Theorie van Kwantumsystemen & Complexe Systemen
Universiteit Antwerpen

*Workshop "Polarons in the 21st Century"*
*ESI, Vienna, December 9-13, 2019*

# Polaron physics through the XX and XXI centuries

***J. T. Devreese, J. Tempere, S. N. Klimin***

***Universiteit Antwerpen***

***Belgium***

Dear Chairman, dear colleagues and participants,

Due to unforeseeable circumstances, I cannot be in Vienna to participate in the Workshop “Polarons in XXI Century”. I would like to send you my greetings on the occasion of this Workshop, which is a prominent page in the history of the polaron physics.

Polarons constituted an essential part of many international conferences in the condensed matter area, particularly the first general EPS-CMD Conference in Antwerp in 1980, where I was the Chairman. From that time, polaron physics continued to intensely develop, involving new areas and testing new powerful methods. Recent discoveries of polarons in a very broad sense, for example, in atomic quantum gases demonstrate the universality of the polaron concept, which can embrace a lot of new unexpected areas of manifestations. It is nice to see that at present, polaron physics is flourishing and demonstrates new fascinating developments. Professor Jacques Tempere has kindly accepted to present the plenary talk for the Workshop.

I wish you all a very fruitful and pleasant meeting.

With friendly greetings,
Jozef T. Devreese

# Outline

Part I Origins - the “traditional polaron”: an electron in a bath of phonons

1. The Fröhlich or “large” polaron
2. Polaron signatures: response (optical absorption)
3. Holstein or “small” polarons
4. Polarons in nanostructures

Part II: Polaronic effects in a broader sense: four examples

1. Ripplopolaron
2. Bose polaron
3. Excitonic polaron
4. Angulon

Part III: From one to many: interacting polarons

1. Many-polaron optical absorption
2. Bipolarons

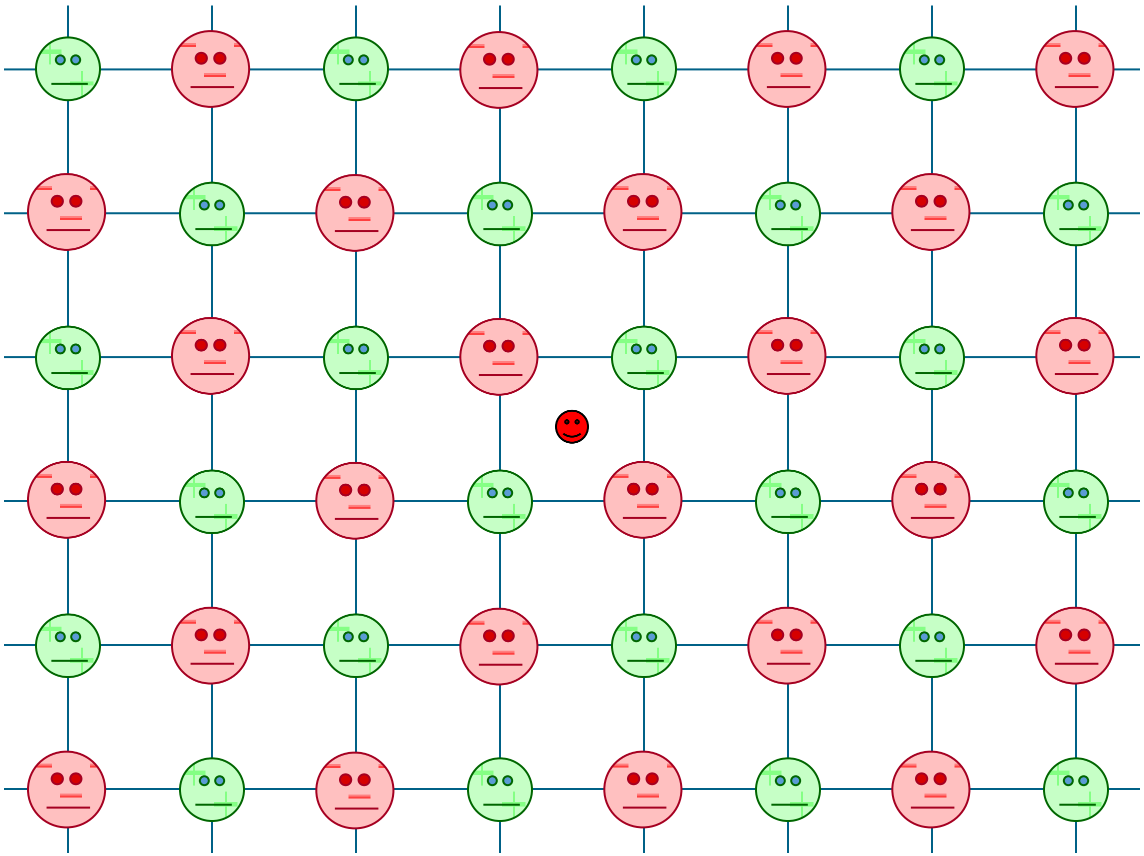
# Introduction

The polaron[1]: an artist's impression[2]

positive ion, for example Na

negative ion, for example Cl

an electron



[1] L. D. Landau, Phys. Z. Sowjetunion **3**, 664 (1933)

[2] J. T. L. Devreese, *Moles agitat mentem. Ontwikkelingen in de fysika van de vaste stof.* Speech on acceptance of the position of full professor of solid physics, in particular solid theory, at the Department of Applied Physics at Eindhoven University of Technology, March 9, 1979

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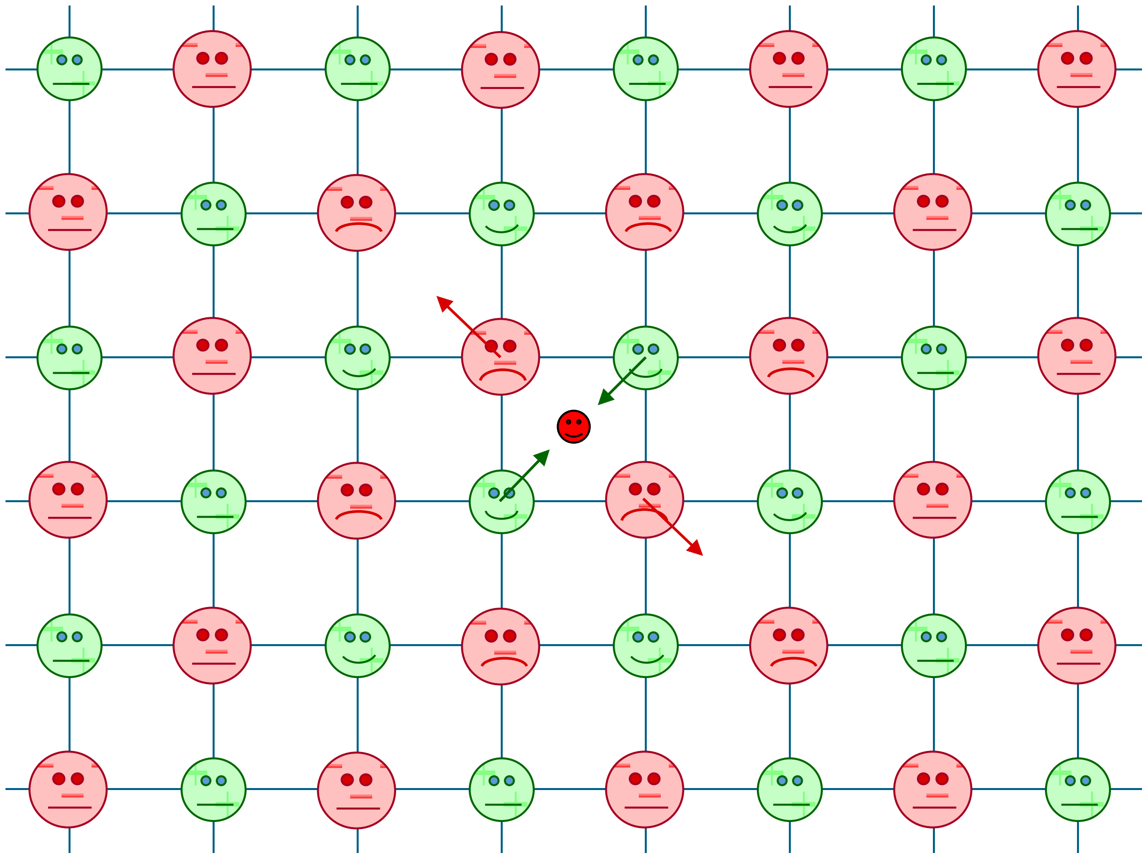

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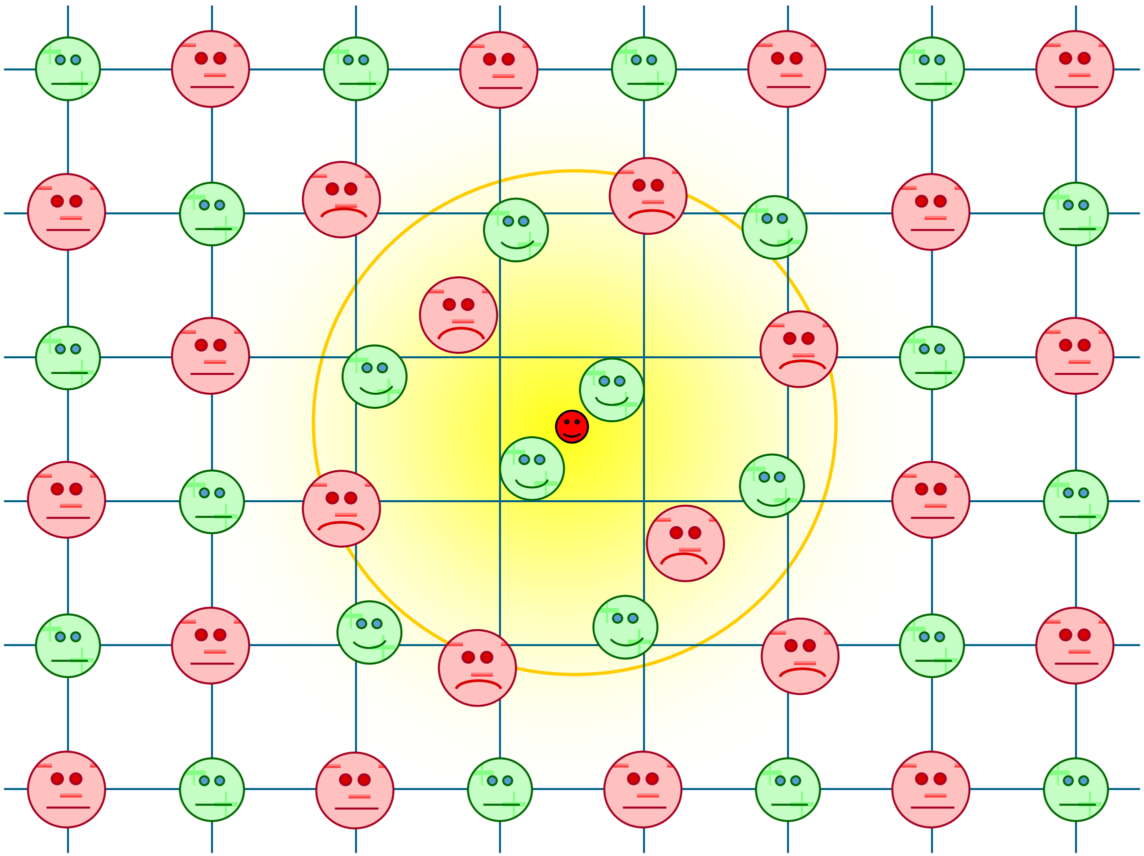
A conduction electron (or hole) together with its self-induced polarization in a polar crystal forms a quasiparticle, which is called a polaron [1-3]



Large vs. small polaron: compare with lattice spacing

[1] L. D. Landau, Phys. Z. Sowjetunion **3**, 664 (1933)
[2] S. I. Pekar, Untersuchungen über die Elektronentheorie der Kristalle, Berlin, Akademie, 1954
[3] H. Fröhlich, Adv. Phys. **3**, 325 (1954)

# Introduction

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img. by J.Ellis

The physical properties of a polaron differ from those of a band-carrier. A polaron is characterized by its binding energy and effective mass and by its characteristic response to external electric and magnetic fields (mobility, optical absorption).

[1] L. D. Landau, Phys. Z. Sowjetunion **3**, 664 (1933)
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# The Fröhlich polaron

Fröhlich[3] derives in 1954 a Hamiltonian for the large polaron,

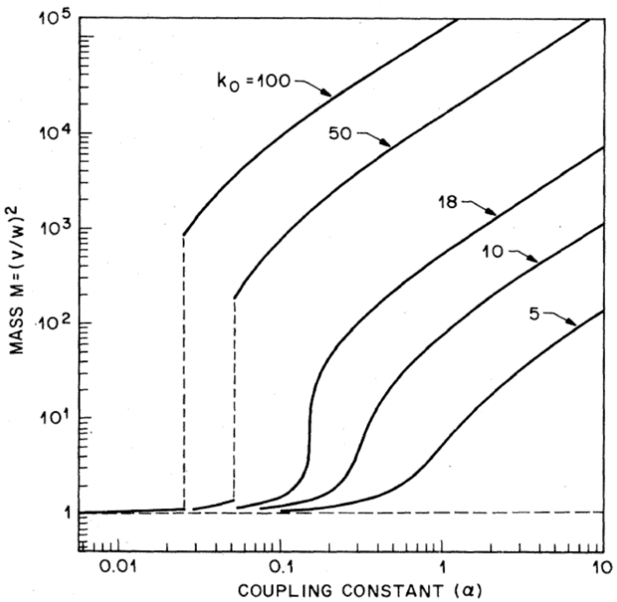
$$\hat{H} = \frac{\hat{p}^2}{2m} + \sum_{\mathbf{k}} V_k \left(\hat{b}_{\mathbf{k}} + \hat{b}^\dagger_{-\mathbf{k}}\right) e^{i\mathbf{k}\cdot\hat{\mathbf{r}}} + \sum_{\mathbf{k}} \hbar\omega_k \hat{b}^\dagger_{\mathbf{k}}\hat{b}_{\mathbf{k}}$$

where the coupling $V_k$ is characterized by a dimensionless coupling constant :

$$\boxed{\alpha = \frac{e^2}{\hbar}\sqrt{\frac{m_b}{2\hbar\omega_{\mathrm{LO}}}}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)}$$

Properties may depend strongly on $\alpha$ !

Example: acoustic polaron effective mass →
[F.M. Peeters, J.T. Devreese, PRB **32**, 3515 (1985)]





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[2] S. I. Pekar, Untersuchungen über die Elektronentheorie der Kristalle, Berlin, Akademie, 1954
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# The Fröhlich polaron at weak and strong coupling

Fröhlich[5] derives in 1954 a Hamiltonian for the large polaron,

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strong coupling (large $\alpha$) expansions[1-4]

$$E^0/\hbar\omega_{\mathrm{LO}} = -0.108513\alpha^2 - 2.836 - \ldots$$
$$m^*/m_b = 1 + 0.0227019\alpha^4 + \ldots$$

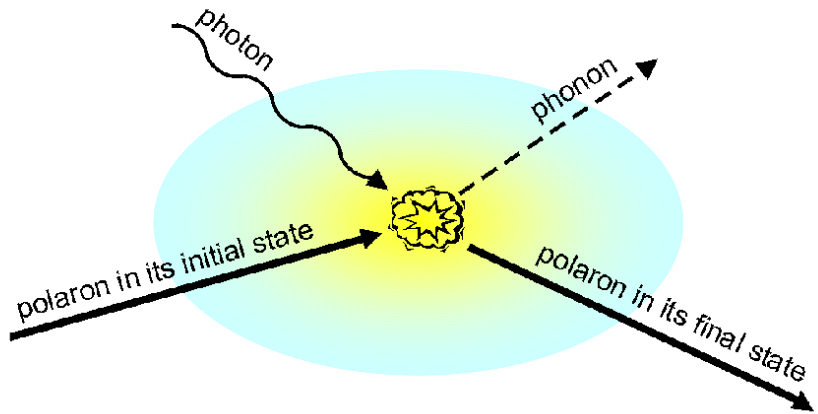
weak coupling (small $\alpha$) expansions[5-8]

$$E^0/\hbar\omega_{\mathrm{LO}} = -\alpha - 0.0159196220\alpha^2 - 0.000806070048\alpha^3 - \ldots$$
$$m^*/m_b = 1 + \frac{1}{6}\alpha + 0.02362763\alpha^2 + \ldots$$


[1] L. D. Landau and S. I. Pekar, Zh. Eksper. Teor. Fiz. **18**, 419 (1948)
[2] S. I. Pekar, *Untersuchungen über die Elektronentheorie der Kristalle*, Akademie Verlag, Berlin, 1951
[3] N. N. Bogolubov, Ukr. Matem. Zh. **2**, 3 (1950)
[4] S. J. Miyake, J. Phys. Soc. Jpn. **38**, 181 (1975)
[5] H. Fröhlich, Adv. Phys. **3**, 325 (1954)
[6] M. A. Smondyrev, Teor. Math. Fiz. **68**, 29 (1986) [English translation: Theor. Math. Phys. **68**, 653 (1986)]
[7] J. Röseler, Phys. Stat. Sol. (b) **25**, 311 (1968)
[8] Wu Xiaoguang, F. M. Peeters, and J. T. Devreese, Phys. Rev. B **31**, 3420 (1985)

# Optical properties of polarons at weak coupling[1,2]

Elementary polaron scattering process




At $T = 0$, the optical absorption coefficient can be expressed in terms of elementary functions in two limiting cases

*High densities*, $\hbar(\Omega - \omega_{LO})/\zeta \ll 1$, where $\zeta$ is the Fermi energy:

$$\Gamma(\omega) = \frac{1}{\epsilon_0 nc} \frac{2^{1/2} N^{2/3} \alpha}{(3\pi^2)^{1/3}} \frac{e^2}{(\hbar m_b \omega_{LO})^{1/2}} \frac{\omega - 1}{\omega^3} \Theta(\omega - 1)$$

*Low densities*, $\hbar(\Omega - \omega_{LO})/\zeta \gg 1$ :

$$\Gamma(\omega) = \frac{1}{\epsilon_0 nc} \frac{2Ne^2\alpha}{3m_b\omega_{LO}} \frac{(\omega - 1)^{1/2}}{\omega^3} \Theta(\omega - 1)$$

where $\omega = \Omega / \omega_{LO}$

[1] V. L. Gurevich, I. G. Lang, and Yu. A. Firsov, Sov. Phys. Solid State **4**, 918 (1962).
[2] J. Devreese, W. Huybrechts, and L. Lemmens, Phys. Stat. Sol. (b) **48**, 77 (1971).

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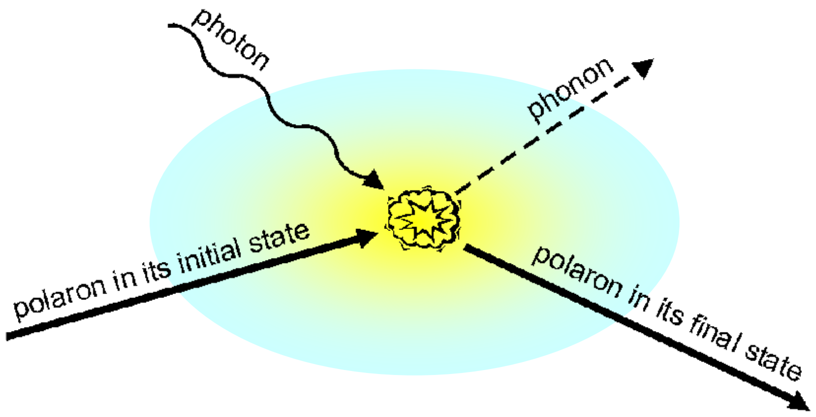


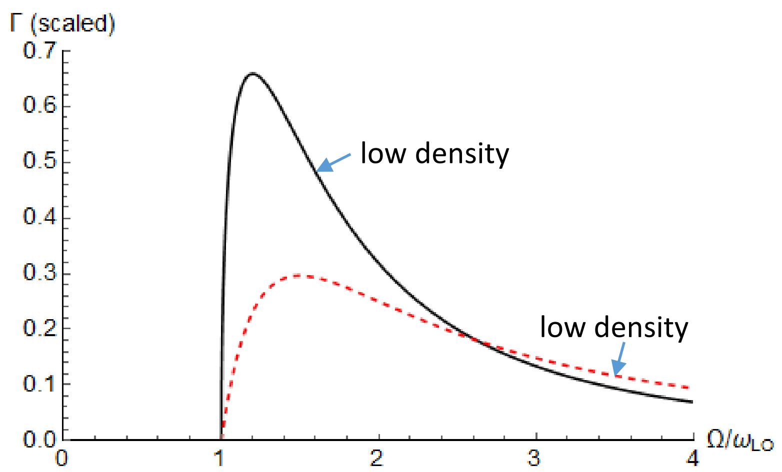


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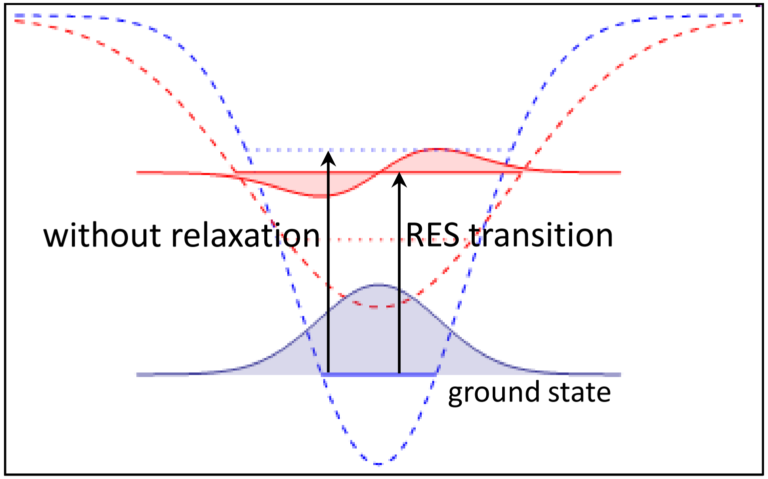
[2] J. Devreese, W. Huybrechts, and L. Lemmens, Phys. Stat. Sol. (b) **48**, 77 (1971).

# Optical properties of polarons at strong coupling[1,2]

At strong coupling, the self-induced potential well for the electron is deep.

Franck-Condon excited states correspond to excitations of the electron in the potential adapted to the ground state

If the lattice polarization is allowed to relax, the relaxed excited state[1, 2] results.




How to reconcile optical absorption results for strong coupling (sharp RES transition peak) and weak coupling (broad absorption band) ?

No known solid has a Fröhlich coupling constant in the strong coupling regime!

[1] R. Evrard, Phys. Lett. **14**, 295 (1965)
[2] J. T. Devreese and R. Evrard, Phys. Lett. **11**, 298 (1966)

# Feynman's all-coupling treatment for the energy

Since the phonon part of the Hamiltonian is quadratic, it can be integrated out exactly, yielding the density matrix (=imaginary time propagator)

$$\rho(0,\beta|0,0) = \int \mathcal{D}\mathbf{r}(\tau)\; e^{-S[\mathbf{r}(\tau)]}$$

as a sum over paths, weighted by the exponential of the action (in units $\hbar = m_b = \omega_{\mathrm{LO}} = 1$)

$$S[\mathbf{r}] = -\frac{1}{2}\int_0^\beta \dot{\mathbf{r}}^2 d\tau + \frac{\alpha}{2^{3/2}}\int_0^\beta\int_0^\beta \frac{\cosh\left(|\tau-\sigma| - \beta/2\right)}{\sinh\left(\beta/2\right)} \frac{1}{|\mathbf{r}(\tau)-\mathbf{r}(\sigma)|} d\tau d\sigma$$

The polaron problem is formulated[1] as an equivalent one-particle problem in which the interaction, non-local in time or "retarded", is between the electron and itself.

This is an all coupling and all temperature $\beta = 1/(k_B T)$ theory.

[1] R. P. Feynman, Phys. Rev. **97**, 660 (1955)

[2] R. P. Feynman, R. W. Hellwarth, C. K. Iddings, and P. M. Platzman, Phys. Rev. **127**, 1004 (1962)

[3] K. K. Thornber and R. P. Feynman, Phys. Rev. B **1**, 4099 (1970)

# The Feynman-Jensen variational principle

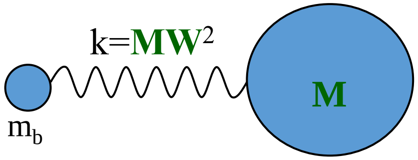
$$\boxed{F \le F_0 + \frac{1}{\beta}\left\langle S - S_0 \right\rangle_{S_0}}$$

Advantages:
- works at finite temperatures
- all-coupling theory
- contains *perturbational* and high-coupling *variational* results

"True" action = Frohlich action:

$$S[\mathbf{r}] = -\frac{1}{2}\int_0^\beta \dot{\mathbf{r}}^2 d\tau + \frac{\alpha}{2^{3/2}}\int_0^\beta\int_0^\beta \frac{\cosh\left(|\tau-\sigma|-\beta/2\right)}{\sinh\left(\beta/2\right)}\frac{1}{|\mathbf{r}(\tau)-\mathbf{r}(\sigma)|}d\tau d\sigma$$

Variational trial action




$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{\hat{P}^2}{2M} + \frac{M\Omega^2}{2}\left(\hat{\mathbf{r}} - \hat{\mathbf{R}}\right)^2$$

$$\begin{aligned} S_0[\mathbf{r}] &= -\frac{1}{2}\int_0^\beta \dot{\mathbf{r}}^2 d\tau \\ &+ \frac{MW^3}{8}\int_0^\beta\int_0^\beta \frac{\cosh\left(W|\tau-\sigma|-\beta/2\right)}{\sinh\left(\beta/2\right)}\left[\mathbf{r}(\tau)-\mathbf{r}(\sigma)\right]^2 d\tau d\sigma \end{aligned}$$

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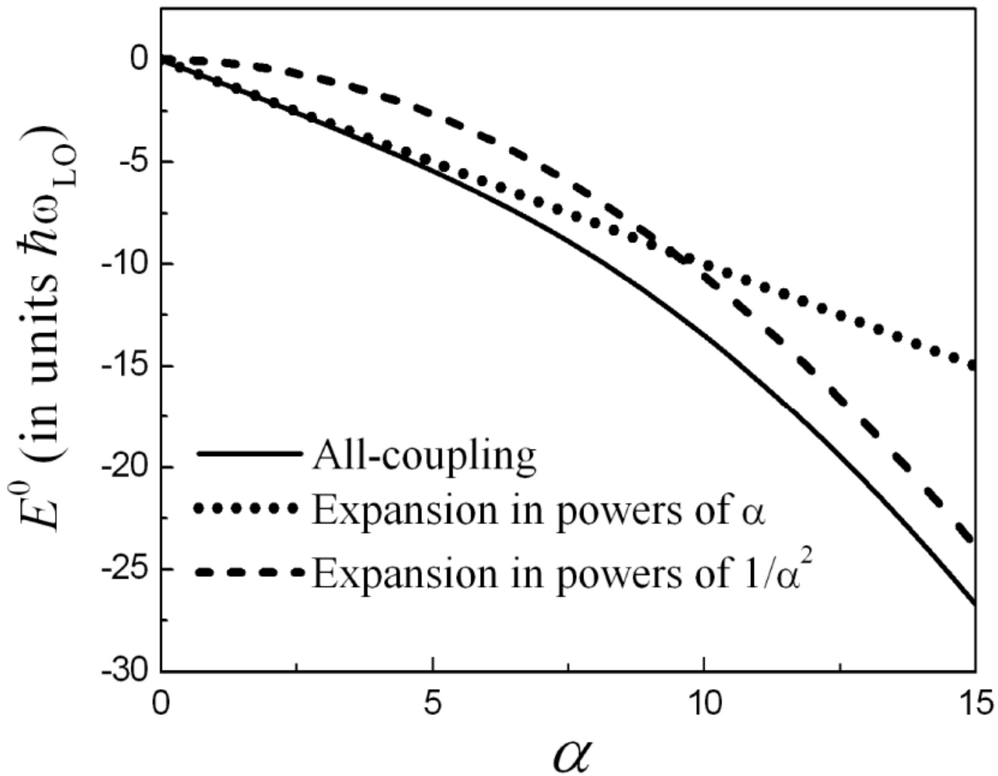


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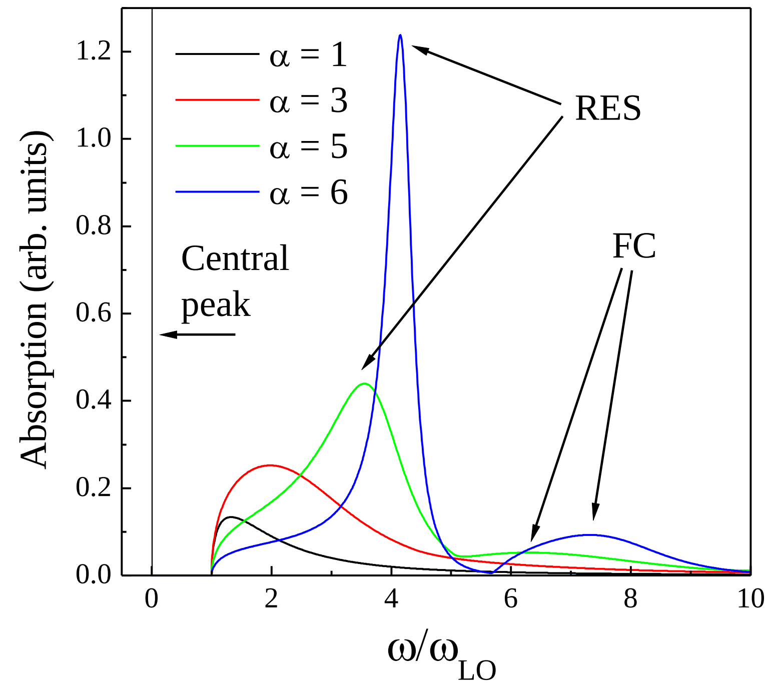
# Single polaron optical absorption at arbitrary coupling

Optical-absorption spectrum of a single large polaron [1]

$$\Gamma_z(\Omega) = \frac{1}{c\epsilon_0 n} \lim_{\beta\to\infty} \frac{\Omega \, \mathrm{Im}\, \chi(\Omega)}{\Omega^4 - 2\Omega^2 \, \mathrm{Re}\, \chi(\Omega) + |\chi(\Omega)|^2}$$

- The memory function $\chi(\omega)$ contains the dynamics of the polaron
- At $T = 0$, there is a $\delta$-like "central peak" at the origin
- For larger $\alpha$, peaks attributed to transitions to RES are more pronounced



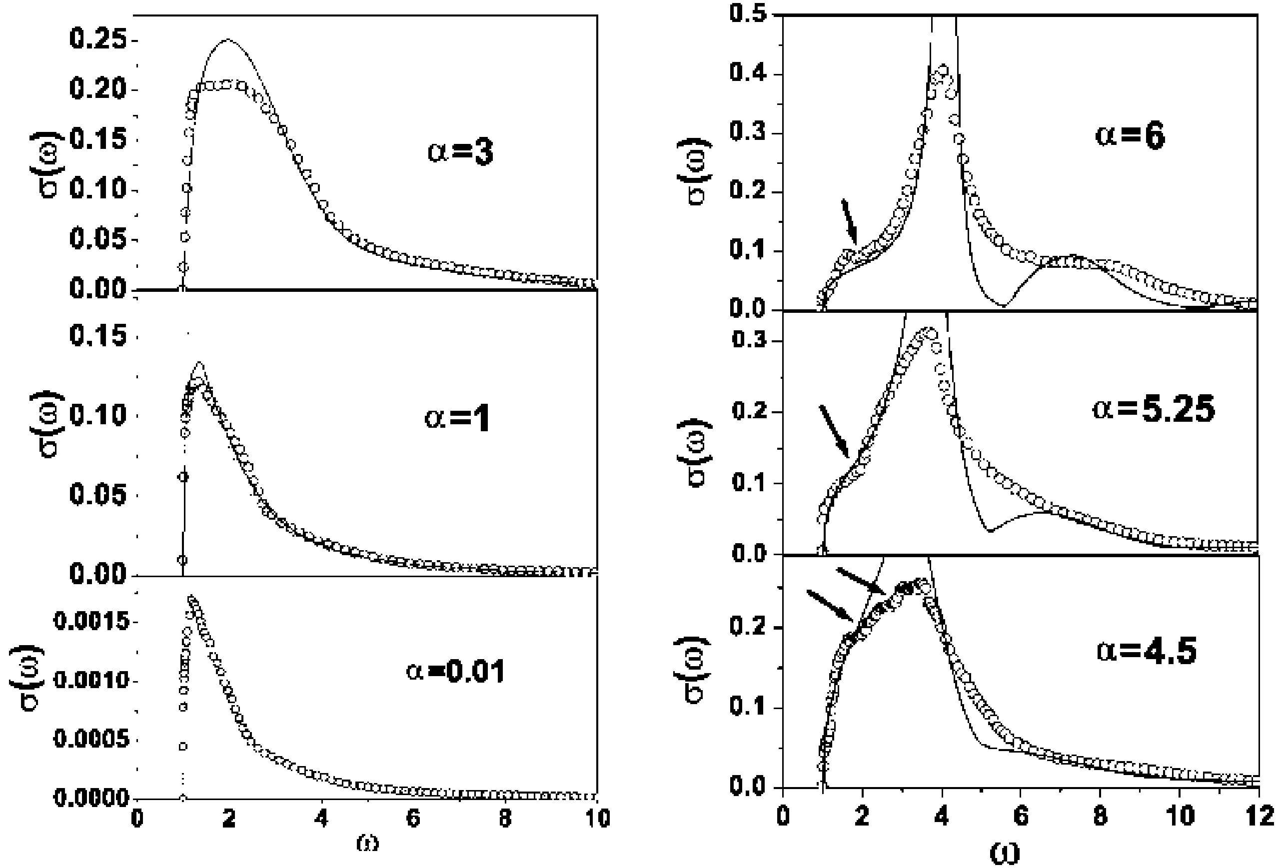

It thus seems that although the FHIP approximation [with expansion of $Z(\Omega)$] gives the gross features of the phonon sidebands, the results are not quantitatively exact. Because the lineshape of the sidebands is related to the lifetime of the RES this would also imply that the shapes of the RES peaks are approximate.

[1] J. Devreese, J. De Sitter, and M. Goovaerts, Phys. Rev. B **5**, 2367 (1972)

# Comparison with diagrammatic Monte-Carlo

DSG approach[1]

Diagrammatic Quantum Monte-Carlo method [2]



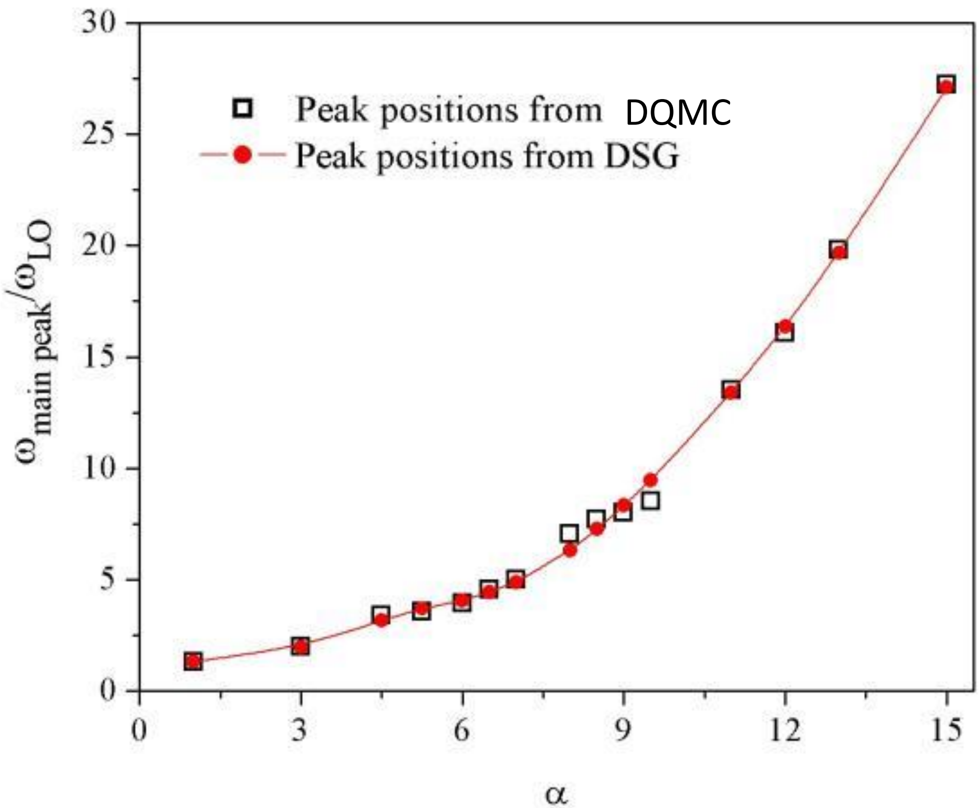

[1] J. Devreese, J. De Sitter, and M. Goovaerts, Phys. Rev. B **5**, 2367 (1972)
[2] A.S. Mishchenko, N. Nagaosa, N. V. Prokof'ev, A. Sakamoto, B. V. Svistunov, Phys. Rev. Lett. **91**, 236401 (2003)
[3] J. T. Devreese and A. S. Alexandrov, *Advances in Polaron Phys*ics, Springer Series in Solid-State Sciences, Vol. 159 (Springer, 2009)

# Comparison with diagrammatic Monte-Carlo

The positions of the main peak of the polaron optical-conductivity band[1], obtained within DSG[2], are in a remarkable agreement with the results of DQMC [3].

The peak width within DSG is smaller than that in DQMC, especially at strong coupling.

The origin of the peak width at strong coupling is not yet understood.

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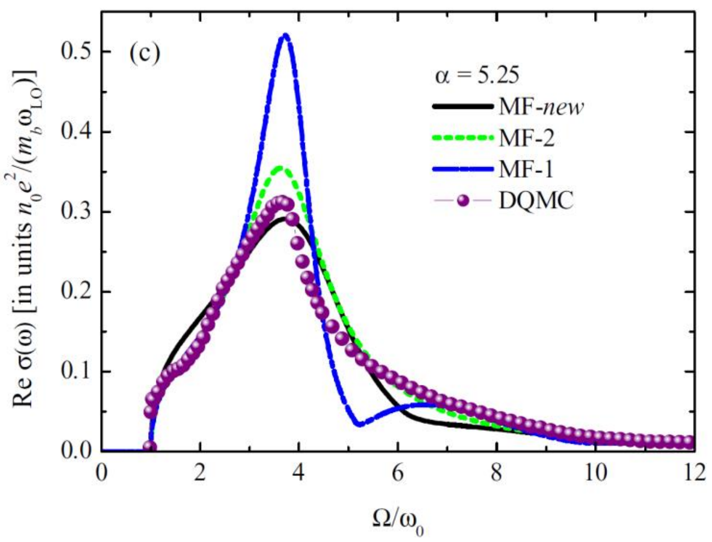
# All coupling approached beyond the adiabatic approximation[1]

***We combined two methods***:

- Weak and intermediate coupling: the memory function formalism with a nonparabolic trial action[1]

- Strong and intermediate coupling: the strong coupling expansion accounting for non-adiabatic transitions[2]




[1] S. N. Klimin, J. Tempere and J. T. Devreese, Phys. Rev. B **94**, 125206 (2016)
[2] S. N. Klimin and J. T. Devreese, Phys. Rev. B **89**, 035201(2014)
[3] J. T. Devreese and A. S. Alexandrov, *Advances in Polaron Phys*ics, Springer Series in Solid-State Sciences, Vol. 159 (Springer, 2009)
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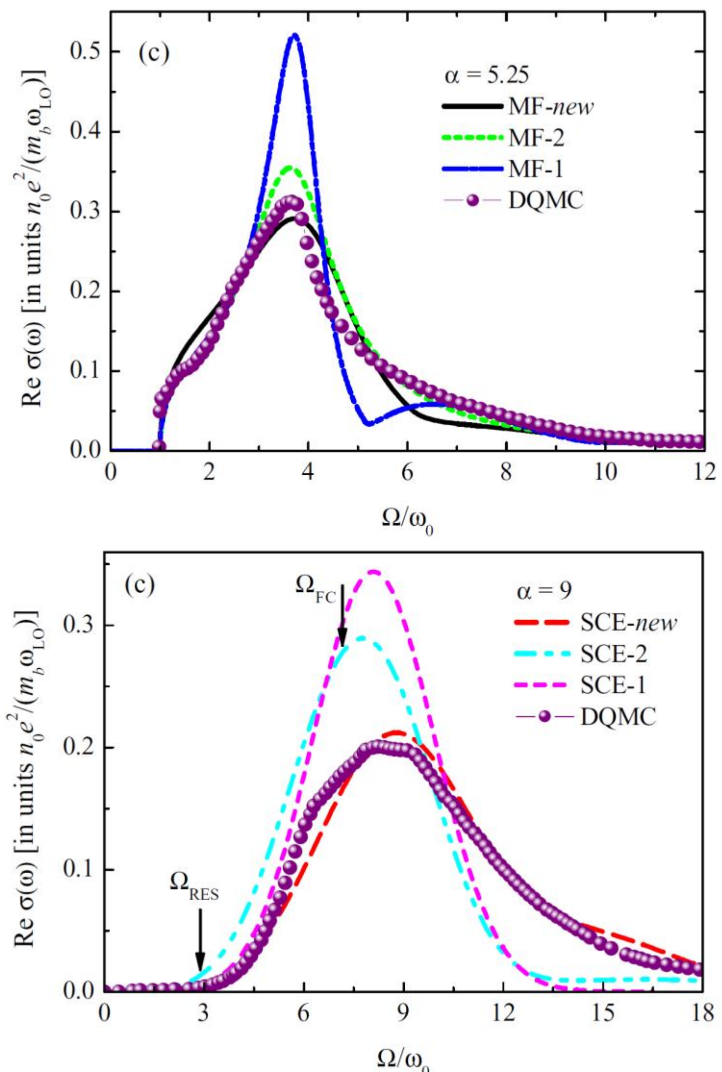


[1] S. N. Klimin, J. Tempere and J. T. Devreese, Phys. Rev. B **94**, 125206 (2016)
[2] S. N. Klimin and J. T. Devreese, Phys. Rev. B **89**, 035201(2014)
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[5] A.S. Mishchenko, N. Nagaosa, N. V. Prokof'ev, A. Sakamoto, and B. V. Svistunov, Phys. Rev. Lett. **91**, 236401 (2003)

# Lattice polarons: the Holstein model

When the electron-phonon coupling strength is driven up, the spatial extension of the polaron becomes comparable to the lattice spacing, and the continuum model at some point is no longer applicable.

The Holstein model model was initially proposed to study molecular crystals[1]. The widely used form of the small polaron Holstein Hamiltonian can be found, e. g., in the recent works [2,3]

$$H = -t \sum_{\langle i,j \rangle} \left( c_i^\dagger c_j + c_j^\dagger c_i \right) + \omega_0 \sum_j a_j^\dagger a_j + g \sum_i c_i^\dagger c_i \left( a_i^\dagger + a_i \right)$$

Here, $t$ is the matrix element for the hopping between sites $i$ and $j$,
$\omega_0$ is the phonon frequency for the $\lambda$-th phonon branch ,
$g$ is the electron-phonon coupling strength

The Holstein Hamiltonian in the momentum representation [2,3]:

$$H = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + \sum_{\mathbf{q}} \hbar\omega_0 a_{\mathbf{q}}^\dagger a_{\mathbf{q}} + \frac{g}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q}} c_{\mathbf{k}-\mathbf{q}}^\dagger c_{\mathbf{k}} \left( a_{\mathbf{q}}^\dagger + a_{-\mathbf{q}} \right)$$

[1] T. Holstein, Ann. Phys. (N.Y.) **8**, 325 (1959); **8**, 343 (1959)
[2] M. Berciu, Phys. Rev. Lett. **97**, 036402 (2006)
[3] G. L. Goodvin, M. Berciu, and G. A. Sawatzky, Phys. Rev. B **74**, 245104 (2006)

# Small polaron transport

From dynamical mean-field theory, three regimes are found for the small polaron DC resistivity.

I. $T<\hbar\omega_0$: heavy particles in a band of renormalized width W, weakly scattered by phonons

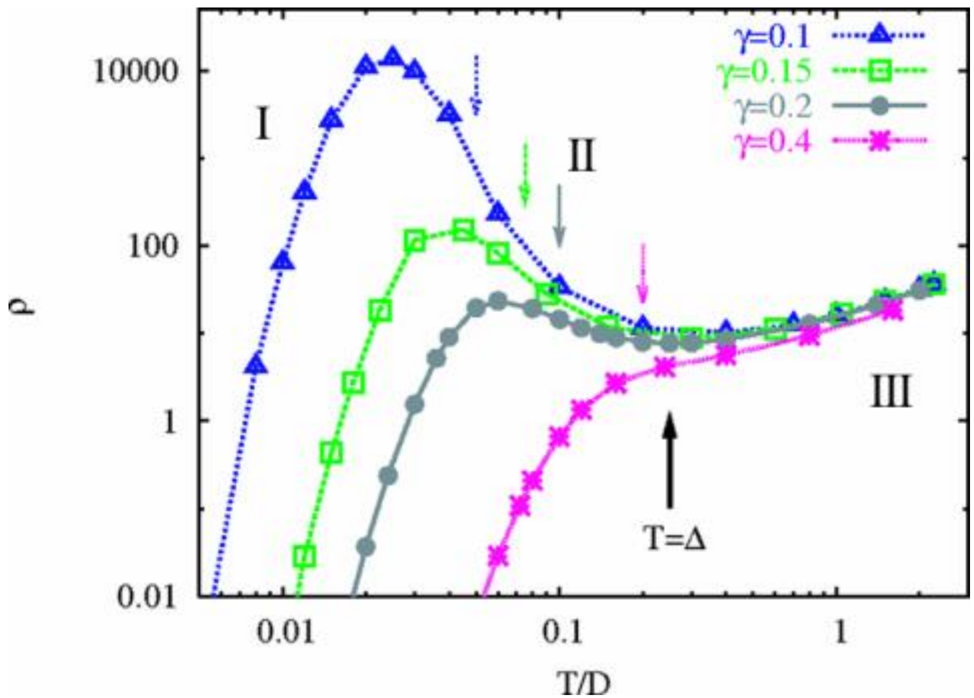
$$\rho \propto \frac{T}{W}\exp\left(-\frac{\hbar\omega_0}{k_B T}\right)$$

II. $\hbar\omega_0<k_B T<E_a$ : Coherent tunnelling breaks down, activated “hopping” sets in

$$\rho \propto e^{E_a/k_B T}$$

III. High temperature: polaron states thermally dissociated

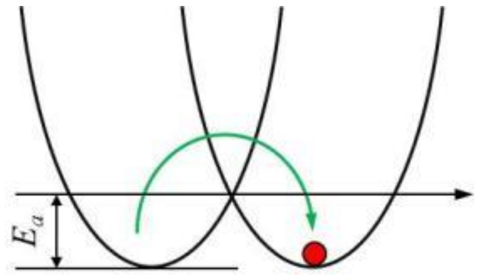
$$\rho \sim T^{3/2}$$




$\gamma$ is the ratio $\gamma = \omega_0/D$ where $D$ is the unrenormalized half bandwidth

S. Fratini and S. Ciuchi, Phys. Rev. Lett. **91**, 256403 (2003)

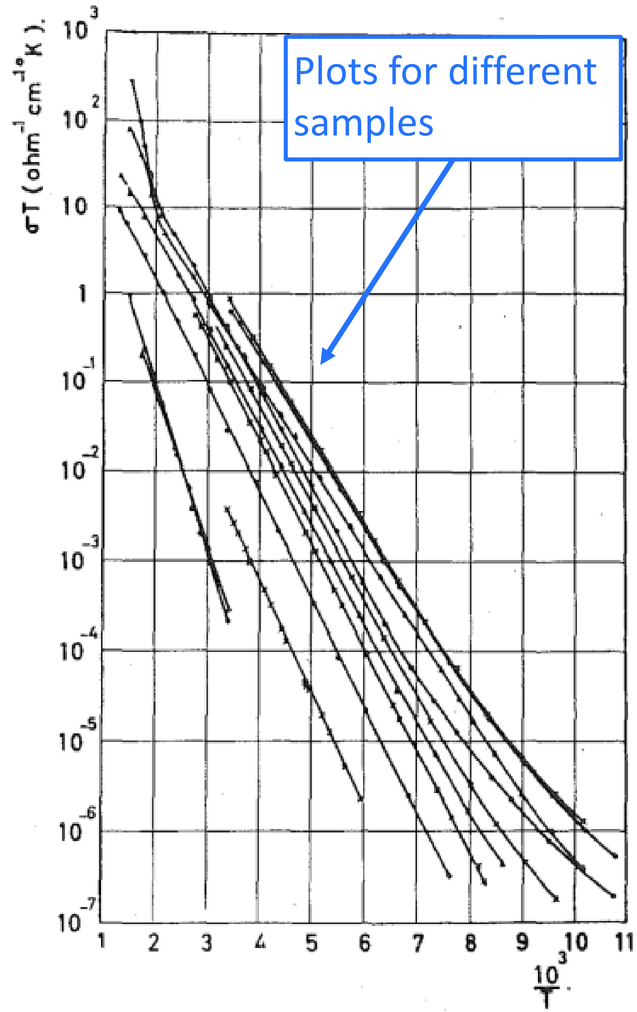
# Thermally activated mobility




II. $\hbar\omega_0 < k_B T < E_a$ : Coherent tunnelling breaks down, activated "hopping" sets in

$$\rho \propto e^{E_a/k_BT}$$

near room temperature

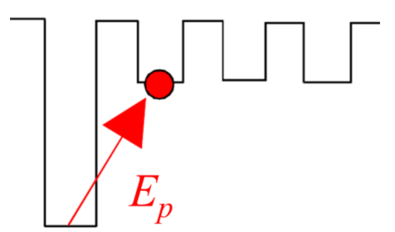



$TiO_2$ : F. J. Morin, Phys. Rev. **93**, 1199 (1954)
$U0_2$ : J. Devreese, *Bull. Soc. Belge de Phys.*, Ser. III, no. 4, 259 (1963)
P. Nagels, M. Denayer, J. Devreese, *Solid State Commun.* **1**, 35 (1963).
P. Nagels, J. Devreese, M. Denayer, *J. Appl. Phys.* **35**, 1175 (1964)
J. Devreese, R. De Coninck, H. Pollak, *Phys. Stat. Sol.* **17**, 825 (1966)
R. De Coninck, J. Devreese, *Phys. Stat. Sol.* **32**, 823 (1969)

# Optical absorption of small polarons

*Early theory (Reik)*

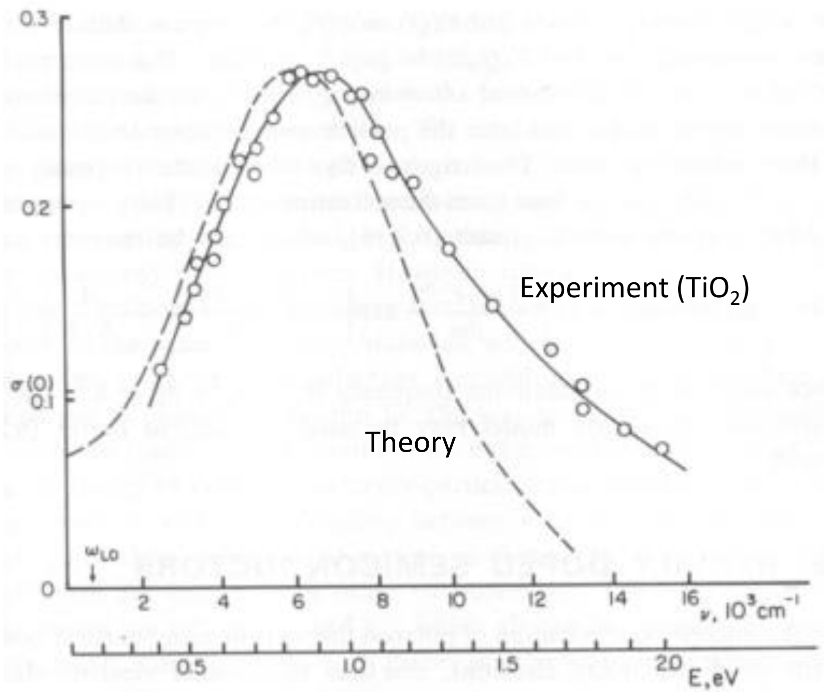
*Photoionization of a small polaron*:




$$\mathrm{Re}\,\sigma(\omega,T) = \sigma(0,T)\,\frac{\sinh\left(\frac{\hbar\omega}{k_B T}\right)}{\frac{\hbar\omega}{k_B T}}\, e^{-\frac{\hbar^2\omega^2}{16 U k_B T}}$$

activation energy

A self-trapped carrier is excited from its localized state to a localized state at a site adjacent to the small polaron's  site.

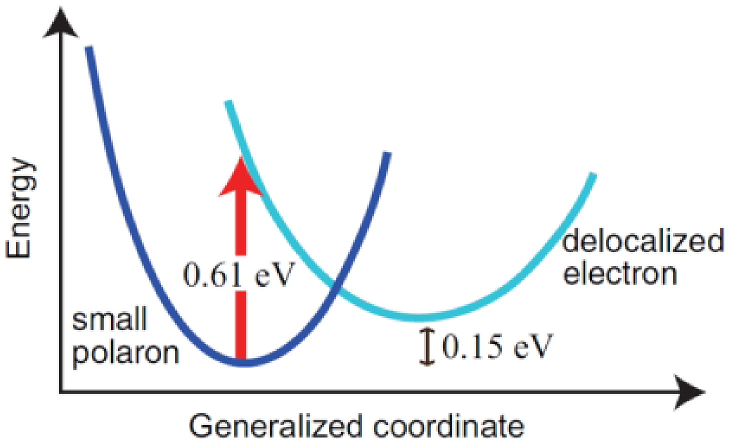




H. Reik, Z. Phys. **203**, 346 (1967)
H. Reik, in Polarons in Ionic Crystals and Polar Semiconductors (North-Holland, Amsterdam, 1972), pp. 679- 714
E. K. Kudinov, D. N. Mirlin and Yu. A. Firsov, Sov. Phys. Solid State **11**, 2257 (1970)
S. Fratini and S. Ciuchi, Phys. Rev. Lett. **91**, 256403

# Small and large polarons in TiO2: recent studies

*Excitation and migration mechanism for a small polaron in $TiO_2$*




Problem:

- optical & spin response indicates small polarons[1]
- mobility indicates large polarons[2]

Solution[3]:

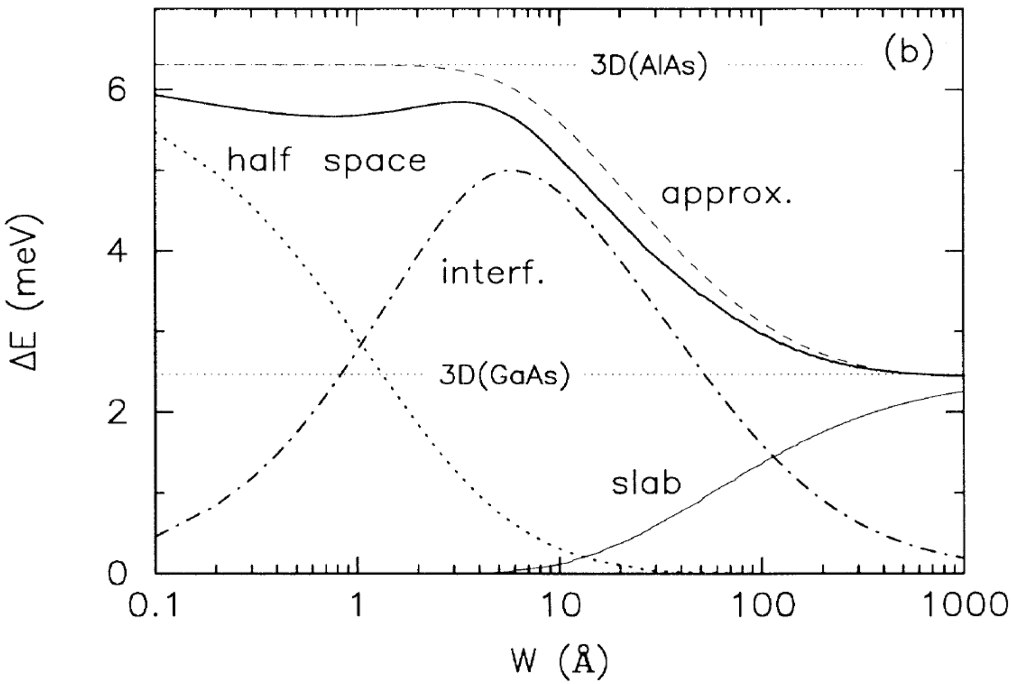
Coexistence of small polarons with delocalized electrons at nearly the same energy.

[1] D. M. Eagles, J. Phys. Chem. Solids25, 1243 (1964).
[2] E. Yagi, R. R. Hasiguti, M. Aono, Phys. Rev. B54, 7945 (1996).
[3] A. Janotti, C. Franchini, J. B. Varley, G. Kresse, and C. G. Van de Walle, Phys. Status Solidi RRL **7**, 199 (2013).

# Polarons in quantum wells

## *Types of optical phonons in QW*

- Confined slab modes
- Interface modes
- Half-space modes




*Contributions to the polaron binding energy in QW (from Ref. 13) as functions of the QW width*

***Some key works***


1. L. Wendler, PSS B **129**, 513 (1985)
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3. N. Mori and T. Ando, PRB **40**, 6175 (1989)
4. K. Huang and B. F. Zhu, PRB **38**, 13377 (1988)
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7. M. H. Degani and O. Hipolito, PRB **35**, 7717 (1987)
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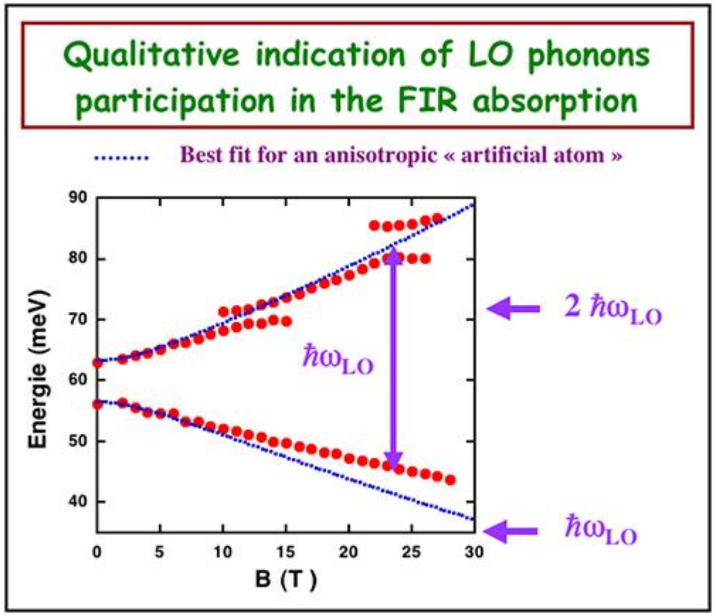
12. S. Adachi, J. Appl. Phys. **58**, R1 (1985)
13. G. Q. Hai, F. M. Peeters, and J. T. Devreese, PRB **48**, 4666 (1993)

# Polarons in quantum dots

## *Types of optical phonons in QD*

- Confined modes
- Interface modes
- Bulk modes

Magneto-optical transitions in self-asssembled InAs QDs: polaron theory vs experiment
[From: *R. Ferreira and G. Bastard, Capture and Relaxation in Self-Assembled Semiconductor Quantum Dots*, IOP, 29015]




*Some key works*


1. R. Englman and R. Ruppin, J. Phys. C **1**, 614 (1968)
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11. R. Fuchs and K.L. Kliewer, Phys. Rev. **140**, A2076 (1965)
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13. A.A. Lucas, E. Kartheuser, and R.G. Badro, Phys. Rev. B **41**, 1439 (1990)
14. L. Wendler, Phys. Status Solidi B **129**, 513 (1985)

# Outline

Part I  Origins - the “traditional polaron”: an electron in a bath of phonons
1. The Fröhlich or “large” polaron
2. Polaron signatures: response (optical absorption)
3. Holstein or “small” polarons
4. Polarons in nanostructures

Part II:  Polaronic effects in a broader sense: four examples
1. Ripplopolaron
2. Bose polaron
3. Excitonic polaron
4. Angulon

Part III:  From one to many: interacting polarons
1. Many-polaron optical absorption
2. Bipolarons

# From electrons in polar solids to a generic model system

The polaron concept has become a generic many-body model that describes a particle interacting with a bath of bosons through absorption or emission of these bosons.

Four examples:

- The ripplopolaron
- The Bose polaron
- Excitonic polarons
- Angulons

# From electrons in polar solids to a generic model system

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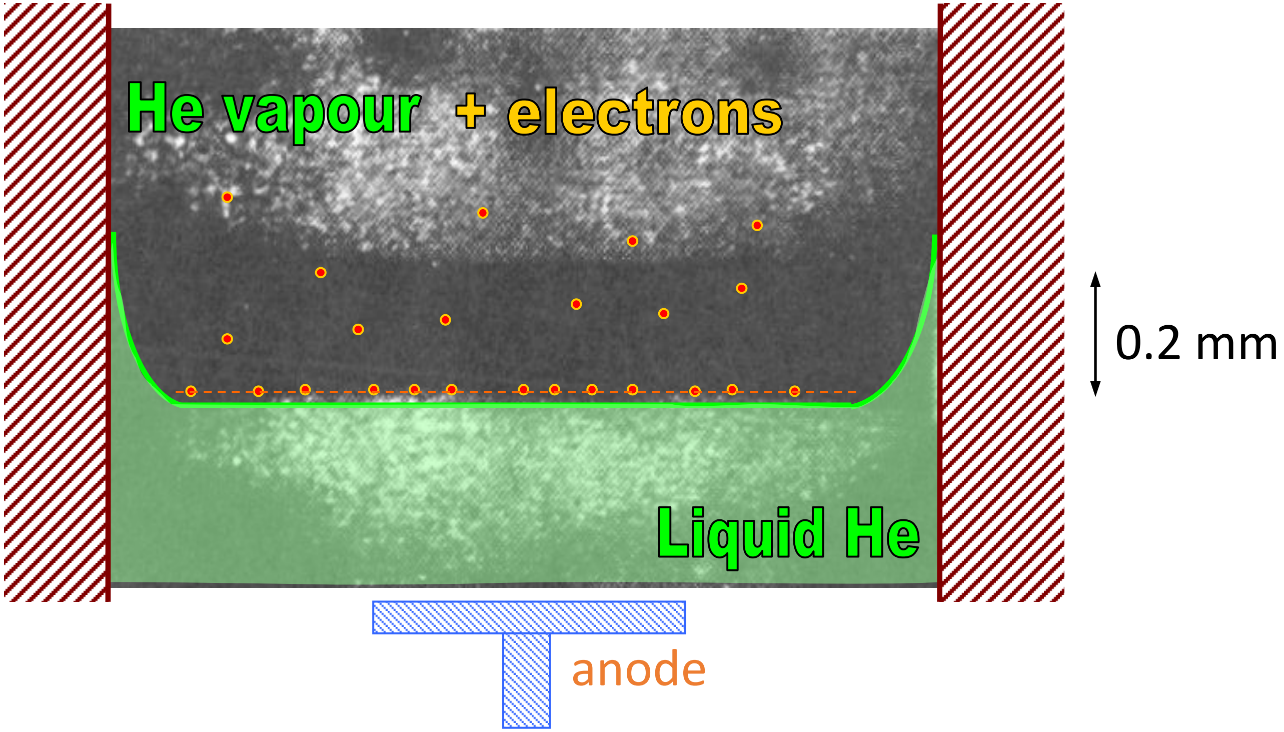
Example: the **ripplopolaron**

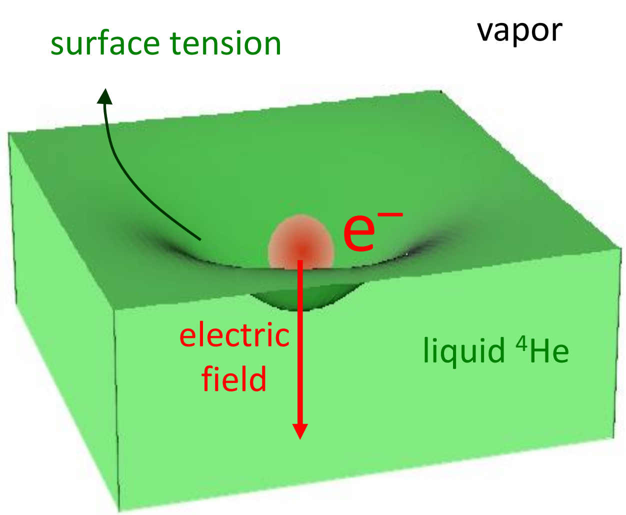



[1] M. W. Cole, Rev. Mod. Phys. **46**, 451 (1974).
[2] *Two-Dimensional Electron Systems on Helium and other Cryogenic Substrates* (ed. E. Y. Andrei, Kluwer Acad. Publ, Dordrecht, The Netherlands, 1997).

# From electrons in polar solids to a generic model system

The polaron concept has become a generic many-body model that describes a particle interacting with a bath of bosons through absorption or emission of these bosons.

Example: the **ripplopolaron**[1-3]




wigner lattice potential

ripplon dispersion $\omega(q) = q\sqrt{\sigma q/\rho}$

$$\hat{H} = \frac{\hat{p}^2}{2m_\mathrm{e}} + V_\mathrm{lat}\left(\hat{\mathbf{r}}\right) + \sum_{\mathbf{q}} \hbar\omega(q)\hat{a}^+_{\mathbf{q}}\hat{a}_{\mathbf{q}} + \sum_{\mathbf{q}} M_q \mathrm{e}^{-\mathrm{i}\mathbf{q}.\mathbf{r}}\left(\hat{a}_{\mathbf{q}} + \hat{a}^+_{-\mathbf{q}}\right),$$

electron-ripplon interaction

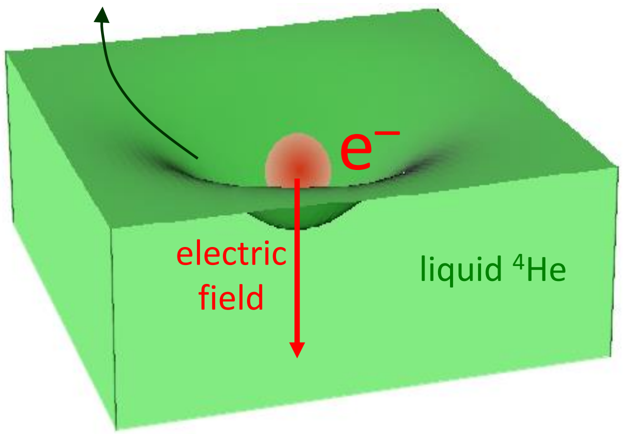
$$M_{\mathbf{q}} = \pi\frac{n\alpha \mathrm{e}^2\lambda^2}{4}A^{-1/2}\sqrt{\frac{\hbar q}{2\rho_\mathrm{He}\omega_{\mathbf{q}}}}$$

[1] O.Hipolito, G.A.Farias, and N.Studart, Surf. Sci. **113**, 394 (1982).
[2] S. A. Jackson and P. M. Platzman, Phys. Rev. B **24**, 499 (1981).
[3] G.E. Marques, N. Studart, Phys. Rev. B **39**, 4133 (1989).

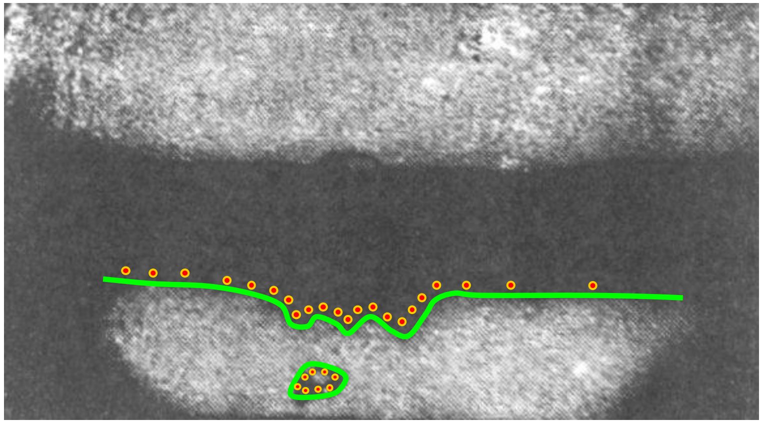
# Strong coupling ripplopolarons ?

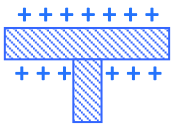
The polaron concept has become a generic many-body model that describes a particle interacting with a bath of bosons through absorption or emission of these bosons.

Example: the **ripplopolaron**[1-3]




Difficulty to reach the strong-coupling regime: the helium surface becomes unstable





[1] O.Hipolito, G.A.Farias, and N.Studart, Surf. Sci. **113**, 394 (1982).
[2] S. A. Jackson and P. M. Platzman, Phys. Rev. B **24**, 499 (1981).
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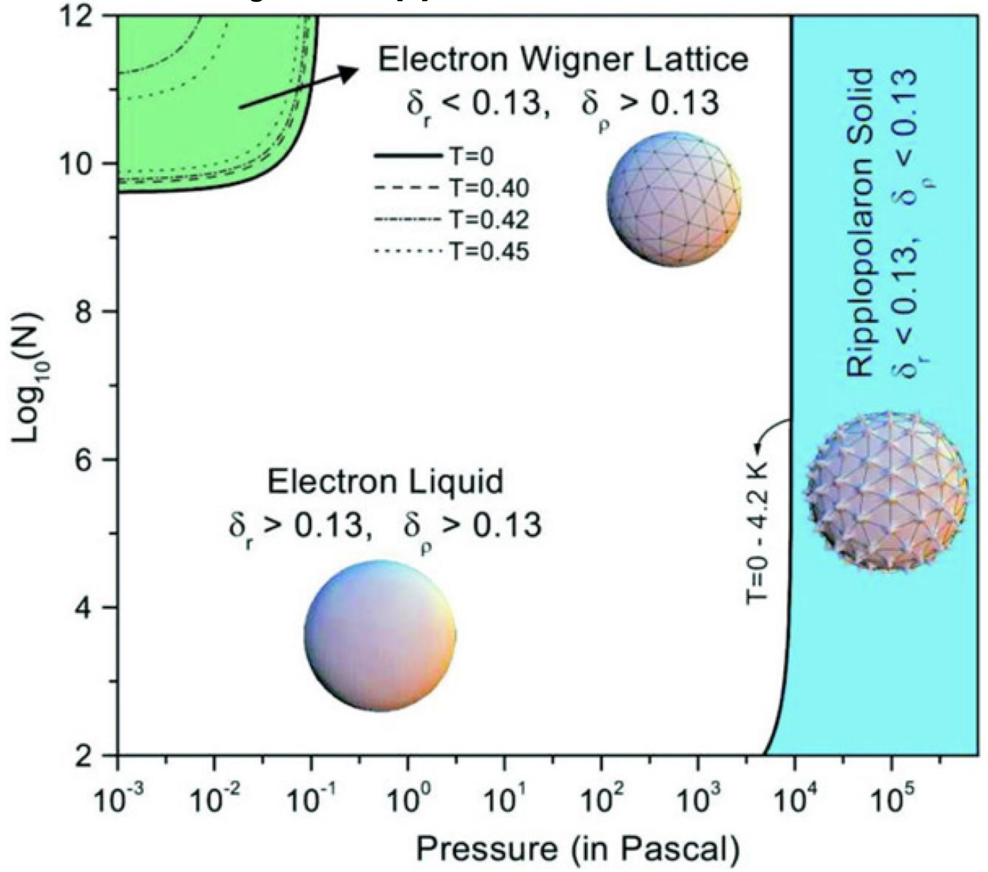
A.P. Volodin, M.S. Khaikin, and V.S. Edelman, JETP **26**, 543 (1977).
U. Albrecht and P. Leiderer, Europhys. Lett. **3**, 705 (1987).
M. M. Salomaa, and G. A. Williams, Phys.Rev. Lett. **47**, 1730 (1981).

# Ripplopolarons in multielectron bubbles

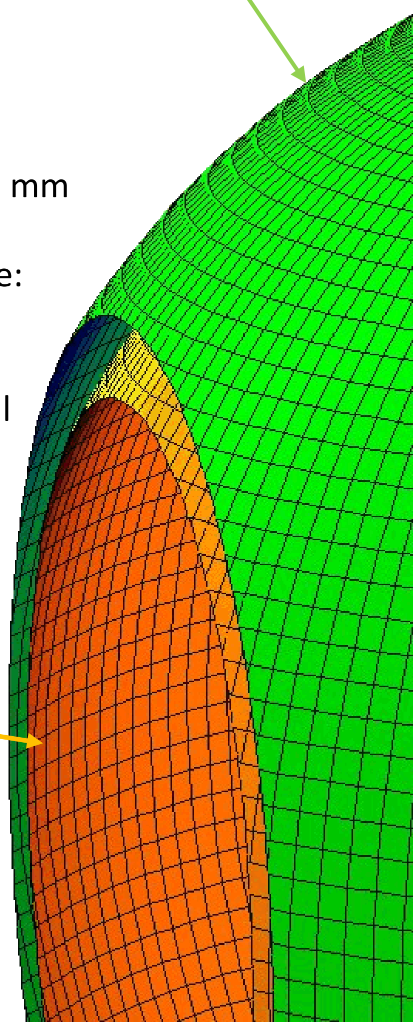
Phase diagram from [2]




typical size:
0.1 μm - 0.1 mm

typical charge:
$10^3$ - $10^8$ e

typical e-shell thickness:
~ 1 nm





[1] S.N. Klimin, V.M. Fomin, 1, J. Tempere, I.F. Silvera, J.T. Devreese, Solid St. Comm. 126 (2003) 409.
[2] J. Tempere, S.N. Klimin, I.F. Silvera, J.T. Devreese, Eur. Phys. J. B 32 (2003) 329.

# From electrons in polar solids to a generic model system

The polaron concept has become a generic many-body model that describes a particle interacting with a bath of bosons through absorption or emission of these bosons.

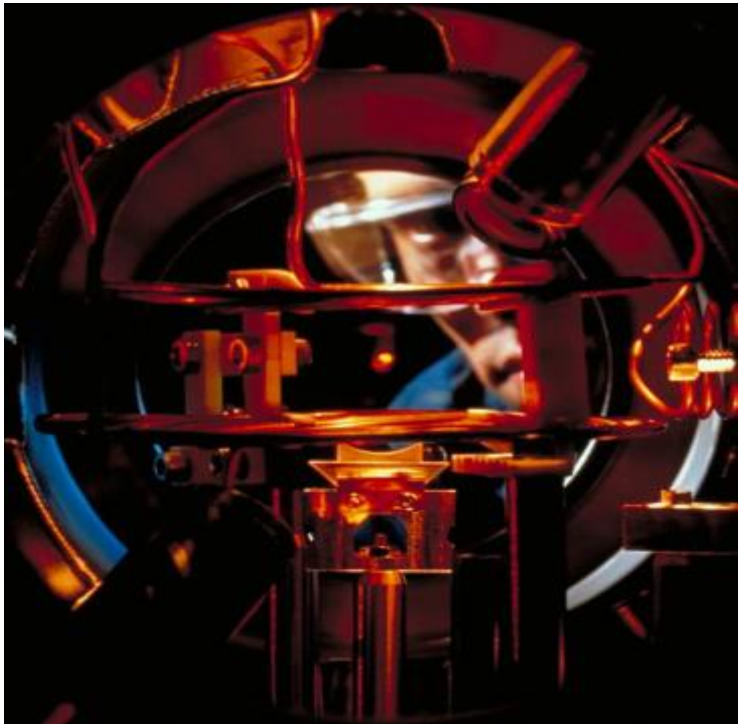
The quest for strong coupling without a lattice and the "**BEC polaron**" [1-2]

Interacting bose gas

$$\hat{H} = \frac{\hat{p}^2}{2m_I} + \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \hat{a}^{\dagger}_{\mathbf{k}} \hat{a}_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{BB}(\mathbf{q}) \hat{a}^{\dagger}_{\mathbf{k}'-\mathbf{q}} \hat{a}^{\dagger}_{\mathbf{k}+\mathbf{q}} \hat{a}_{\mathbf{k}} \hat{a}_{\mathbf{k}'}$$

$$+ \sum_{\mathbf{k},\mathbf{q}} V_{IB}(\mathbf{q}) \hat{\rho}_I(\mathbf{q}) \hat{a}^{\dagger}_{\mathbf{k}'-\mathbf{q}} \hat{a}_{\mathbf{k}'}$$

Interatomic interaction between
Impurity and bosonic atoms



[1] F. M. Cucchietti and E. Timmermans, Phys. Rev. Lett. **96**, 210401 (2006).
[2] J. Tempere, W. Casteels, M. K. Oberthaler, S. Knoop, E. Timmermans, and J. T. Devreese, Phys. Rev. B **80**, 184504 (2009).

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The quest for strong coupling without a lattice and the "**BEC polaron**" [1-2]

In the Bogoliubov approximation, the Hamiltionian maps onto a Frohlich form:

$$\hat{H}_{pol} = \frac{\hat{p}^2}{2m_I} + \sum_{\mathbf{k}\neq 0} \hbar\omega_{\mathbf{k}} \hat{b}^{\dagger}_{\mathbf{k}} \hat{b}_{\mathbf{k}} + \sum_{\mathbf{k}\neq 0} V_{\mathbf{k}} e^{i\mathbf{k}\cdot\hat{\mathbf{r}}} (\hat{b}_{\mathbf{k}} + \hat{b}^{\dagger}_{-\mathbf{k}})$$

Bogoliubov dispersion

$$\hbar\omega_{\mathbf{k}} = ck\sqrt{1 + (\xi k)^2/2}$$

Interaction

$$V_{\mathbf{k}} = \sqrt{N_0}\left[\frac{(\xi k)^2}{(\xi k)^2 + 2}\right]^{1/4} g_{IB}$$

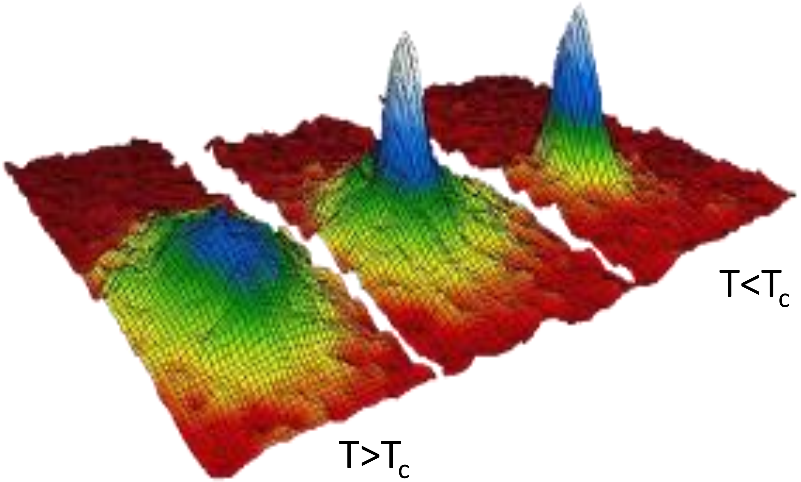
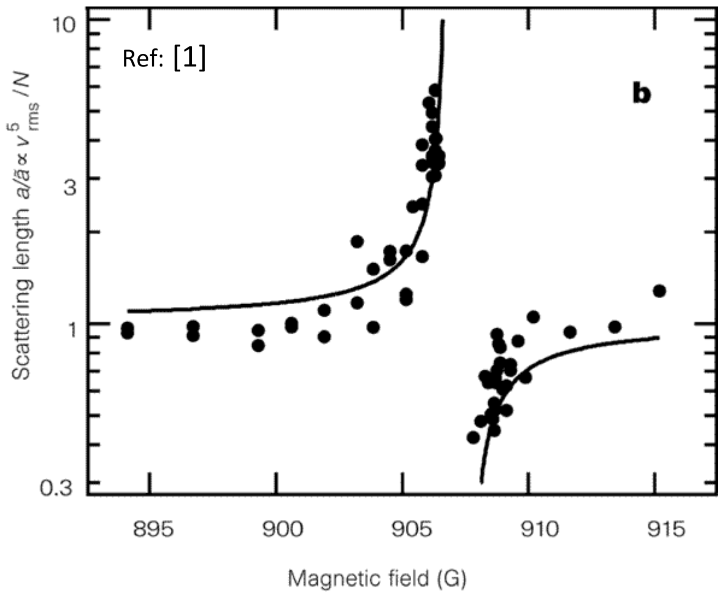


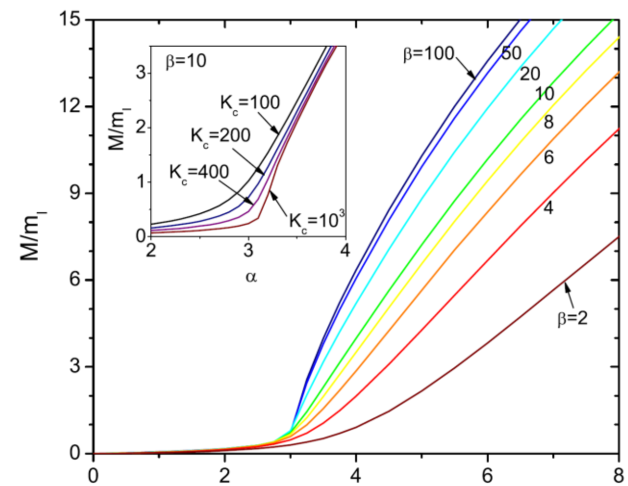

Image source: JILA BEC & Ultracold atoms

[1] F. M. Cucchietti and E. Timmermans, Phys. Rev. Lett. **96**, 210401 (2006).
[2] J. Tempere, W. Casteels, M. K. Oberthaler, S. Knoop, E. Timmermans, and J. T. Devreese, Phys. Rev. B **80**, 184504 (2009).

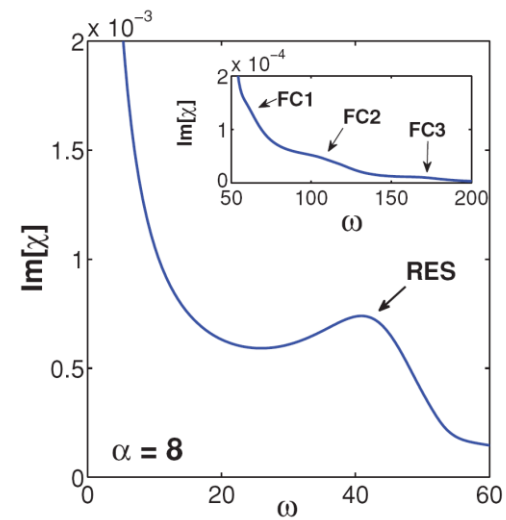
# Feshbach resonances

In ultracold atomic gases, the interatomic scattering lengths can be experimentally modified.
This leads to a tunable Fröhlich coupling constant in this system: $\alpha = a_{IB}^2/(a_{BB}\xi)$




Ref: [2]



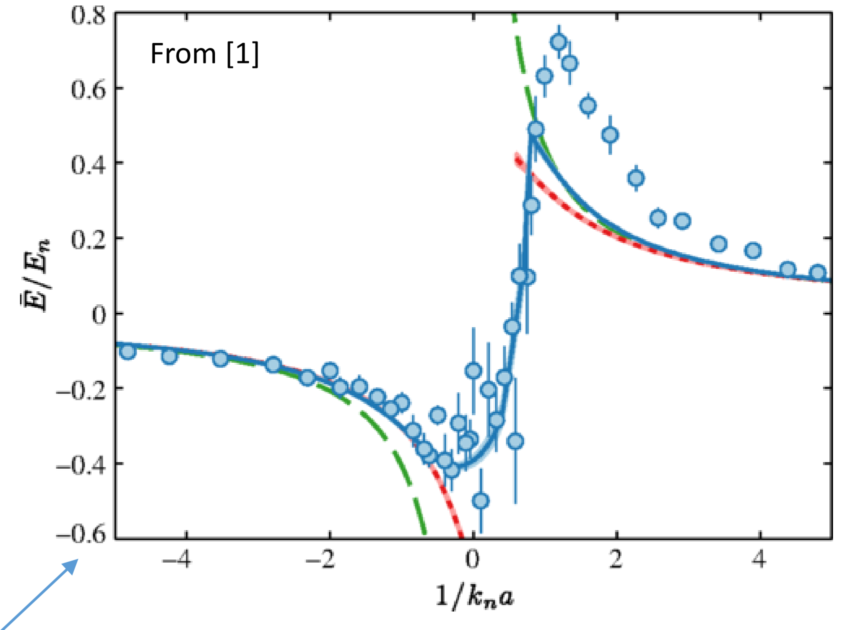

Ref: [3]

[1] S. Inouye et al., Nature **392**, 151 (1998).
[2] J. Tempere, W. Casteels, M. K. Oberthaler, S. Knoop, E. Timmermans, and J. T. Devreese, Phys. Rev. B **80**, 184504 (2009)
[3] W. Casteels, J. Tempere, and J. T. Devreese, Phys. Rev. A **84**, 063612 (2011).

# Experimental observation of Bose polarons

Processes beyond those included in the Frohlich model cannot be neglected!

- Vertices that couple the impurity to two phonons
- Not just coupling to unbound (free phonon) states, also negative bound-energy states matter




<u>Seminal Bose ppolaron experiments in quantum gases:</u>

[1] N. B. Jorgensen, L. Wacker, K. T.Skalmstang, M. M. Parish, J. Levinsen, R. S. Christensen, G. M. Bruun, and J. J. Arlt, Phys. Rev. Lett. **117**, 055302 (2016).
[2] M.-G. Hu, M.J. Van de Graaff, D. Kedar, J.P. Corson, E.A. Cornell, and D.S. Jin, Phys. Rev. Lett. **117**, 055301 (2016).

<u>Additional cold gas experiments :</u>

**Rydberg atoms** («very large» polaron) : F. Camargo, R. Schmidt, J. D. Whalen, R. Ding, G. Woehl Jr., S. Yoshida, J. Burgdörfer,
F. B. Dunning, H. R. Sadeghpour, E. Demler, T. C. Killian, Phys. Rev. Lett. 120, 083401 (2018)

**Polaron mass measurement**: T. Rentrop, A. Trautmann, F. A. Olivares, F. Jendrzejewski, A. Komnik, and M. K. Oberthaler Phys. Rev. X 6, 041041 (2016).

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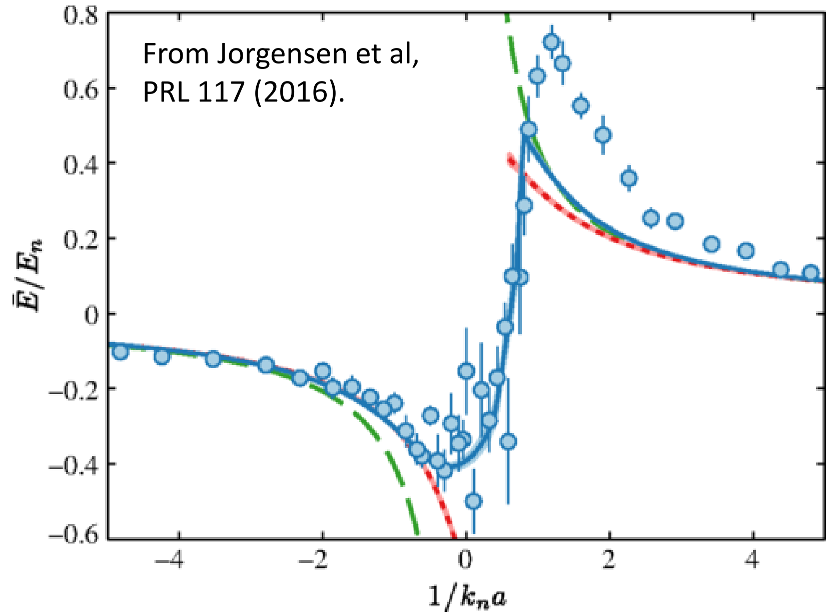


A selection of theory papers:

S. P. Rath and R. Schmidt, Phys. Rev. A88, 053632 (2013).
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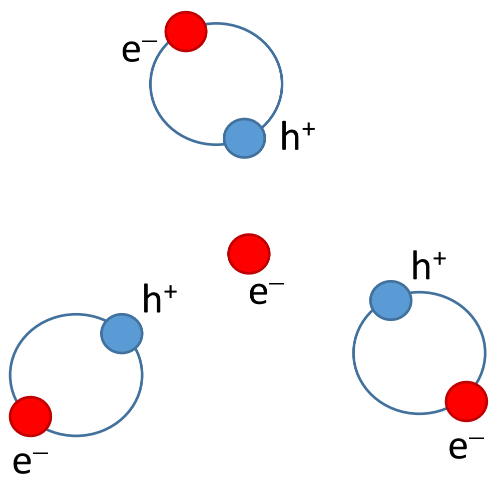
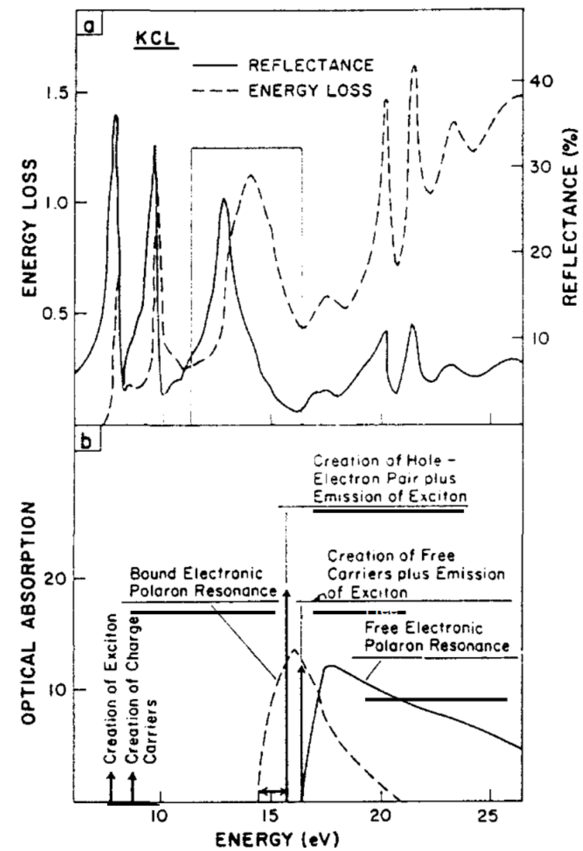
R. S. Christensen, J. Levinsen, and G. M. Bruun, Phys. Rev. Lett.115, 160401 (2015).
F. Grusdt, Y. E. Shchadilova, A. N. Rubtsov, and E. Demler, Scientific Reports5, 12124 EP (2015)
J. Levinsen, M. M. Parish, and G. M. Bruun, Phys. Rev. Lett.115, 125302 (2015).
L. A. Pena Ardila and S. Giorgini, Phys. Rev. A 92, 033612 (2015).
Y. E. Shchadilova, R. Schmidt, F. Grusdt, and E. Demler, Phys. Rev. Lett. 117, 113002 (2016).
Y. E. Shchadilova, F. Grusdt, A. N. Rubtsov, and E. Demler, Phys. Rev. A93, 043606 (2016).
F. Grusdt, Phys. Rev. B93, 144302 (2016).
F. Grusdt, R. Schmidt, Y. E. Shchadilova, and E. Demler, Phys. Rev. A 96, 013607 (2017).
S. Van Loon, W. Casteels, and J. Tempere, Phys. Rev. A 98, 063631 (2018).
R. Schmidt, J. D. Whalen, R. Ding, F. Camargo, G. Woehl, S. Yoshida, J. Burgd˙orfer, F. B. Dunning, E. Demler,H. R. Sadeghpour, and T. C. Killian, Phys. Rev. A97, 022707 (2018).
L. A. P. Ardila and T. Pohl, Journal of Physics B: Atomic, Molecular and Optical Physics 52, 015004 (2018).
L. A. Pena Ardila, N. B. Jørgensen, T. Pohl, S. Giorgini, G. M. Bruun, and J. J. Arlt, Phys. Rev. A 99, 063607(2019).

# The "electronic" or "exciton-" polaron

The polaron concept has become a generic many-body model that describes a particle interacting with a bath of bosons through absorption or emission of these bosons.

Back in solids, any source of polarization can contribute to a polaronic effect: virtual excitons can take the role of the phonons[1-2].

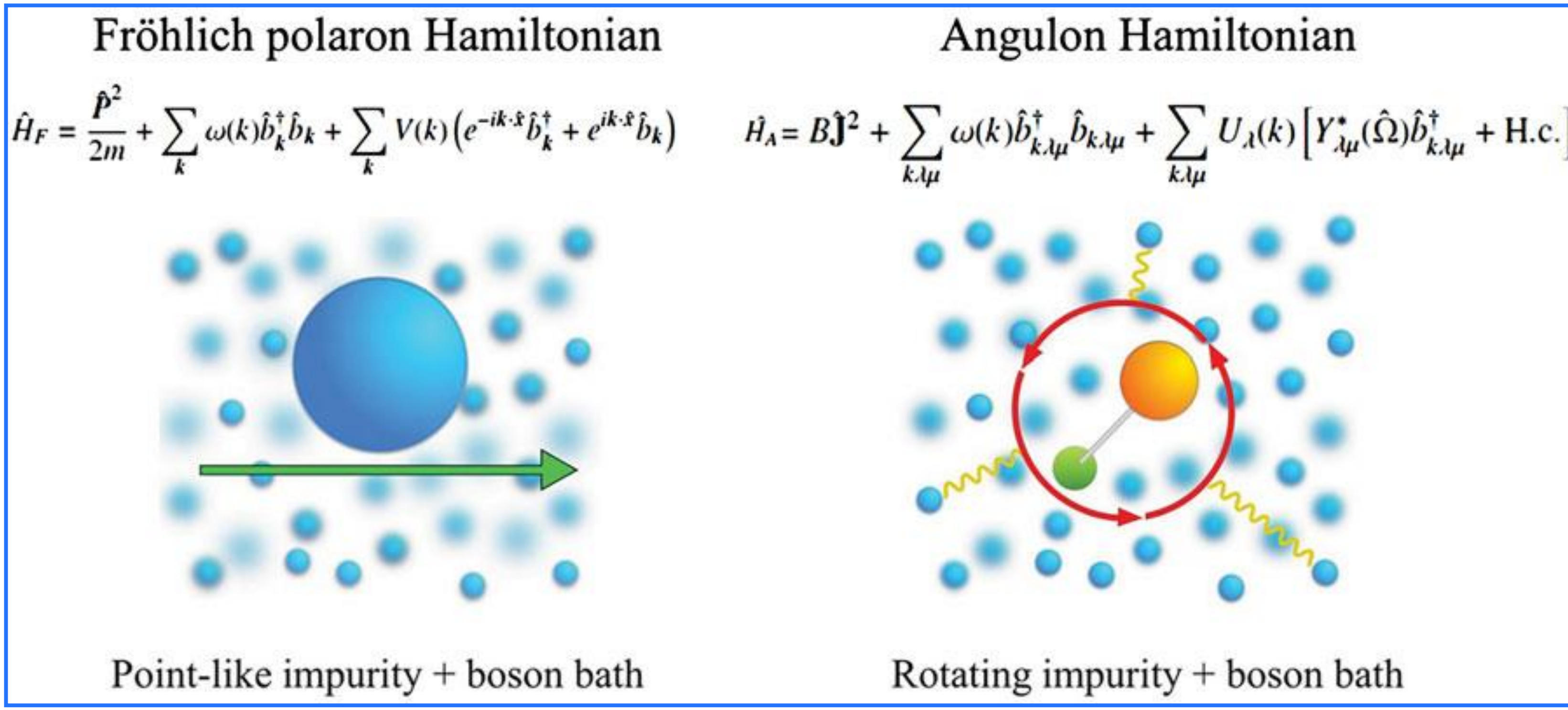



[1] J. T. Devreese, A. B. Kunz and T. C. Collins, Sol. St. Comm. **11**, 673 (1972)
[2] A. B. Kunz, J. T. Devreese, and T. C. Collins, J. Phys. C **5**, 3259 (1972)

# The Angulon[1]

The polaron concept has become a generic many-body model that describes a particle interacting with a bath of bosons through absorption or emission of these bosons.




From: Mol. Phys. **117**, 1981 (2019)

[1] R. Schmidt and M. Lemeshko, PRL **114**, 203001 (2015).
[2] G. Bighin, T. V. Tscherbul, and M. Lemeshko, PRL **121**, 165301 (2018).
[3] J. H. Mentink, M. I. Katsnelson, and M. Lemeshko, PRB **99**, 064428 (2019).
[4] X. Li, G. Bighin, E. Yakaboylu and M. Lemeshko, Mol. Phys. **117**, 1981 (2019).

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## From one to many

Frohlich many-polaron Hamiltonian:

$$H_0=\sum_{j=1}^{N}\frac{p_j^2}{2m_b}+\sum_{\mathbf{k}}\hbar\omega_{\mathrm{LO}}a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+\sum_{\mathbf{k}}\sum_{j=1}^{N}[e^{i\mathbf{k}.\mathbf{r}_j}a_{\mathbf{k}}V_{\mathbf{k}}+e^{-i\mathbf{k}.\mathbf{r}_j}a_{\mathbf{k}}^{+}V_{\mathbf{k}}^{*}]+\frac{e^2}{2\varepsilon_\infty}\sum_{j=1}^{N}\sum_{l(\neq j)=1}^{N}\frac{1}{|\mathbf{r}_l-\mathbf{r}_j|}$$

phonon dispersion

electron-phonon coupling

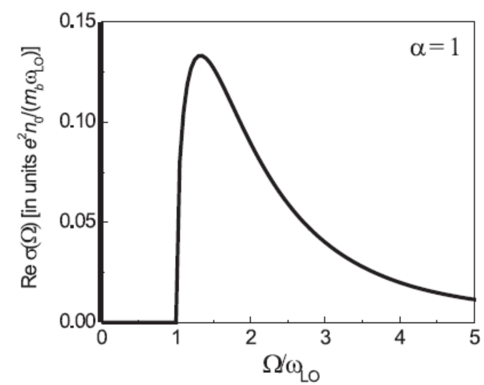
Note that this problem can be generalized from electrons in a bath of LO phonons to any other boson bath (ripplons, acoustic phonons, ...) through a change in the coupling amplitude and the dispersion.

The electron-electron interactions in this problem can be "factorized" into the problem through the dynamic structure factor:

$$\boxed{\mathrm{Re}[\sigma(\omega)]=\frac{n}{\hbar\omega^3}\frac{e^2}{m_b^2}\sum_{\mathbf{k}}k_x^2|V_{\mathbf{k}}|^2S(\mathbf{k},\omega-\omega_{\mathrm{LO}})}$$

$$\delta[\hbar k^2/(2m_{\mathrm{b}})-(\omega-\omega_{\mathrm{LO}})]$$

retrieves the well-known 1 polaron result

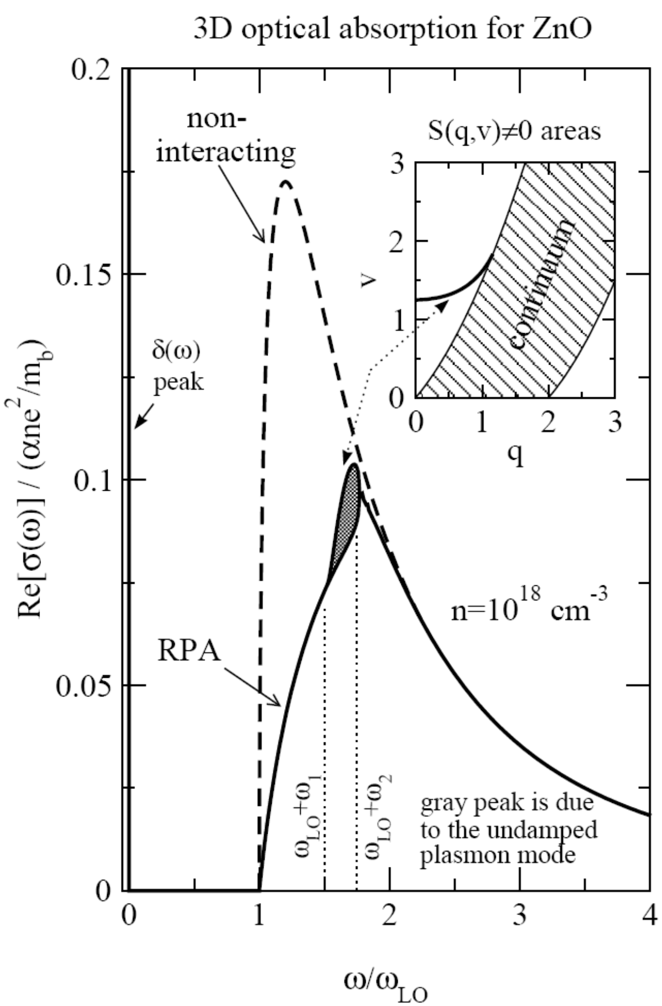


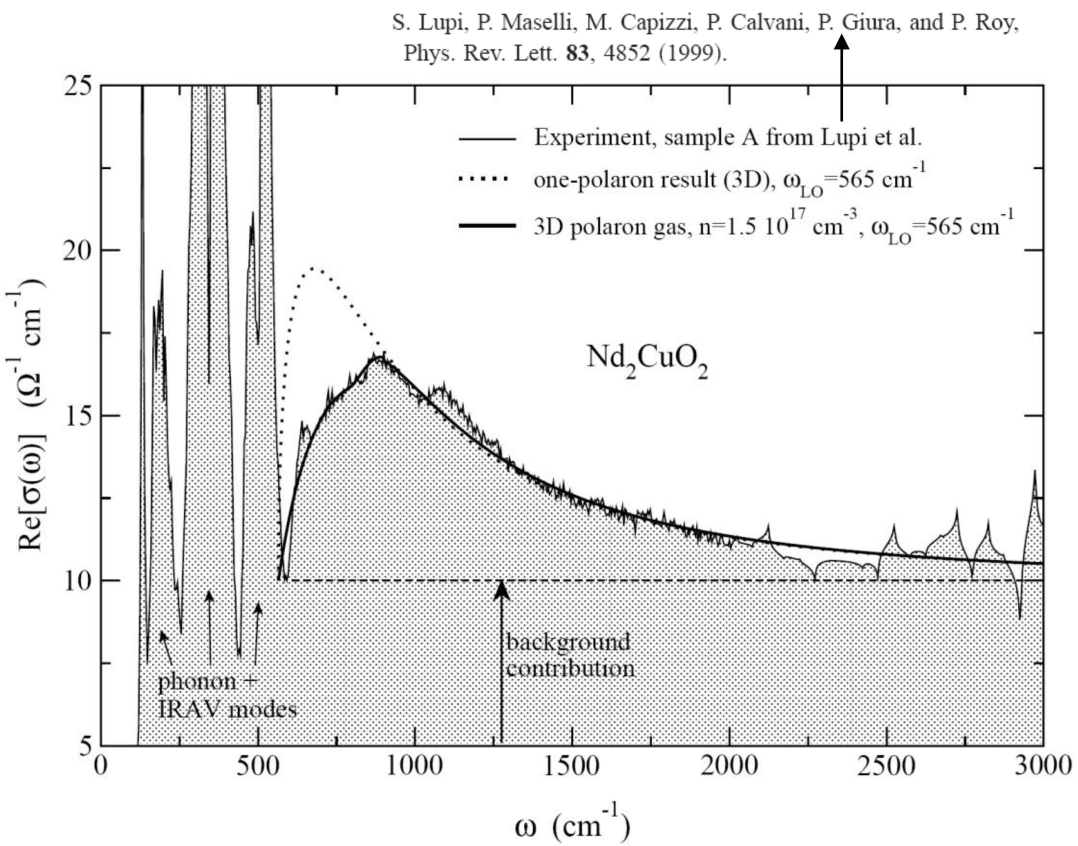

Ground state energy: L. F. Lemmens, J. T. Devreese, and F. Brosens, Phys. Status Solidi B **82**, 439 (1977).
Optical absorptiom: J. Tempere, J.T. Devreese, Phys. Rev. B **64**, 104504 (2001).

# Many-polaron optical response

$$\mathrm{Re}[\sigma(\omega)] = \frac{n}{\hbar\omega^3}\frac{e^2}{m_b^2}\sum_{\mathbf{k}} k_x^2 |V_{\mathbf{k}}|^2 S(\mathbf{k}, \omega - \omega_{\mathrm{LO}})$$

Using the second "simplest" structure factor (RPA) in this formula allows already for a nice agreement with experiment:



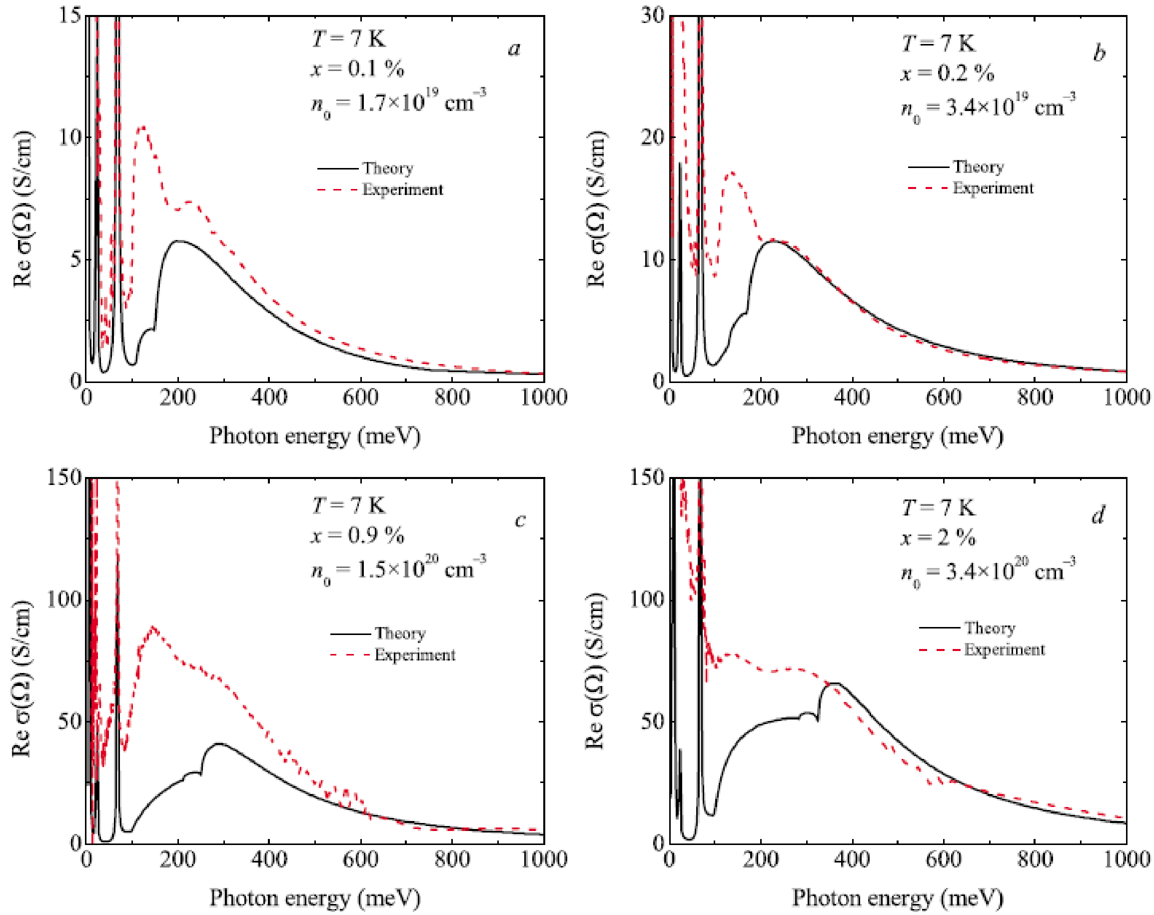

J. Tempere, J.T. Devreese, Phys. Rev. B **64**, 104504 (2001).

# Many-polaron optical response

Application to doped strontium titanate (JTD et al. 2010) using a random-phase approximation for the many-polaron density-density Green's function (Cataudella et al. 1999)

The mid-infrared optical conductivity band is attributed to large polarons,

The 130 meV feature remains unexplained.





V. Cataudella, G. De Filippis and G. Iadonisi, EPJB **12**, 17 (1999).
J. T. Devreese and J. Tempere, Phys. Rev. B B **64**, 104504 (2001).
J. T. Devreese, S. N. Klimin, J. L. M. van Mechelen, and D. van der Marel, Phys. Rev. B **81**, 125119 (2010).

# From many back down to two

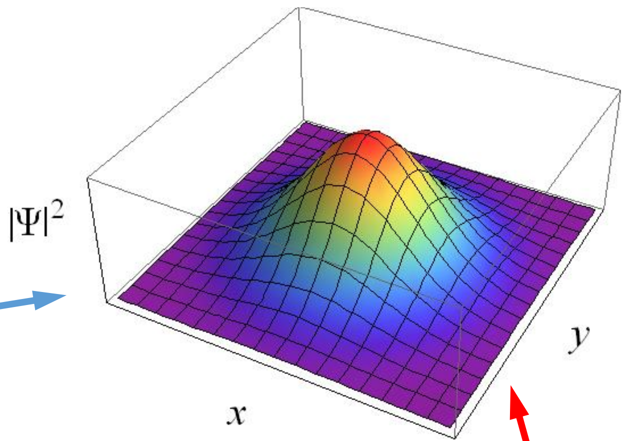
***Fröhlich bipolaron***:
When two polarons are near each other, their potential wells and polarization clouds overlap and can form a "joint" potential well.

Trial wave function for a large bipolaron

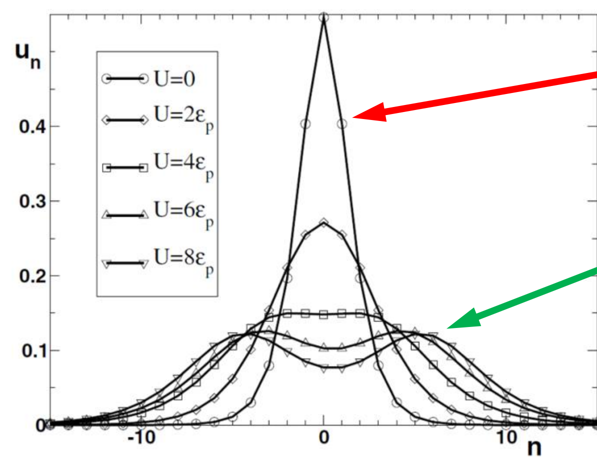
$$|\Psi\rangle = |f\rangle \left[\frac{\gamma\beta}{\pi}\right]^{3/2} e^{-(\gamma^2 r^2/2)} e^{-(\beta^2 R^2/2)}$$

(from F. Bassani et al., PRB 1991)

Density profile for a large bipolaron




***Holstein bipolaron***:
When the on-site repulsion is overscreened by strong electron-phonon coupling, the polarons attract each other through the effective potential, bind into pairs, and form small bipolarons.




One-center bipolaron

Two-center bipolaron

O. S. Barišić and S. Barišić, Eur. Phys. J. B **85**, 111 (2012)

# Fröhlich Bipolarons

Key parameters:

(1) the electron-phonon coupling constant
$$\alpha = \frac{e^2}{\hbar}\sqrt{\frac{m_b}{2\hbar\omega_{LO}}}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)$$

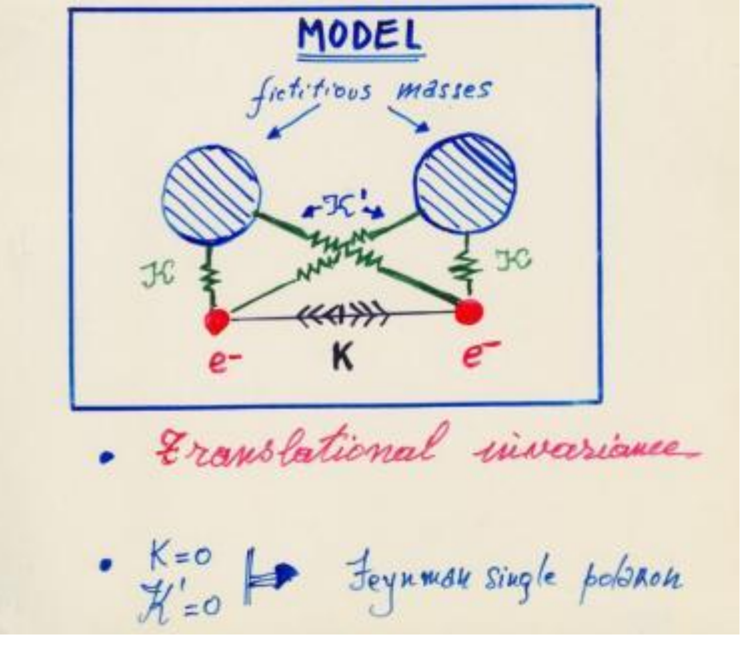
(2) The dimensionless strength of the Coulomb repulsion between the two electrons
$$U = \frac{1}{\hbar\omega_{\mathrm{LO}}}\frac{e^2}{\varepsilon_\infty}\sqrt{\frac{m_b\omega_{\mathrm{LO}}}{\hbar}}$$

(3) The ratio of the dielectric constants:
$$\eta = \frac{\varepsilon_\infty}{\varepsilon_0}$$

They are related by $U = \dfrac{\sqrt{2}\alpha}{1-\eta}$.

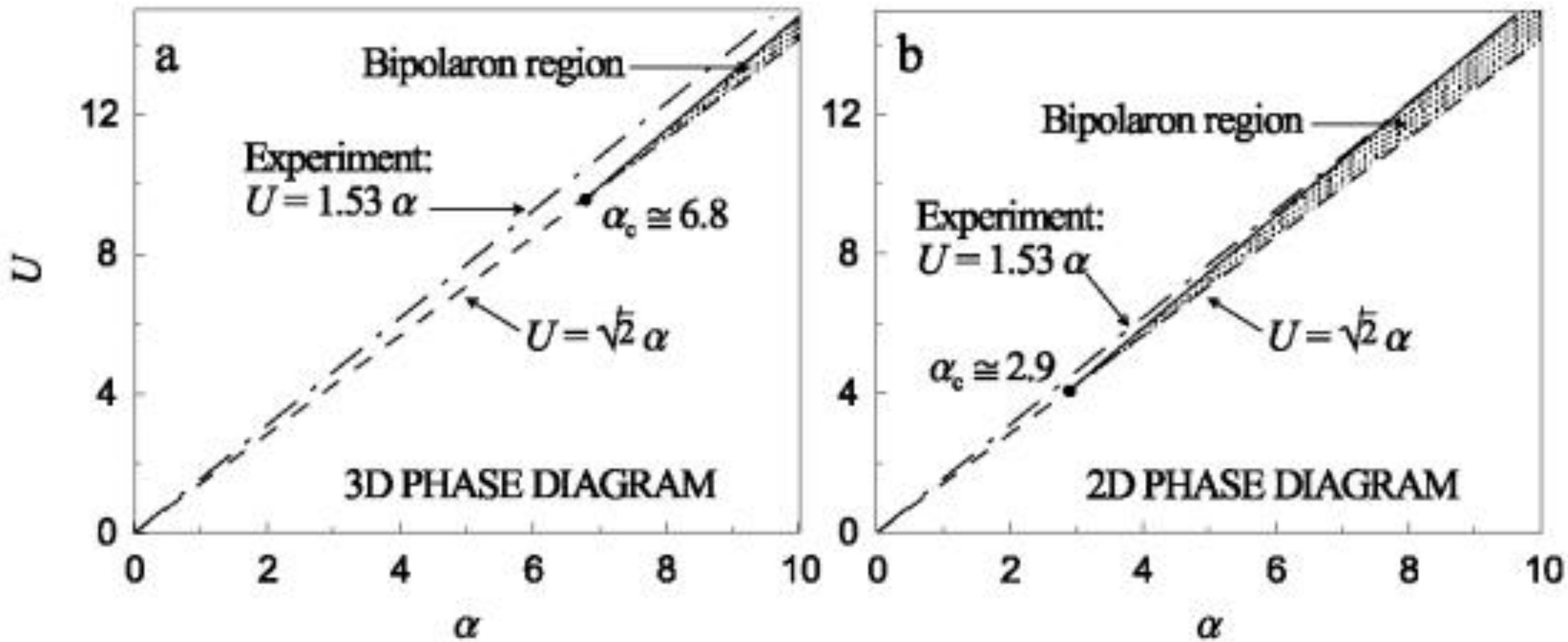
The criterion of the bipolaron formation: $E_{\mathrm{bip}} \leq 2E_{\mathrm{pol}}$

Calculated with the Feynman path integral formalism :




J. Adamowski, Phys. Rev. B **39**, 3649 (1989)
F. Bassani, M. Geddo, G. Iadonisi, and D. Ninno, Phys. Rev. B **43**, 5296 (1991)
G. Verbist, F. M. Peeters, and J. T. Devreese, Phys. Rev. B **43**, 2712 (1991)

# Fröhlich Bipolarons

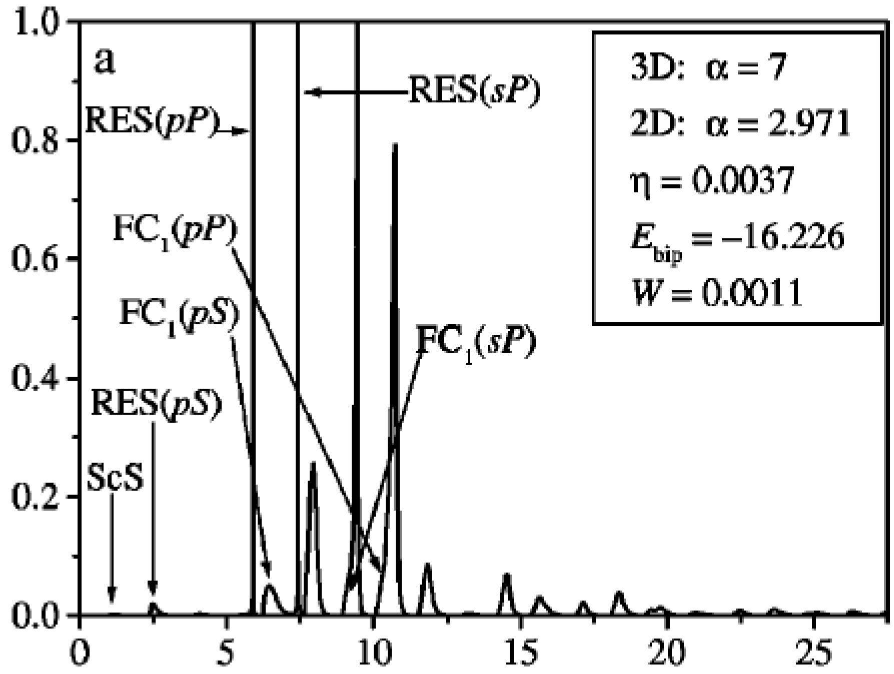



The phase diagram[1] for bipolaron formation for three (a) and two (b) dimensions. Bipolarons are formed in the shaded areas. The critical values of the electron-phonon coupling constant $\alpha$ are $\alpha_c$ = 6.8 (3D) and $\alpha_c$ = 2.9 (2D).

G. Verbist, F. M. Peeters, and J. T. Devreese, Phys. Rev. B **43**, 2712 (1991)

# Bipolaron optical absorption

A similar calculation for polarons, using the path integral formalism, leads for bipolarons to a series of sharp peaks in far IR regime, hard to distinguish from IR active phonon modes.




Up till now there has been no experimental signature of large bipolarons in solids.


[1] A.S. Mishchenko, N. Nagaosa, N. V. Prokof'ev, A. Sakamoto, and B. V. Svistunov, Phys. Rev. Lett. **91**, 236401 (2003);
[2] G. De Filippis, V. Cataudella, A. S. Mishchenko, C. A. Perroni, and J. T. Devreese, Phys. Rev. Lett. **96**, 136405 (2006).

# Conclusions and open problems

- It is remarkable how the Fröhlich continuum polaron, one of the simplest examples of a Quantum Field Theoretical problem, has resisted full analytical solution at all coupling since ~1950, when its Hamiltonian was first written.
- Although a mechanism for the optical absorption of Fröhlich polarons was already proposed a long time ago, some subtle characteristics were only clarified very recently by combining numerical DQMC studies and improved analytical methods.
- Of special interest are several sum rules derived for the optical conductivity spectra of arbitrary-coupling polarons.
- A variety of magneto-optical and transport experiments were successfully analyzed with polaron theory.
- The charge carriers in a rich variety of systems of reduced dimension and dimensionality turn out to be polarons.
- The richness and profundity of Landau–Pekar's polaron concept is further illustrated by its extensions to lattice polarons.
- The finite-temperature polaron mobility still needs a deeper clarification.
- The multipolaron problem remains a challenging one when electron-phonon interaction competes with sometimes strong electronic correlations.
- There are a lot of new fields for the application of the polaron theory.

# Some key works for this talk:

- J. T. Devreese, S. N. Klimin, J. L. M. van Mechelen, and D. van der Marel, Phys. Rev. B **81**, 125119 (2010)
  - *explains observed optical absorption spectra in terms of many large polaron optical response.*
- G. De Filippis, V. Cataudella, A. S. Mishchenko, C. A. Perroni, and J. T. Devreese, Phys. Rev. Lett. **96**, 136405 (2006)
  - *all-coupling analytic polaron optical conductivity which compares well with the Diagrammatic Quantum Monte Carlo results.*
- J. Tempere and J. T. Devreese, Phys. Rev. B **64**, 104504 (2001)
  - *many large polaron optical response is treated.*
- A. S. Alexandrov and J. T. Devreese, *Advances in Polaron Physics*, Springer Series in Solid-State Sciences, Vol. 159 (Springer, 2009)
  - *a review of the state-of-the art of polaron physics*
- S. N. Klimin and J. T. Devreese, Phys. Rev. B **94**, 125206 (2016)
  - *All-coupling polaron optical response: Analytic approaches beyond the adiabatic approximation.*
- J. Vlietinck ,W. Casteels, K. Van Houcke, J. Tempere, J. Ryckebusch and J. T. Devreese, New. J. Phys. **17**, 033023 (2015)
  - *Diagrammatic Monte Carlo study of the acoustic and the Bose-Einstein condensate polaron.*
- T. Hahn, S. Klimin, J. Tempere, J. T. Devreese, and C. Franchini, Phys. Rev. B **97**, 134305 (2018)
  - *Diagrammatic Monte Carlo study of Fröhlich polaron dispersion in two and three dimensions.*

# Title

# Title