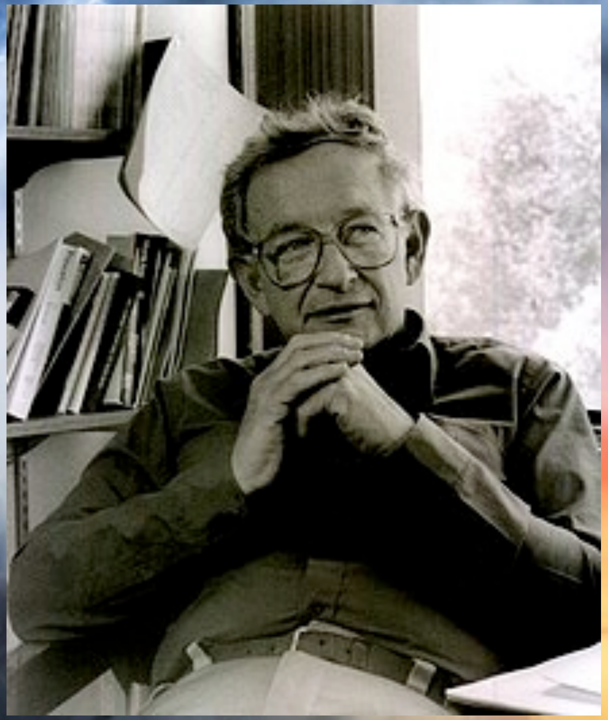
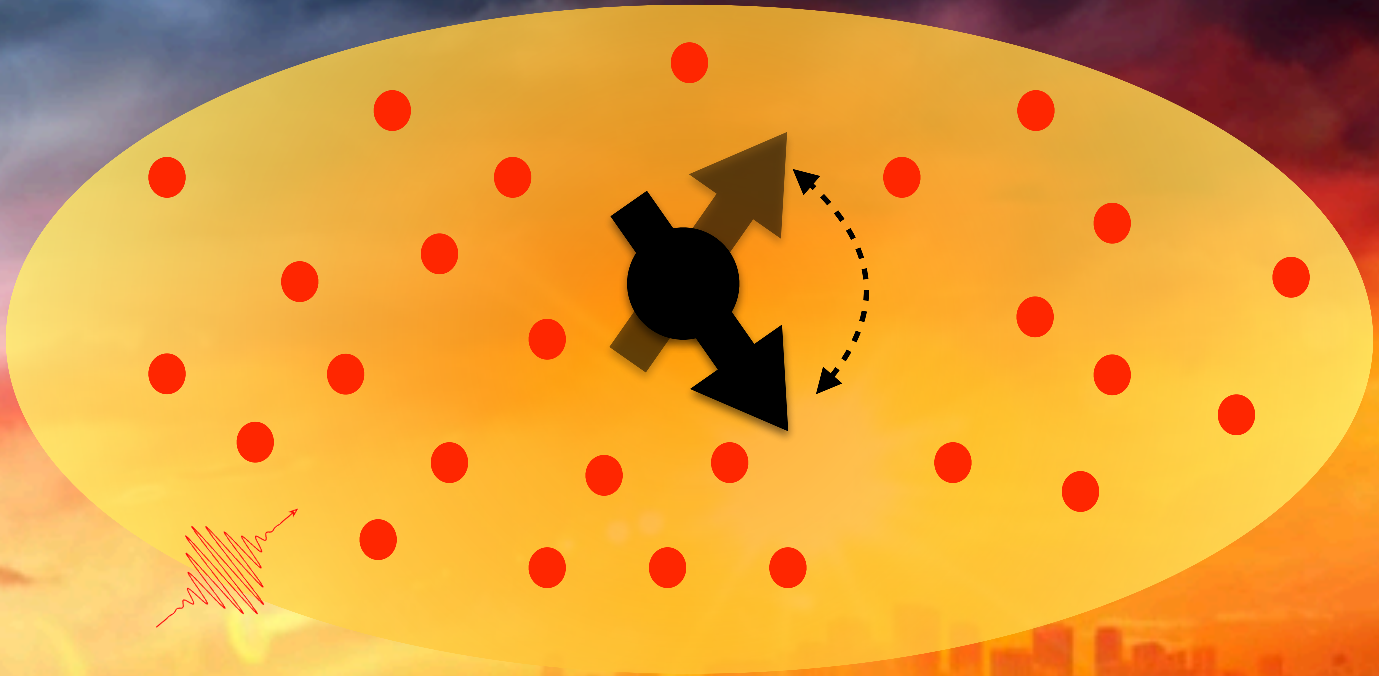
The Exact Properties of Ultracold Polarons

—- and how to Prevent a Catastrophe Predicted by Anderson





Jia Wang ,
Xia-Ji Liu,
Hui Hu
Centre for Quantum Technology Theory,
Swinburne University of Technology

[1] PRA **105**, 023317 (2022)
[2] PRL **128**, 175301 (2022)
[3] PRA **105**, 043320 (2022)
[4] arXiv: 2207.10501

AIP Congress, 13/12/2022

Impurity-Medium Systems

L. Landau, "Uber die Bewegung der Elektronen im Kristallgitter," (1933)

10. ELECTRON MOTION IN CRYSTAL LATTICES

It is well known that in a periodic field an electron can move without resistance. When the lattice is slightly distorted at a point, this only leads to scattering of the electrons at this point. This, however, does not mean the electron is trapped at this point. According to a familiar theorem in wave mechanics this will only be possible if, in addition possible if, in addition to continuous eigenvalues, the distorted lattice would also have discrete eigenvalues. But this is not the case for slight distortions.

Let us consider a free electron, subjected in a certain region to a weak field. we can then demonstrate in accordance with Peierls[1] that the solution of the Schrödinger equation at $E = 0$ has no nodes at weak fields, that is it corresponds to the lowest possible eigenvalue. For, when determining the solution of the Schrödinger equation

$$\nabla^2 \psi = \frac{2mU}{\hbar^2}\psi \tag{1}$$

for small U in the form

$$\psi = 1 + \chi, \tag{2}$$

where χ is also small, one obtains:

$$\nabla^2 \chi = \frac{2mU}{\hbar^2}. \tag{3}$$

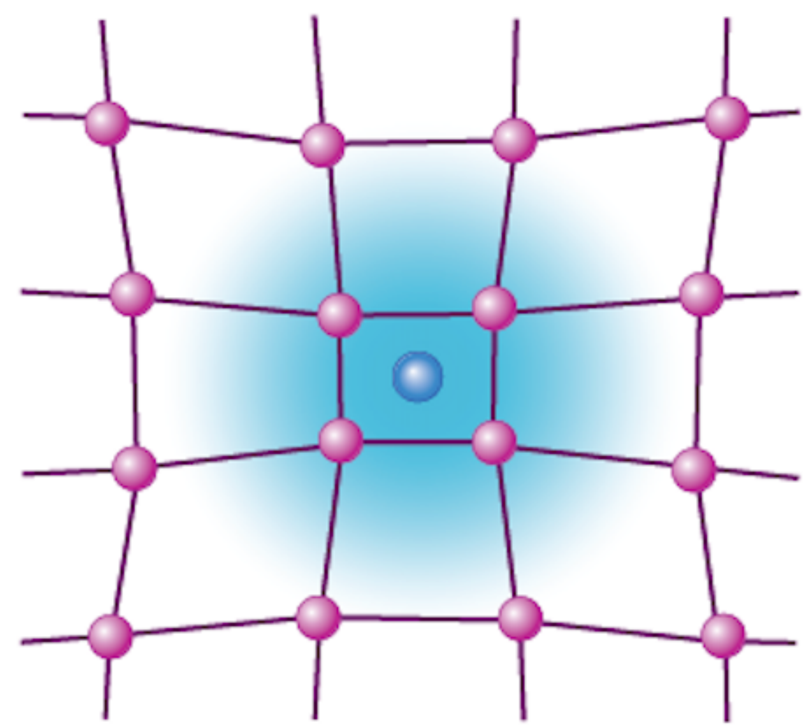
If U decreases at infinity more rapidly than $1/r^2$, then this equation has a solution finite throughout, and whose values are proportional to those of U. For a sufficiently small U one therefore has $|\chi| < 1$ hence $1 + \chi$ vanishes nowhere. (When denoting the dimension of the region where U is different from zero by a, we find that a discrete eigenvalue can only exist when $mUa^2/\hbar^2$ is of the order of unity.)

An analogous proof is possible for a periodic lattice by taking as starting point the solution corresponding to the lowest eigenvalue which is consequently nodeless for a strictly periodic field, and by writing the "distorted" ψ in the form $\psi = \psi_0 + \chi$.

Hence a small distortion does not yet lead to the possible trapping of the electron. This possibility only exists for large distortions. We can now differentiate between two essentially different cases. For, the energetically most favourable state of the total system may correspond, firstly, to the undistorted lattice and the electron moving about "freely" and, secondly, the electron

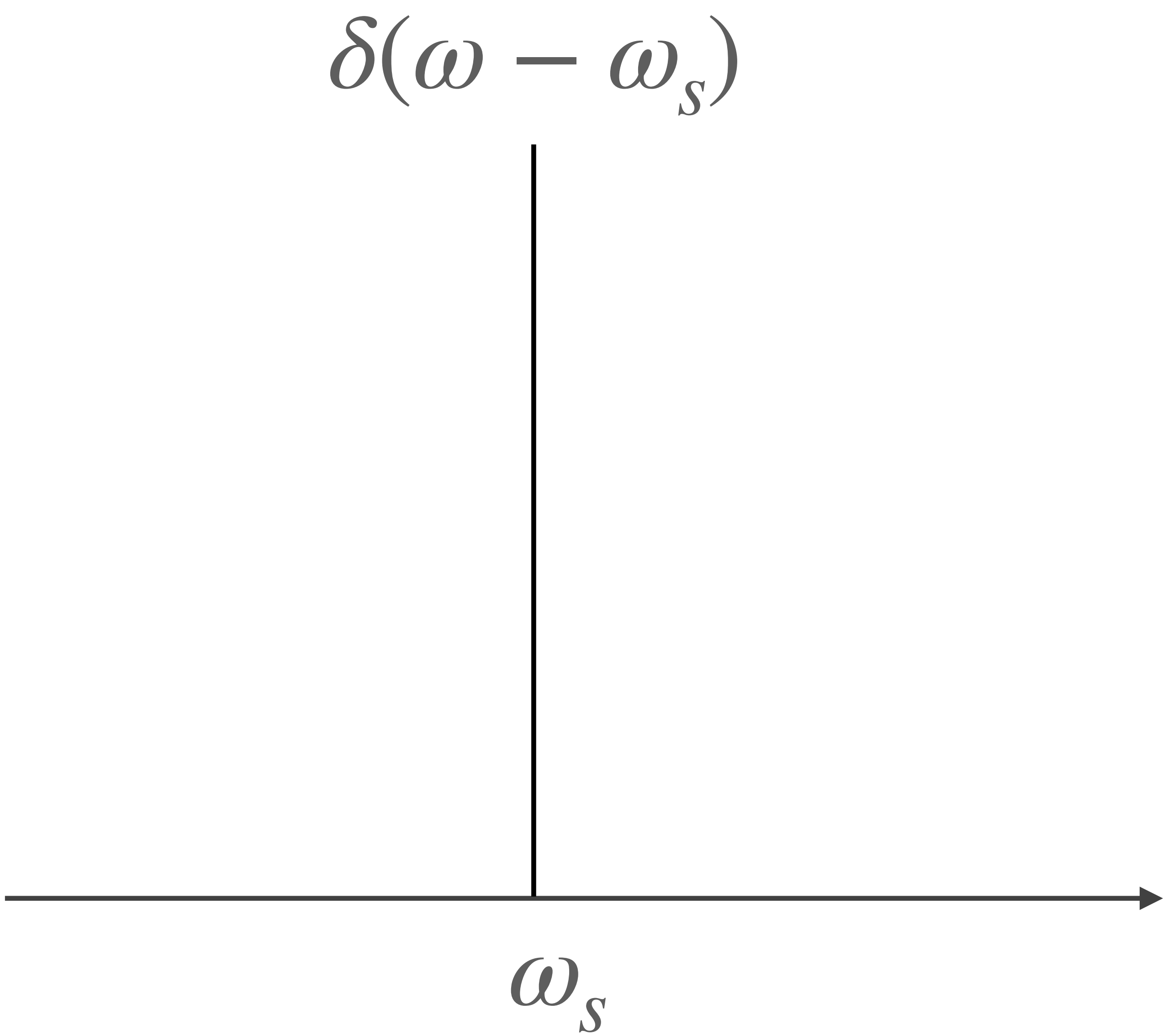
trapped at a strongly distorted region. In the first case, the electron cannot be trapped at all by the lattice. This situation seems to be realised in the case of diamond. In the second case, the electron can only be trapped when passing over an energy barrier. For, as already stated, in the case of a small distortion, the eigenvalues of the electron are not changed. Hence the energy variation of the total system consists solely in the distortion energy and thus is essentially positive. We must therefore expect that the trapping of the electron is associated with activation effects. This corresponds to the situation in the case of NaCl which cannot be discoloured by X-rays at low temperatures. It would be interesting to verify in this effect the $\exp(-A/kT)$ law and to determine the value of the activation energy A.

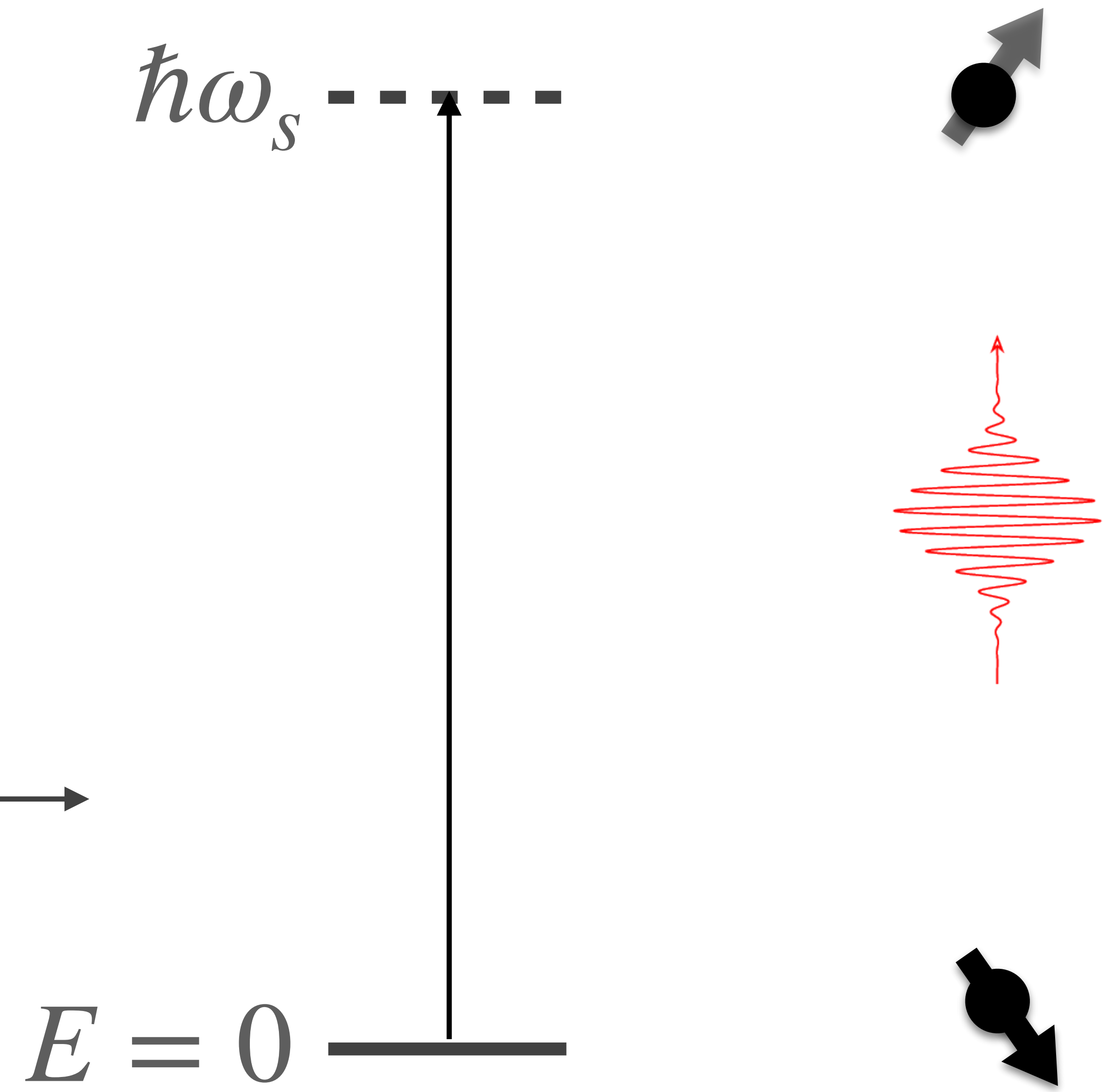
Peker (1946) Landau & Peker (1948) Fröhlich(1950)



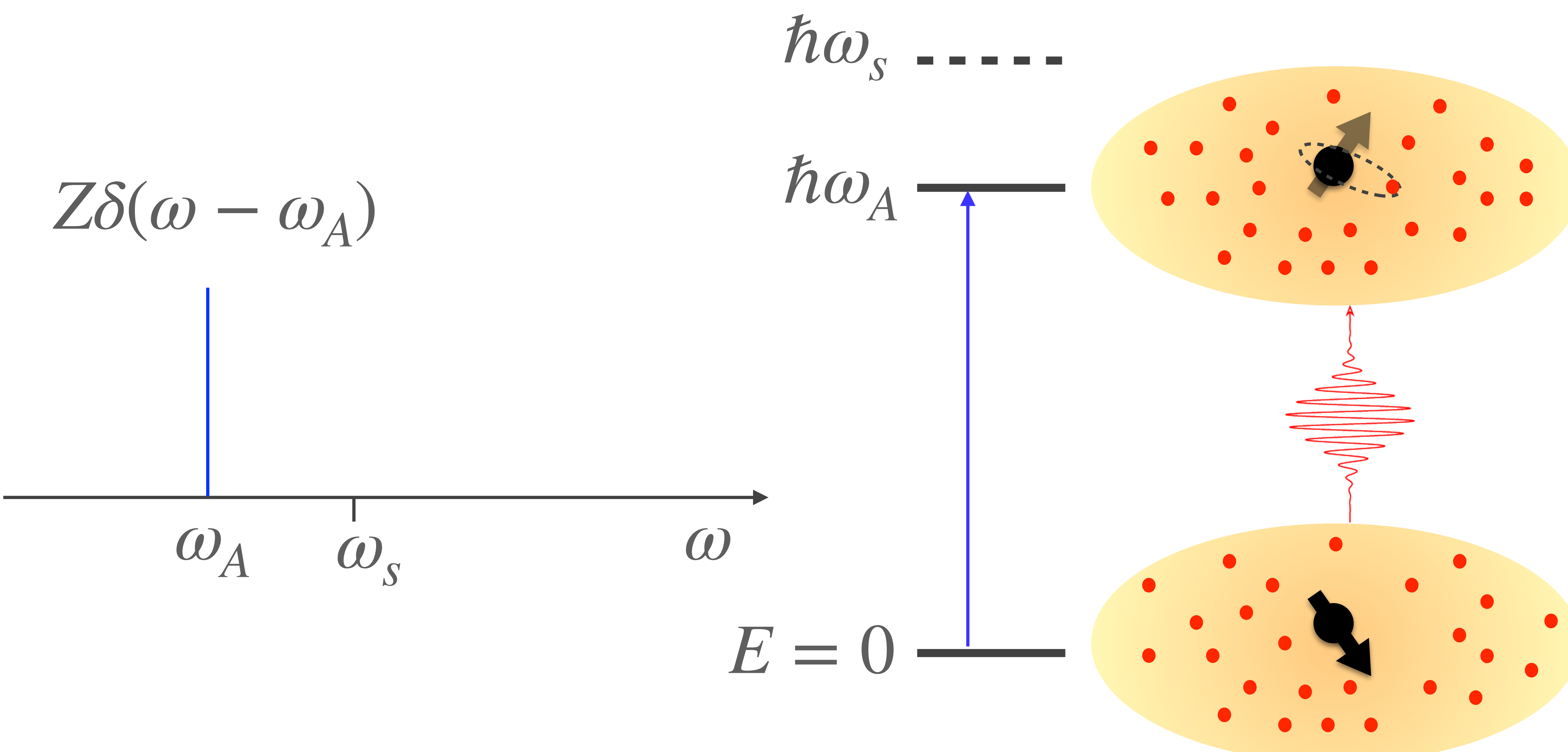
Polaron: impurity + quantum medium

Quasi-particle & Absorption Spectrum

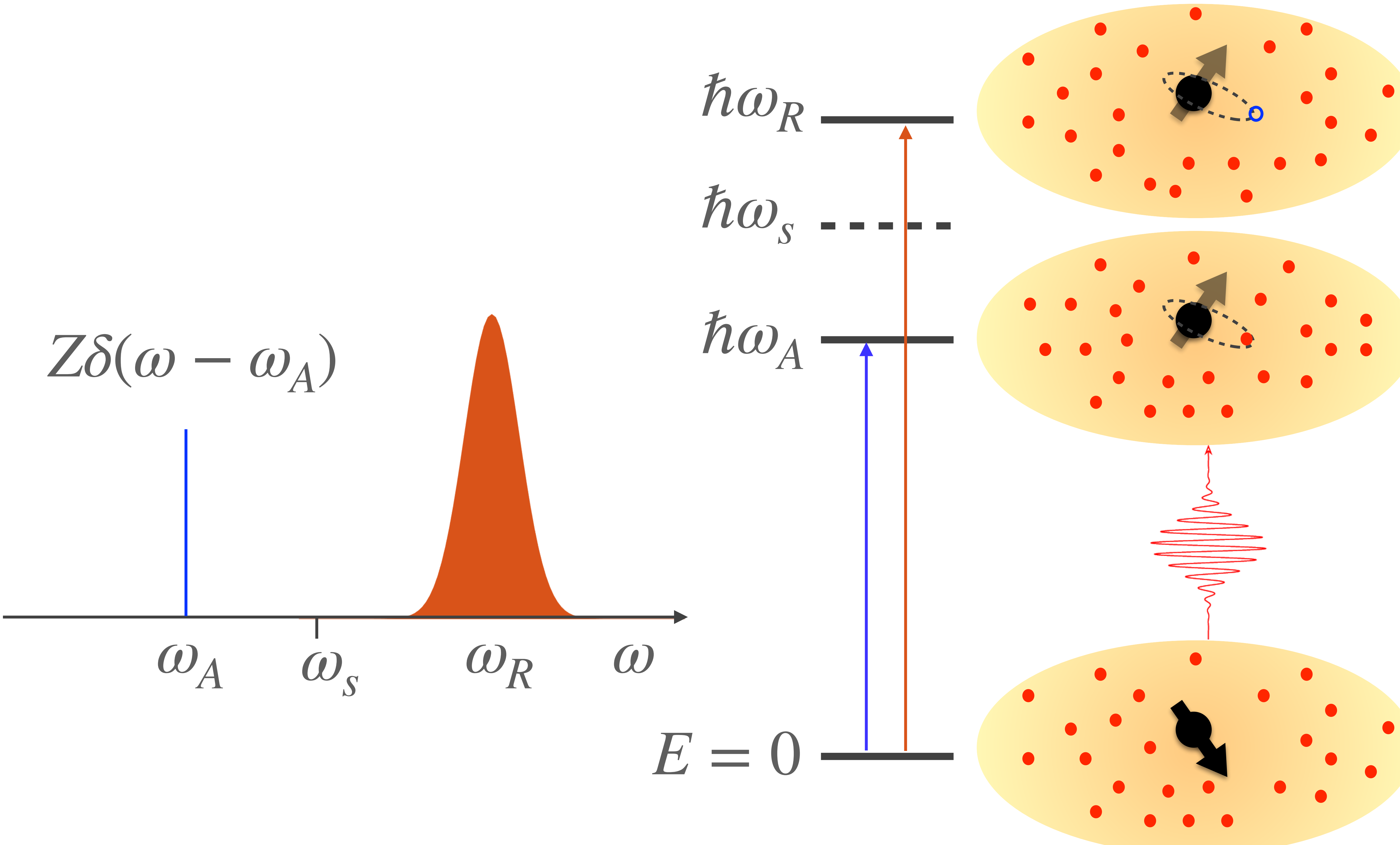




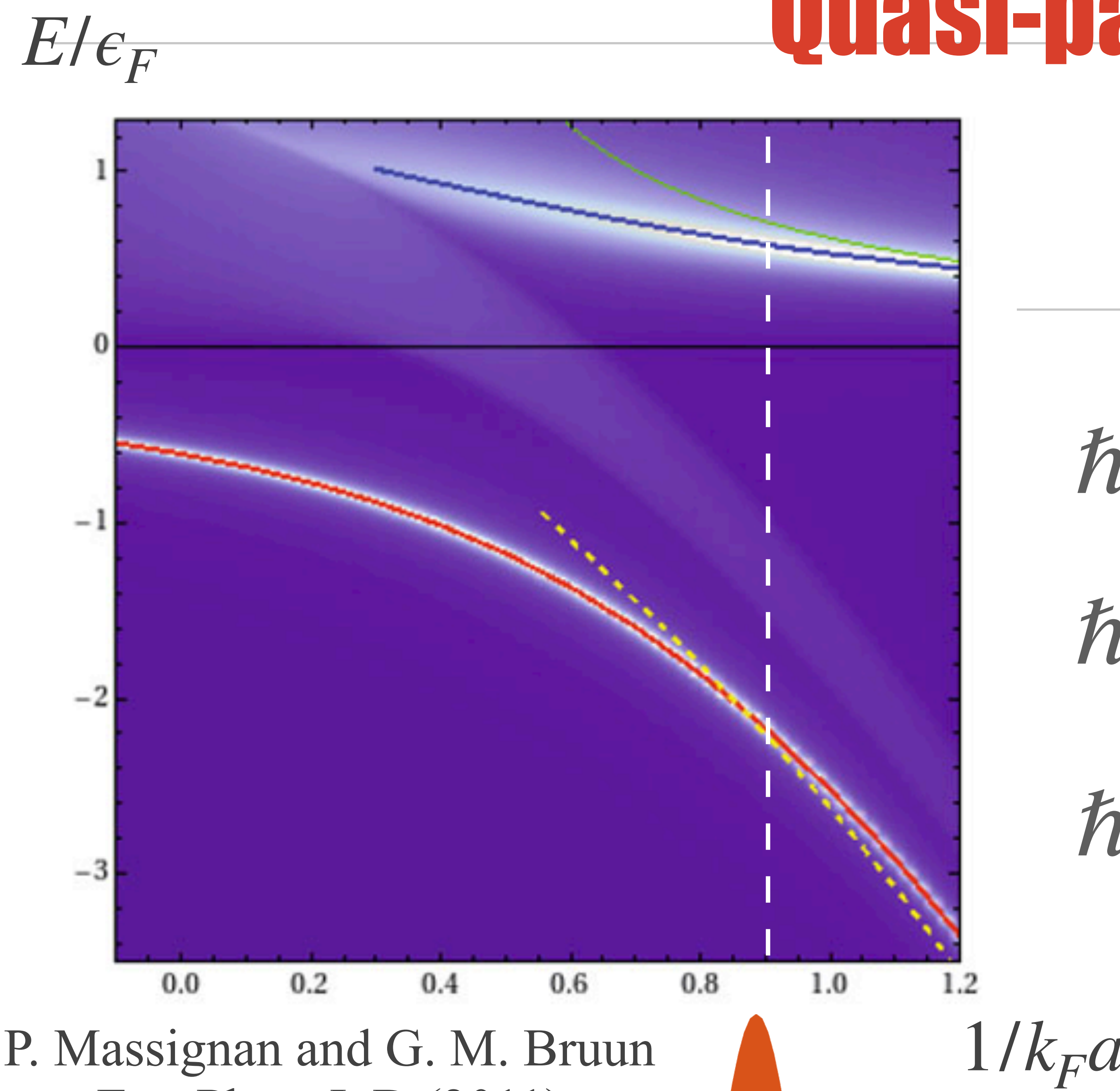
Quasi-particle & Absorption Spectrum



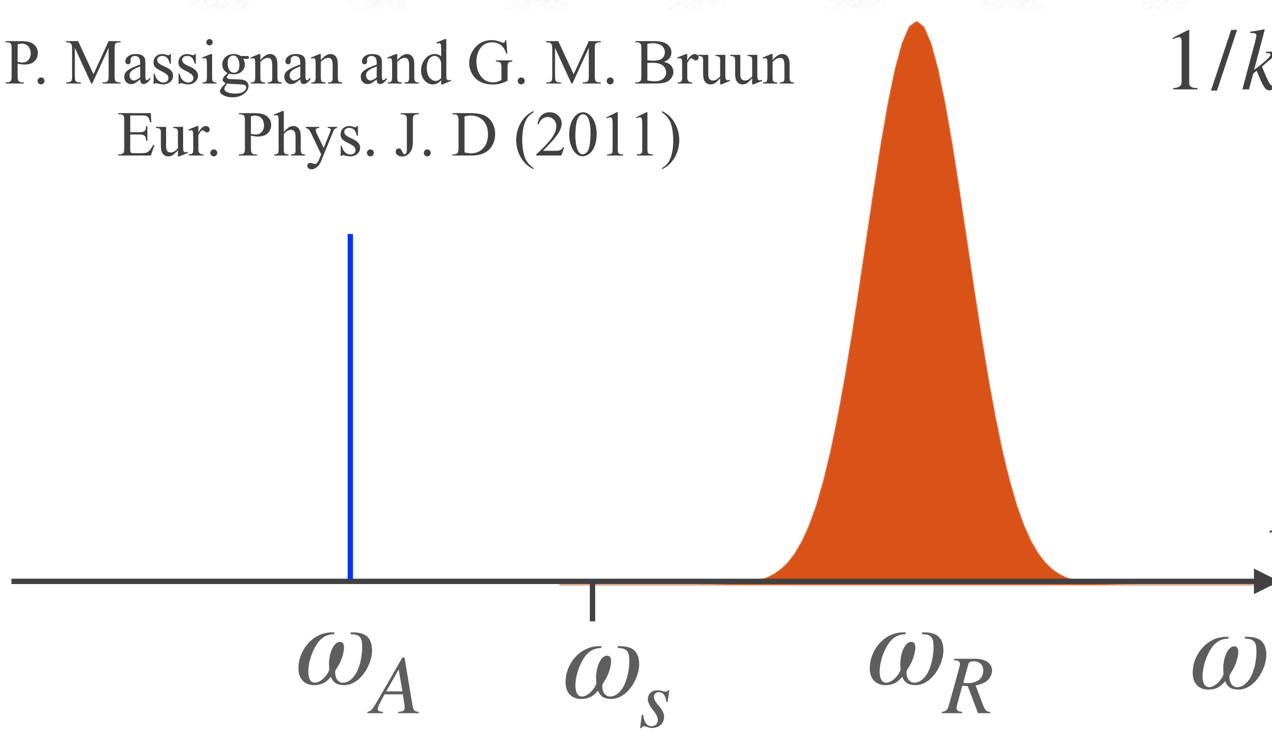
Quasi-particle & Absorption Spectrum

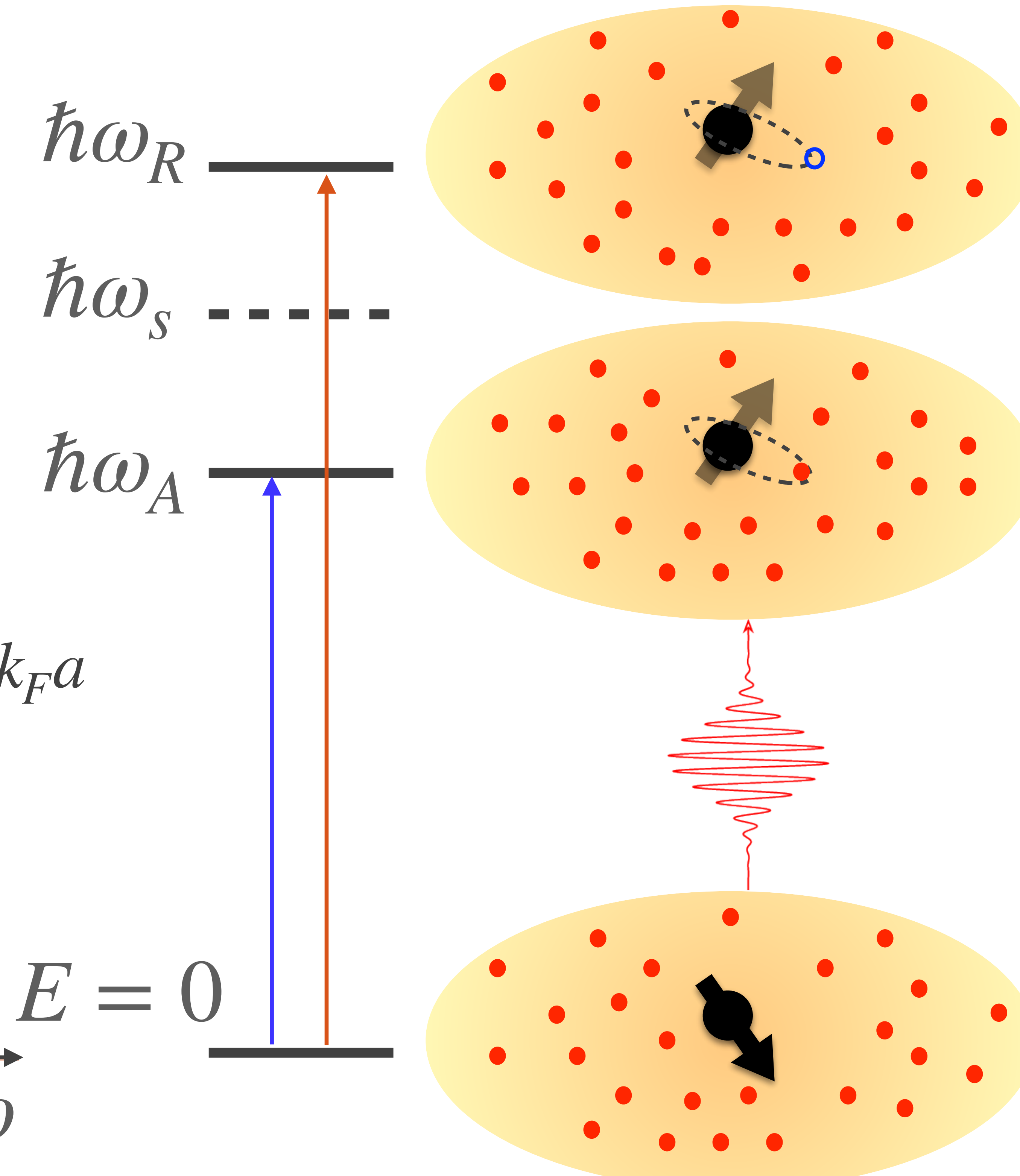


Quasi-particle & Absorption Spectrum

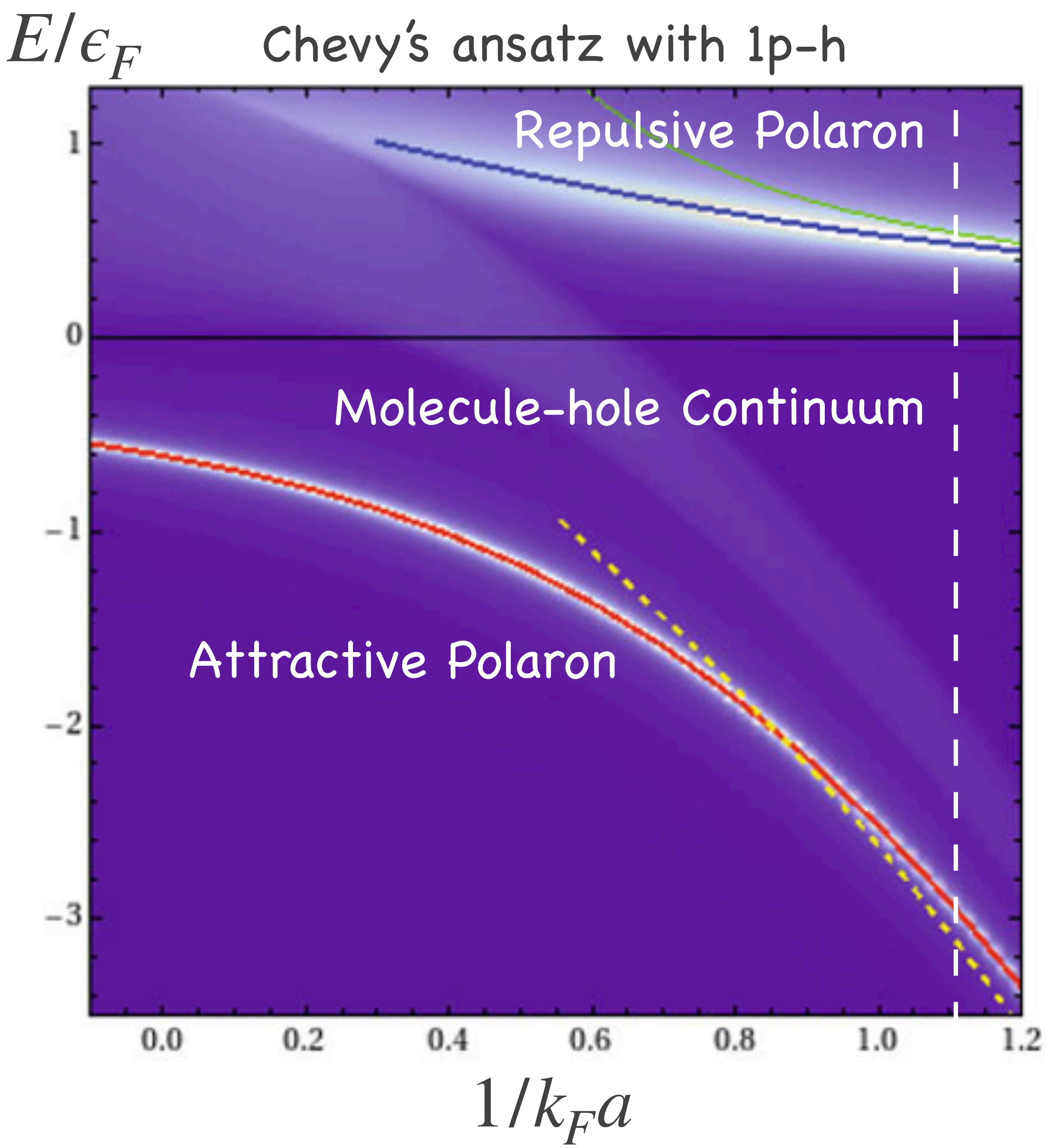


P. Massignan and G. M. Bruun
Eur. Phys. J. D (2011)





Salient Features of Polaron



P. Massignan and G. M. Bruun
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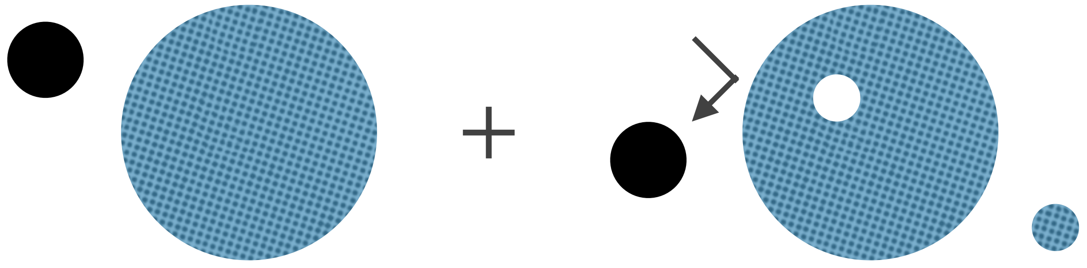
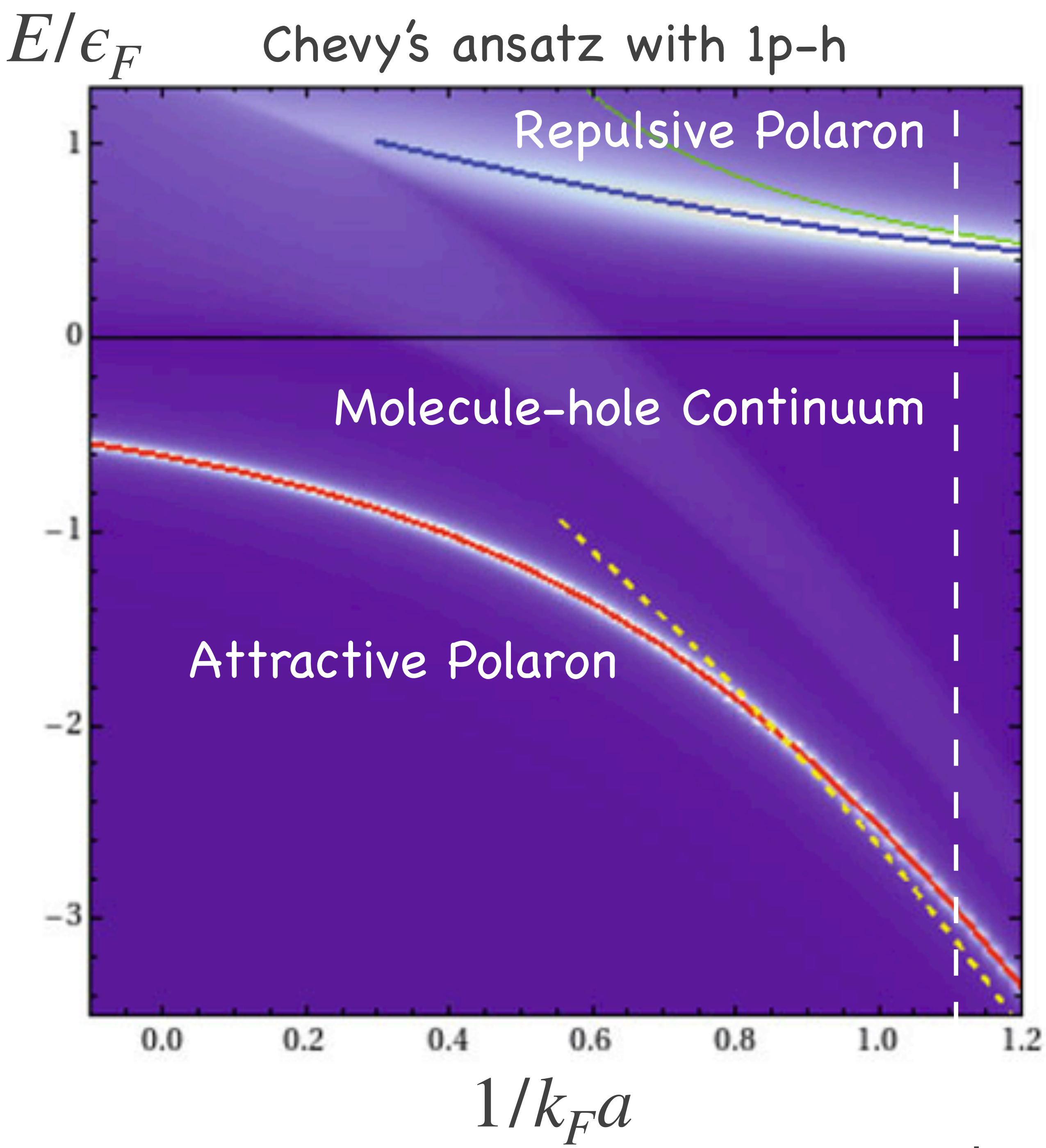


Salient Features of Polaron



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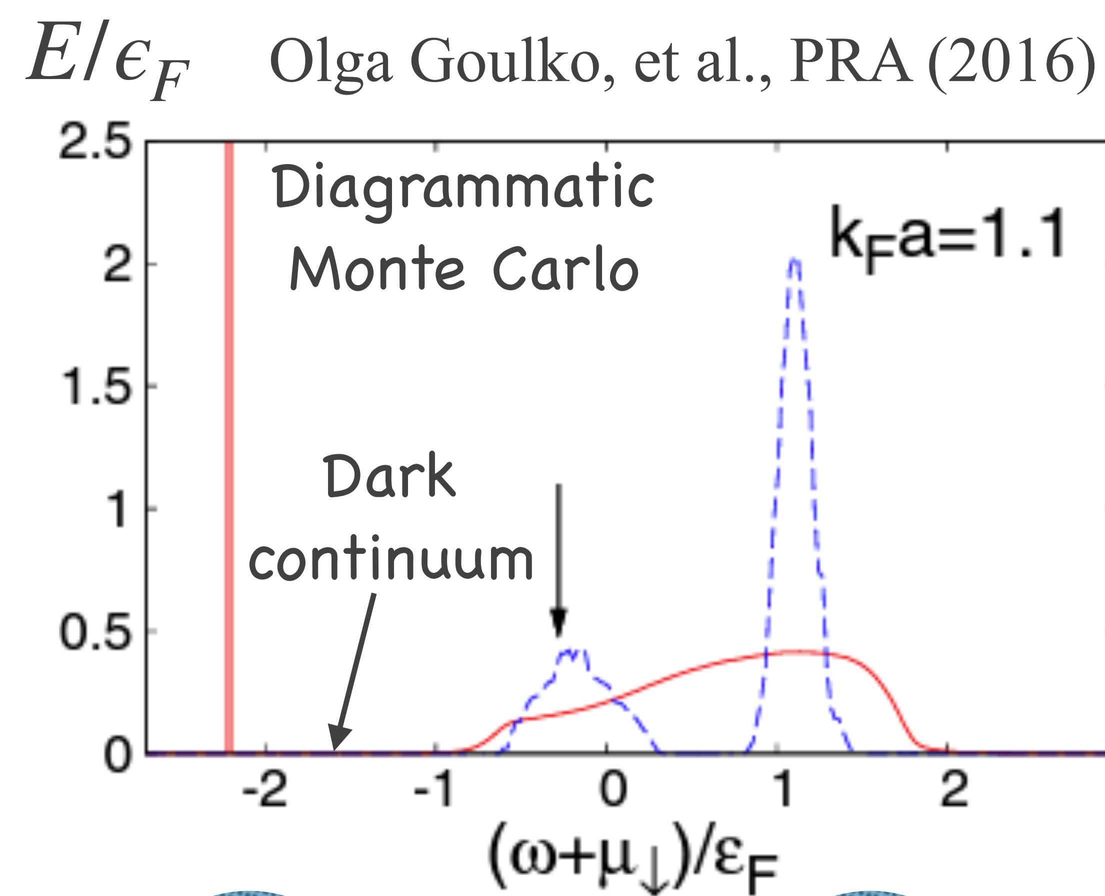
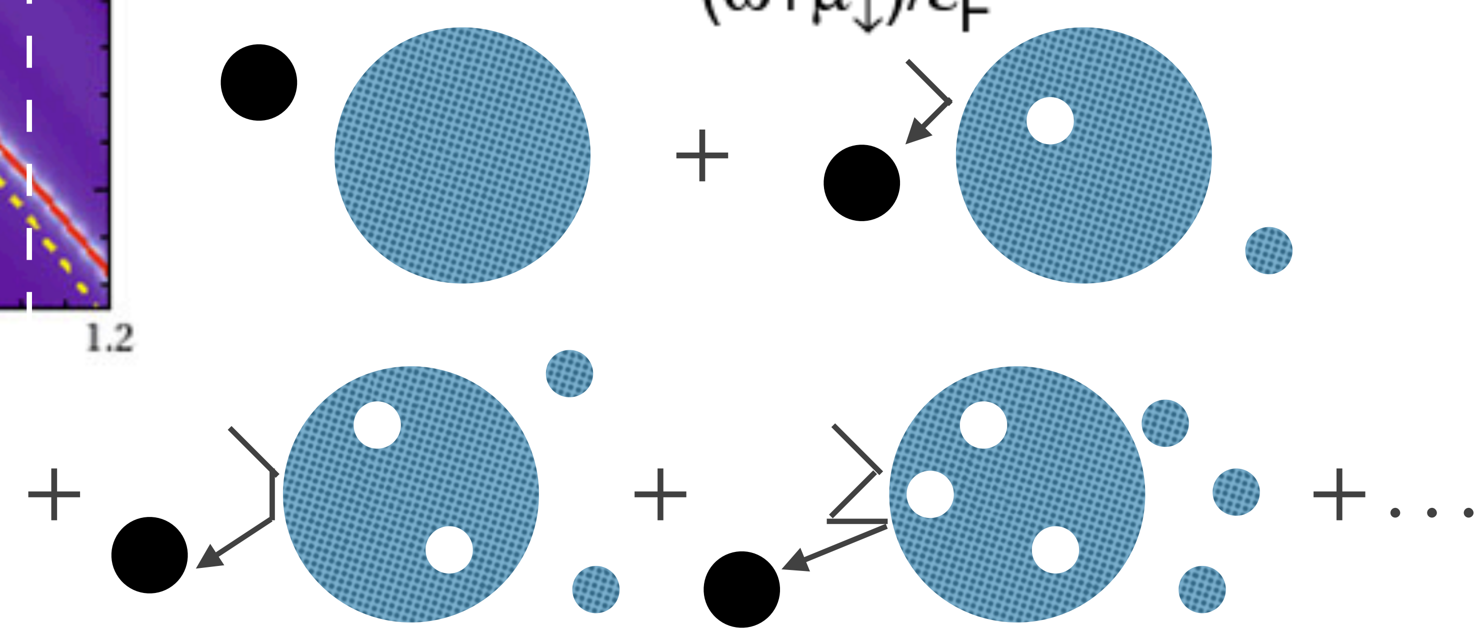
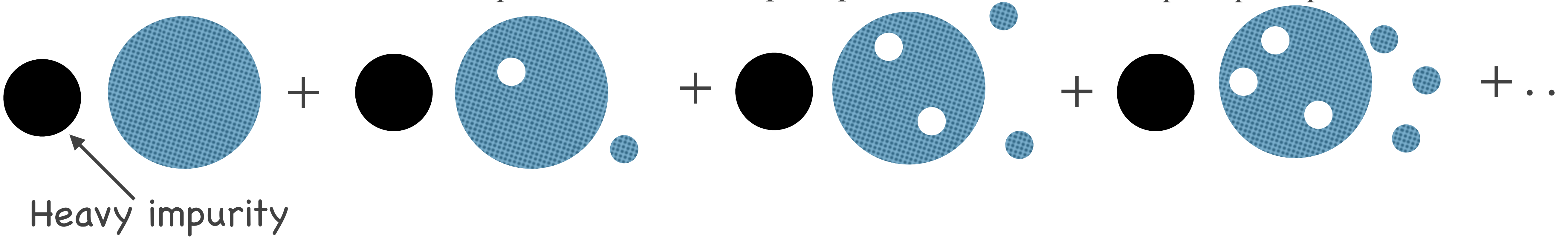
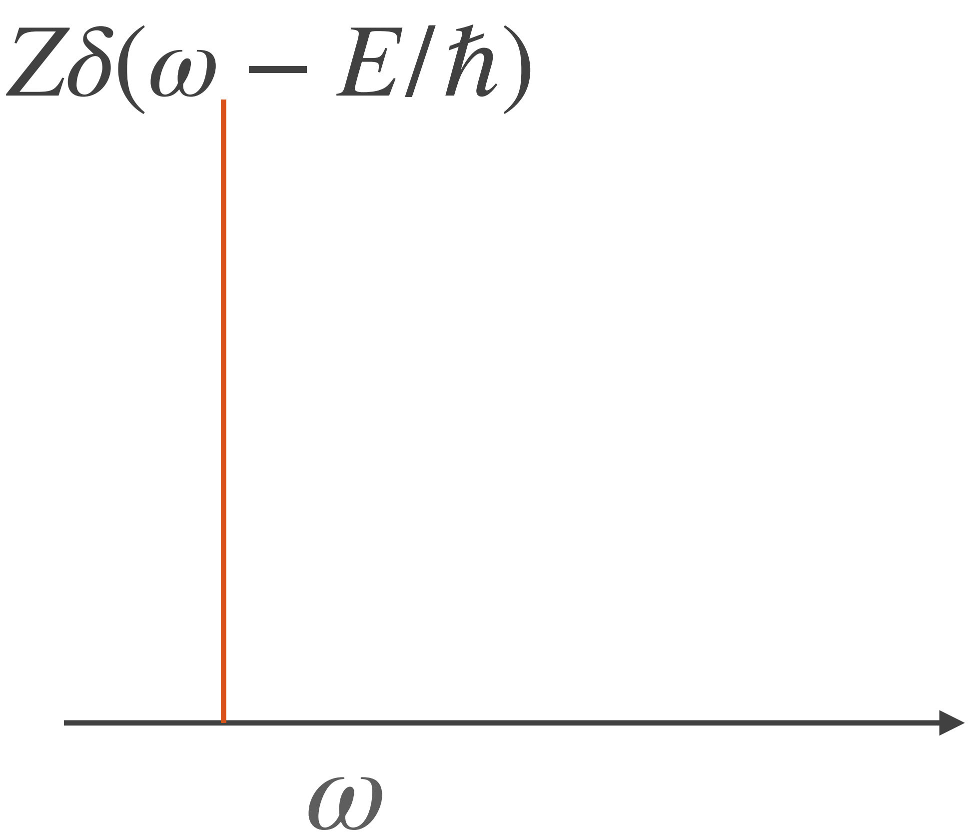




Anderson's Orthogonality Catastrophe

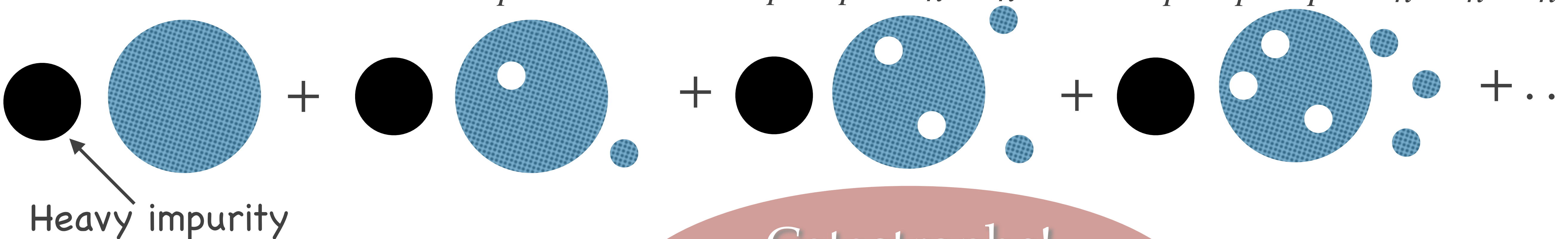
ϕ_0 $\phi_{\mathbf{k}_p,\mathbf{k}_h}$ $\phi_{\mathbf{k}_p^{(1)}\mathbf{k}_p^{(2)},\mathbf{k}_h^{(1)}\mathbf{k}_h^{(2)}}$ $\phi_{\mathbf{k}_p^{(1)}\mathbf{k}_p^{(2)}\mathbf{k}_p^{(3)},\mathbf{k}_h^{(1)}\mathbf{k}_h^{(2)}\mathbf{k}_h^{(3)}}$





Anderson's Orthogonality Catastrophe

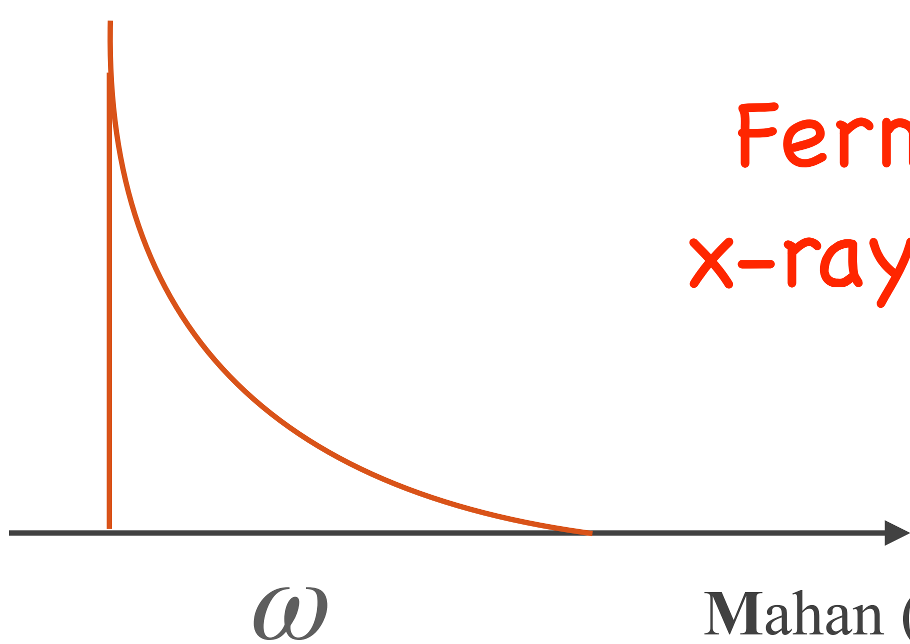
$$\phi_0 \qquad \phi_{\mathbf{k}_p,\mathbf{k}_h} \qquad \phi_{\mathbf{k}_p^{(1)}\mathbf{k}_p^{(2)},\mathbf{k}_h^{(1)}\mathbf{k}_h^{(2)}} \qquad \phi_{\mathbf{k}_p^{(1)}\mathbf{k}_p^{(2)}\mathbf{k}_p^{(3)},\mathbf{k}_h^{(1)}\mathbf{k}_h^{(2)}\mathbf{k}_h^{(3)}}$$



$$\frac{A_0}{(\omega - E/\hbar)^\alpha}\theta(\omega - E/\hbar)$$

Catastrophe!

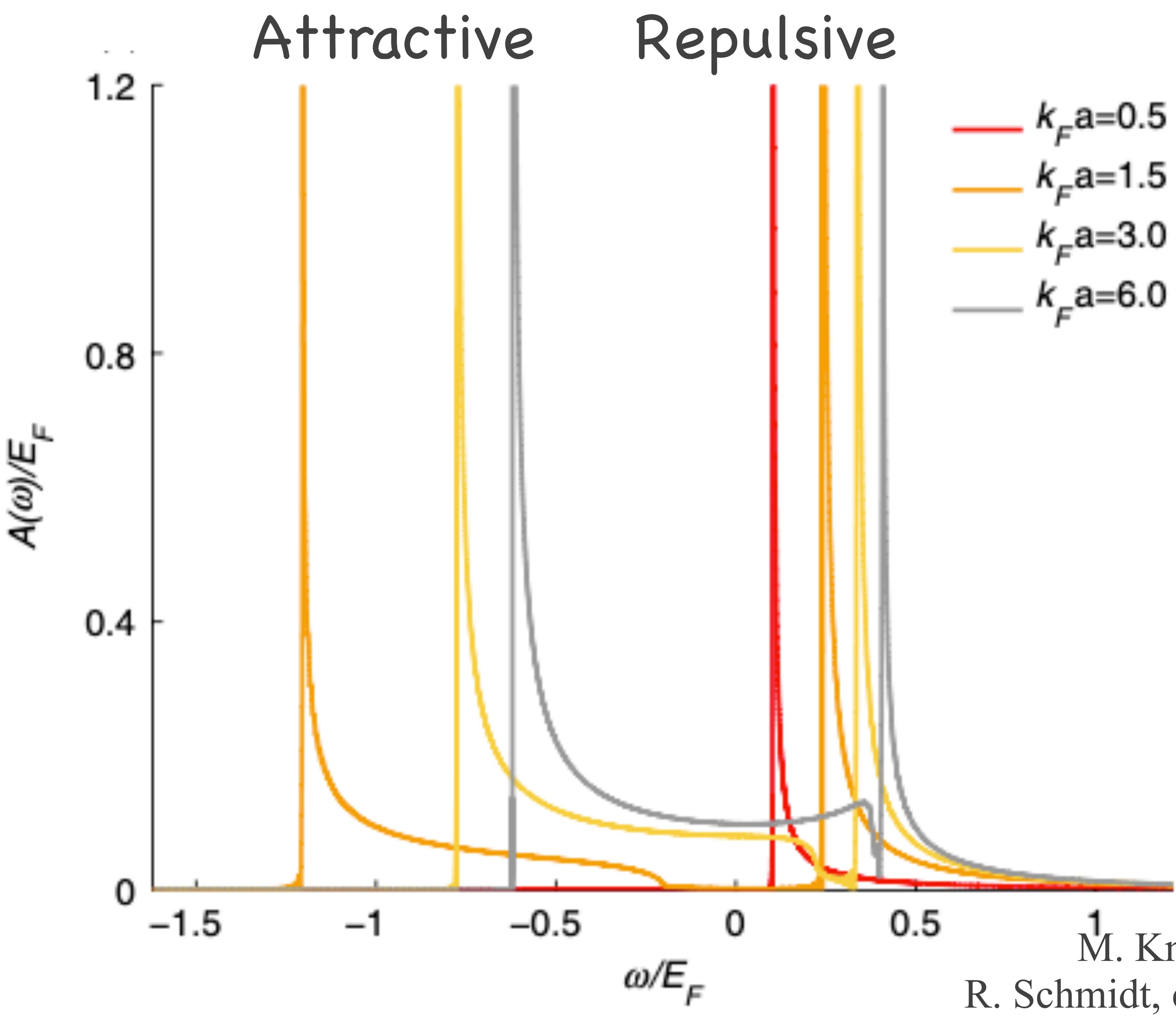
$$Z = |\phi_0|^2 \to 0$$

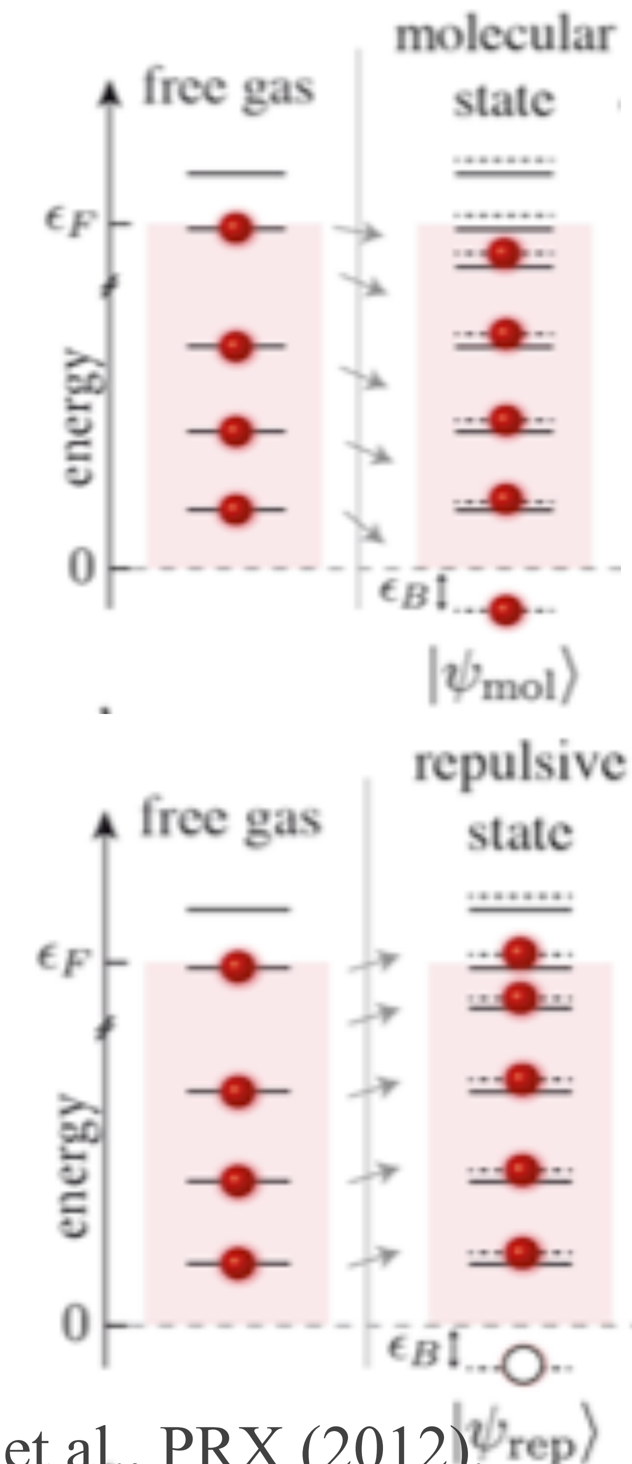


Fermi-edge singularity
x-ray absorption spectra
in metals

Mahan (1967) **N**oziers and de**D**ominicis (1969)

Fermi Edge Singularity



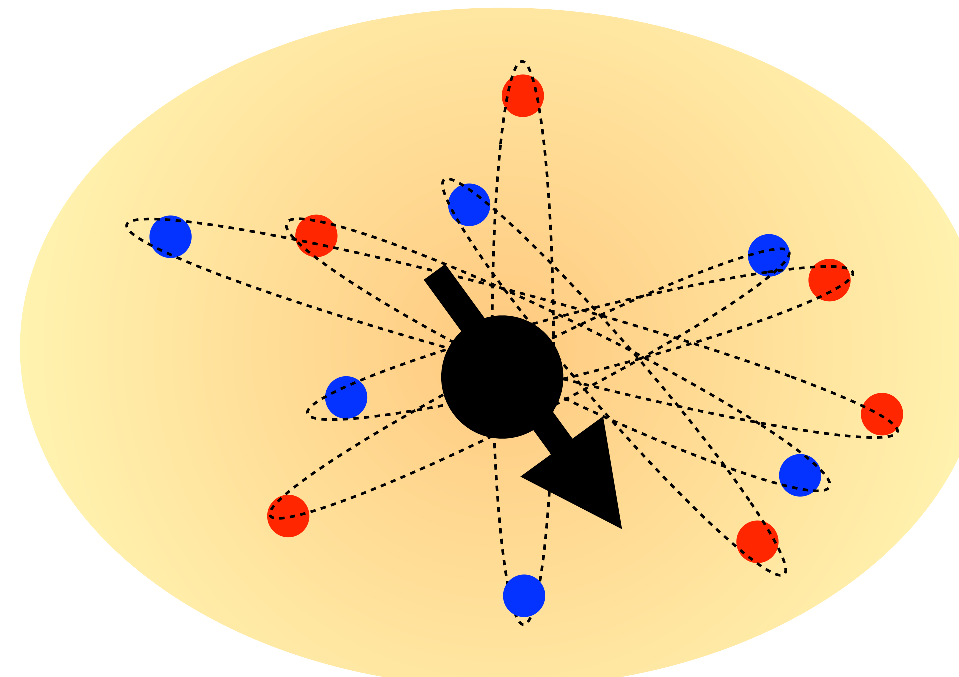


M. Knap, et al., PRX (2012).
R. Schmidt, et al., Rep. Prog. Phys. (2018)

BCS superfluid

Chevy's ansatz /T-matrix approach for mobile impurity:

Nishida, PRL (2015); Yi & Cui, PRA (2015);
Pierce, Leyronas , and Chevy, PRL (2019);
Hu, JW, Zhou, and Liu, PRA (2022)

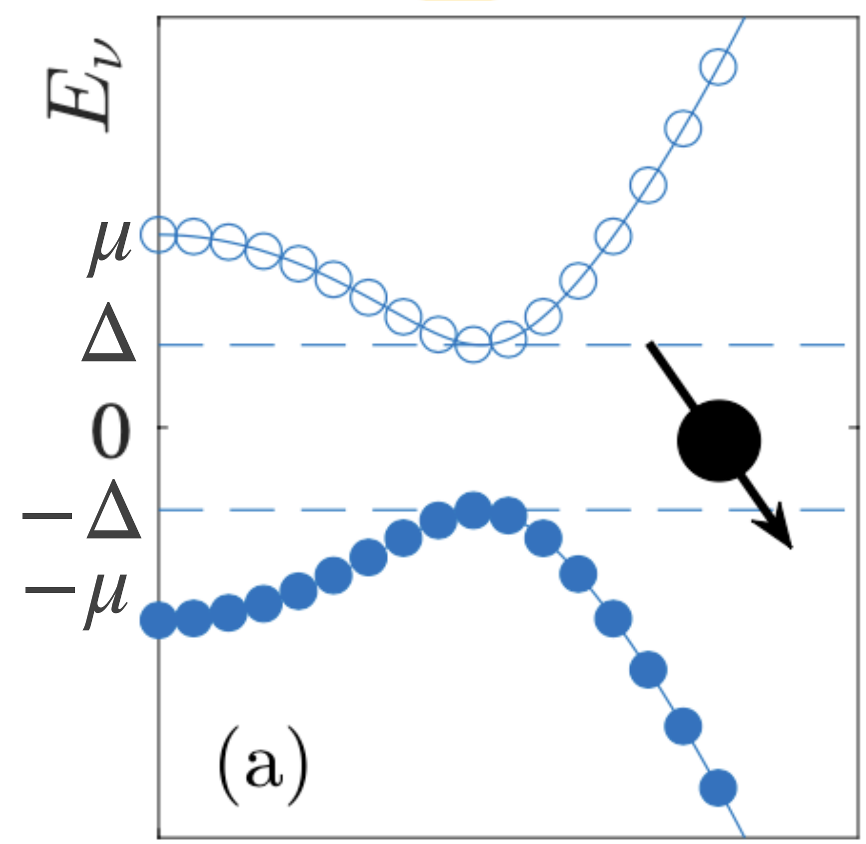


BCS Hamiltonian in Nambu spinor representation: $\hat{\psi}^{\dagger}_{\mathbf{k}} = (c^{\dagger}_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow}) \equiv (c^{\dagger}_{\mathbf{k}}, h^{\dagger}_{\mathbf{k}})$

$$\hat{\mathscr{H}}_i = K_0 + \sum_{\mathbf{k}} \hat{\psi}^{\dagger}_{\mathbf{k}} h_i(\mathbf{k}) \psi_{\mathbf{k}}$$

$$h_i(\mathbf{k}) = \begin{bmatrix} \xi_{\mathbf{k}} & \Delta \\ \Delta & -\xi_{\mathbf{k}} \end{bmatrix}, \qquad \xi_{\mathbf{k}} \equiv \epsilon_{\mathbf{k}} - \mu$$

Bogolyubov spectrum $\quad E_\nu = \pm \mathscr{E}_{k_\nu} = \pm \sqrt{\xi^2_{k_\nu} + \Delta^2}$

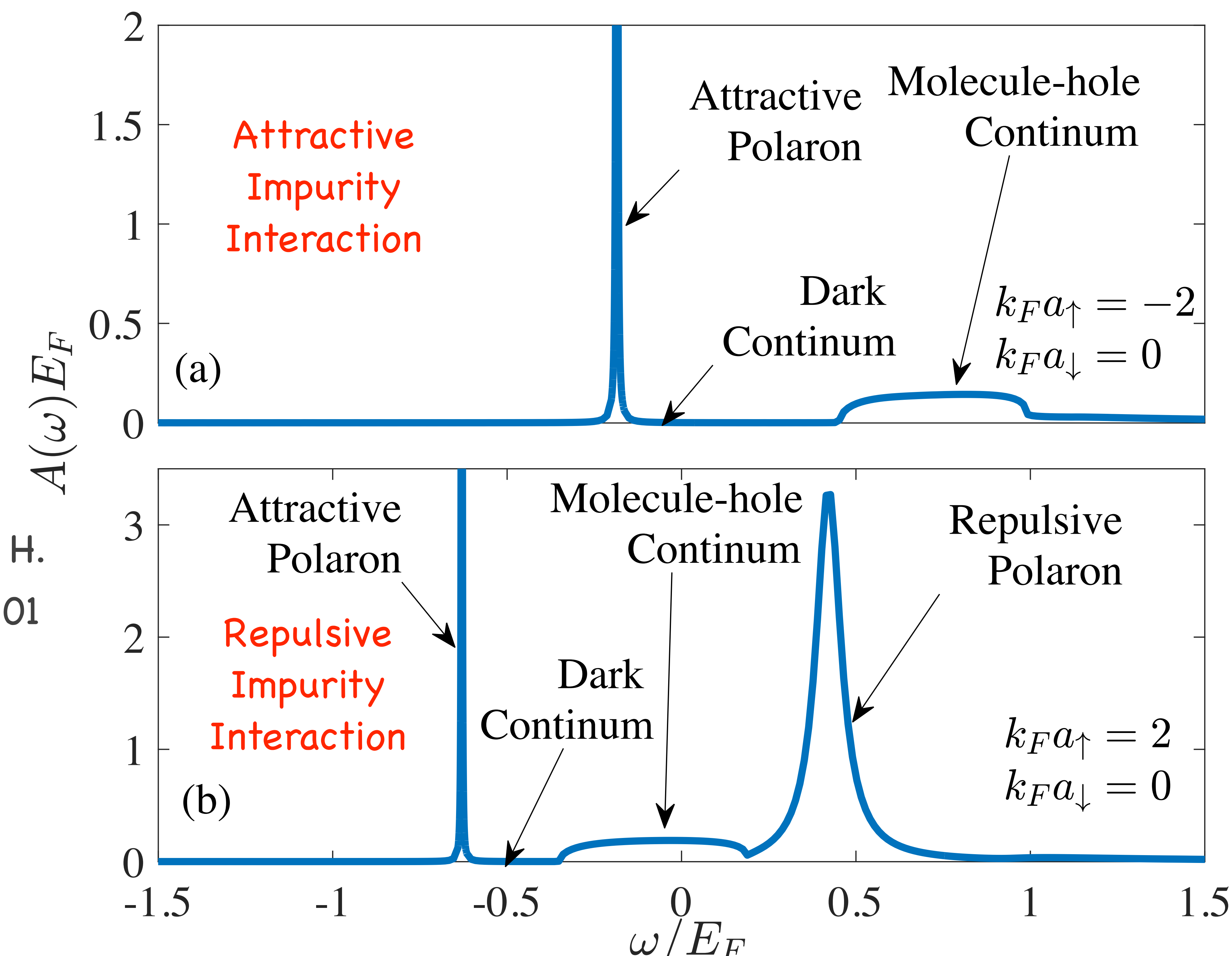


Spectral Function

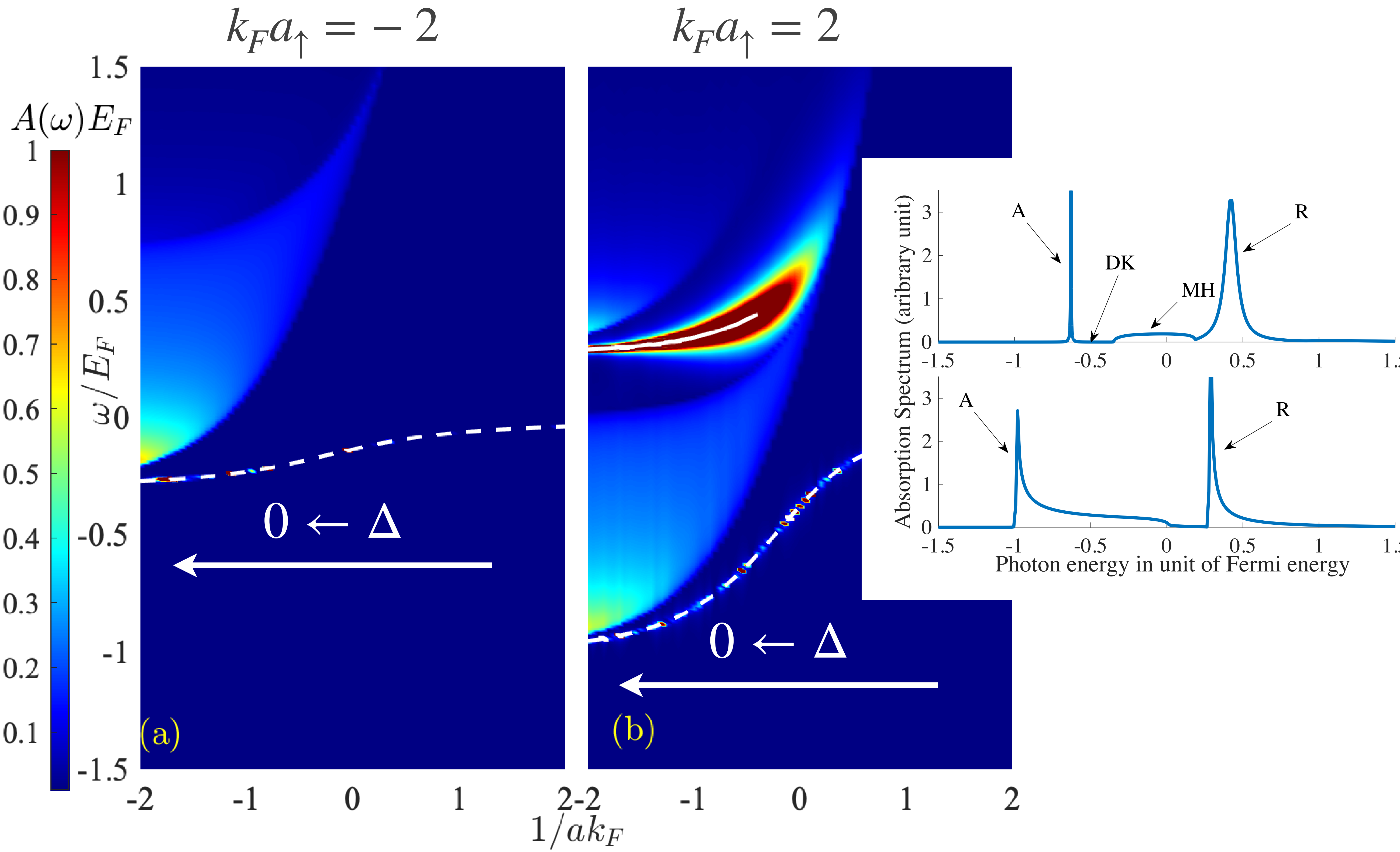
$k_F a = -2$

$\Delta \approx 0.4 E_F$

JW, X.-J. Liu, and H. Hu, PRL **128**, 175301 (2022); PRA **105**, 043320 (2022)



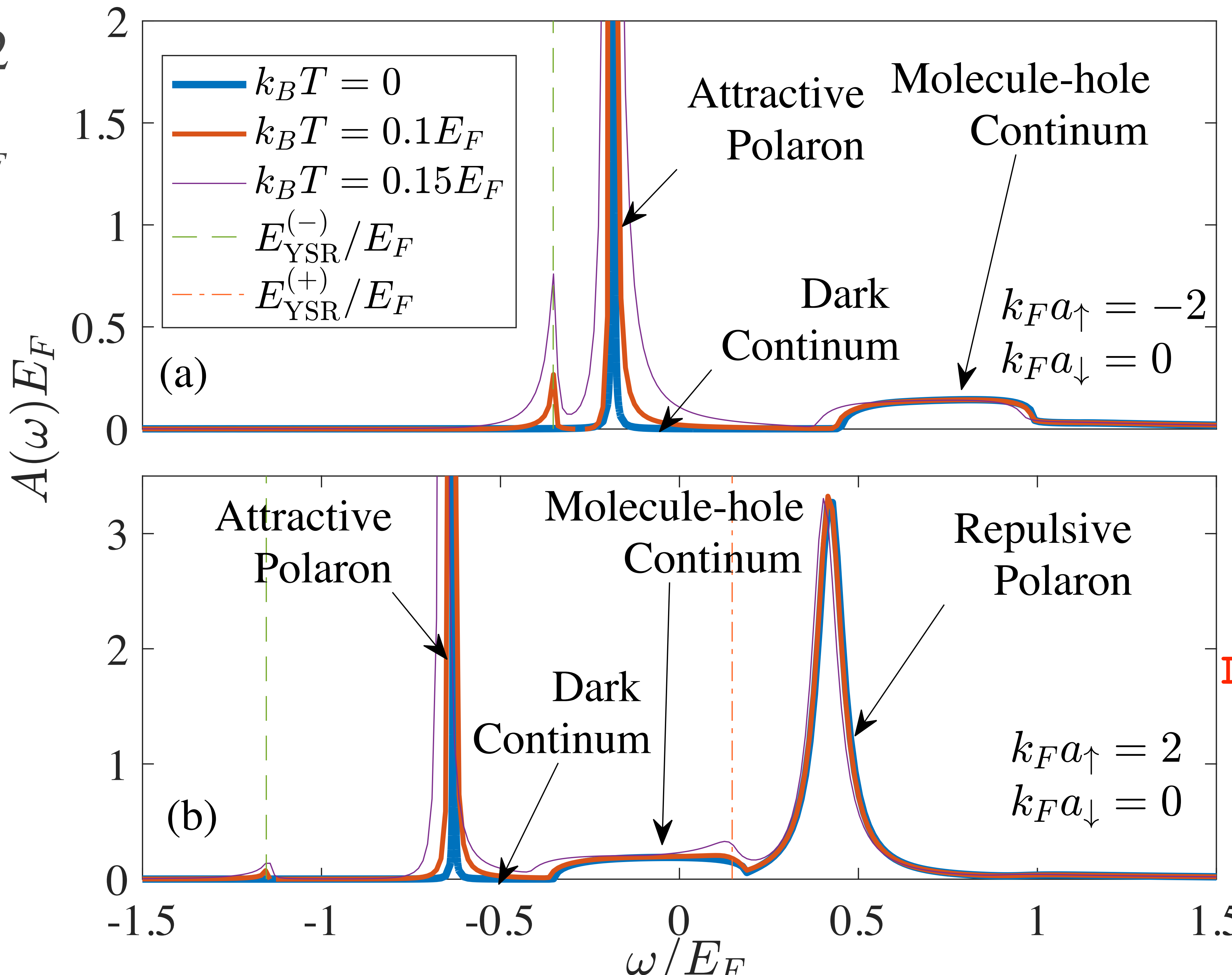
Superfluid Gap Dependence



Finite Temperature

$k_F a = -2$

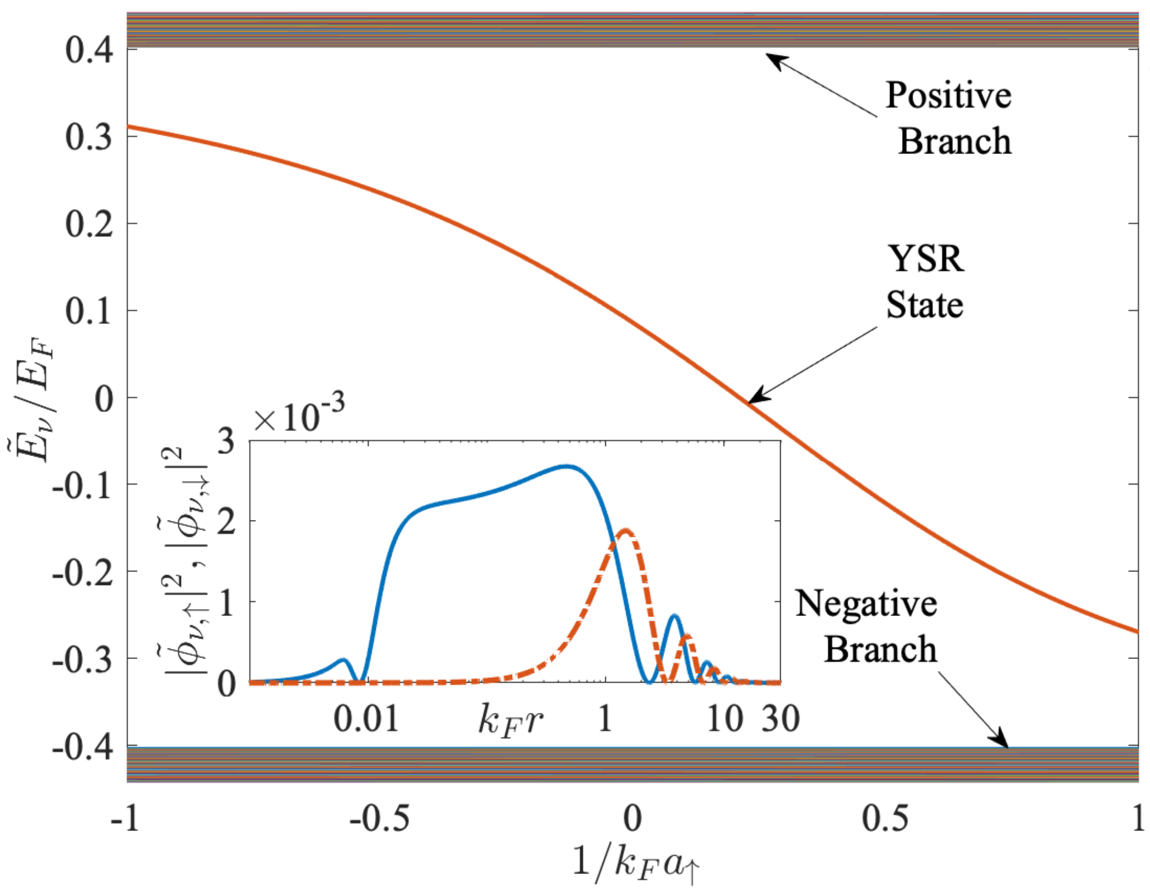
$\Delta \approx 0.4 E_F$

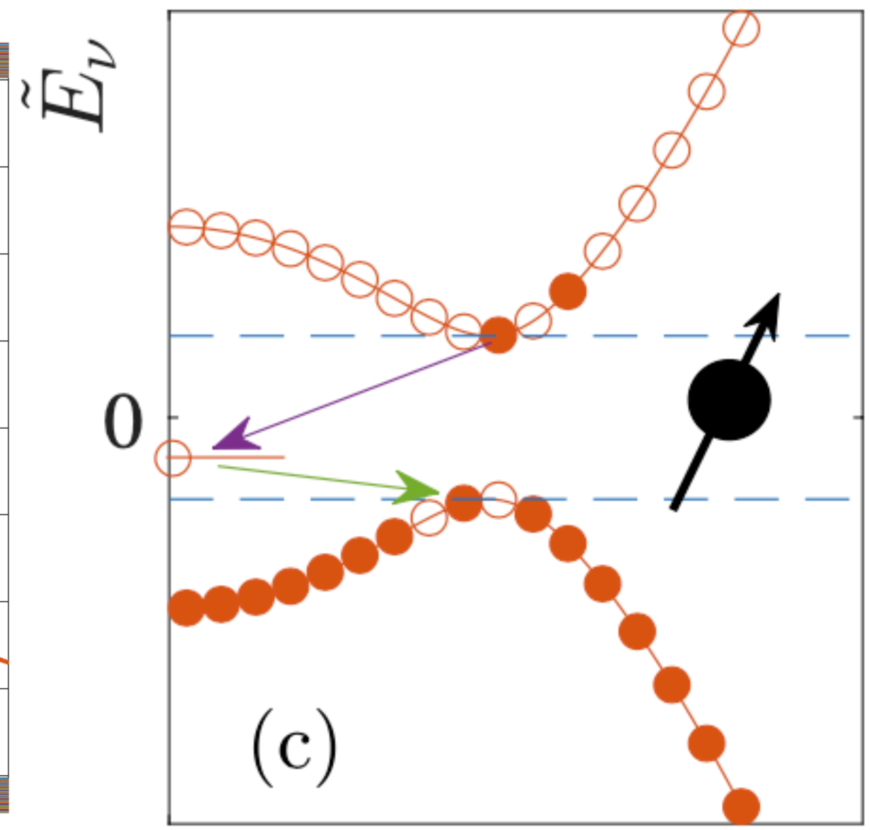


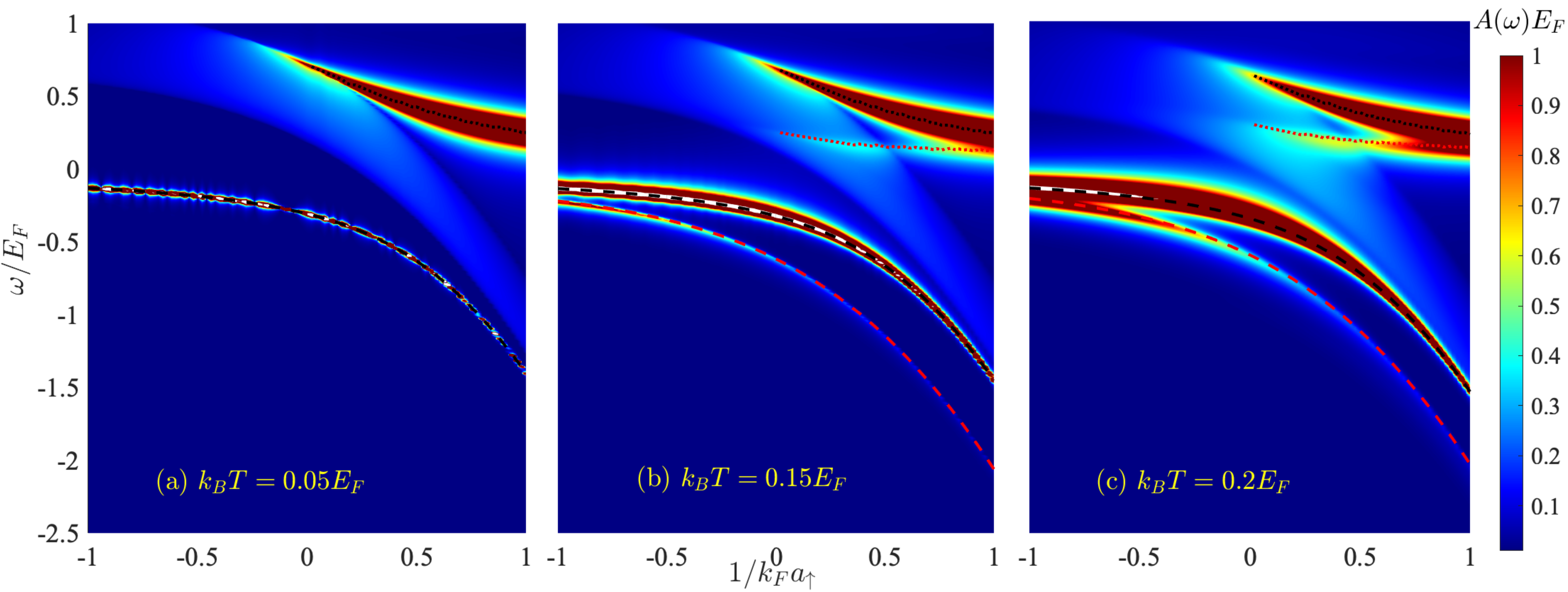
Attractive Impurity Interaction

Repulsive Impurity Interaction

Yu Shiba Rusinov Features







Conclusion

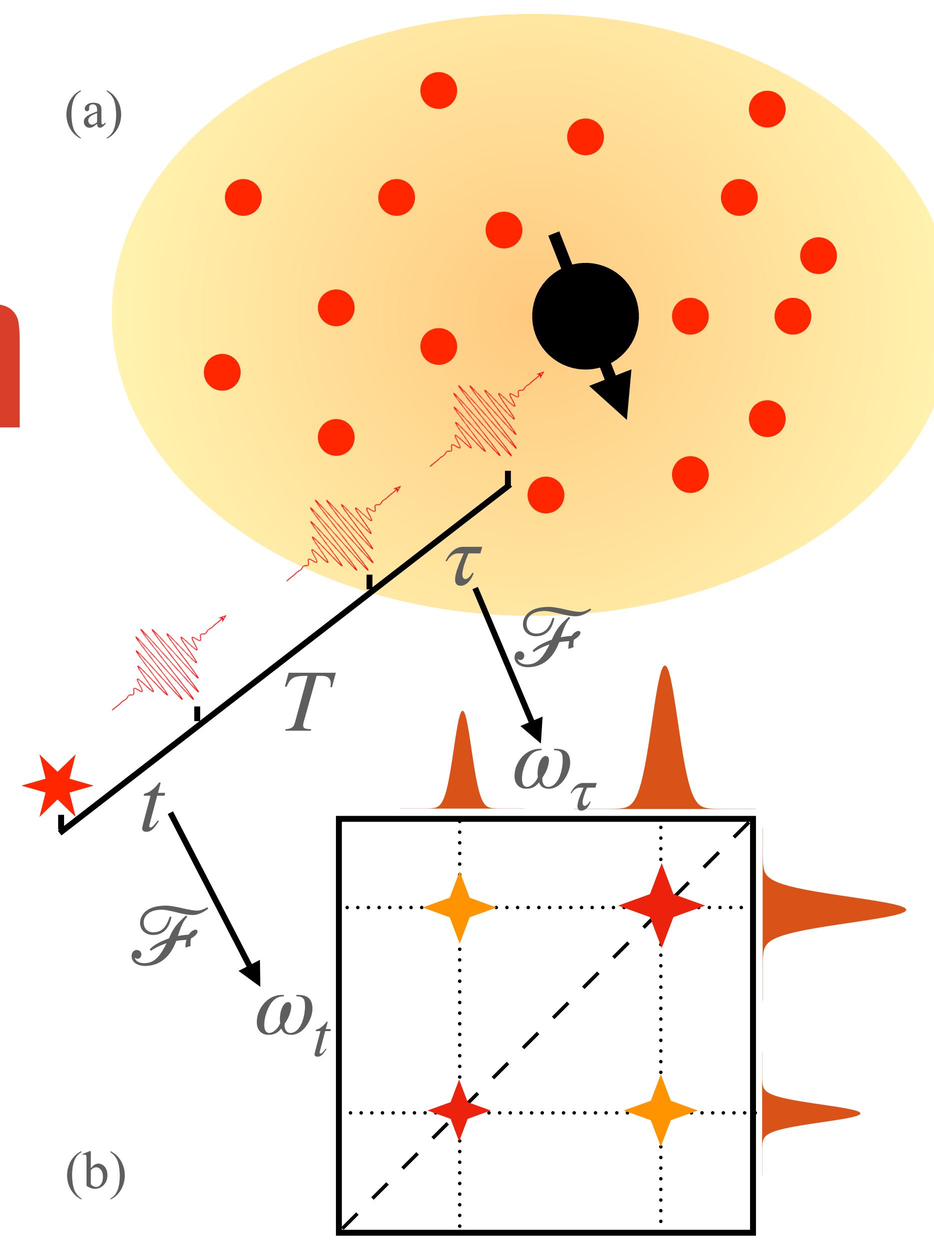
- An exact model to investigate polaron physics;
- YSR features for magnetic impurity;
- Experimental realizable: ^{6}Li-^{133}Cs

Future Extension

- Multidimensional Spectrum.

[1] arXiv: 2207.10501
[2] arXiv: 2207.14509
[3] arXiv: 2208.03599

- p+ip topology superfluid.



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Thank You!

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Feshbach Resonance

van-der-Waals potential

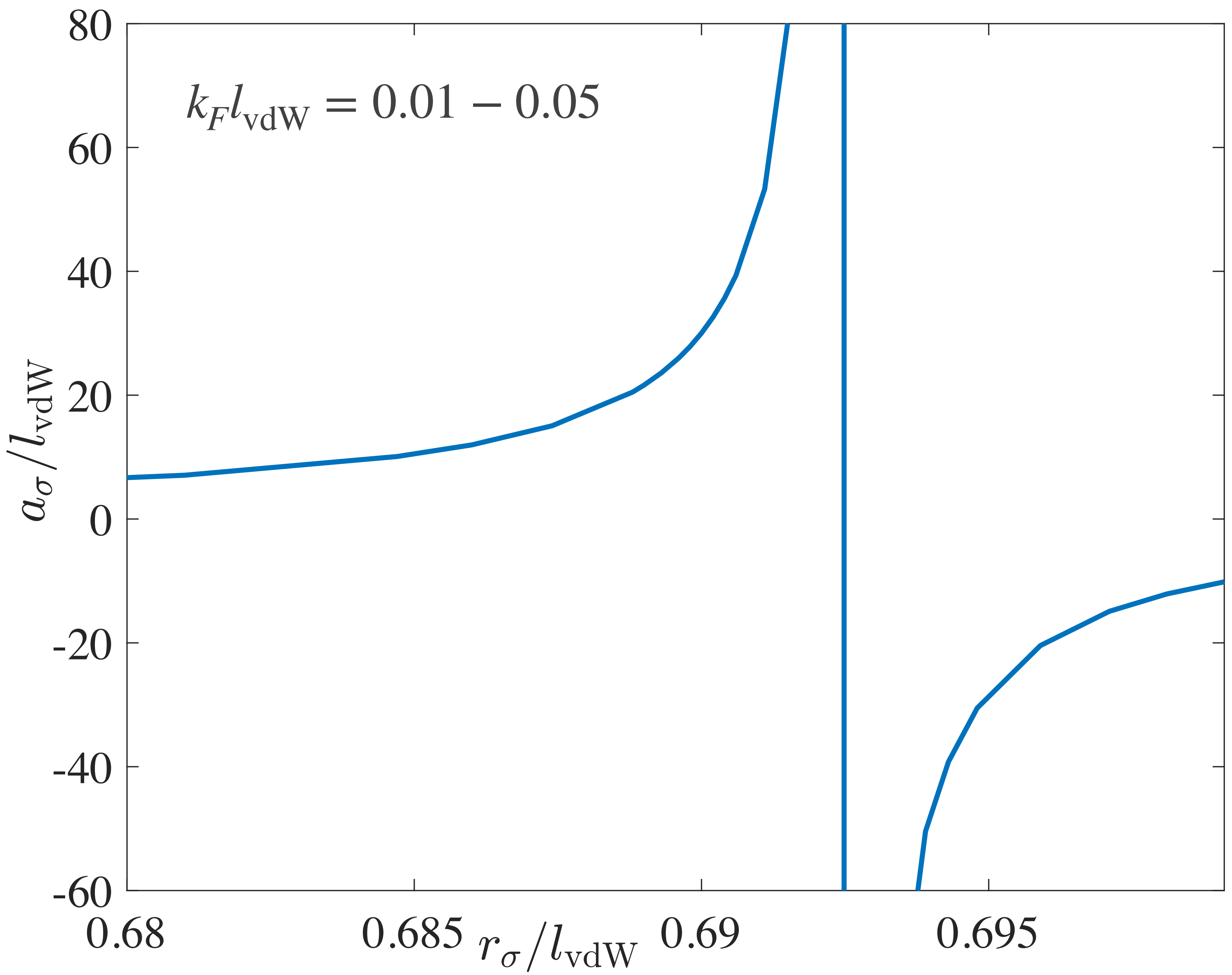
$$V_\sigma(r) = -\frac{C_6}{r^6}\exp\left[-\frac{r_\sigma^6}{r^6}\right]$$

van-der-Waals length

$$l_{\mathrm{vdW}} = (2mC_6)^{1/4}/2$$

scattering length:

$$a_\sigma(E_F) = -\frac{\tan\eta_\sigma(k_F)}{k_F}$$



A Heavy Impurity in a BCS superfluid

Interacting Hamiltonian: $\hat{\mathscr{H}}_f = \hat{H}_i + \hat{V} \equiv \hat{H}_i + \sum_{\sigma,\mathbf{k},\mathbf{q}} \tilde{V}_\sigma(\mathbf{k}-\mathbf{q}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{q}\sigma},$

$$(c^\dagger_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow}) \equiv (c^\dagger_{\mathbf{k}}, h^\dagger_{\mathbf{k}})$$

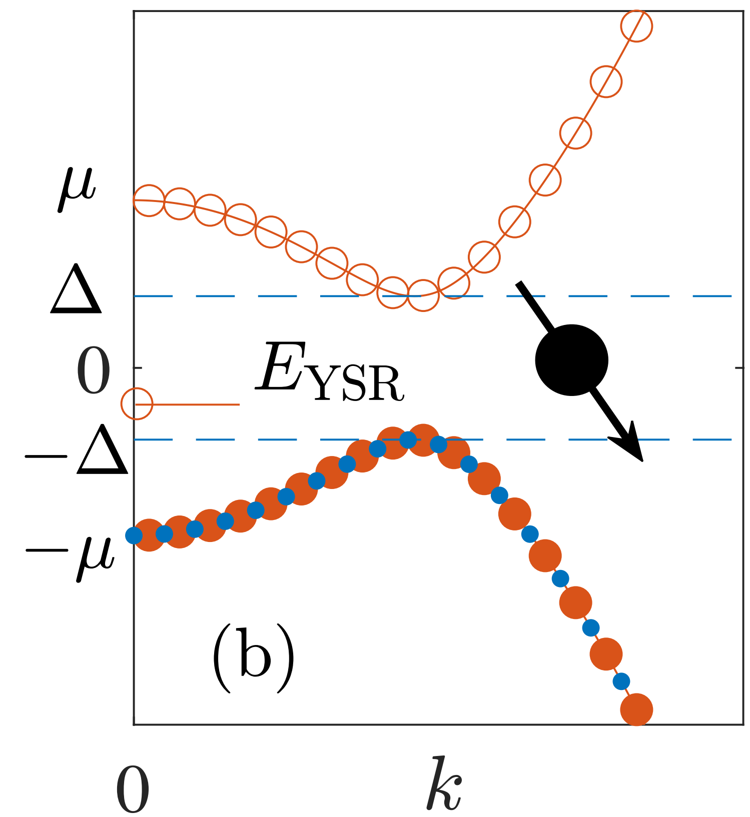
$$\hat{V} = \sum_{\mathbf{kq}} \left[\tilde{V}_\uparrow(\mathbf{k}-\mathbf{q}) c^\dagger_{\mathbf{k}} c_{\mathbf{q}} - \tilde{V}_\downarrow(\mathbf{q}-\mathbf{k}) h^\dagger_{\mathbf{k}} h_{\mathbf{q}} \right] + \sum_{\mathbf{k}} \tilde{V}_\downarrow(0)$$

Bilinear Form:

$$\hat{\mathscr{H}}_f = K_0 + \omega_0 + \sum_{\mathbf{kq}} \hat{\psi}^\dagger_{\mathbf{k}} \underline{h_f(\mathbf{k},\mathbf{q})} \hat{\psi}_{\mathbf{q}}$$

Single-particle Hamiltonian:

$$\underline{h_f(\mathbf{k},\mathbf{q})} = \underline{h_i(\mathbf{k})}\delta_{\mathbf{kq}} + \begin{bmatrix} \tilde{V}_\uparrow(\mathbf{k}-\mathbf{q}) & 0 \\ 0 & -\tilde{V}_\downarrow(\mathbf{q}-\mathbf{k}) \end{bmatrix}$$



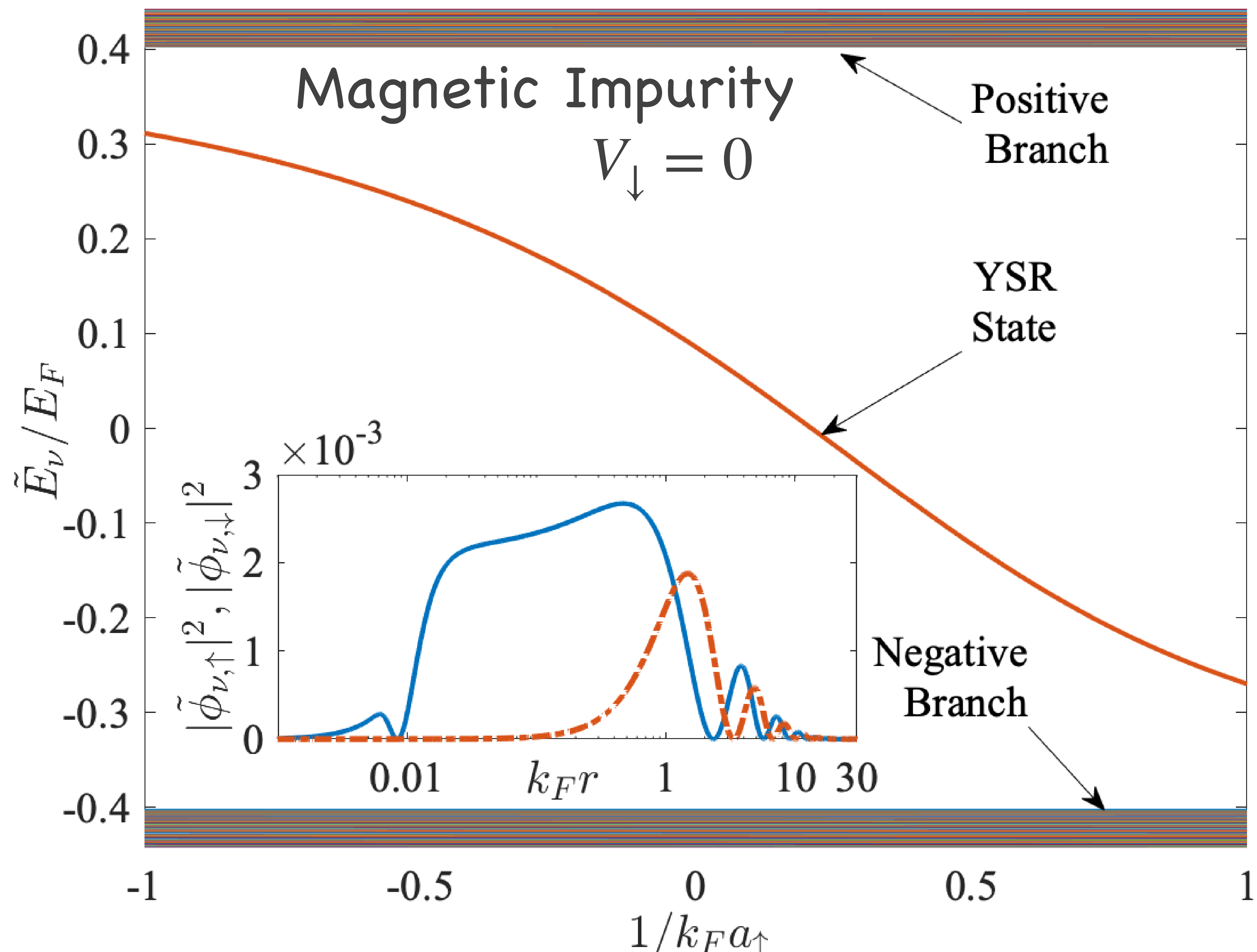
exact formula of FDA:

$$S(t) = e^{-i\omega_0 t} \det[1 - \hat{n} + e^{i\hat{h}_i t} e^{-i\hat{h}_f t} \hat{n}]$$

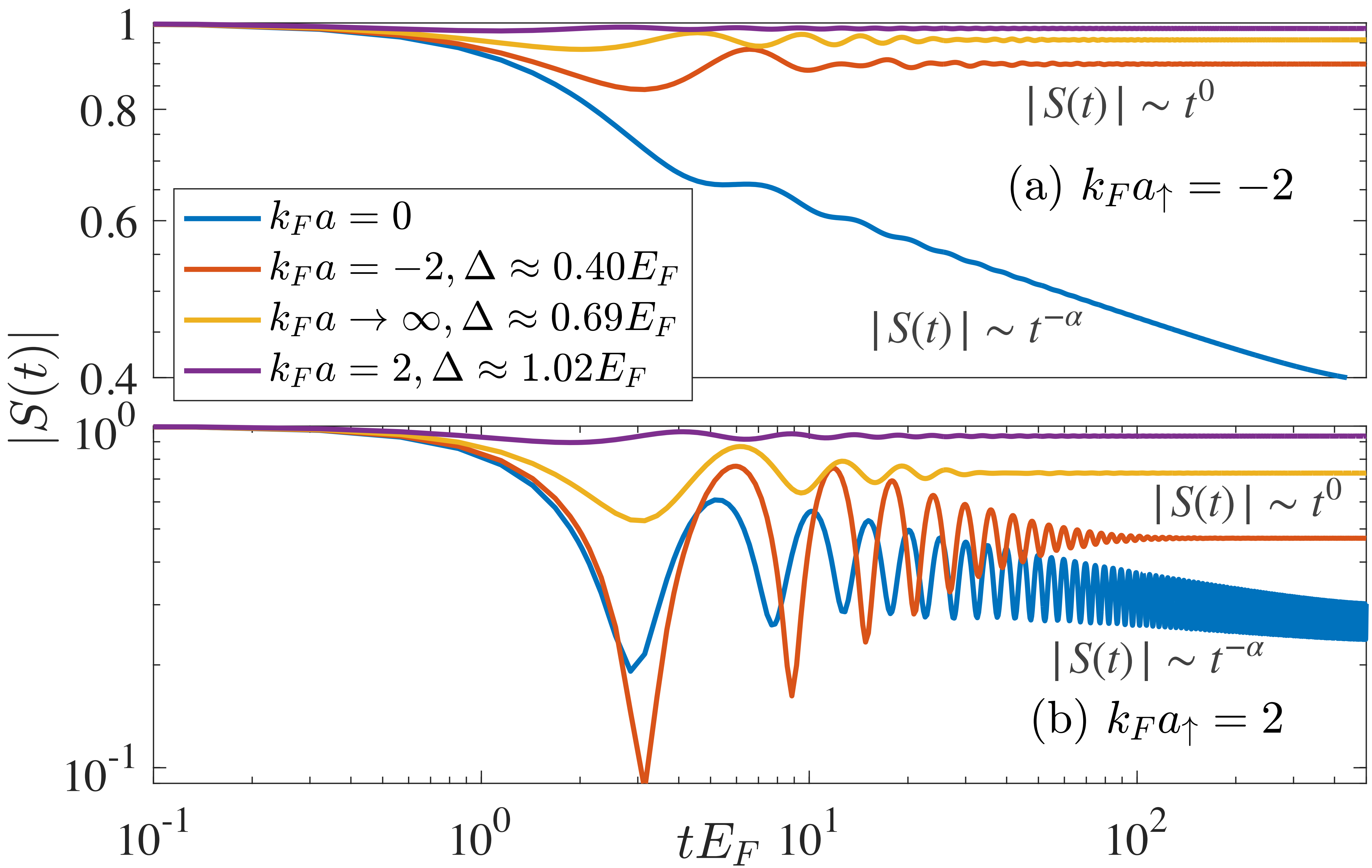
$$\omega_0 = \sum_{\mathbf{k}} \tilde{V}_\downarrow(0)$$

$$V_\downarrow = 0 \rightarrow \omega_0 = 0$$

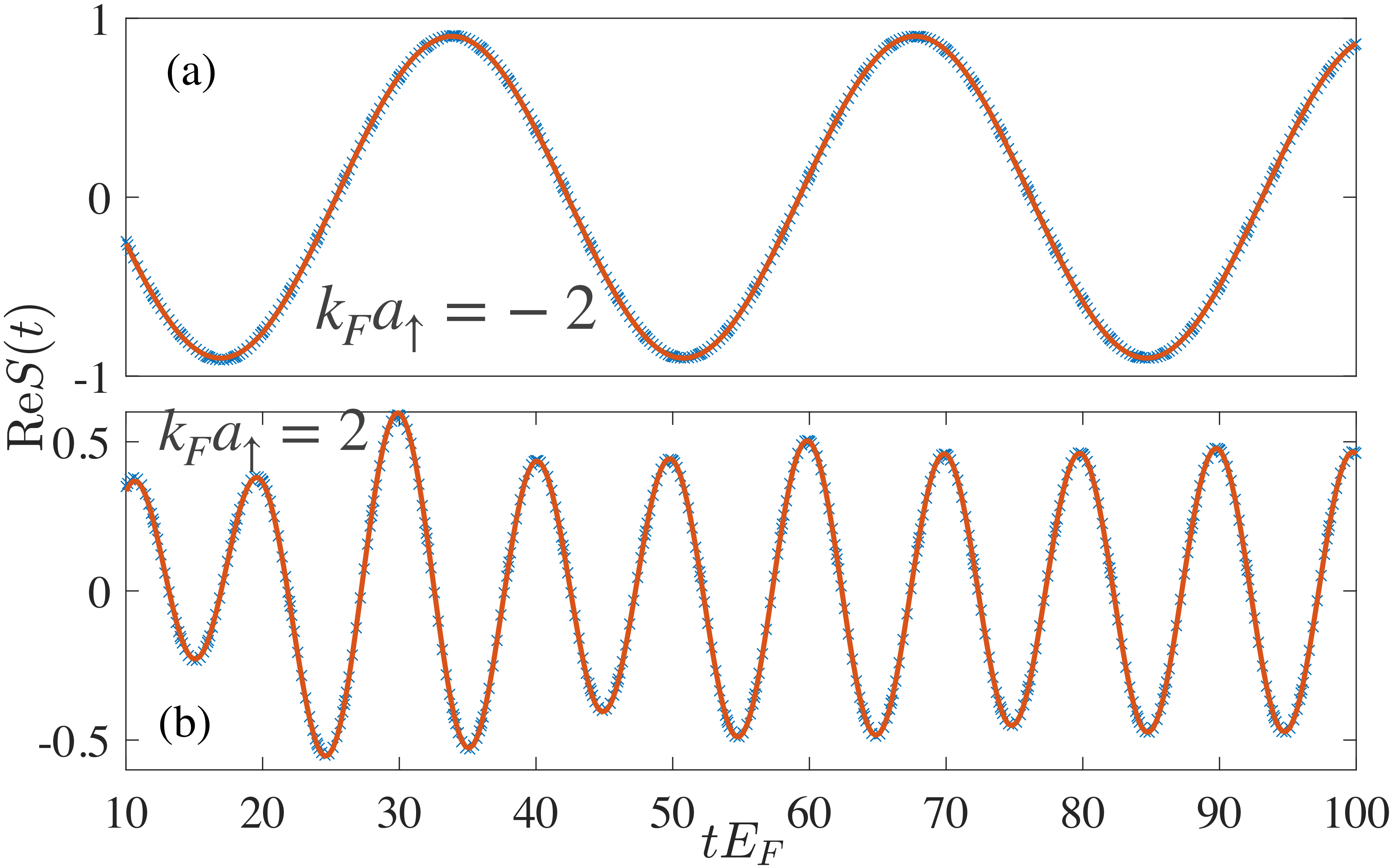
Yu-Shiba-Rusinov bound state

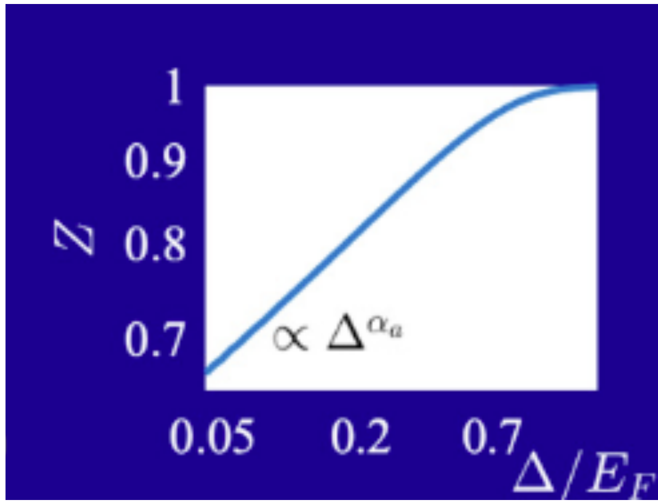


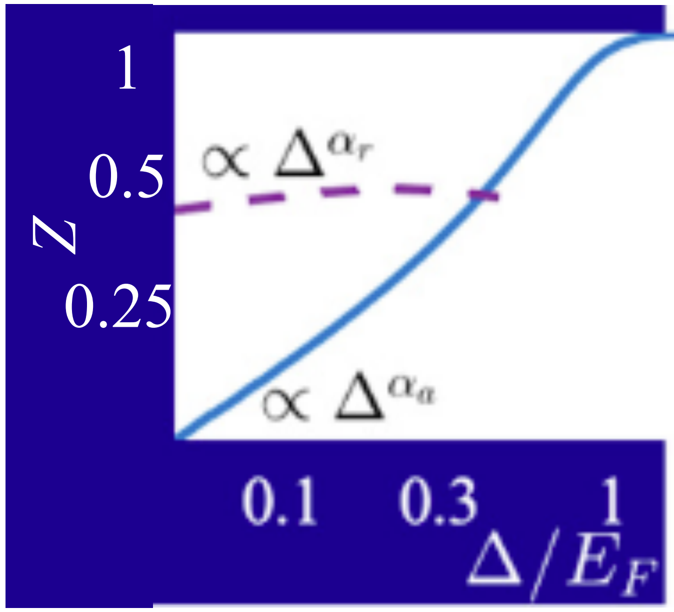
Ramsey Responses



Asymptotic Behaviour





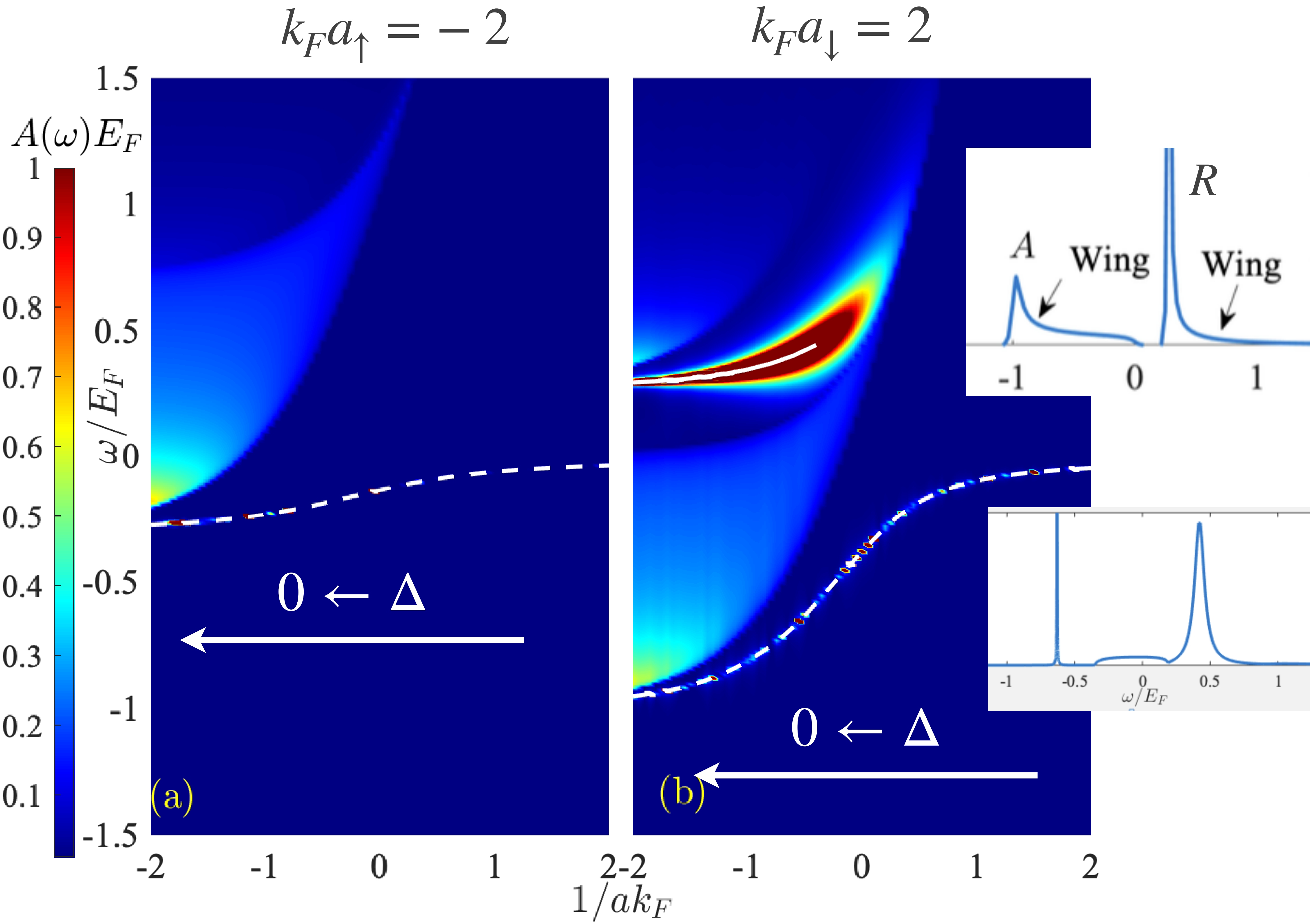


$$S(t) \approx D_a e^{-iE_a t} + D_r e^{-iE_r t}$$

$$Z = |D|$$

$$A(\omega) \propto \begin{cases} Z_a \delta(\omega - E_a) & \omega \approx E_a \\ Z_r \frac{|\mathrm{Im}E_r|/\pi}{(\omega - \mathrm{Re}E_r)^2 + (\mathrm{Im}E_r)^2} & \omega \approx \mathrm{Re}E_r \end{cases}$$

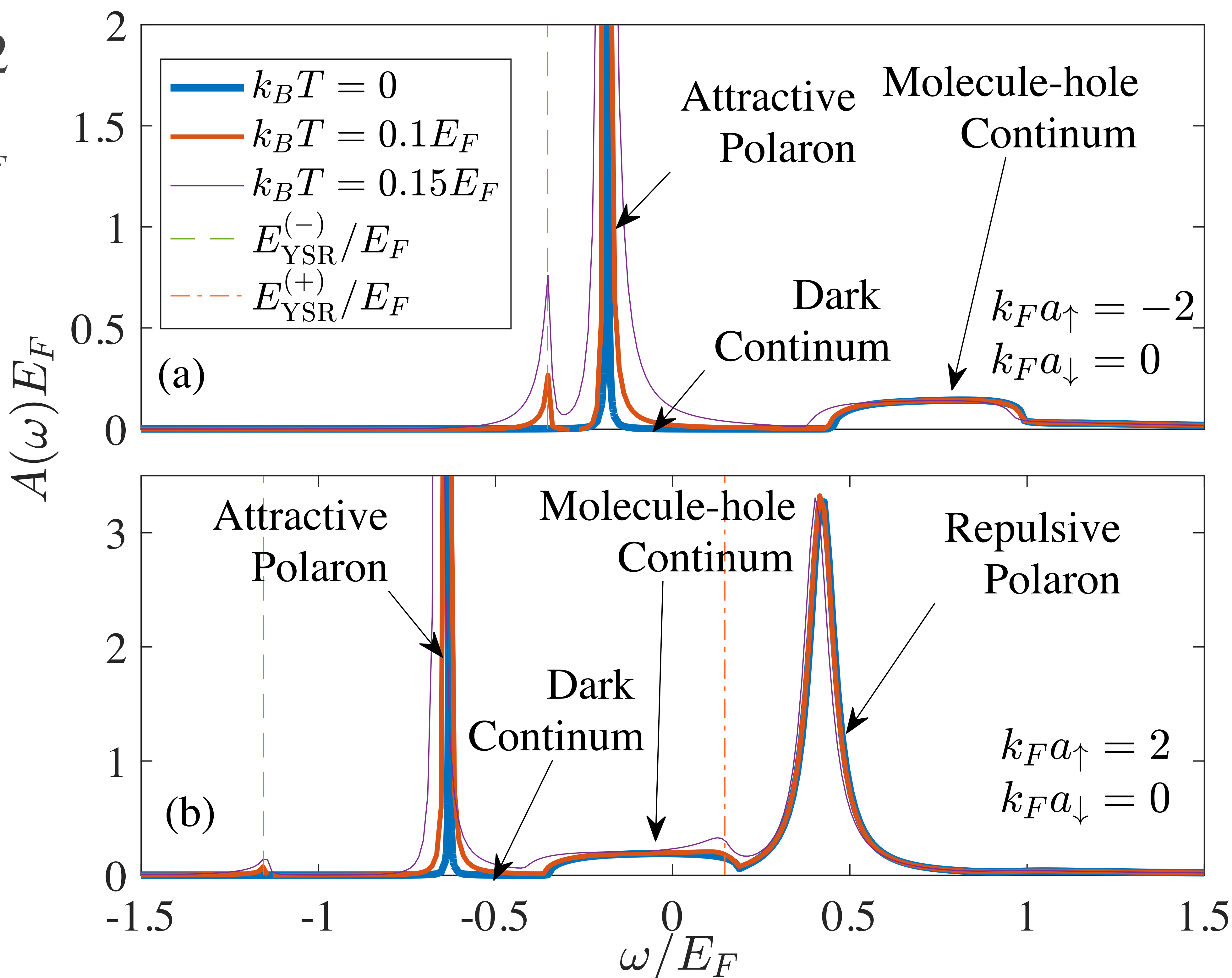
Superfluid Gap Dependence

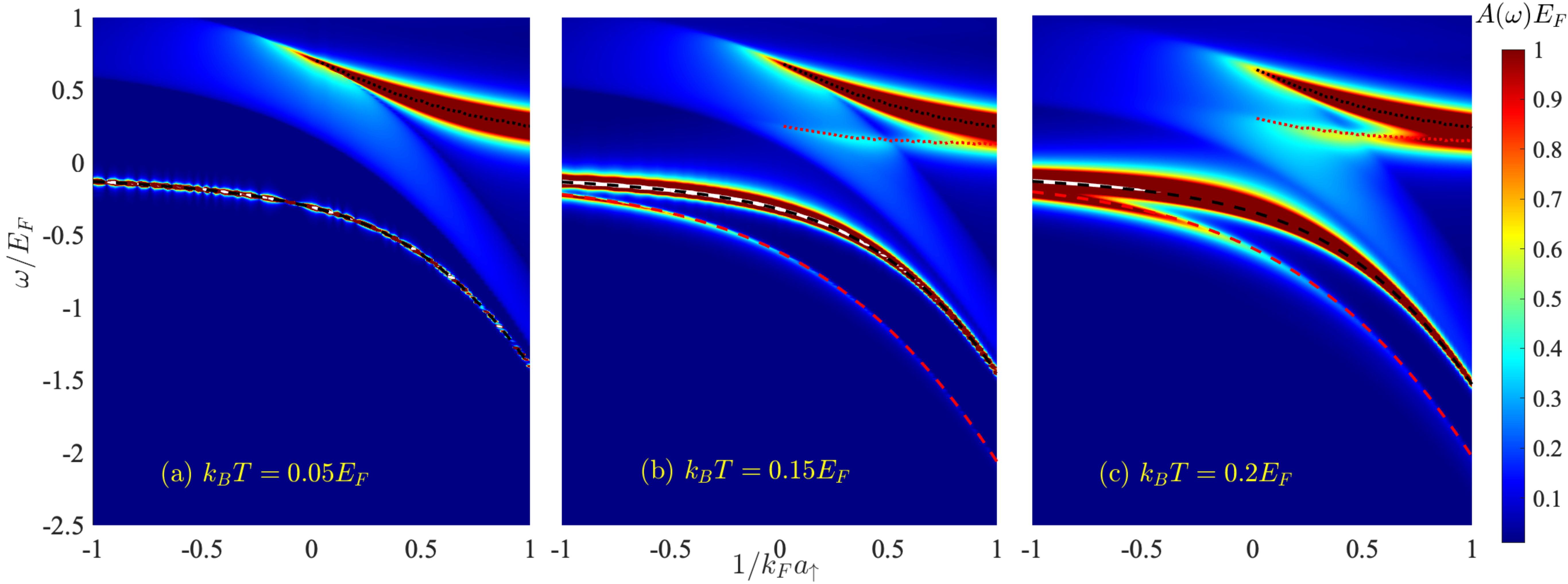


Finite Temperature

$k_F a = -2$

$\Delta \approx 0.4 E_F$



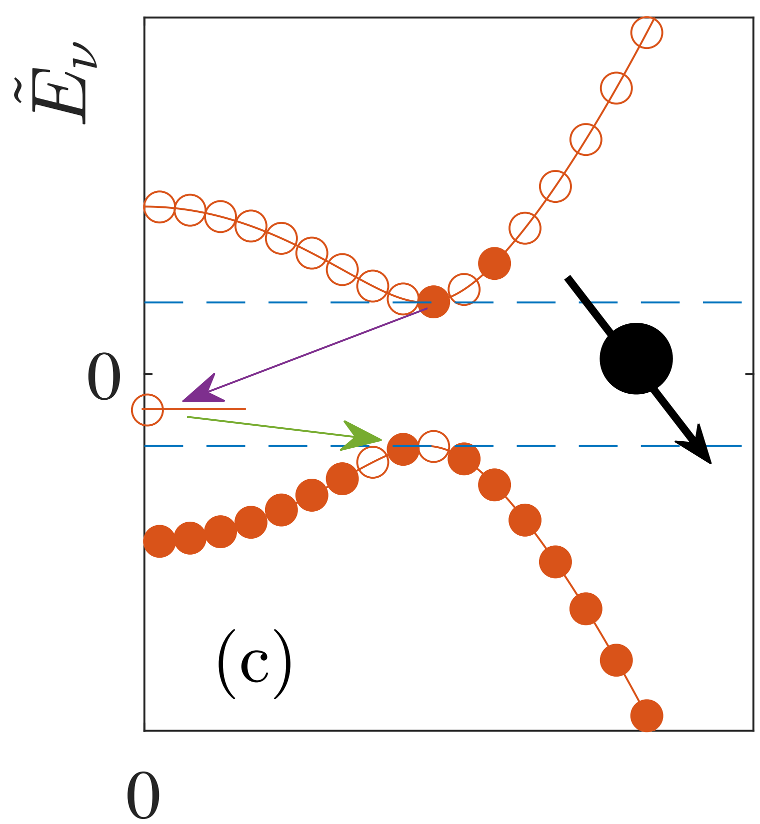


YSR Features

$$E_{\text{YSR}}^{(-)} = E_a - (\Delta - E_{\text{YSR}})$$

$$E_{\text{YSR}}^{(+)} = \text{Re}(E_r) - (E_{\text{YSR}} + \Delta)$$

$$2\Delta = E_a + \text{Re}(E_r) - E_{\text{YSR}}^{(-)} - E_{\text{YSR}}^{(+)}$$



Nonmagnetic impurity $a_\uparrow = a_\downarrow$

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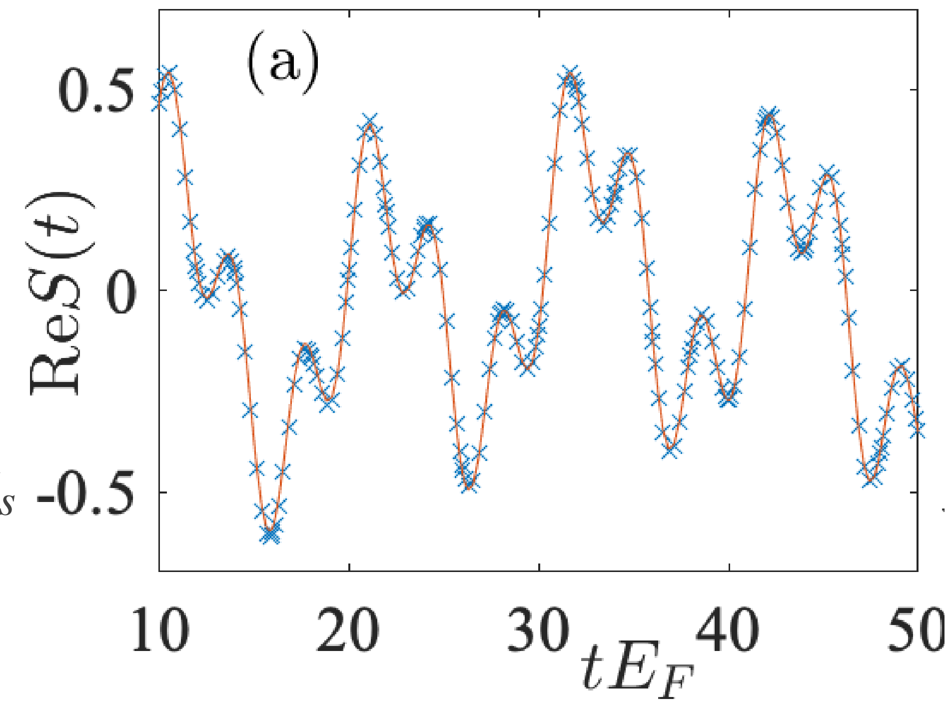
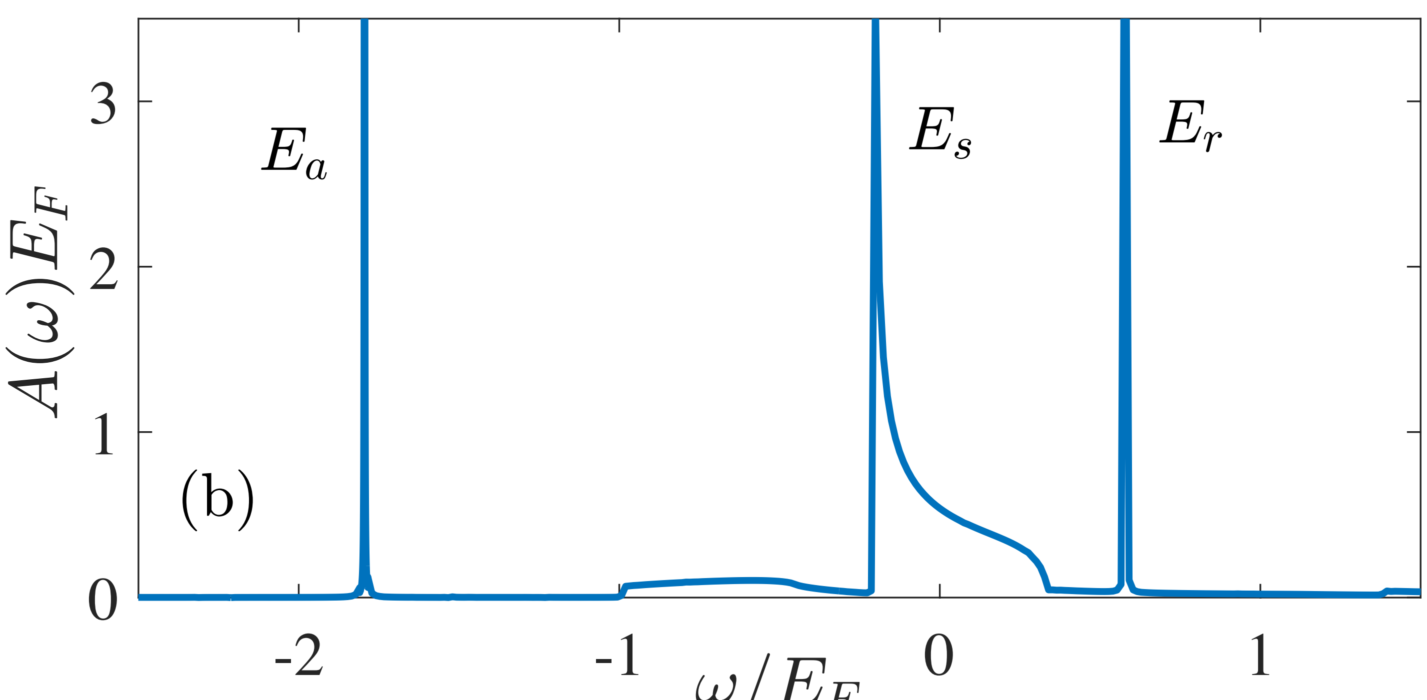
$$S(t) = e^{-i\omega_0 t}\det[1 - \hat{n} + e^{i\hat{h}_i t}e^{-i\hat{h}_f t}\hat{n}]$$

$$\omega_0 = \sum_{\mathbf{k}} \tilde{V}_\downarrow(0) = \sum_{\mathbf{k}} \left\langle \mathbf{k} \middle| \hat{V}_\downarrow \middle| \mathbf{k} \right\rangle$$

Asymptotic Behaviour:

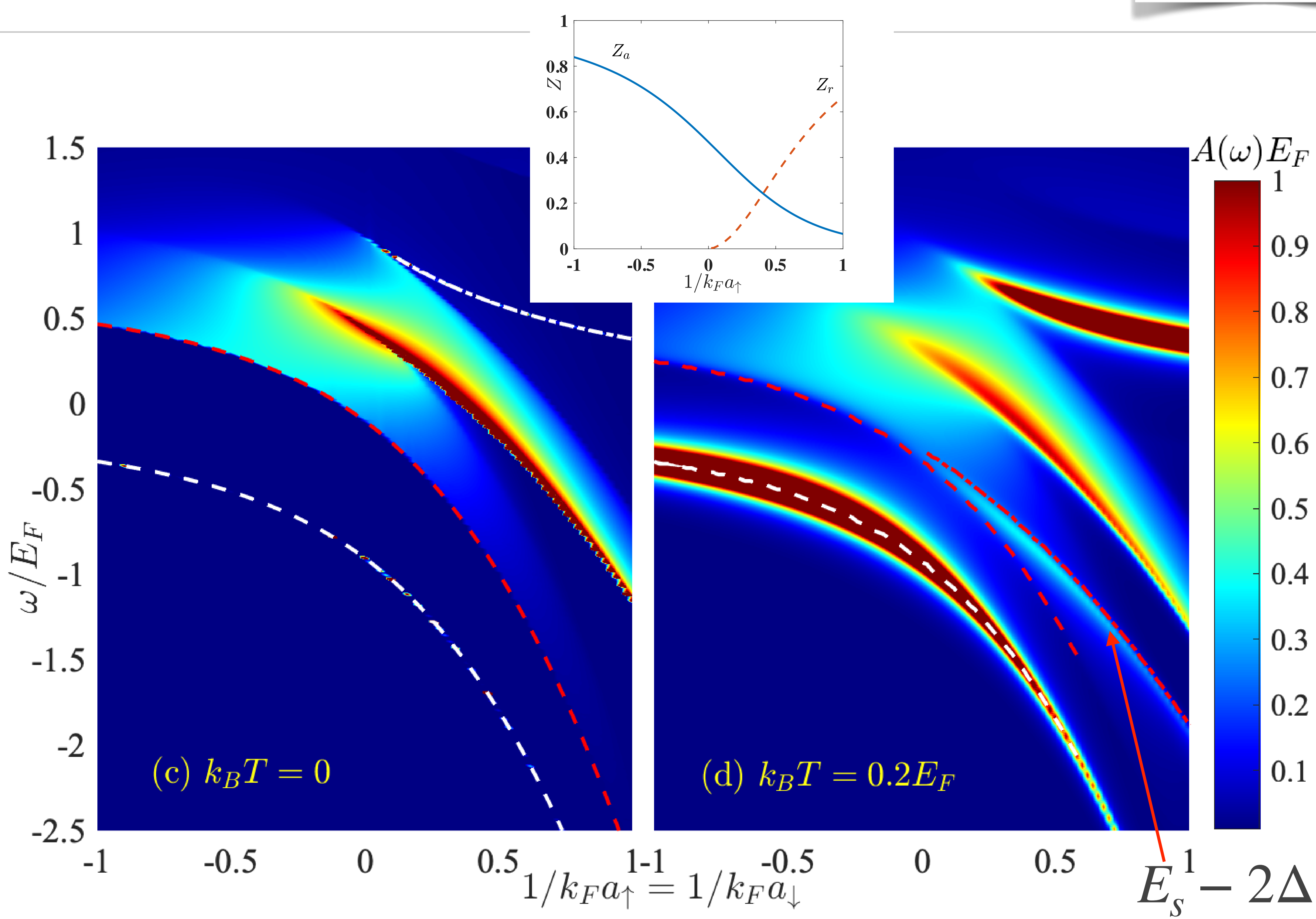
$$S(t) \approx D_a e^{-iE_a t} + D_r e^{-iE_r t} + D_s e^{-iE_s t}\left(\frac{1}{iE_F t}\right)^{\alpha_s}$$





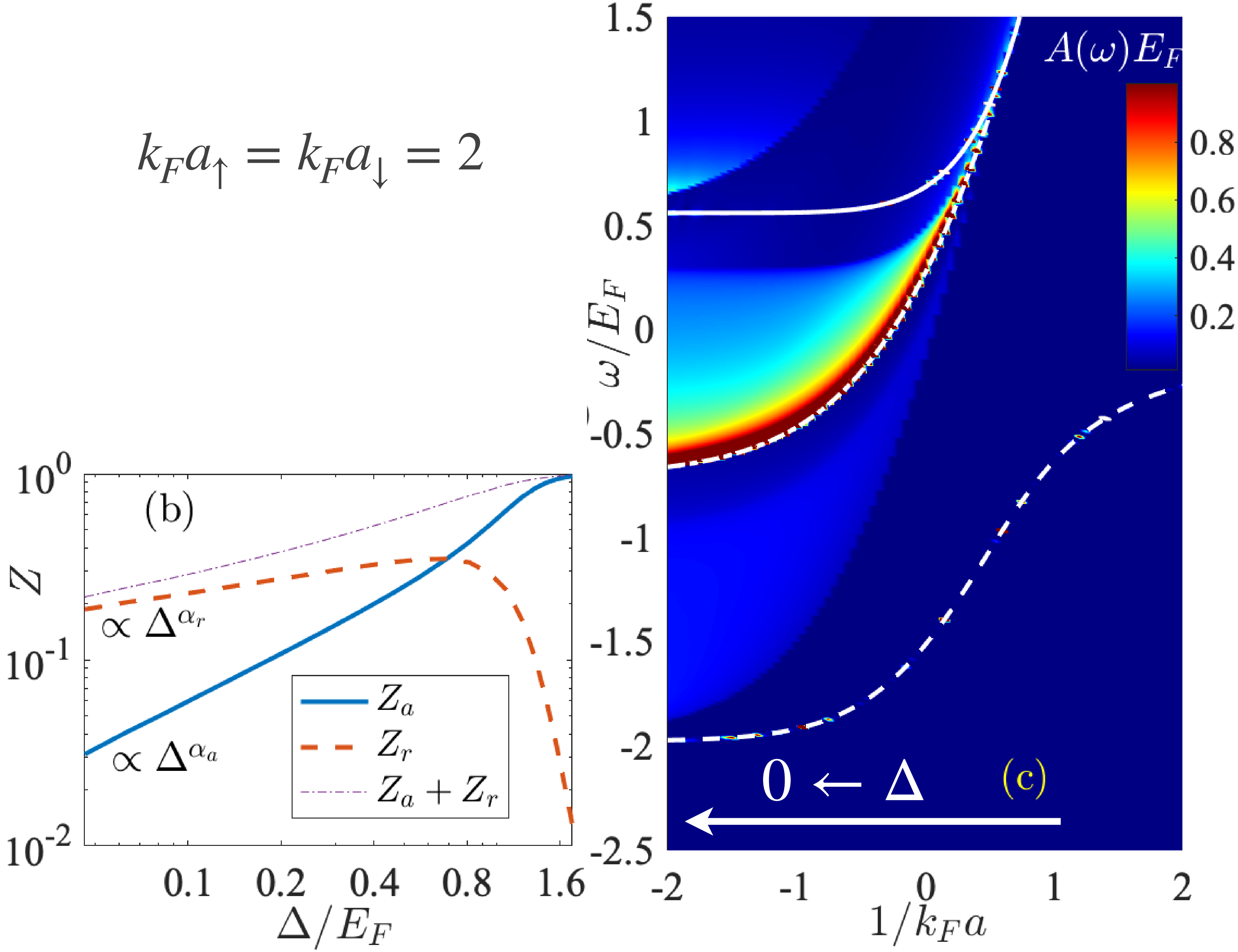
$$k_F a_\uparrow = k_F a_\downarrow = 2$$

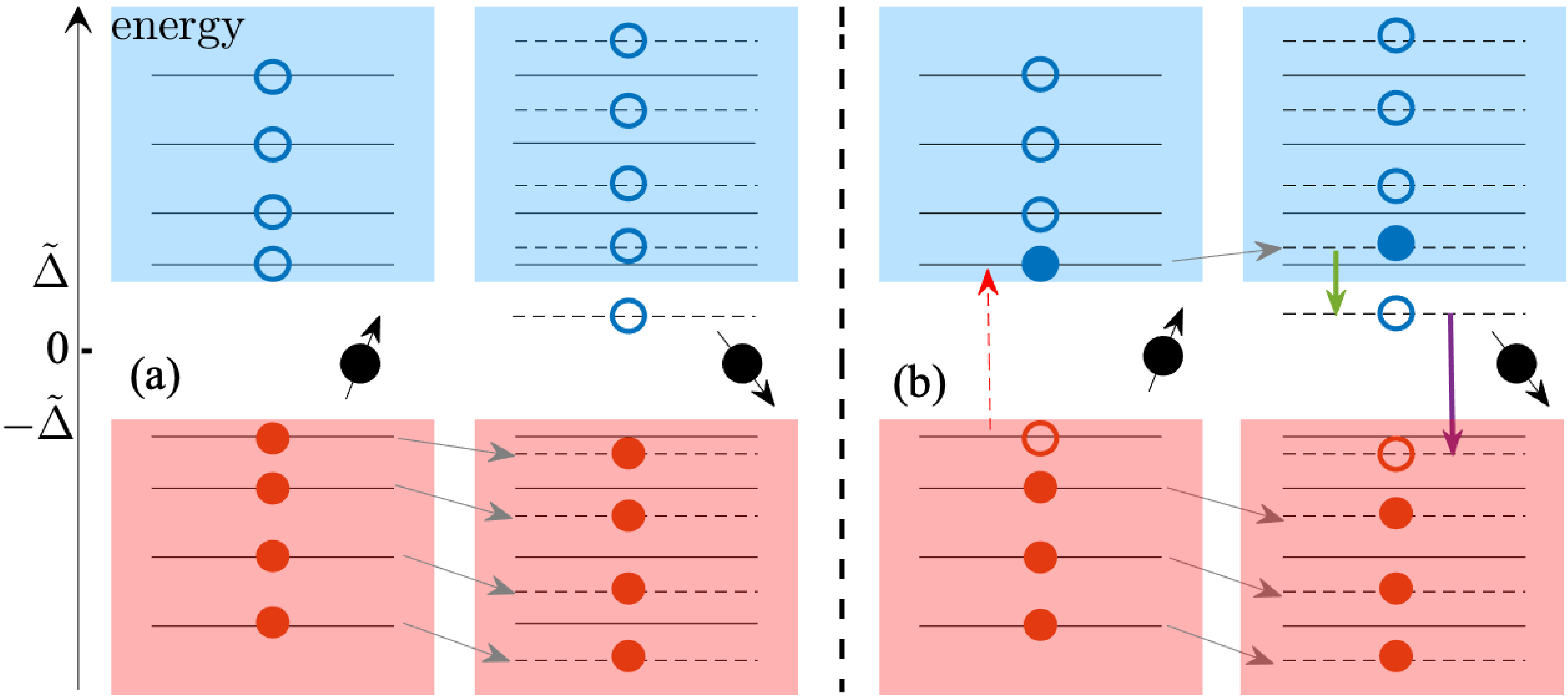
Nonmagnetic impurity



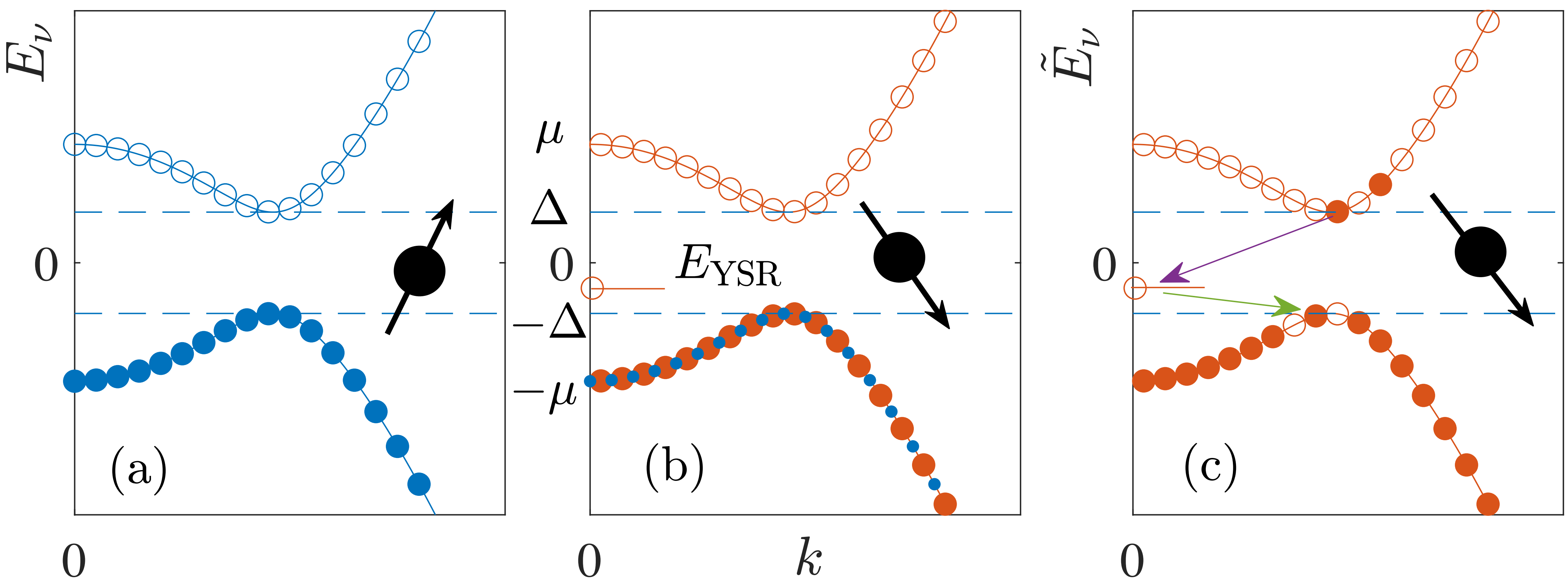
Superfluid Gap Dependence

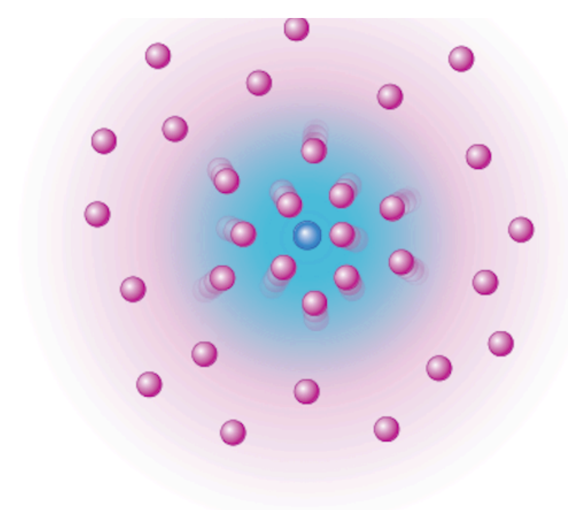
$k_F a_\uparrow = k_F a_\downarrow = 2$





energy
$\tilde{\Delta}$
0
$-\tilde{\Delta}$
(a)
(b)





$$\det(\exp(\mathbf{A})) = \exp(\mathrm{tr}(\mathbf{A})).$$

Yu-Shiba-Rusinov bound state