Model for the inverse field dependence in N-doped cavities

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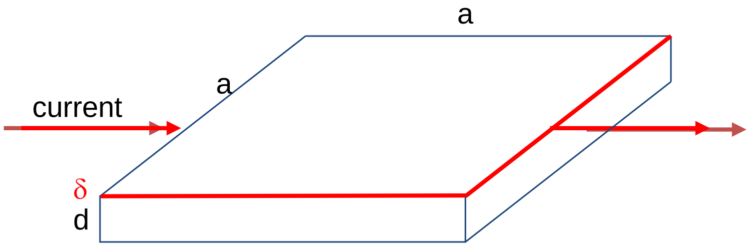
Outline

- RF surface impedance
- BCS theory, Mattis-Bardeen (M-B) theory and extension
- Calculation results and explanation
- Theory vs. experiments
- Summary

J. Bardeen, L. N. Cooper, and J. R. Schrieffer, *Physical Review* **108**, 1175 (1957)
D. C. Mattis and J. Bardeen, *Physical Review* **111**, 412 (1958)
B.P. Xiao, C.E. Reece, M.J. Kelley, *Physica C* **490** (2013) 26–31

RF surface impedance model



- RF surface impedance of a superconductor caused by the inertia (mass) of the Cooper pairs: they cannot follow the RF oscillation.
- Incomplete shielding of RF field allows the superconductor to store RF energy inside its surface - surface reactance.
- The RF field that enters the superconductor will interact with quasi-particles, causing RF power dissipation - surface resistance.

$$Z_s = R_s + iX_s$$

BCS, M-B and extension

- **Each Cooper pair was assumed to have zero net momentum. By minimizing the free energy one get a single particle distribution function *f* and Density of State (DoS), represented by *h*.**
- **Considering that a single particle scattering from one energy state to another one, by considering the energy of each state (with one photon added to either the initial state or the final state.), the probability of initial state and the possibility of scattering, a scattering form was calculated using *f* and *h*.**
- **This scattering form was then applied to the anomalous skin effect to get the surface impedance.**
- **We assume that all Cooper pairs move with the same velocity *Vs*, and apply this assumption to BCS theory to get new *f* and *h*.**[*]
- **These new *f* and *h* are applied to get a new scattering form, thus a new surface impedance.**
- **We average these effects over both RF cycle and depth into the surface to get the effective surface resistances (Rs) under different fields.**[**]

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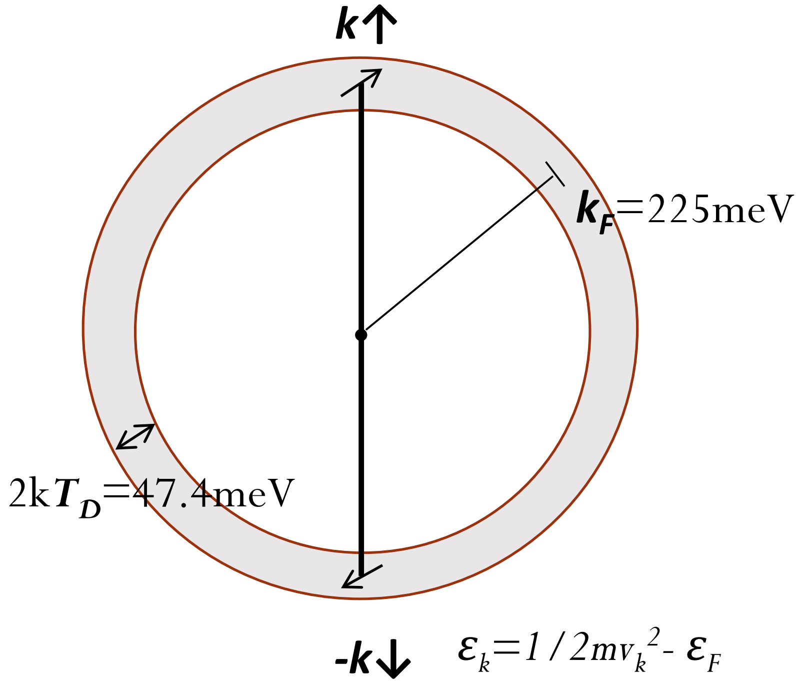
[*] J. Bardeen, Reviews of Modern Physics 34 (1962) 667.

[**] I.O. Kulik, V. Palmieri, Particle Accelerators 60 (1998) 257.

Cooper pair with zero momentum



$\varepsilon_k = 1/2mv_k^2 - \varepsilon_F$

(Energies are based on Nb with selected parameters)

Two particles can be attractive to each other with electron-phonon interaction, if they have:

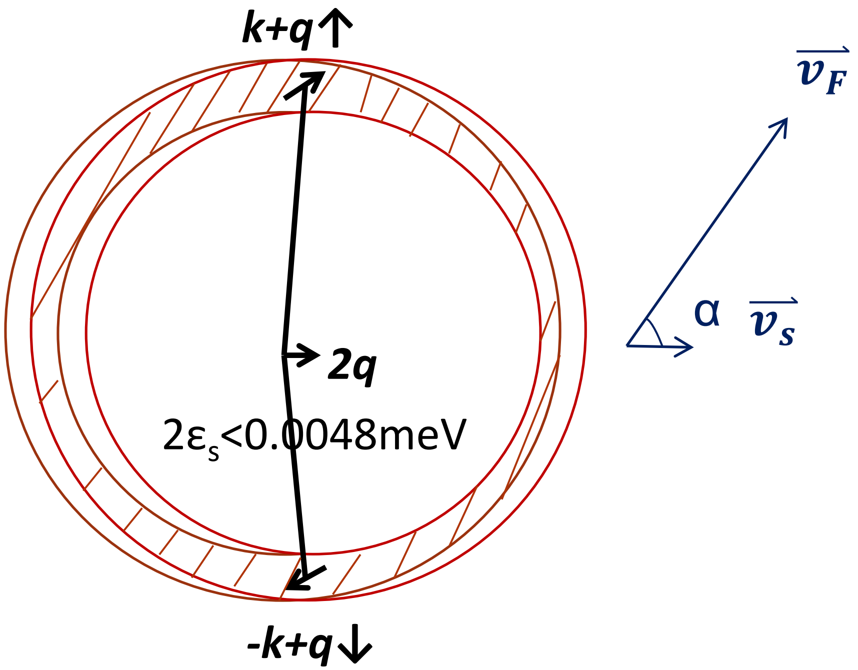
- **momentums in opposite direction**
- **same energy state k (one ↑ the other ↓)**
- **k in a shell nearby Fermi level k_F, with its thickness determined by Debye energy**

Consequence of attraction:

- **Bonded particles become Bosons and get condensed**
- **Excited particles obey Fermi-Dirac distribution**
- **A "forbidden zone" appears nearby k_F, with its thickness to be 2Δ (energy gap)**
- **Energy of excited particle (hole below k_F and electron above k_F) changes from $|\varepsilon_k| = |1/2mv_k^2 - \varepsilon_F|$ before condensation to $E_k = \sqrt{\varepsilon_k^2 + \Delta^2}$ after condensation**

A macroscopic quantum effect!

Cooper pair with a net momentum



$$\varepsilon_{k+q} = 1/2m(\overrightarrow{v_k} + \overrightarrow{v_s})^2 - \varepsilon_F = \varepsilon_k + \varepsilon_s + \varepsilon_{ext}$$

$$\varepsilon_{-k+q} = 1/2m(\overrightarrow{v_k} - \overrightarrow{v_s})^2 - \varepsilon_F = \varepsilon_k + \varepsilon_s - \varepsilon_{ext}$$

$$\varepsilon_{ext} = m v_F v_s \cos\alpha = p_F v_s x$$

“States with a net current flow can be obtained by taking a pairing (*k1*↑, *k2*↓) with *k1*+*k2* =*2q*, and *2q* the same for all virtual pairs” – quoted from **BCS theory**

A small net momentum appears

Consequence:

- **Energy split appears for ↑ and ↓**
- **The energy split is angle dependent**
- **This angle can be any number**

Energy split caused by moving Cooper pairs

BCS theory

Before condensation ε_k

After condensation $E_k = [\varepsilon_k{}^2 + \Delta^2]^{\frac{1}{2}}$

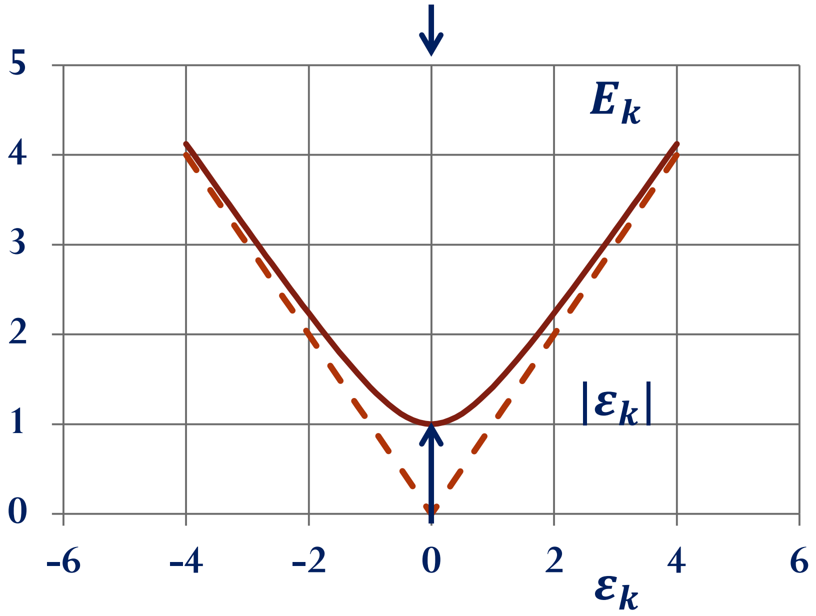
extension

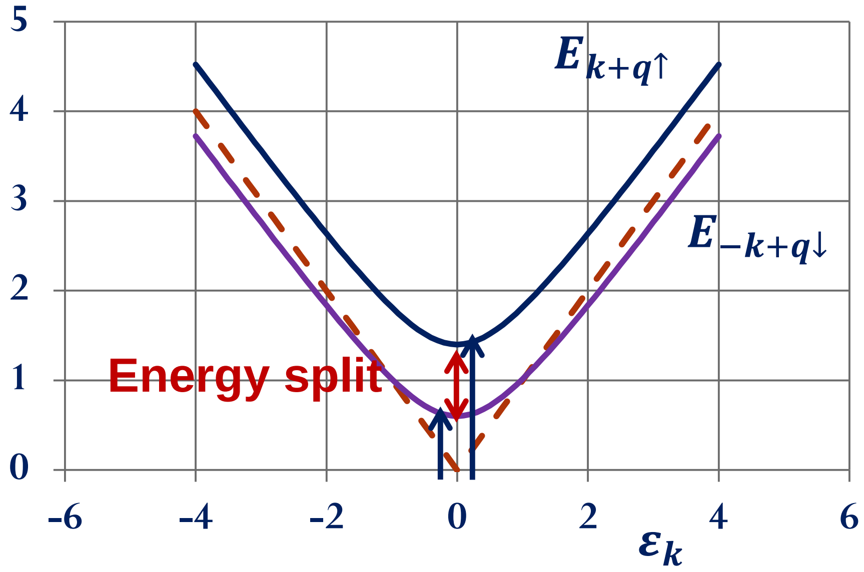
$\varepsilon_{-k+q} = \varepsilon_k + \varepsilon_s - \varepsilon_{ext}, \varepsilon_{k+q} = \varepsilon_k + \varepsilon_s + \varepsilon_{ext}$

$E_{-k+q\downarrow} = E_k - \varepsilon_{ext},\ E_{k+q\uparrow} = E_k + \varepsilon_{ext}$

with $E_k = [(\varepsilon_k + \varepsilon_s)^2 + \Delta^2]^{\frac{1}{2}}$

$ref: \varepsilon_F$





Energy needed to break a Cooper pair,
Δ for ↑, and the same for ↓

$\Delta - \varepsilon_{ext}$ for ↑, $\Delta + \varepsilon_{ext}$ for ↓

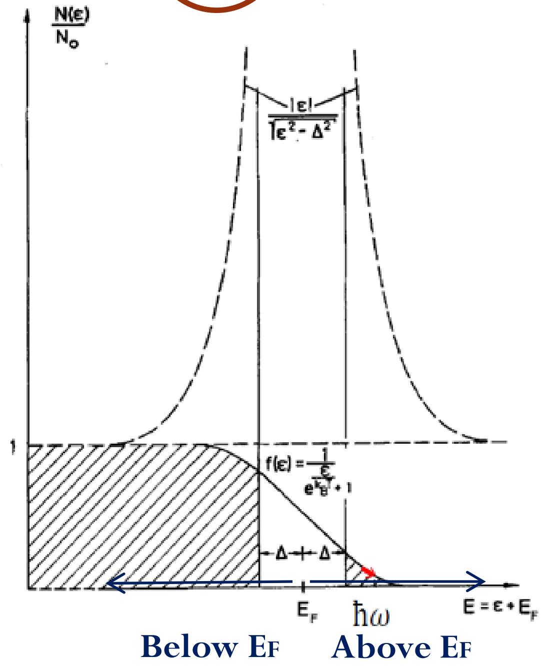
f and *h* modified by moving Cooper pairs

Modified density of states and probability of single occupation at $T<T_c$:

$$\frac{1}{N(0)}\frac{dN(E)}{dE}=\frac{d\varepsilon}{dE}$$

$$f_{-k+q\downarrow}=\begin{cases} f(E_{-k+q\downarrow}), k>k_F & \textbf{For electron} \\ f(E_{k+q\uparrow}),\ \ k<k_F & \textbf{For hole}\end{cases}$$

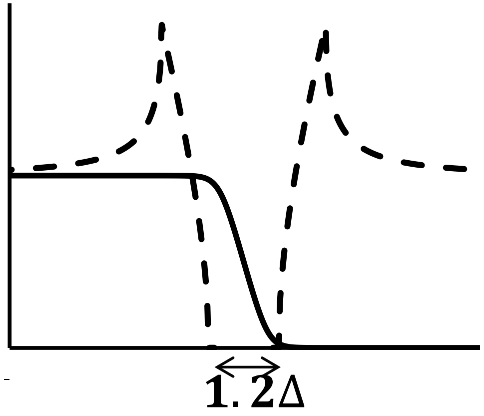
$$f_{k+q\uparrow}=\begin{cases} f(E_{k+q\uparrow}), k>k_F & \textbf{For electron} \\ f(E_{-k+q\downarrow}),\ \ k<k_F & \textbf{For hole}\end{cases}$$



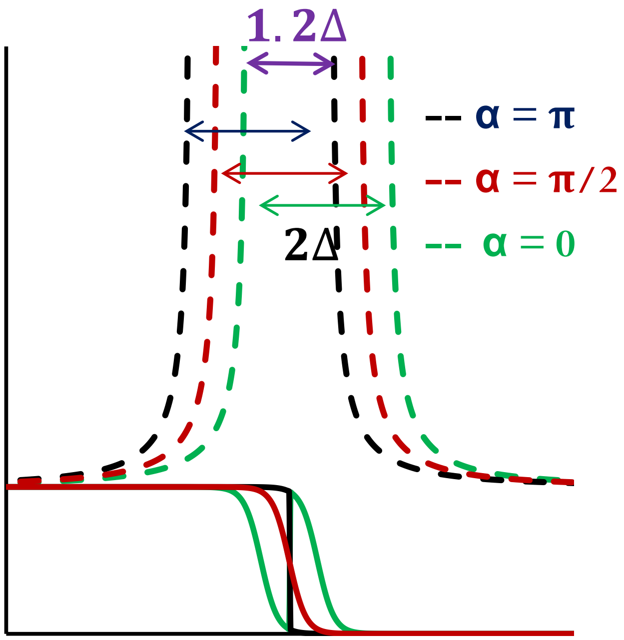
Low field limit density of states and distribution function

Also appeared in I.O. Kulik, V. Palmieri, Particle Accelerators 60 (1998) 257.

Plots with $P_F V_s = 0.4\Delta$ and $T/T_c=0.97$



Density of states and distribution function with moving cooper pairs, angle averaged



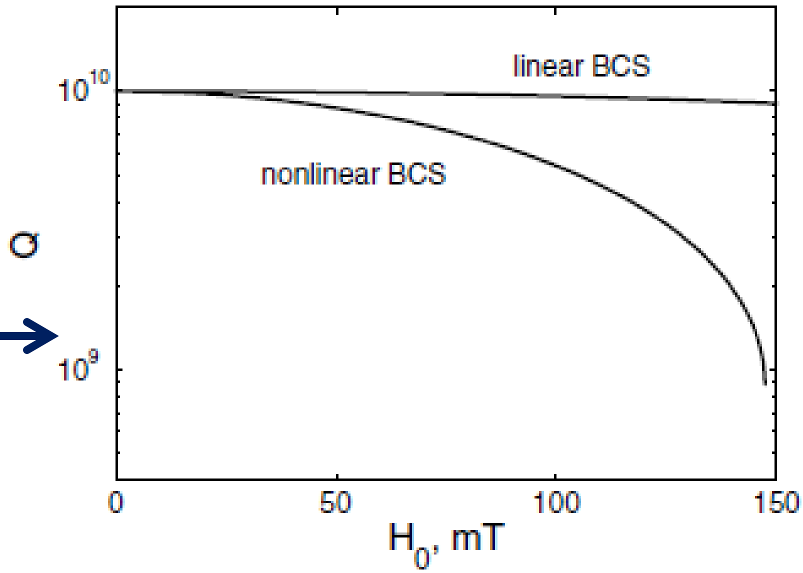
Density of states and distribution function with moving cooper pairs, angle-dependent

J. P. Turneaure, J. Halbritter, and H. A. Schwettman, *Journal of Superconductivity* 4, 341 (1991)

Modification of M-B theory by moving Cooper pairs

- **Till now, there is nothing new.**
- **Modification of M-B theory by moving Cooper pairs were previously considered:***

$$n(J) = \frac{n_{eq}}{2}\int_0^{\pi} exp(P_F V_S cos\alpha/k_B T) sin\alpha d\alpha$$



- **Why these considerations failed?**
  Considering scattering from k to k',
  even the direction of Cooper pair velocity V_s keeps the same,
  the directions of the Fermi velocities (V_F for k and V_F' for k') could be different.
  The angle between V_s and V_F changes after scattering: $\alpha \neq \alpha'$
- **Systematic consideration is needed**

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*I.O. Kulik, V. Palmieri, Particle Accelerators 60 (1998) 257.
and A. Gurevich, Physica C 441 (2006) 38.

Modification of M-B theory by moving Cooper pairs

		BCS/M-B	Extension
Net momentum		0	$2q$
Initial	*X0* *00*	$(k\uparrow, -k\downarrow)$ $(k'\uparrow, -k'\downarrow)$	$(k+q\uparrow, -k+q\downarrow)$ $(k'+q\uparrow, -k'+q\downarrow)$
Final	*00* *X0*	$(k\uparrow, -k\downarrow)$ $(k'\uparrow, -k'\downarrow)$	$(k+q\uparrow, -k+q\downarrow)$ $(k'+q\uparrow, -k'+q\downarrow)$
Ground(+) or excited(-)	+ +	$(k\uparrow, -k\downarrow)$ $(k'\uparrow, -k'\downarrow)$	$(k+q\uparrow, -k+q\downarrow)$ $(k'+q\uparrow, -k'+q\downarrow)$
Energy difference	$W_i - W_f$	$E_{k\uparrow} - E_{k'\uparrow}$	$E_{k+q\uparrow} - E_{k'+q\uparrow}$
Probability of initial state		***f* dependent**	**Modified *f* dependent**
Scattering matrix elements		***h* dependent**	**Modified *h* dependent**

Absorbing/releasing one photon: additional energy difference $\pm\hbar(\omega - is)$, $s \rightarrow 0$

Scattering happens between
any two *k* and *k'*

⇨

any two *k* and *k'* with *q*,
$E_k + \varepsilon_{ext}$ and $E_k' + \varepsilon_{ext}'$

Final expression

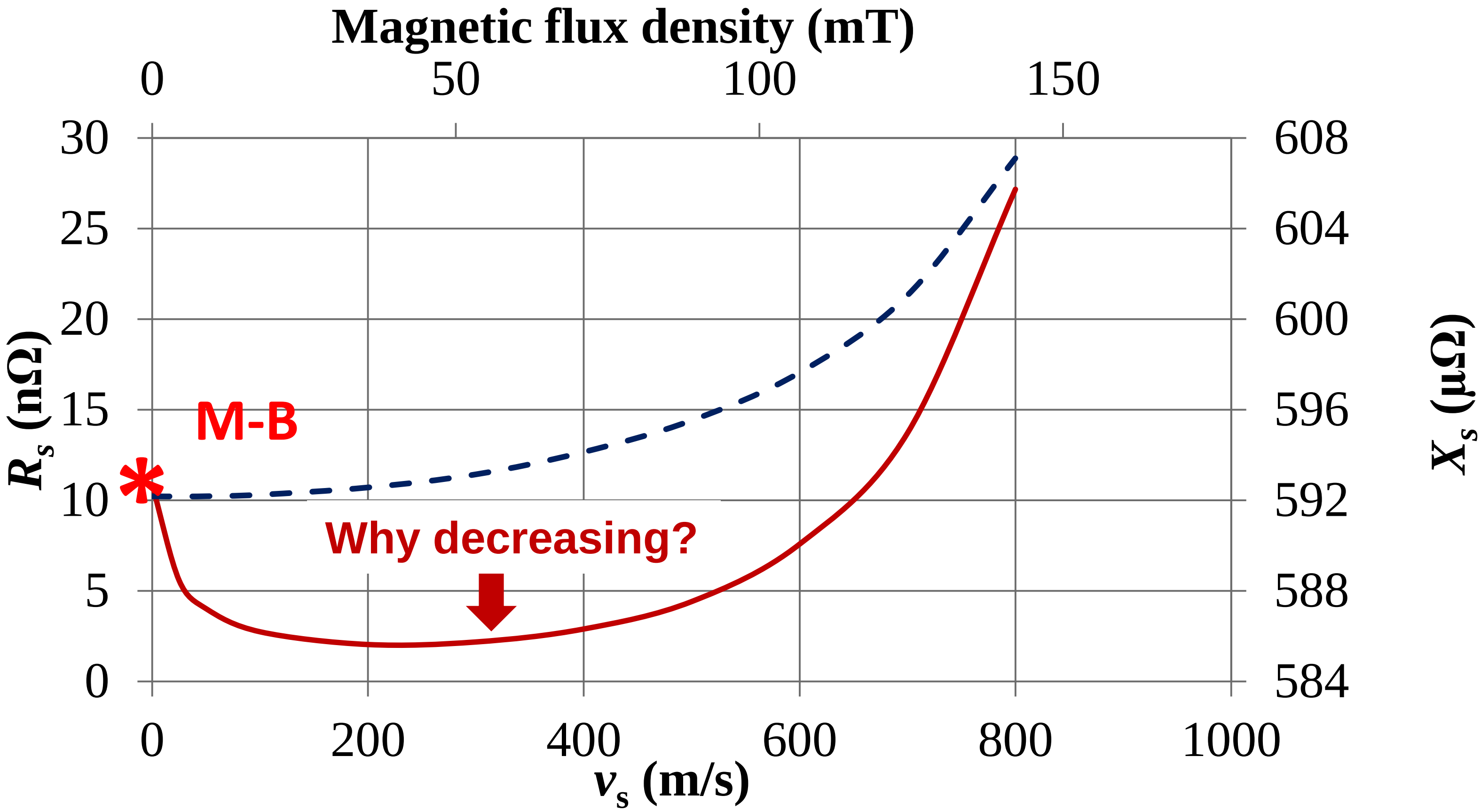
- The final expression is a quadruple integration, besides the integrations in energy and in reciprocal space shown in M-B theory, the extension has two additional integrations in angles, related to *k* and *k'*.

- The averaging over both RF cycle and depth into the surface requires two additional integrations.

- A Mathematica^{TM} script was developed to calculate the R_s vs B_{pk}. It is slow, but it works.

- No parameter fittings can be done using current script due to the slow calculation speed.

Calculation result and explanation (1)



Surface resistance, R_s, (**red line**) and reactance, X_s, (**blue dashed line**) versus Cooper pair velocity and corresponding magnetic field for Nb at 2 K and 1.5 GHz.

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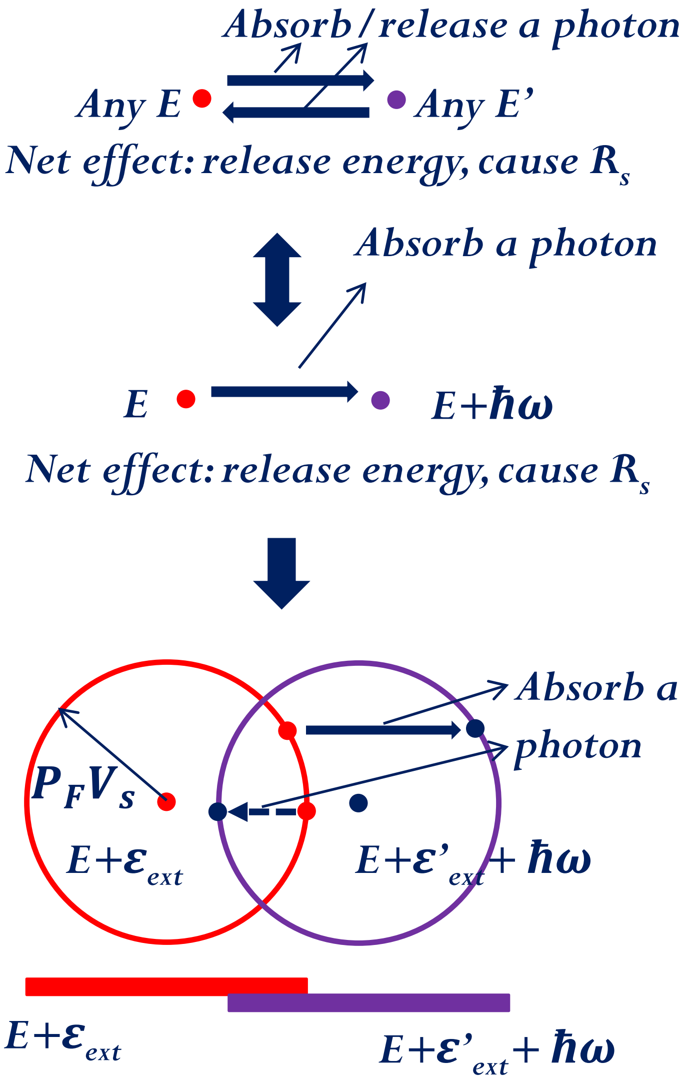
Calculation result and explanation (2)

- In M-B theory, mathematically, the scattering between any two *k* and *k'* with photon interaction equals to the scattering between *E* and $E+\hbar\omega$.
- With moving Cooper pairs, mathematically, the scattering between any two *k* and *k'* with photon interaction equals to the scattering between $E+\varepsilon_{ext}$ and $E+\varepsilon'_{ext}+\hbar\omega$.

Note that $P_F V_s >> \hbar\omega$ could happen, the overlap between red and purple could be significant.



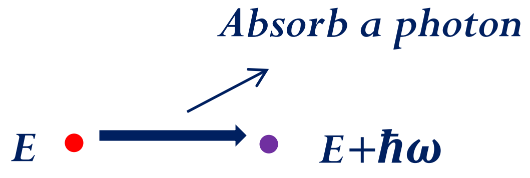
Net effect: release energy, cause R_s

Net effect: release energy, cause R_s

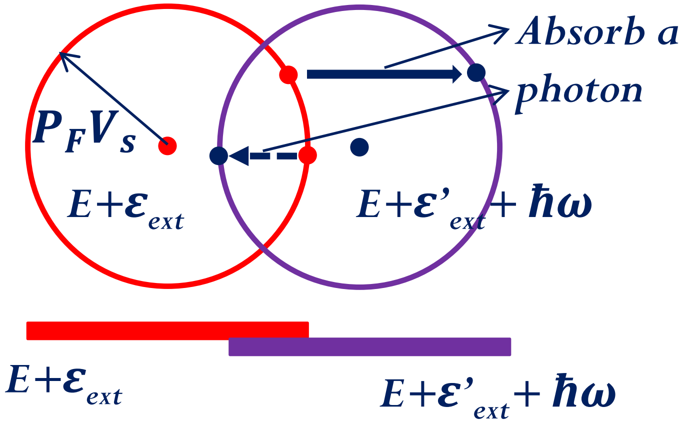
Calculation result and explanation (3)

The “golden rule” in extreme anomalous limit and low temperature approximation

$$R \propto \int [f(E) - f(E+\hbar\omega)]\, g\, dE$$



Net effect: release energy, cause R_s



R_s decreasing?

- Source: angle between V_F (any direction) and V_s cause energy split with angle dependence.
- Consequence: Energy split and modified single particle distribution function cause an overall reduction effect in scattering.

$$R \propto \int \overbrace{[f(E+\varepsilon_{ext}) - f(E+\varepsilon'_{ext}+\hbar\omega)]}^{\text{Term 1}}\; \underbrace{g(h)}_{\text{Term 2}} \underbrace{[f(\varepsilon_{ext})+f(-\varepsilon_{ext})]}_{\text{Term 3}}\, dE$$

Justifications of this extension

- **A mean (phonon) field theory, same as BCS theory, differs from Eliashberg.**
- **Consider single photon absorption only, same as M-B theory, which is good for Nb, differs from de Visser[*] who considered multi photo absorption, which is good for Al.**
- **However the conclusion is the same as de Visser that the reduction comes from the Fermi-Dirac distribution. Differs from Gurevich who believes that the reduction comes from DoS.**
- **Dealing with moving Cooper pairs, same as Bardeen[**].**
- **The way to deal with mean free path, same as M-B theory.**
- **Calculates the "ideal" case, which means the best performance a cavity can achieve.**
- **A cavity with short mean free path is not necessary to be a "non-ideal" cavity.**
- **No extra parameters needed except those in M-B theory + residual**
- **How good it can explain experimental results?**

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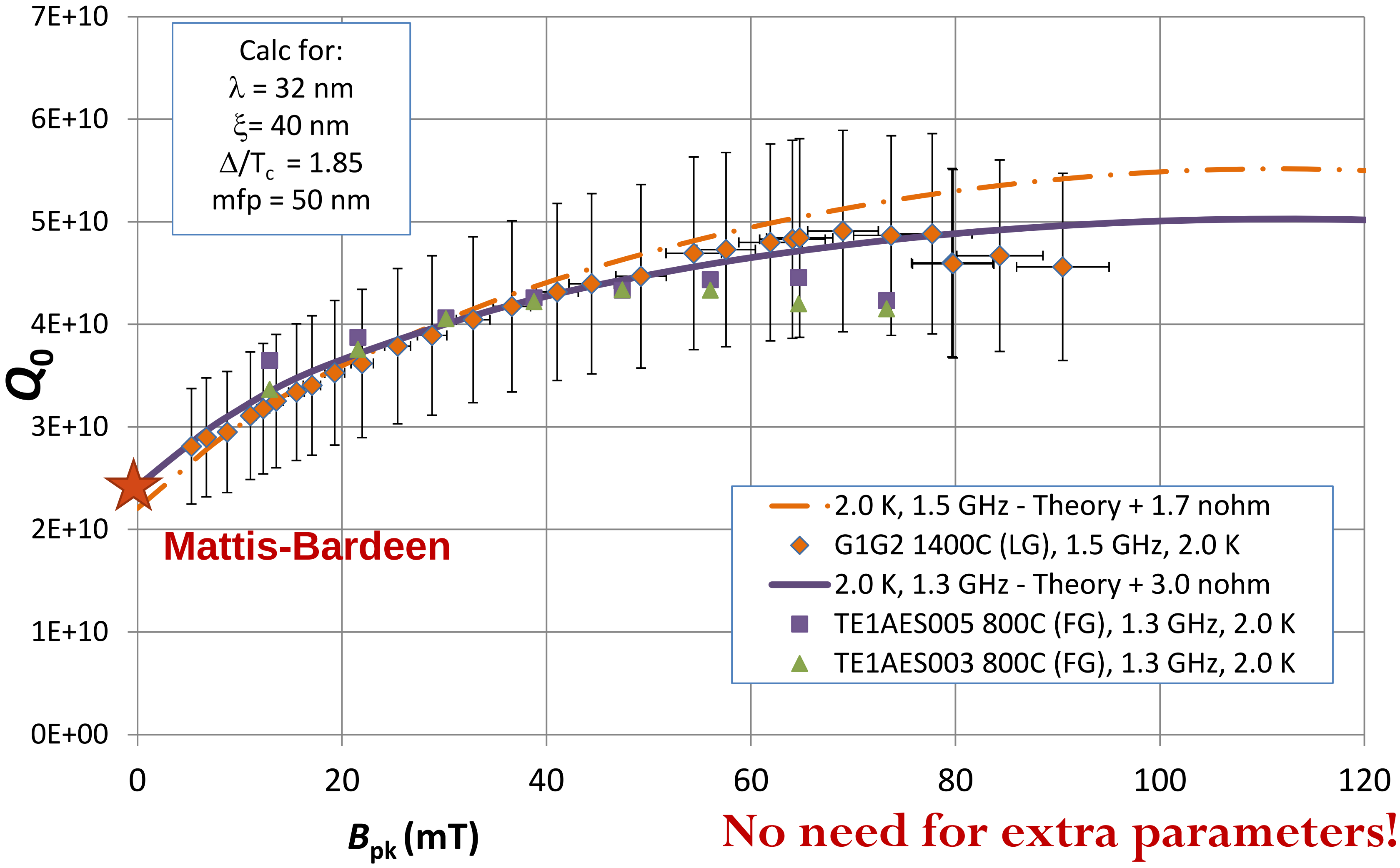
[*] de Visser, P.J., et al., physical review letters, 2014. **112**: p. 047004.

[**] Bardeen, J., Reviews of Modern Physics, 1962. **34**(4): p. 667.

Theory vs Experiments

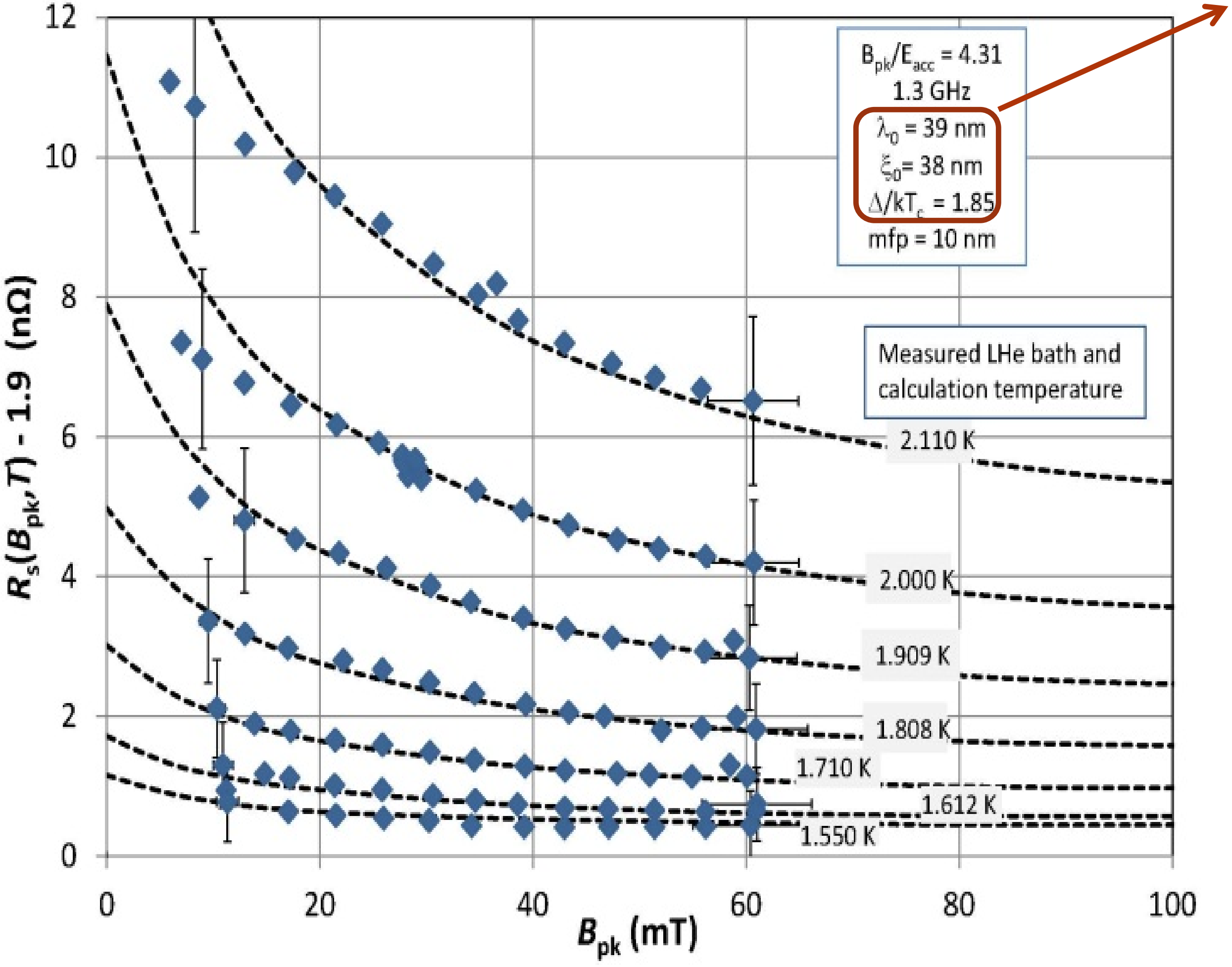
P. Dhakal, *et al.*, PRST-AB, 2013. **16**(4): p. 042001.
A. Grassellino, *et al.*, *Supercon. Sci.and Tech.*, 2013. **26**(10): p. 102001.



No need for extra parameters!

More data…

Palczewski *et al.*, LINAC2014



"Textbook" values

About the inconsistency at the beginning, there are several possibilities:

1, The choose of parameters

2, Measurement errors

3, Cavity performance could be further improved

4, Some facts that are not considered in this model: phonon distribution, multiple photo absorption, additional non-linear effects, etc.

We actually predicted the behavior at low temperatures

Why N-doping works?

- First of first, this theory predicted that NOT ONLY short mean free path, but also long mean free path, should give an "inverse field dependent"
- Why ONLY those with short mean free path worked? Could it be Hydrogen?

Summary

- **Previous surface impedance calculations are available only for the low field limit.**

- **A field-dependent derivation of the Mattis-Bardeen theory of SRF surface impedance has been developed.**

- **The extended range of gradients is treated for the first time.**

- **Without any extra parameters except those from original M-B theory, field-dependent R_s agreement with experiment with recent heat-treated/Nb-doping Nb with unusual surface loading is excellent at different temperatures, with residual resistance to be constant.**

- **The reduction in resistance with increasing field is seen to be an intrinsic effect.**
  - **For type-I, and type-II under H_{c1}.**
  - **What is going to happen between H_{c1} and H_{c2}?**

Thank you for your attention!

In order to understand the reduction of the surface resistance with increasing field (to a certain level), it is necessary to compare the following expressions and analytically show a reduction of R_s with increasing V_s,

$$R_s \propto 2\int_{\Delta}^{\infty}\left[f(E)-f\left(E+\hbar\omega\right)\right]g(E)dE \qquad [1]$$

$$R_s \propto 2\int_{\max(\Delta-\varepsilon_{\text{ext}},\Delta-\varepsilon'_{\text{ext}}-\hbar\omega)}^{\infty}[\mathrm{f}(E_1)-f(E_2)][\mathrm{f}(\varepsilon_{\text{ext}})+\mathrm{f}(-\varepsilon_{\text{ext}})]\mathrm{g}(E,\alpha,\alpha')\mathrm{d}E \qquad [2]$$

It is hard to directly compare these two expressions since the lower limit of the integration is different. Now we consider that at field level just above zero, which means V_s is a small number (it does not matter whether it is positive or negative) that $|2p_F v_s| < \hbar\omega$. In this case $\Delta-\varepsilon'_{\text{ext}}-\hbar\omega$ is always smaller than $\Delta-\varepsilon_{\text{ext}}$ and $R_s \propto 2\int_{\Delta-\varepsilon_{\text{ext}}}^{\infty}[f(E_1)-f(E_2)][\mathrm{f}(\varepsilon_{\text{ext}})+\mathrm{f}(-\varepsilon_{\text{ext}})]\mathrm{g}(E,\alpha,\alpha')\mathrm{d}E$.

At this point we change the integration from E to E_1, so the above expression changes to:

$$R_s \propto 2\int_{\Delta}^{\infty}[f(E_1)-f(E_1+\varepsilon'_{\text{ext}}-\varepsilon_{\text{ext}}+\hbar\omega)][\mathrm{f}(\varepsilon_{\text{ext}})+\mathrm{f}(-\varepsilon_{\text{ext}})]\mathrm{g}(E_1-\varepsilon_{\text{ext}},\alpha,\alpha')\mathrm{d}E_1 \qquad [3]$$

Expression [3] and expression [1] now have the same range of integration and can be directly compared.

In [3], the angle integration of $[\mathrm{f}(\varepsilon_{\text{ext}})+\mathrm{f}(-\varepsilon_{\text{ext}})]$ and $\mathrm{g}(E_1-\varepsilon_{\text{ext}},\alpha,\alpha')$ do not reduce with increasing V_s.

Now we evaluate the change brought by the single particle distribution function:

$$1/4\int_{-1}^{1}\int_{-1}^{1}[f(E_1)-f(E_1+\varepsilon'_{\text{ext}}-\varepsilon_{\text{ext}}+\hbar\omega)]\mathrm{d}x\,\mathrm{d}x' = f(E_1)-\left[\frac{Sinh(p_F v_s)}{p_F v_s}\right]^2 f(E_1+\hbar\omega)$$

with $\mathrm{x}=\cos\alpha$ and $\mathrm{x}'=\cos\alpha'$.

The expression $\frac{Sinh(p_F v_s)}{p_F v_s}$ is increasing with increasing V_s, thus with increasing V_s, the R_s reduces, and the reduction comes from the angle-dependent modified single particle distribution function providing on average reduced opportunities for transitions.

averaging effect of the angle dependent single particle distribution.

Calculation result and explanation (2)

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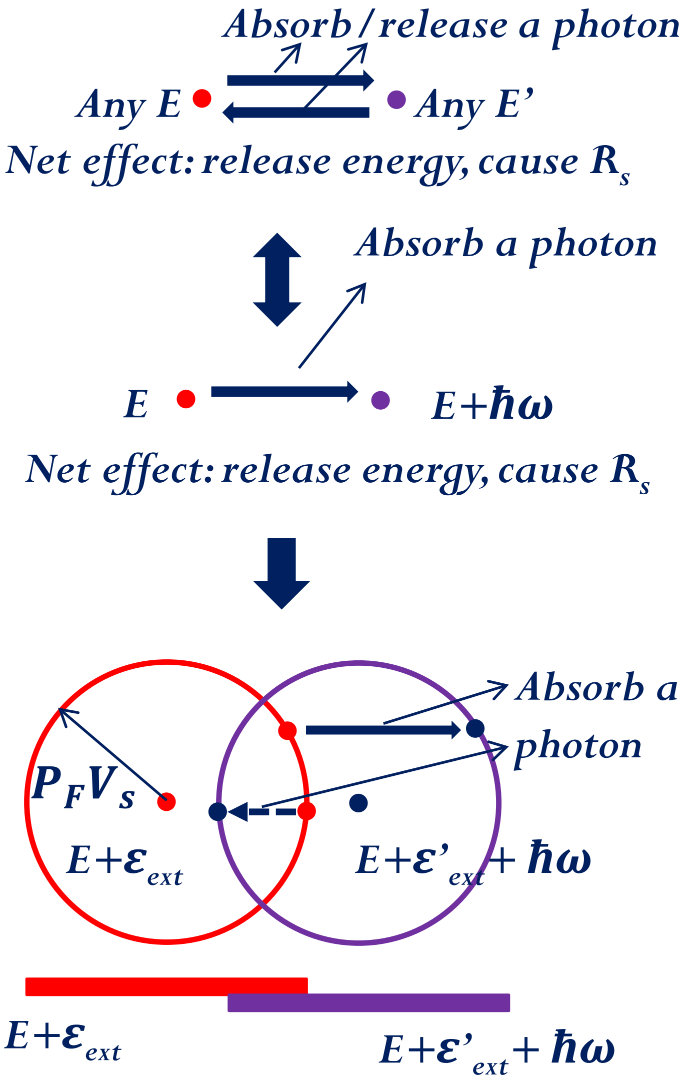

Absorb / release a photon

Any E

Any E'

Net effect: release energy, cause R_s

Absorb a photon

E

$E+\hbar\omega$

Net effect: release energy, cause R_s

Absorb a photon

$P_F V_s$

$E+\varepsilon_{ext}$

$E+\varepsilon'_{ext}+\hbar\omega$

$E+\varepsilon_{ext}$

$E+\varepsilon'_{ext}+\hbar\omega$

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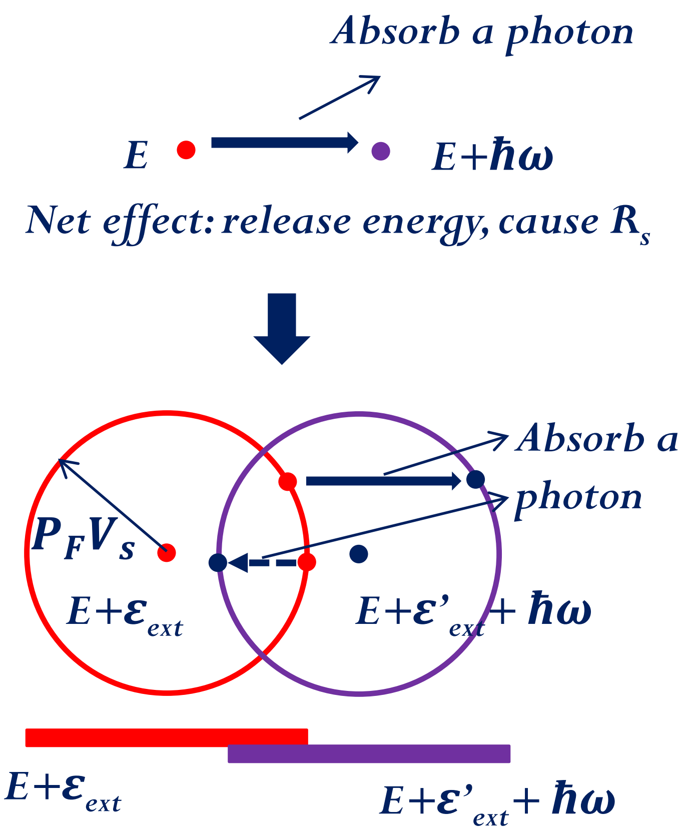

Net effect: release energy, cause R_s