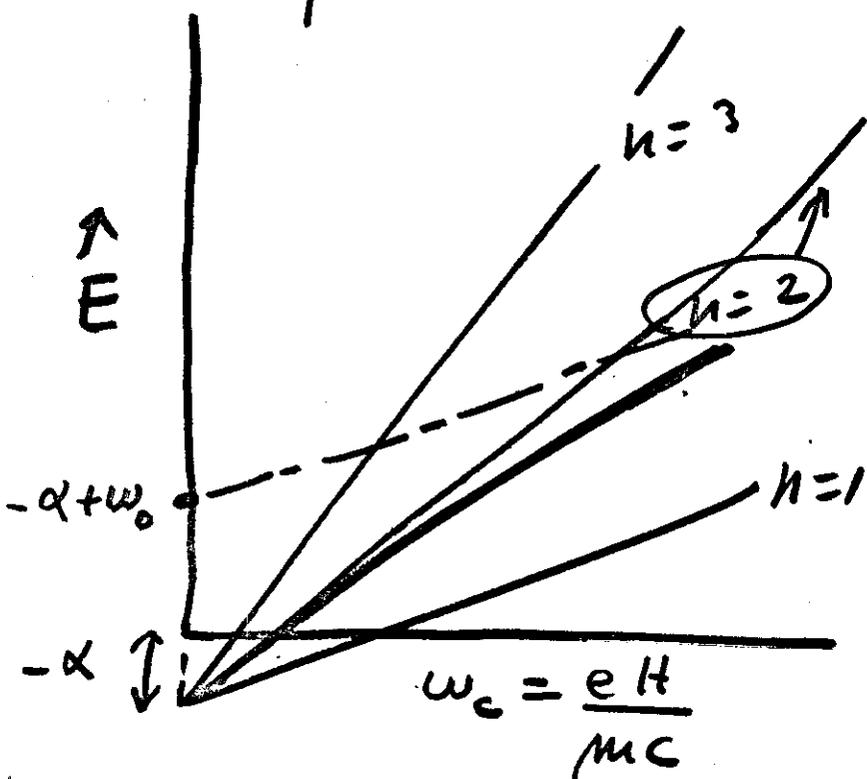
Experiment: Until now only weak coupling behaviour (eq 7) seems to have been observed [REF 5]

② POLARONS IN MAGNETIC FIELDS // [REF 6, 7]

ELECTRON-PHONON interaction modifies the Landau levels and adds extra levels.

1) Weak coupling (REF 6)

The spectrum becomes:



→ The $n=2$ level is "pinned" by the scattering state at $-\alpha + \omega_0$.

→ The slope of the LANDAU LEVELS is determined by the polaron mass, instead

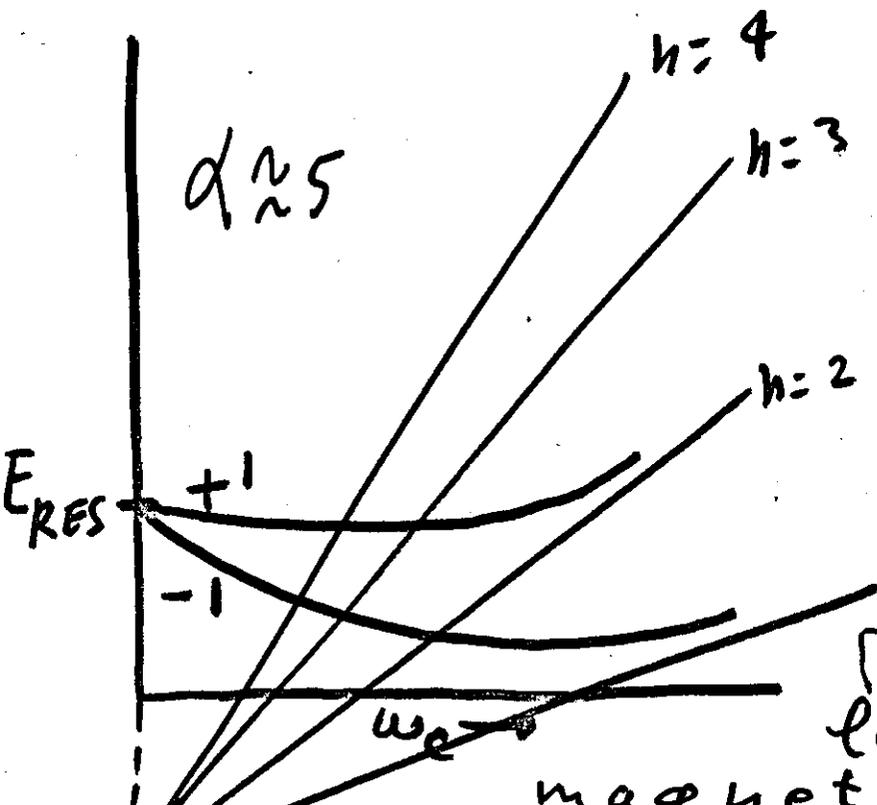
of the bare mass. Brown's [7] measurements are based on this fact. LARSEN, LAX et al. [8] have studied the pinning.

Also R.E.S. modify the LANDAU LEVEL SCHEME.

LEE, LOW PINES

In L.L.P. approximation for z-direction Landau Product - Ansatz for wave functions ($\Psi = |\text{field}\rangle |\text{electr.}\rangle$)

we obtain:



There is a Zeeman splitting of RES.

The state belonging to $l_z = +1$ ($l_z = \text{angular momentum}$ of the electron)

tends to the $n=2$ Landau level for large magnetic field.

The state belonging to $l_z = -1$ tends to the $n=1$ Landau level for $H \rightarrow \infty$.

Recent calculations have shown that the $l_z = +1$ state gets stabilized if the field increases.

Therefore: HIGH MAGNETIC FIELDS ARE A TOOL TO OBSERVE R.E.S. (PRESUMABLY ONLY IF $\alpha \geq 3$)
 EXPER. EVIDENCE: KOBAYASHI (REF 9) observed stabilization of

③ INTERMEDIATE COUPLING; PATH INTEGRALS.

//

A short survey of path integral techniques is given. [see 9]

Advantages: - No operators involved.
- One can rely on classical intuition
- phonons can be exactly eliminated
(transformation of many body problem to one-particle problem)
- path integrals might even be calculated by computer.

Disadvantages: - Until now spin could not be treated.
- Involved mathem.

One can treat exactly with path-integrals:

- a) Harmonic oscillator (1948)
- b) now progress: Coulomb potential
ref 10, 11, 12.

The only existing intermediate coupling theory is due to Feynman, F.H.I.P. [14], Feynman Thornber [15]. [13]

It is based on a quadratic approximation.
after the elimination of the phonons one concentrates on the motion of one particle.

One supposes that the electron moves in a quadratic potential.

FHIP calculated:

$$\frac{1}{z(\Omega)} = \Omega G(\Omega) \quad z(\Omega) = \text{impedance function}$$

harmonic approximation:

$$\frac{1}{z(\Omega)} = \Omega G_0(\Omega)$$

then they go one order further:

$$\frac{1}{z(\Omega)} = \Omega (G_0 + G_1)$$

G_1 is a linear function of $S - S_0$:
the difference between exact and trial action.

FHIP then consider:

$$\bar{z}(\Omega) = \frac{1}{\Omega G(\Omega)} \approx \frac{1}{\Omega(G_0 + G_1)} \quad (3)$$

and the "development"

$$\bar{z}(\Omega) = \frac{1}{\Omega} \left(\frac{1}{G_0} - \frac{G_1}{G_0^2} \right) \quad (4)$$

They have no real justification for (4).

From (4) they obtain $\lim_{\Omega \rightarrow 0} \bar{z}(\Omega) = \frac{1}{\mu}$ ($\mu =$ the mobility) and they also plot $\text{Re } \bar{z}(\Omega)$. $\text{Re } \bar{z}(\Omega)$ shows structure at FRANCK-CONDON STATES.

It seems that no lattice relaxation is taken into account.

We calculated [16]

$$\Gamma \sim \text{Re } \frac{1}{\bar{z}(\Omega)} = \text{Re } \frac{-\Omega}{\frac{1}{G_0} - \frac{G_1}{G_0^2}} \quad (5)$$

This leads to cumbersome analytical & numerical work.

References.

1. Gurevich et al: Sov. Phys. Sol. St., 4, 918 (1962).
2. Devreese, Huybrechts, Lemmens: Phys. Stat. Sol. (1971)
(to be published).
3. E. Kartheuser, R. Evrard, J. Devreese: Phys. Rev. Letters,
22, 94 (1969).
4. M. Goovaerts, J. De Sitter, J. Devreese: B.L.G., 439,
Internal Report, Atomic Energy Center, Mol, Belgium (1969).
5. Finkenrath et al: Solid State Communications, 7, 11 (1969).
6. D. Larsen: Phys. Rev., 135, 1, 419 (1967).
7. Brown et al: in "Polarons and Excitons", Kuper editor,
Oliver Boyd (1962).
8. Lax et al: Phys. Rev. Lett., 23, 1033 (1969).
9. Kobayashi et al: J. Phys. Soc. Japan, 28, 1096 (1970).
10. Gutzwiller: J. Math. Phys., 8, 1979 (1967).
11. C.C. Grosjean: Lecture presented at the Royal Flemish Academy
(1970).
12. M. Goovaerts, J. Devreese: J. Math. Phys. (to appear May 1972).
13. Feynman: Phys. Rev., 97, 660 (1955).
14. Feynman et al: Phys. Rev., 128, 1599 (1962).
15. Thornber, Feynman: Phys. Rev. B. 1, 4099 (1970).