Laboratoire Kastler Brossel
Physique quantique et applications

MARIE CURIE ACTIONS

# An impurity in a Fermi sea on a narrow Feshbach resonance: A variational study of the polaronic and dimeronic branches

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cnrs
dépasser les frontières

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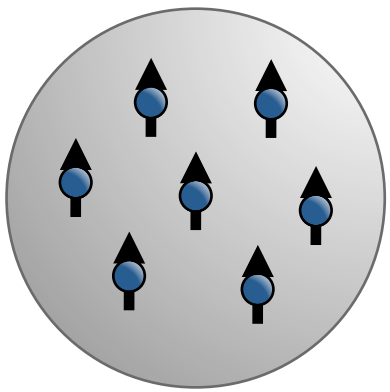
IFRAF

# Introduction: The system

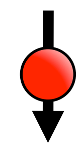
Homogeneous (3D) Fermi gas
of particles of same spin state

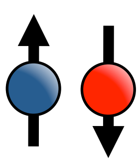
$m, k_{\mathrm{F}}$



Distinguishable impurity
(boson/fermion)

$M, \mathbf{K}$





s-wave interactions are described by two parameters:

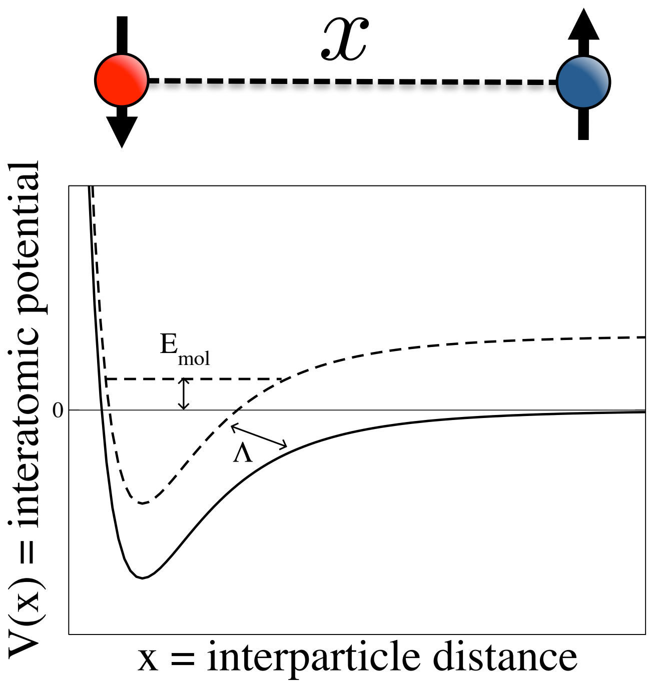
Scattering length

$a$

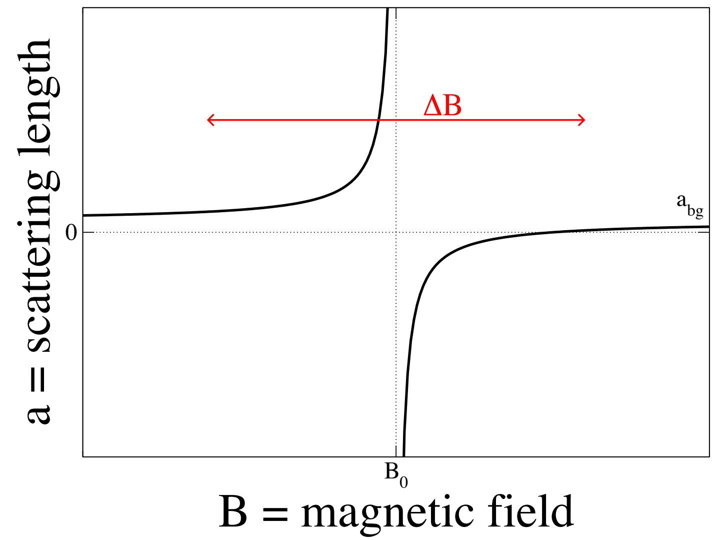
Feshbach length

$R_*$

# The Narrow Feshbach resonance




$$\boxed{a = a_{\mathrm{bg}}\left(1 - \frac{\Delta B}{B - B_0}\right)}$$




$$\boxed{\text{The resonance width : } \quad \Delta B \quad \Longrightarrow \quad R_* \propto 1/\Delta B}$$

(i) Theoretically: Competition of $a, R_*$

(ii) Experimentally: $^{40}\mathrm{K} - {}^{6}\mathrm{Li}$ narrow Feshbach resonances

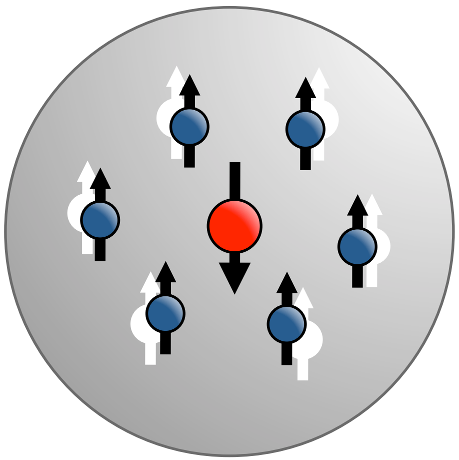
$$R_* > 100\mathrm{nm} \gg R_{\mathrm{VdW}} \simeq 2\mathrm{nm}$$

# Ground state

The ground state has two quasi-particle branches:

$$1/(k_{\mathrm{F}}a)_{\mathrm{c}}$$

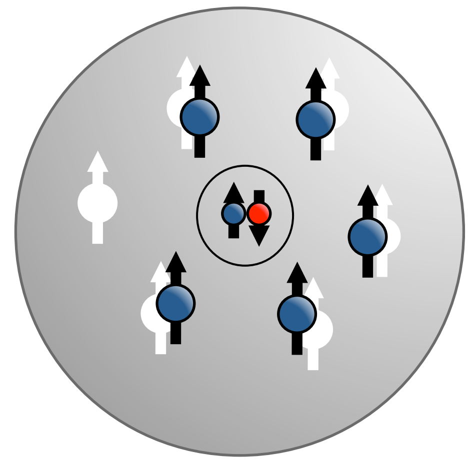
POLARONIC | DIMERONIC $\longrightarrow 1/k_{\mathrm{F}}a$



C. Lobo *et. al.*, PRL **97**, 200403 (2006)

F. Chevy, PRA **74**, 063628 (2006)

N. Prokof’ev, B. Svistunov, PRB **77**, 020408 (2008)



M. Punk *et. al.*, PRA **80**, 053605 (2009)

C. Mora, F. Chevy, PRA **80**, 033607 (2009)

R. Combescot *et. al.*, EPL **88**, 60007 (2009)

# Outlook

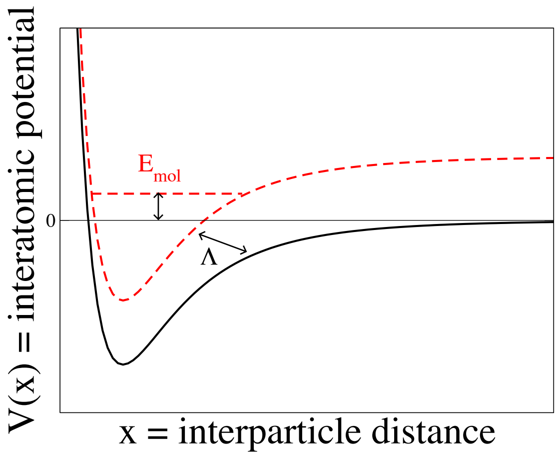
1. Two-channel model Hamiltonian
2. Variational ansätze, integral equations
3. Properties of the two branches at $\hbar K=0$
   a. Polaron-to-dimeron crossing point
   b. Non-trivial weakly interacting limit
4. Polaronic quasi-particle residue
5. Polaronic pair correlation function
6. A moving polaron

# Hamiltonian of the system

Two-channel model

$$\hat{H} = \sum_{\mathbf{k}} \left[ \varepsilon_{\mathbf{k}} \hat{u}^\dagger_{\mathbf{k}} \hat{u}_{\mathbf{k}} + E_{\mathbf{k}} \hat{d}^\dagger_{\mathbf{k}} \hat{d}_{\mathbf{k}} + \left( \frac{\varepsilon_{\mathbf{k}}}{1 + M/m} + E_{\text{mol}} \right) \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} \right]$$

$$+ \frac{\Lambda}{\sqrt{V}} \sum_{\mathbf{k},\mathbf{k}'} \chi(\mathbf{k}_{\text{rel}}) (\hat{b}^\dagger_{\mathbf{k}+\mathbf{k}'} \hat{u}_{\mathbf{k}} \hat{d}_{\mathbf{k}'} + \text{h.c.})$$



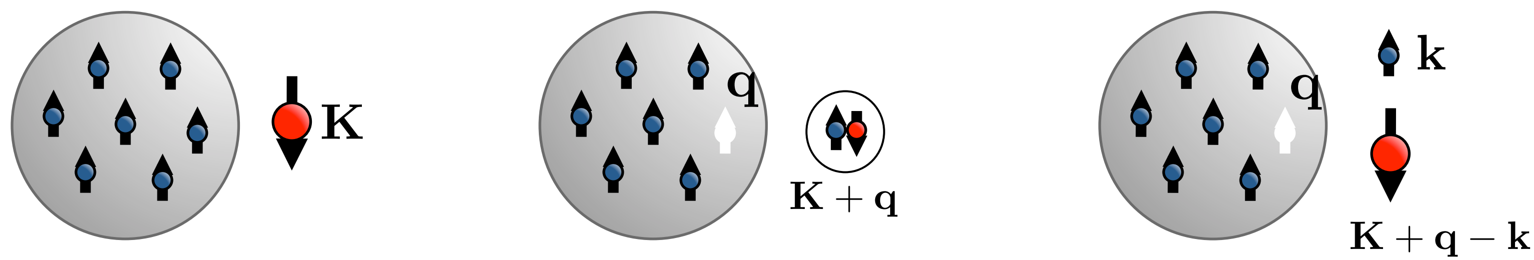

Kinetic energies in the open channel

$$\varepsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m} \qquad E_{\mathbf{k}} = \frac{\hbar^2 k^2}{2M}$$

$$\frac{E_{\text{mol}}}{\Lambda^2} = -\frac{\mu}{2\pi\hbar^2 a} + \int \frac{d^3k}{(2\pi)^3} \chi^2(k) \frac{2\mu}{\hbar^2 k^2}$$

# Polaron: Integral equations

$$|\psi_{\rm pol}(\hbar\mathbf{K})\rangle = \Big(\phi\,\hat{d}^\dagger_{\mathbf{K}} + {\sum_{\mathbf{q}}}' \phi_{\mathbf{q}}\hat{b}^\dagger_{\mathbf{K}+\mathbf{q}}\hat{u}_{\mathbf{q}} + {\sum_{\mathbf{k},\mathbf{q}}}' \phi_{\mathbf{k}\mathbf{q}}\hat{d}^\dagger_{\mathbf{K}+\mathbf{q}-\mathbf{k}}\hat{u}^\dagger_{\mathbf{k}}\hat{u}_{\mathbf{q}}\Big)|{\rm FS}\rangle$$



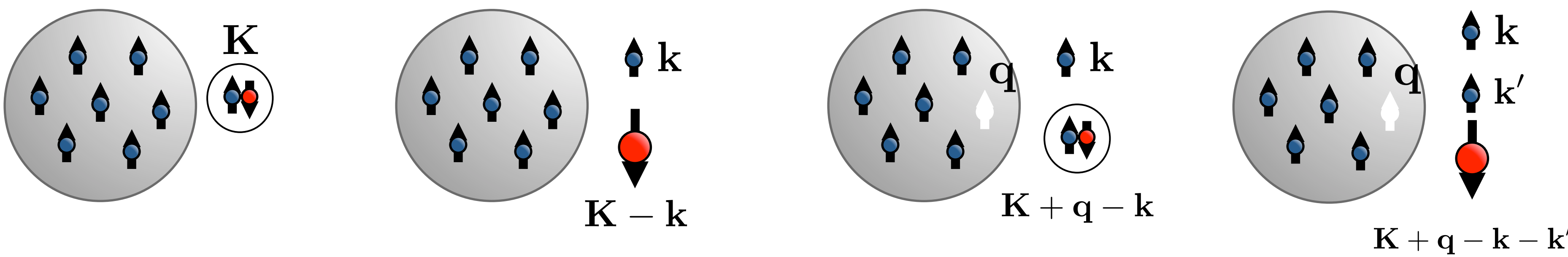

Minimise: $\langle\psi_{pol}(\hbar\mathbf{K})|\hat{H}|\psi_{pol}(\hbar\mathbf{K})\rangle$, with respect to $\phi, \phi_{\mathbf{q}}, \phi_{\mathbf{k},\mathbf{q}}$

Thermodynamic limit:

$$\boxed{\Delta E_{\rm pol}(\hbar\mathbf{K}) = E_{\mathbf{K}} + \int' \frac{d^3q}{(2\pi)^3}\frac{1}{D_{\mathbf{q}}[\Delta E_{\rm pol}(\hbar\mathbf{K}), \hbar\mathbf{K}]}}$$

# Dimeron: Integral equations

$$|\psi_{\mathrm{dim}}(\hbar\mathbf{K})\rangle = \Big(\eta\, \hat{b}^\dagger_{\mathbf{K}} + \sum_{\mathbf{k}}{}' \eta_{\mathbf{k}} \hat{d}^\dagger_{\mathbf{K}-\mathbf{k}} \hat{u}^\dagger_{\mathbf{k}} + \sum_{\mathbf{k},\mathbf{q}}{}' \eta_{\mathbf{kq}} \hat{b}^\dagger_{\mathbf{K}+\mathbf{q}-\mathbf{k}} \hat{u}^\dagger_{\mathbf{k}} \hat{u}_{\mathbf{q}} + \sum_{\mathbf{k}',\mathbf{k},\mathbf{q}}{}' \eta_{\mathbf{k}'\mathbf{kq}} \hat{d}^\dagger_{\mathbf{K}+\mathbf{q}-\mathbf{k}-\mathbf{k}'} \hat{u}^\dagger_{\mathbf{k}'} \hat{u}^\dagger_{\mathbf{k}} \hat{u}_{\mathbf{q}}\Big)|\mathrm{FS}: N-1\rangle$$

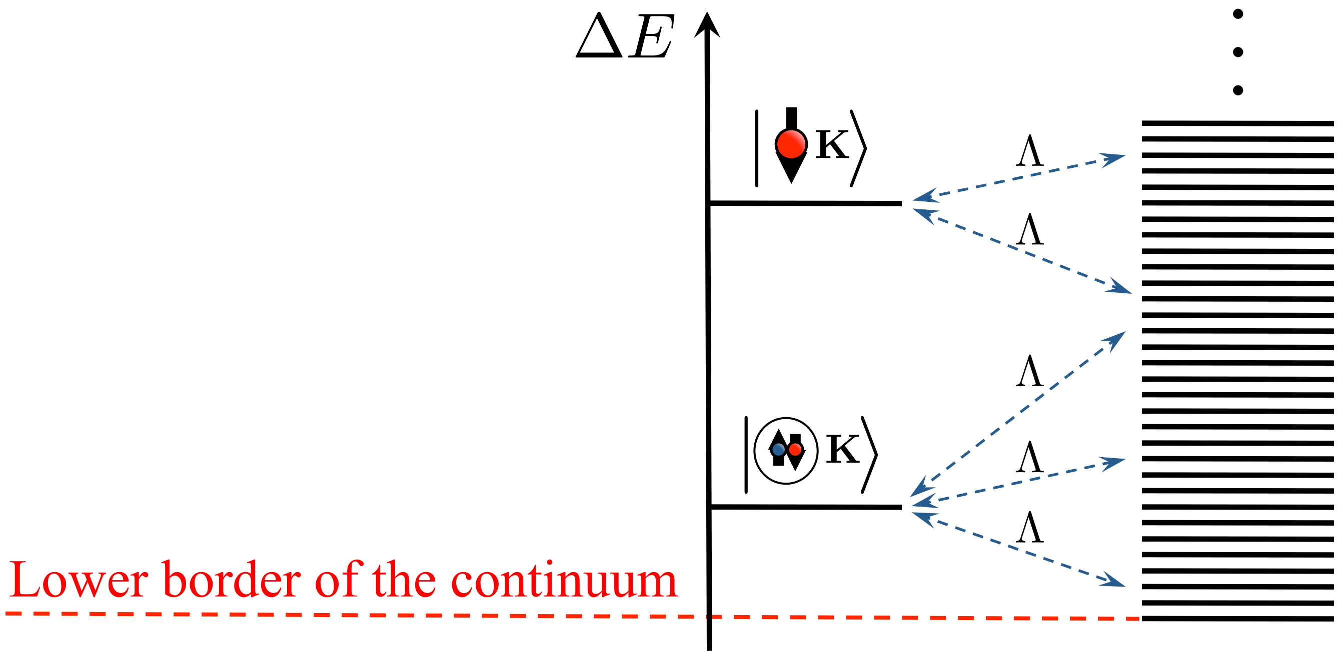



Minimise: $\langle\psi_{\mathrm{dim}}(\hbar\mathbf{K})|\hat{H}|\psi_{\mathrm{dim}}(\hbar\mathbf{K})\rangle$, with respect to $\eta,\ \eta_{\mathbf{k}},\ \eta_{\mathbf{kq}},\ \eta_{\mathbf{k}'\mathbf{kq}}$

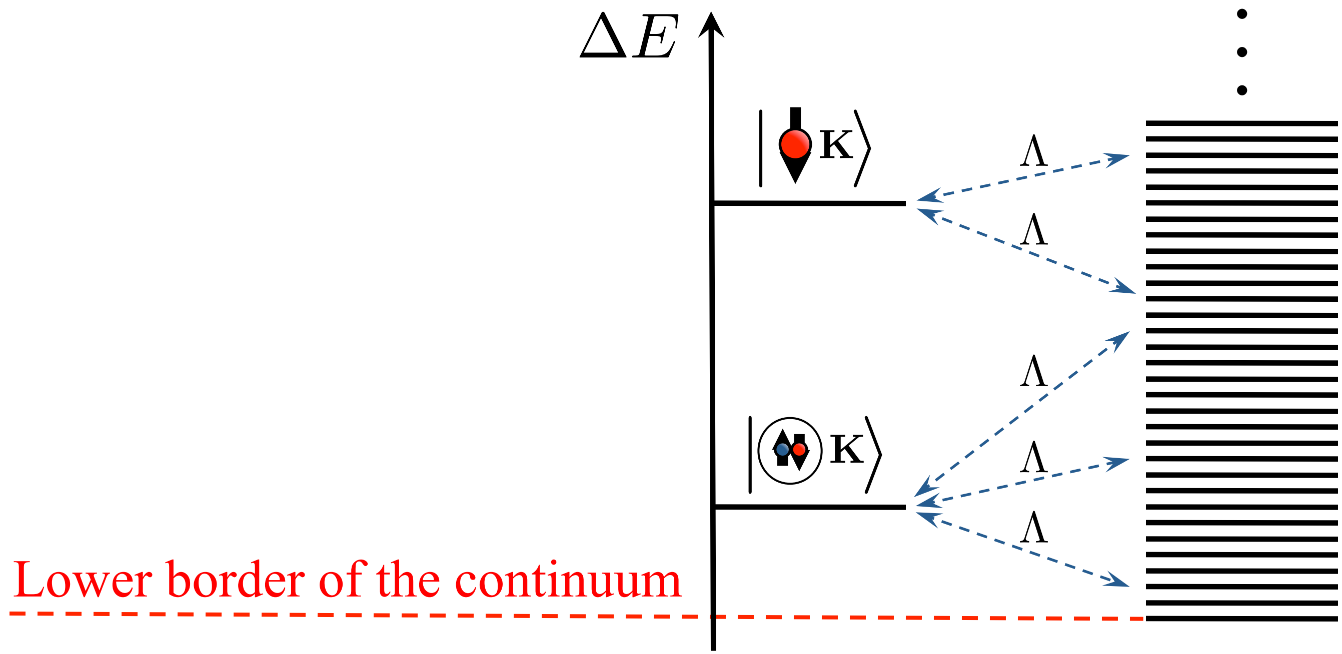
Thermodynamic limit:

$$\boxed{\int' \frac{d^3k'\,d^3q'}{(2\pi)^6} \mathcal{M}[\Delta E_{\mathrm{dim}}(\hbar\mathbf{K}), \mathbf{K}; \mathbf{k}, \mathbf{q}; \mathbf{k}', \mathbf{q}']\, \eta_{\mathbf{k}'\mathbf{q}'} = 0}$$

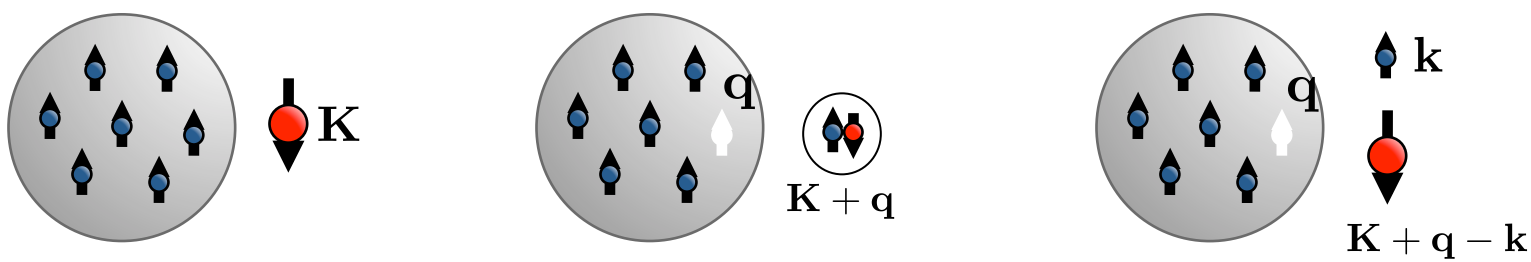
# A discrete state coupled to a continuum



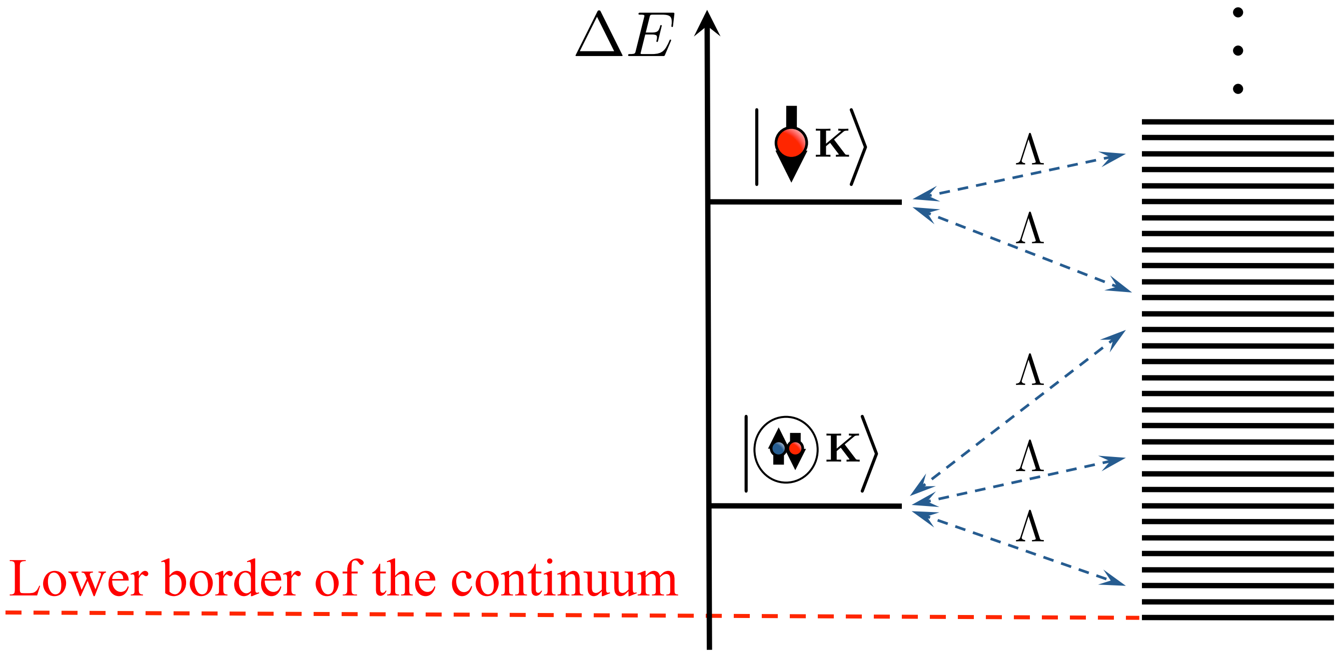
# A discrete state coupled to a continuum



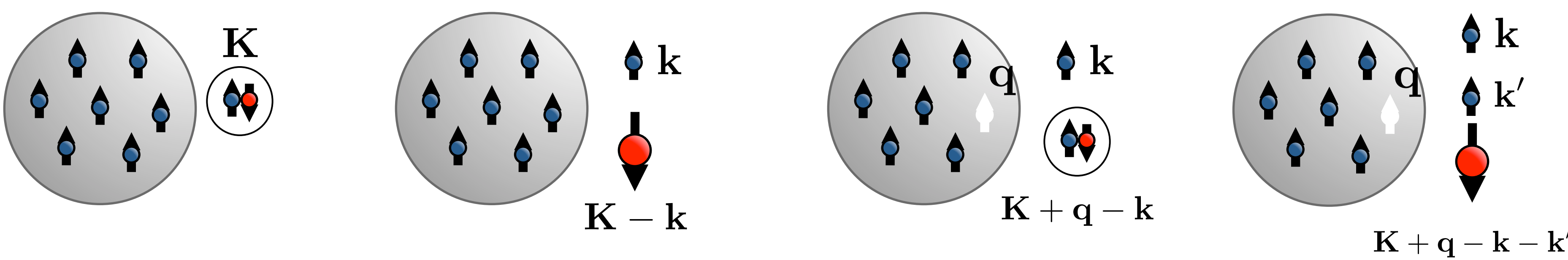

$$|\psi_{\rm pol}(\hbar\mathbf{K})\rangle = \left(\phi\,\hat{d}^\dagger_{\mathbf{K}} + {\sum_{\mathbf{q}}}' \phi_{\mathbf{q}}\hat{b}^\dagger_{\mathbf{K}+\mathbf{q}}\hat{u}_{\mathbf{q}} + {\sum_{\mathbf{k},\mathbf{q}}}' \phi_{\mathbf{kq}}\hat{d}^\dagger_{\mathbf{K}+\mathbf{q}-\mathbf{k}}\hat{u}^\dagger_{\mathbf{k}}\hat{u}_{\mathbf{q}}\right)|\mathrm{FS}\rangle$$



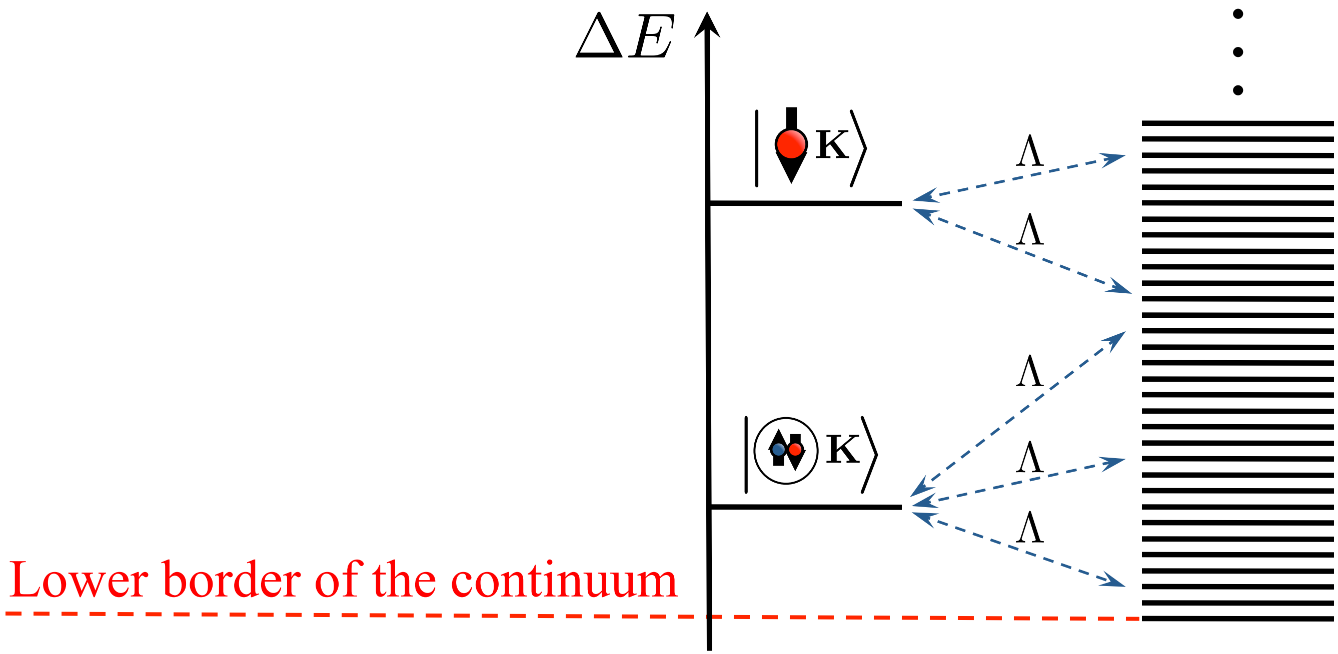
# A discrete state coupled to a continuum




$$|\psi_{\mathrm{dim}}(\hbar\mathbf{K})\rangle = \Big(\eta\,\hat{b}^{\dagger}_{\mathbf{K}} + {\sum_{\mathbf{k}}}' \eta_{\mathbf{k}}\hat{d}^{\dagger}_{\mathbf{K}-\mathbf{k}}\hat{u}^{\dagger}_{\mathbf{k}} + {\sum_{\mathbf{k},\mathbf{q}}}' \eta_{\mathbf{kq}}\hat{b}^{\dagger}_{\mathbf{K}+\mathbf{q}-\mathbf{k}}\hat{u}^{\dagger}_{\mathbf{k}}\hat{u}_{\mathbf{q}} + {\sum_{\mathbf{k}',\mathbf{k},\mathbf{q}}}' \eta_{\mathbf{k}'\mathbf{kq}}\hat{d}^{\dagger}_{\mathbf{K}+\mathbf{q}-\mathbf{k}-\mathbf{k}'}\hat{u}^{\dagger}_{\mathbf{k}'}\hat{u}^{\dagger}_{\mathbf{k}}\hat{u}_{\mathbf{q}}\Big)|\mathrm{FS}:N-1\rangle$$



# A discrete state coupled to a continuum




(1) Discrete state EXPELLED from the continuum, remains a discrete state.

(2) Discrete state DILUTED in the continuum, becomes a resonance:

$$\boxed{\Delta E = \Re \Delta E + i \Im \Delta E}$$

Of physical interest if $\Im \Delta E \ll \Re \Delta E$

# Outlook

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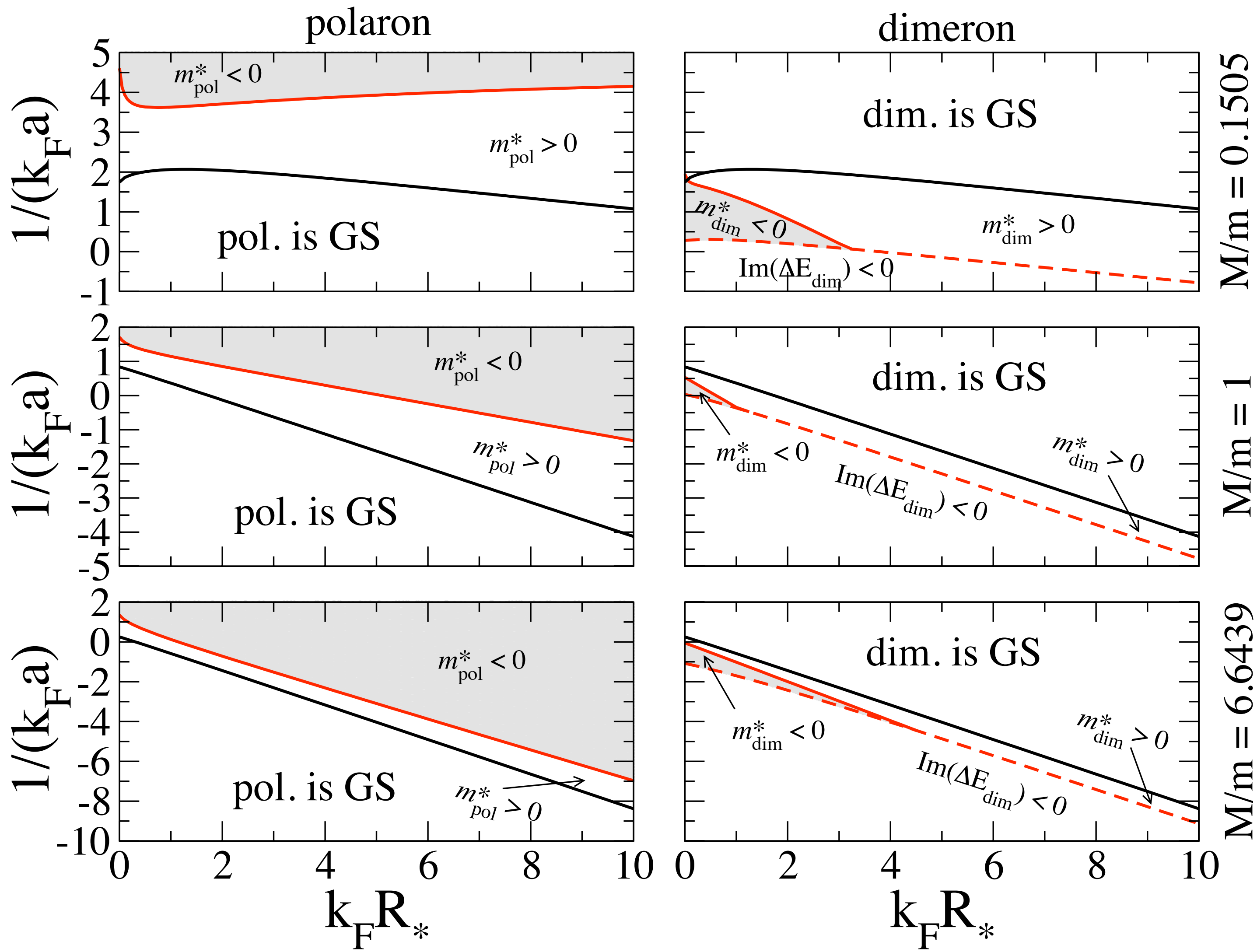
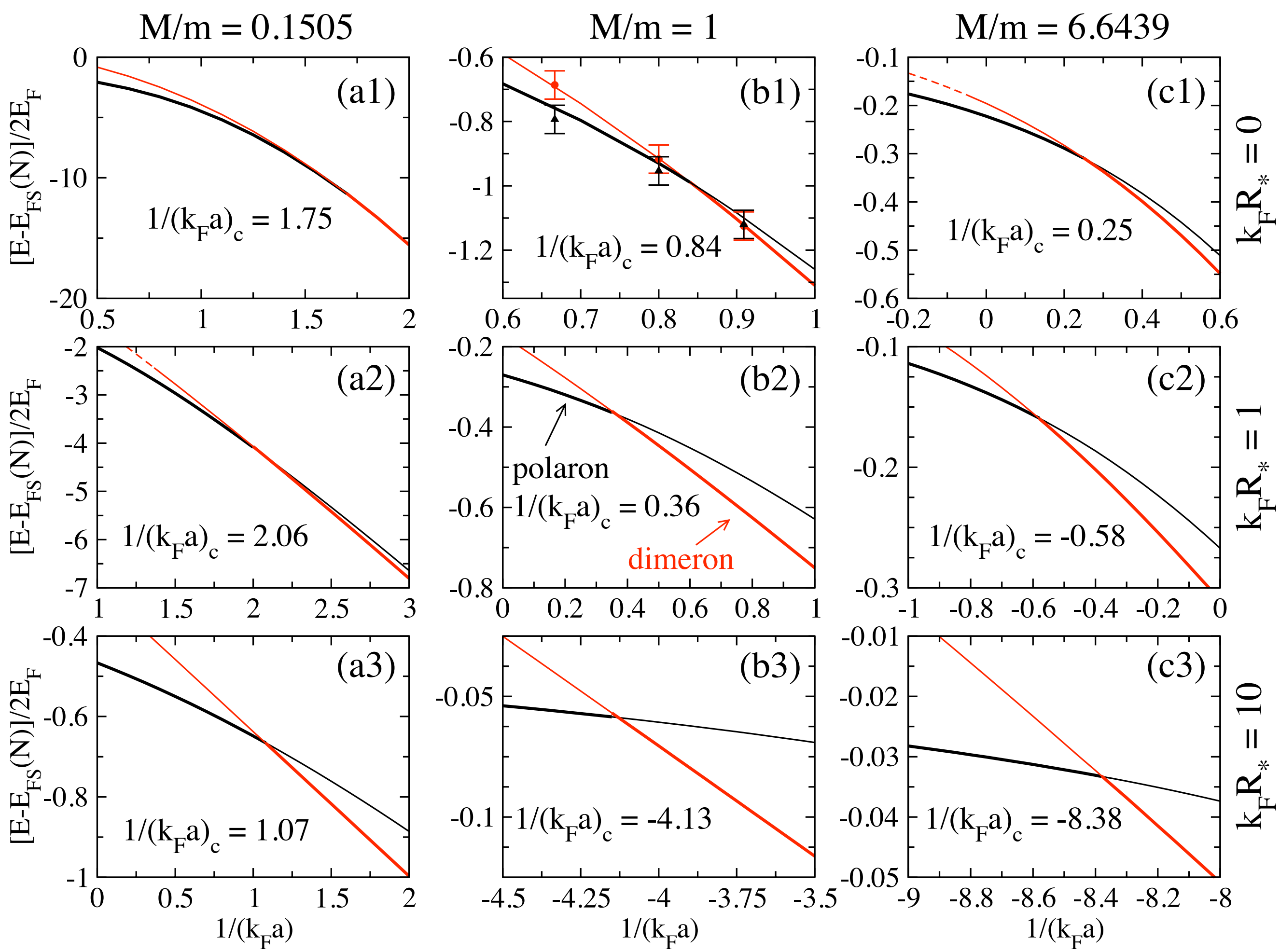
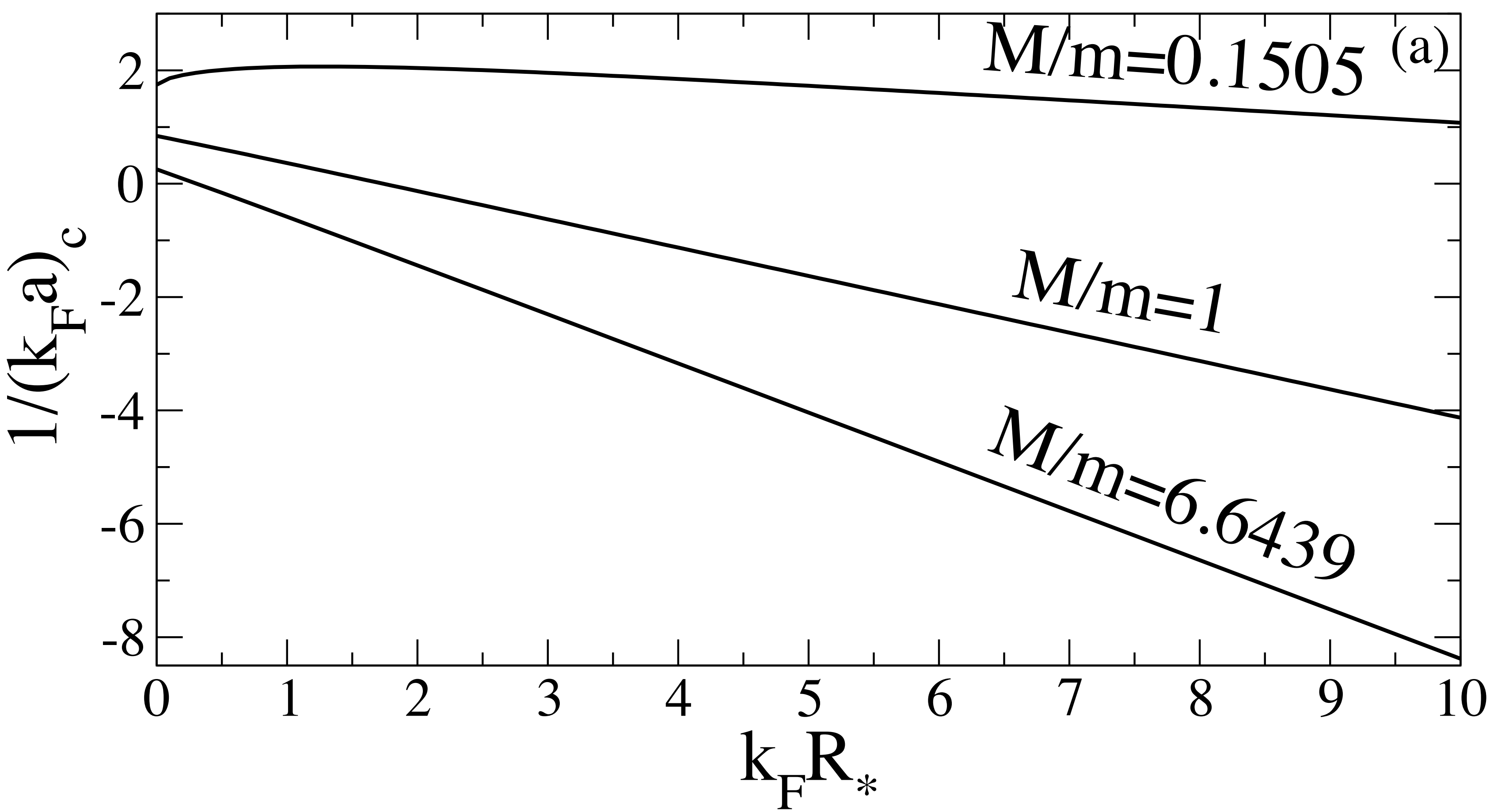
# Properties of the two branches at ħK=0



# (a) Polaron-to-dimeron crossing point



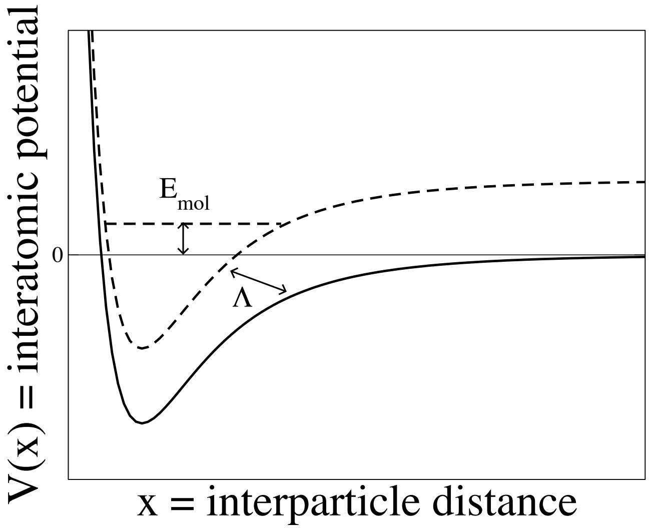
# (a) Polaron-to-dimeron crossing point



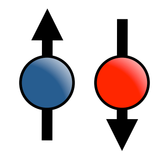

In vacuum, for ANY value of $R_*$, one has a two-body bound state iff $a > 0$

# Intuitive picture

Question: When do we have a two-body bound state ?




(1) Two particles in vacuum:



(i) Naïve answer: $E_{\mathrm{mol}} < 0$

(ii) Lamb shift due to vacuum fluctuations in the open channel:

$$\widetilde{E}_{\mathrm{mol}} = E_{\mathrm{mol}} - \int \frac{d^3k}{(2\pi)^3} \frac{\chi(k)^2 \Lambda^2}{\frac{\hbar^2 k^2}{2\mu}} \;\Rightarrow\; \widetilde{E}_{\mathrm{mol}} = -\frac{\Lambda^2 \mu}{2\pi \hbar^2 a}$$

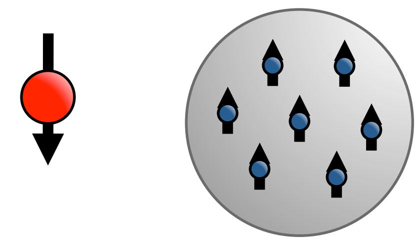
$$\boxed{\widetilde{E}_{\mathrm{mol}} < 0 \iff a > 0}$$

# Intuitive picture

Question: When do we have a two-body bound state ?

(2) One impurity in a Fermi sea:

TWO EFFECTS



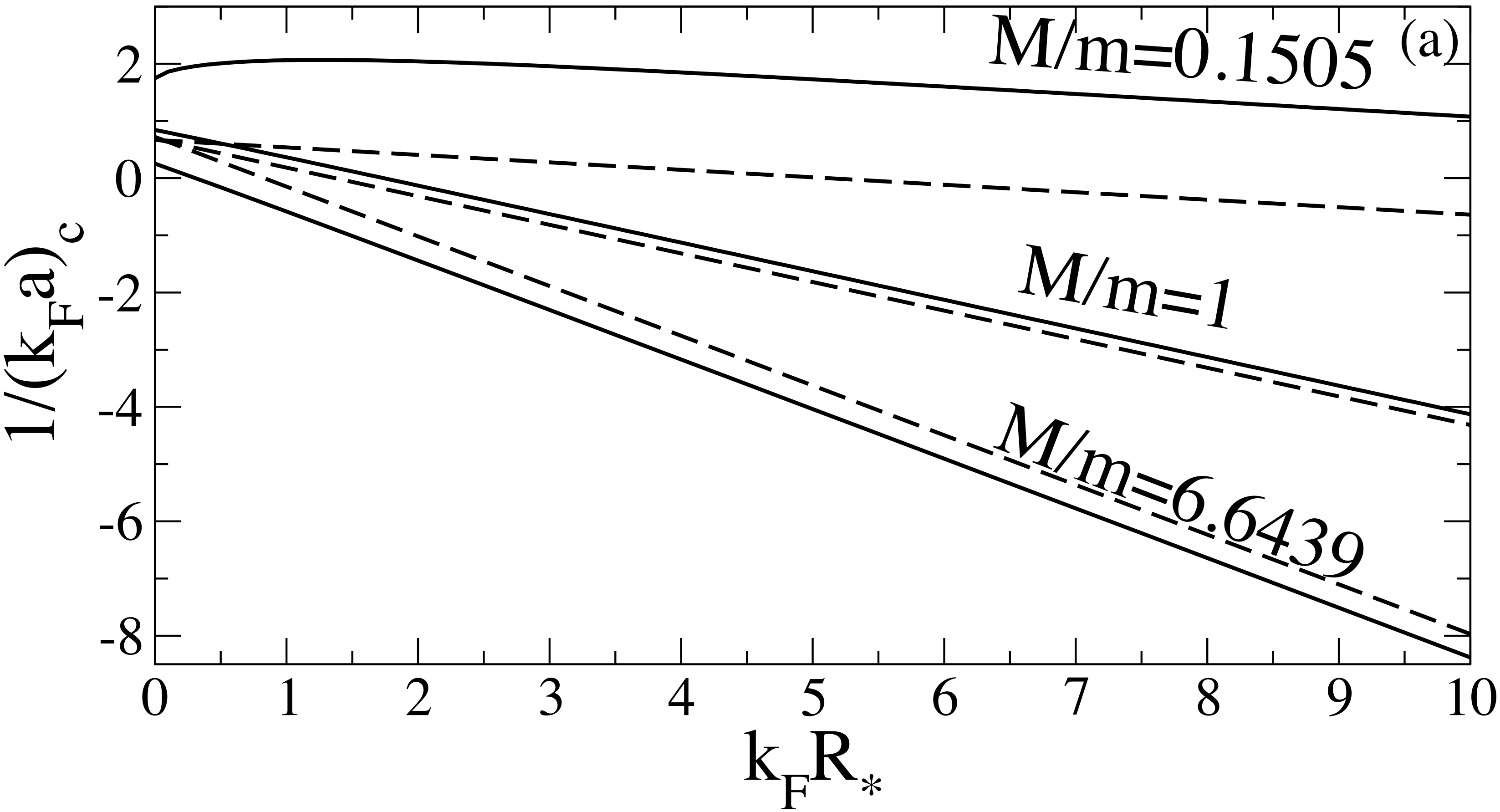
(i) Effect on the Lamb shift

$$\widetilde{E}'_{\mathrm{mol}} = E_{\mathrm{mol}} - \int_{k>k_{\mathrm{F}}} \frac{d^3k}{(2\pi)^3} \frac{\chi(\mathbf{k})\Lambda^2}{\frac{\hbar^2 k^2}{2\mu}}$$

(ii) Change of the dissociation threshold, $E_{\mathrm{F}}$

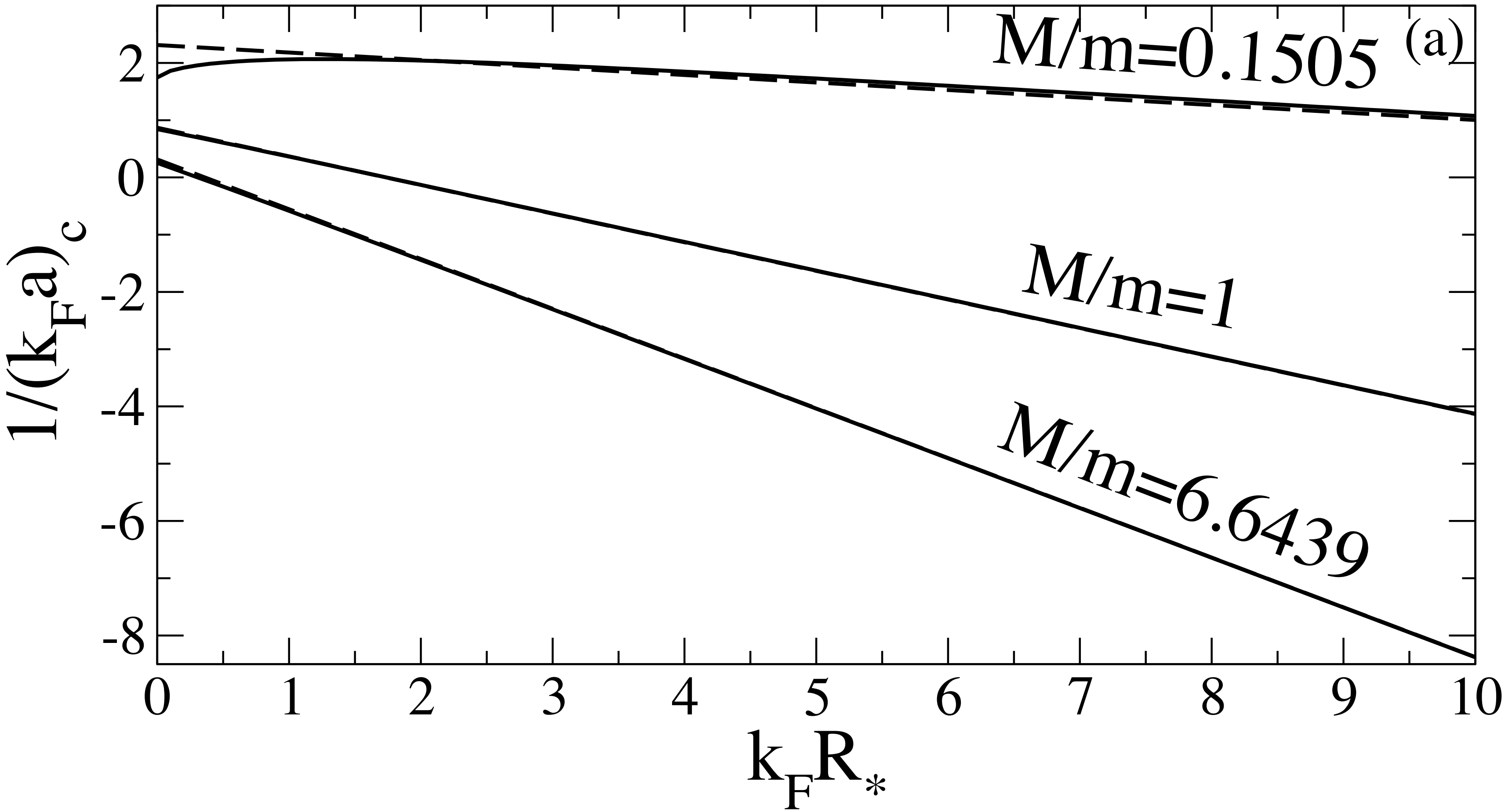
$$\widetilde{E}'_{\mathrm{mol}} < E_{\mathrm{F}} \Longrightarrow \quad \frac{1}{k_{\mathrm{F}} a} > \frac{2}{\pi} - \frac{M}{m+M} k_{\mathrm{F}} R_*$$

# Test of intuitive picture




$$\frac{1}{k_{\mathrm{F}}a} = \frac{2}{\pi} - \frac{M}{m+M} k_{\mathrm{F}} R_*$$

# Quantitative analytical result described later




Same slope as intuitive picture, but exact calculation of the INTERCEPT of the asymptote

# (b) Non-trivial weakly interacting limit

Standard weakly interacting limit:

$$a \to 0^-, R_* \ \text{ fixed!}$$

Loose information on the narrowness of the resonance

$$f_{\mathbf{k}} = \frac{-1}{\frac{1}{a} + ik + k^2 R_*}$$

Non-trivial weakly interacting limit:

$$\boxed{a \to 0^-, \frac{1}{a} \ \text{ and } \ R_* \ \text{ proportional}}$$

# (b) Non-trivial weakly interacting limit

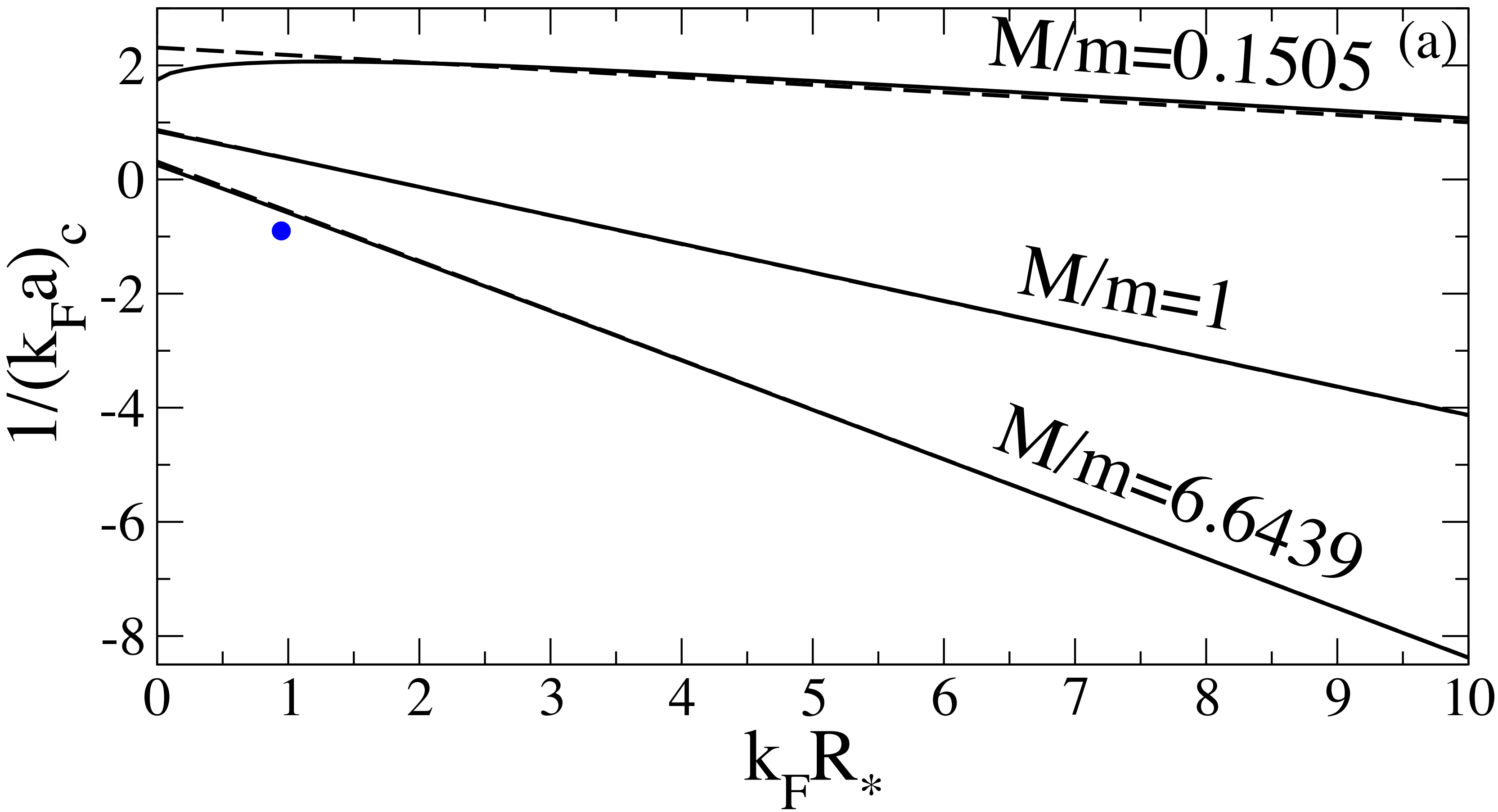
$$\boxed{a \to 0^-, \qquad aR_* = \text{const.}}$$

$$\Delta E^{(0)}_{\text{pol}} + \Delta E^{(1)}_{\text{pol}}\, k_F a \quad = \quad \Delta E^{(0)}_{\text{dim}} + \Delta E^{(1)}_{\text{dim}}\, k_F a$$

$$\left(\frac{1}{k_{\mathrm{F}} a}\right)_c \underset{R_* \to +\infty}{=} -\frac{r}{1+r} k_{\mathrm{F}} R_* + \frac{2}{\pi}\left\{1 - \left(\frac{1+r}{r}\right)^2 + \frac{1}{2}\left[\left(\frac{1+r}{r}\right)^{5/2} - \left(\frac{r}{1+r}\right)^{1/2}\right] \ln \frac{1+\left(\frac{r}{1+r}\right)^{1/2}}{1-\left(\frac{r}{1+r}\right)^{1/2}}\right\}$$

# (b) Non-trivial weakly interacting limit

C.T. and Yvan Castin, Phys. Rev. A **85**, 053612 (2012)




$M/m = 1,\ R_* = 0:$ analytics $\neq$ numerics $\rightarrow 3\%$

● R. Grimm, Nature **485**, 615-618 (2012)

# Outlook

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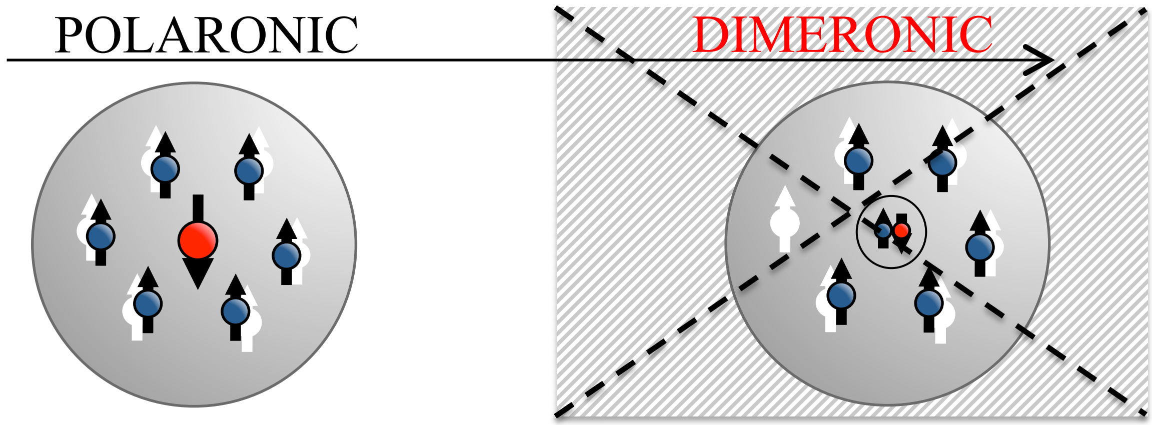
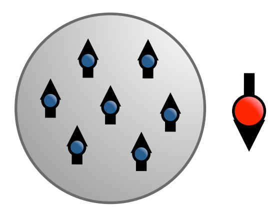
# Polaronic quasi-particle residue




The quasi-particle residue Z quantifies the quasi-particle nature of the ground state of the system

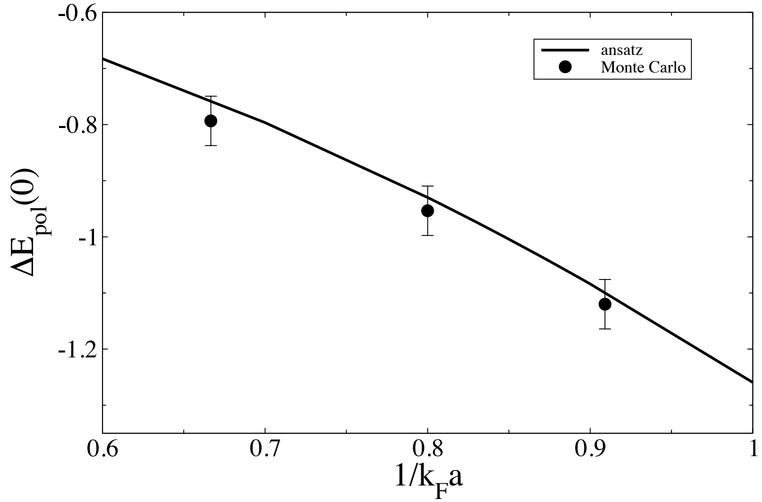
$$Z = |\phi|^2 = \Big|$$  $$\kappa \Big|^2$$

| $Z$ | **MEANING** |
|---|---|
| 1 | Free Impurity |
| 0 | No Quasi-Particle |

# Polaron: Test the ansatz

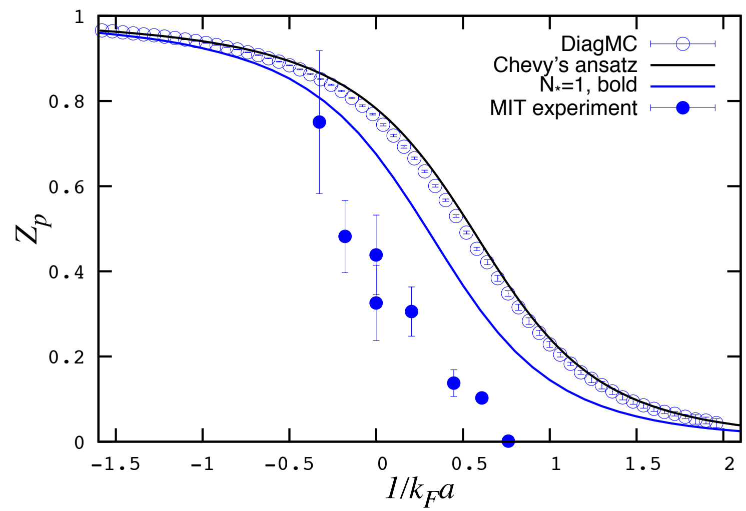
Test the ansatz with quantum Monte Carlo results for equal masses and wide resonance: $m = M, R_* = 0$

Test: Energy




N. Prokof' ev, B. Svistunov, PRB **77**, 020408 (2008)

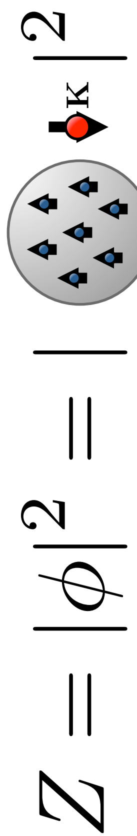
Test: State

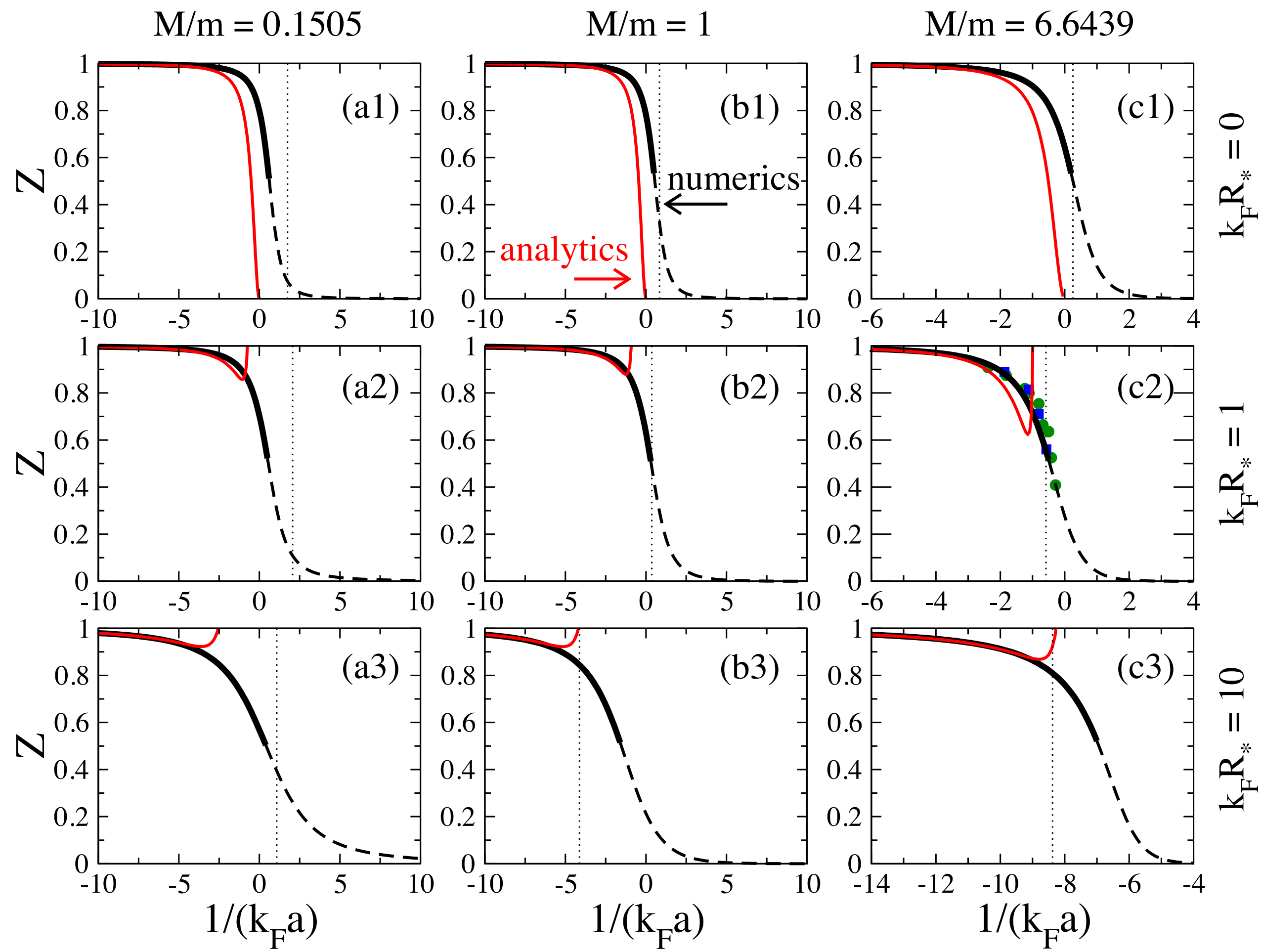



J. Vlietinck, J. Ryckebusch, K. Van Houcke, Phys. Rev. B **87**, 115133 (2013)

The variational ansatz seems to be good to describe both the ground energy and the ground state of the system

# Polaronic quasi-particle residue






C.T. and Yvan Castin, Europhys. Lett. **101**, 30006 (2012)

# Polaronic quasi-particle residue

Non-trivial weakly attractive limit

$$\boxed{a \to 0^-, \qquad\qquad aR_* = \text{const.}}$$

$$\left(\frac{1}{Z}\right)_{\text{exact}} \stackrel{a\to 0^-}{=} 1 + \left(\frac{M}{M+m}\right)^2 \left[c_1 \frac{k_F a}{\pi} + c_2 \left(\frac{k_F a}{\pi}\right)^2 + O(k_F a)^3\right]$$

Compare with an exactly solvable model:
The infinite-mass impurity

$$c_2 \underset{M/m\to+\infty}{\sim} \ln(M/m)$$

The divergence is a signature of the Anderson ortogonality catastrophe

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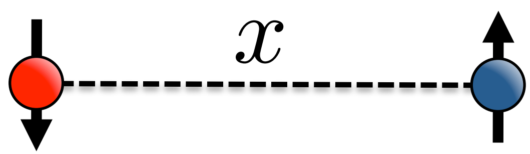
# Pair correlation function

Due to the symmetry of interactions, the density that surrounds the impurity is a spherically symmetric function of the radial coordinate




$$\mathbf{x} = \mathbf{x}_u - \mathbf{x}_d$$

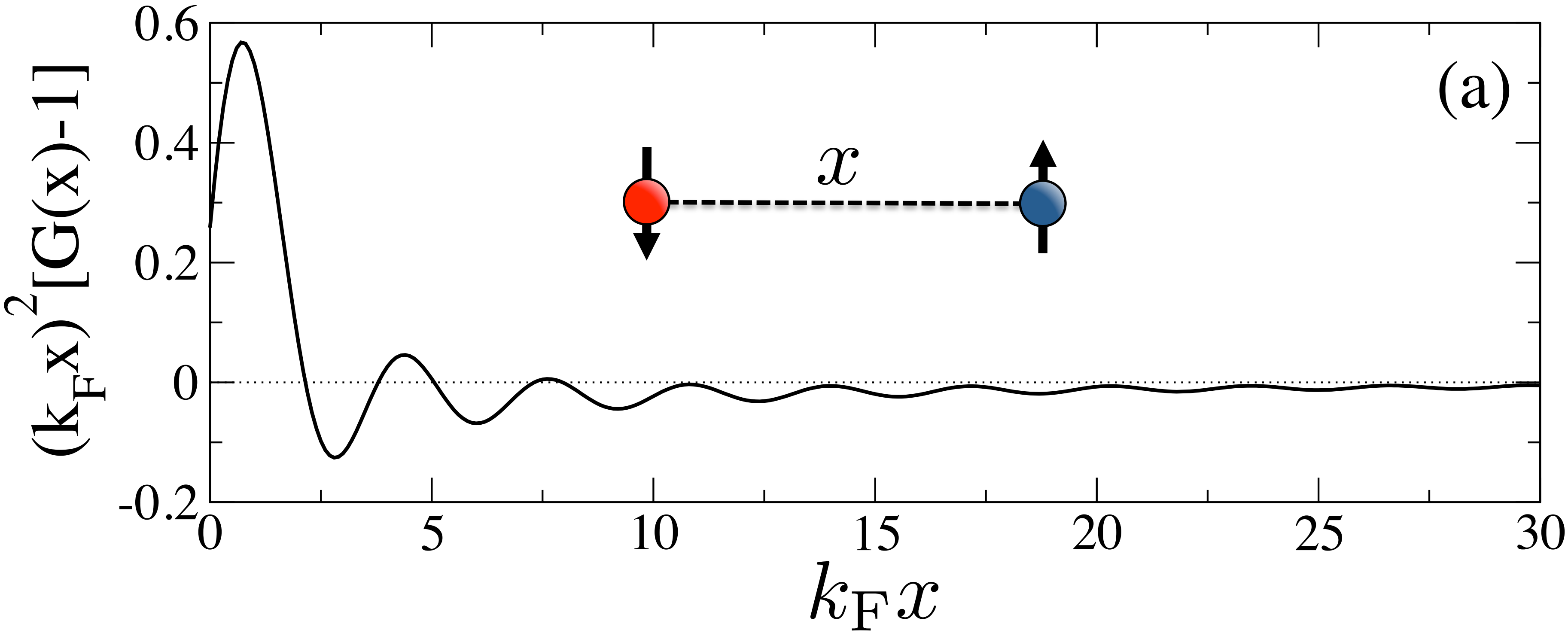
$$G(\mathbf{x}_u - \mathbf{x}_d) = \frac{\langle \hat{\psi}_u^\dagger(\mathbf{x}_u)\hat{\psi}_d^\dagger(\mathbf{x}_d)\hat{\psi}_d(\mathbf{x}_d)\hat{\psi}_u(\mathbf{x}_u)\rangle}{\rho\rho_d}$$

$\hat{\psi}_u(\mathbf{x}_u)$ Fermion field operator

$\hat{\psi}_d(\mathbf{x}_d)$ Impurity field operator

G(x) is a measure of the spatial extension of the polaron in a Fermi gas, G(x) presents Friedel-like oscillations and a multiscale structure

# Pair correlation function

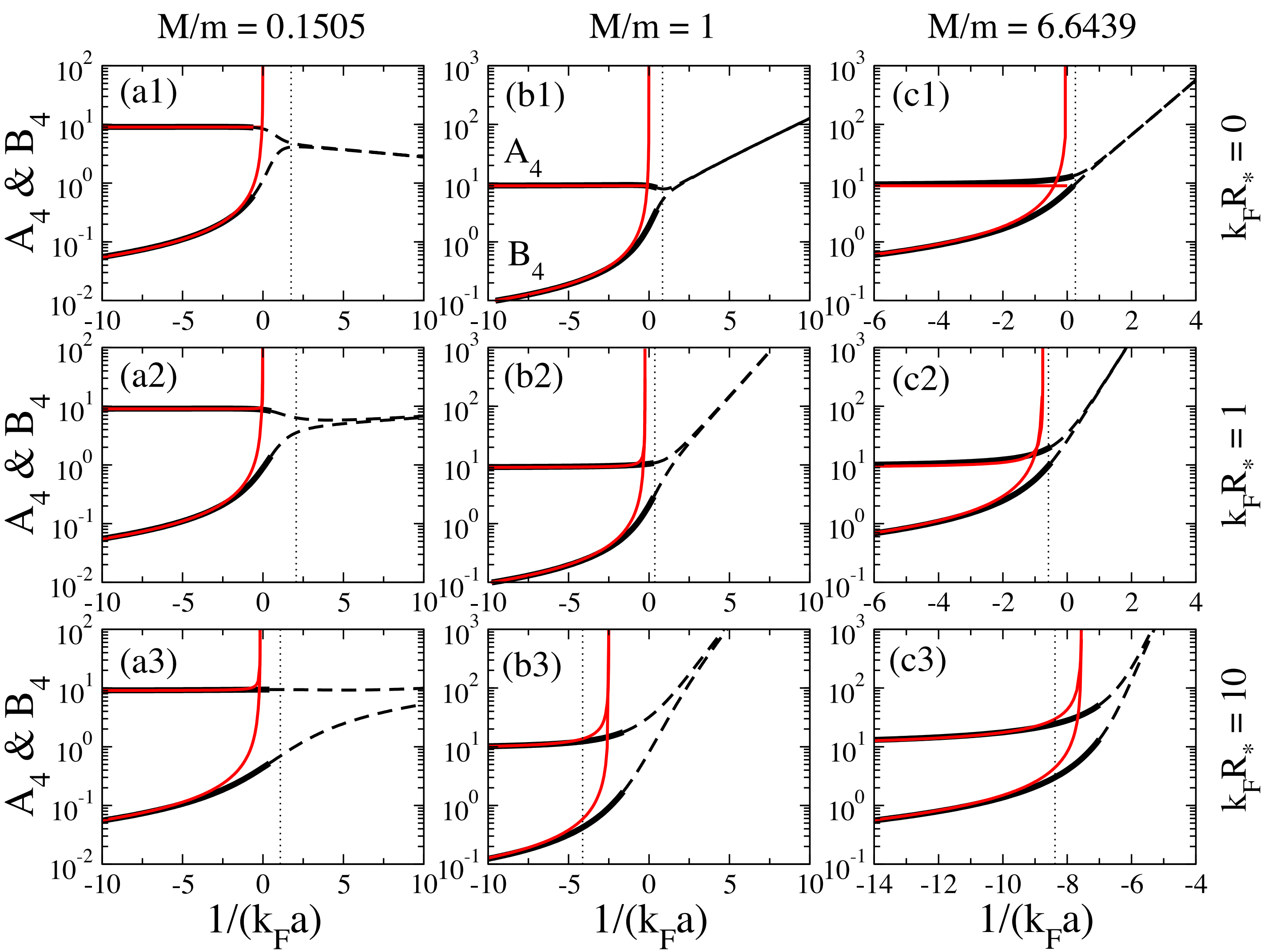



At large distance

$$G(x) - 1 \underset{x\to+\infty}{\sim} -\frac{A_4 + B_4\cos(2k_F x)}{(k_F x)^4}$$

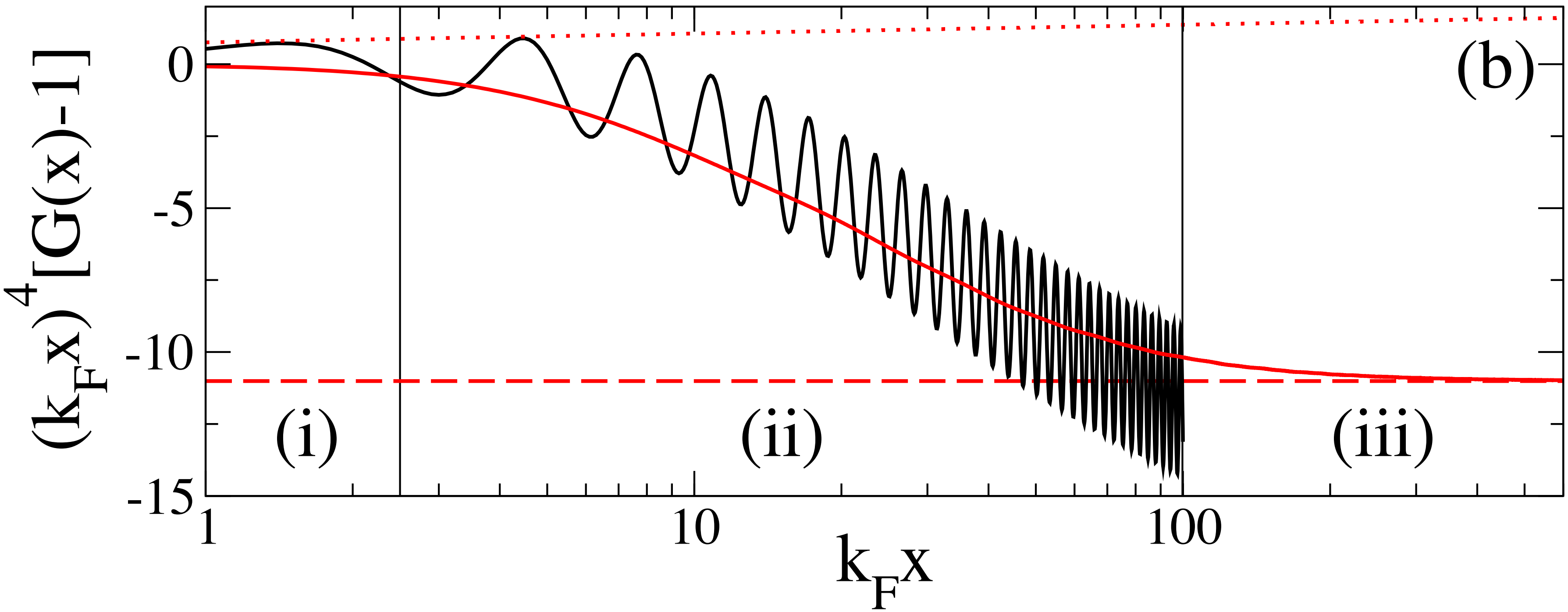
$$\langle x \rangle = \int d^3x\, x[G(x)-1] \underset{x\to+\infty}{\sim} -A_4 \int_0^{+\infty} \frac{x^3}{(k_{\mathrm{F}} x)^4} \underset{x\to+\infty}{\sim} A_4 \ln(x)$$

# Pair correlation function




C.T. and Yvan Castin, Europhys. Lett. **101**, 30006 (2012)

# Multiscale structure




$$\frac{\ln x}{x^4}$$

intermediate

$$\mathrm{Ci}(x),\ \mathrm{Si}(x)$$

$$\frac{1}{x^4}$$

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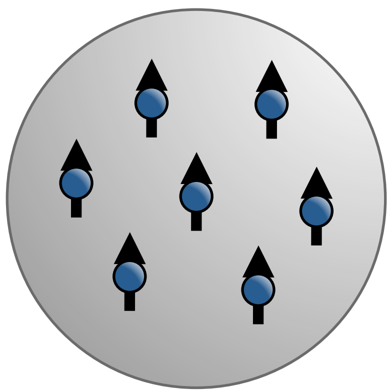
# A moving polaron

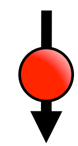
Homogeneous (3D) Fermi gas
of same spin state

$$m, k_{\mathrm{F}}$$

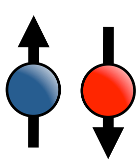


Distinguishable impurity
(boson/fermion)

$$M, \mathbf{K}$$



No interaction between the Fermions



Attraction $\boxed{g \to 0^{-}}$ $\boxed{R_*}$

# What do we know ($R_* \to 0$) ?

$(\mathbf{K} = \mathbf{0})$ The ground state is the Fermi polaron

N. Prokof'ev, B. Svistunov, PRB **77**, 020408 (2008)

1) Perturbative regime: R.F. Bishop, Nucl. Phys B **17**, 573 (1970)

2) Any regime: Variational ansatz F. Chevy, PRA **74**, 063628 (2006)

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$(\mathbf{K} \neq \mathbf{0})$ The energy of the polaron becomes complex

$$\boxed{\Delta E(\mathbf{K}) = \Re\Delta E(\mathbf{K}) + i\,\Im\Delta E(\mathbf{K})}$$

3) Perturbative regime: R.F. Bishop, Nucl. Phys B **17**, 573 (1970)

$$M = m: \qquad \Im\Delta E(\mathbf{K}) \propto K^4 \qquad \text{for} \qquad K < k_F$$

NOT REPRODUCED BY THE ANSATZ

# A moving polaron ($R_* = 0$)

$$\boxed{\Delta E(\mathbf{K}) \underset{g\to 0^-}{=} \frac{\hbar^2 K^2}{2M} + \rho g + \frac{(\rho g)^2}{E_F} f(K/k_F) + O(g^3)}$$

$f(\kappa)$

Sextuple integral (over the momenta of particle-hole pair)

Presents singularities of the nth-order derivative

$\kappa = 0 \qquad \kappa = 1 \qquad \kappa = r \equiv M/m$

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Presents singularities of the nth-order derivative

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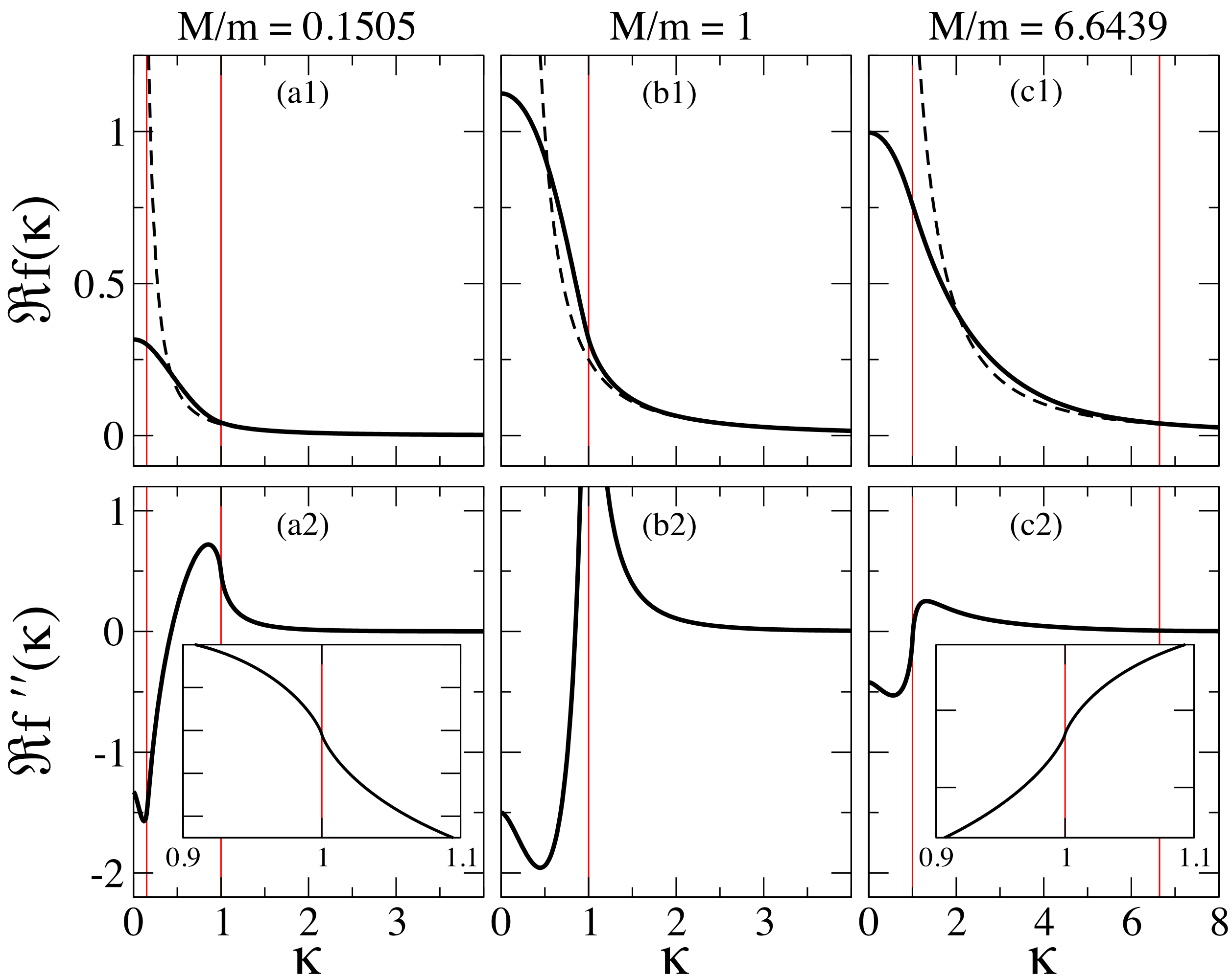
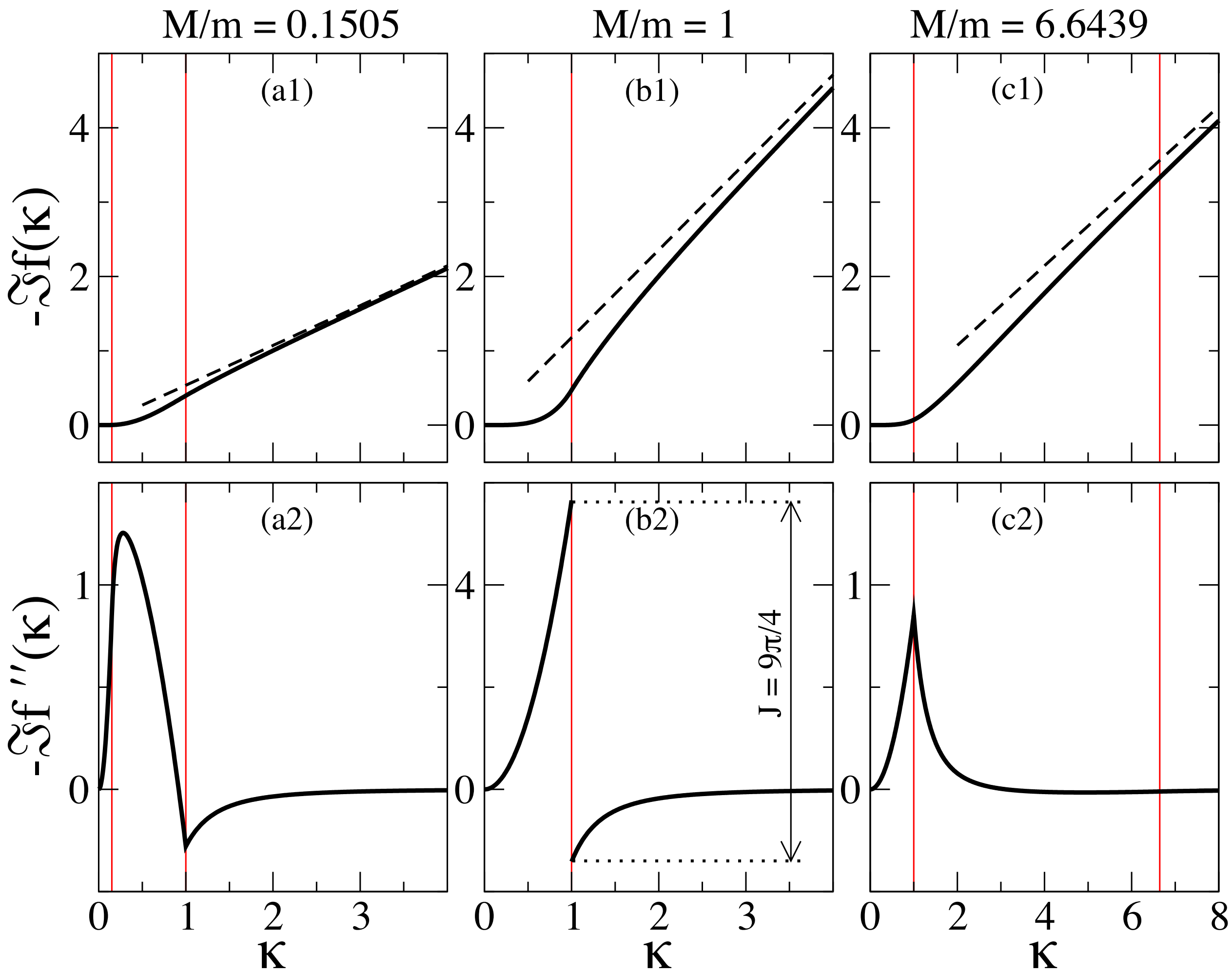
$$\begin{aligned}
\Re f(\kappa) &= \frac{3r}{r+1} - \frac{3r}{20(r^2-1)^2}\Bigg\{\Bigg[\frac{(r^2-1)}{2}(\kappa^2+20r-9) \\
&+ \frac{(\kappa-1)^3}{\kappa}[\kappa(\kappa+3)(r^2-2)+6r^2-2]\ln\left|\frac{\kappa-1}{\kappa}\right| \\
&+ \frac{(\kappa-r)^4}{\kappa}\left(\frac{\kappa+4r}{r^2}\right)\ln\left|\frac{\kappa-r}{\kappa}\right|\Bigg] + \Big[\kappa\to-\kappa\Big]\Bigg\}.
\end{aligned}$$

# A moving polaron ($R_* = 0$)




$\boxed{K = k_F \ (\kappa = 1)}$ Effective mass divergence is an artifact of the perturbative approach. We expect a behavior $g^2 \ln(g^2)$

# A moving polaron ($R_* = 0$)



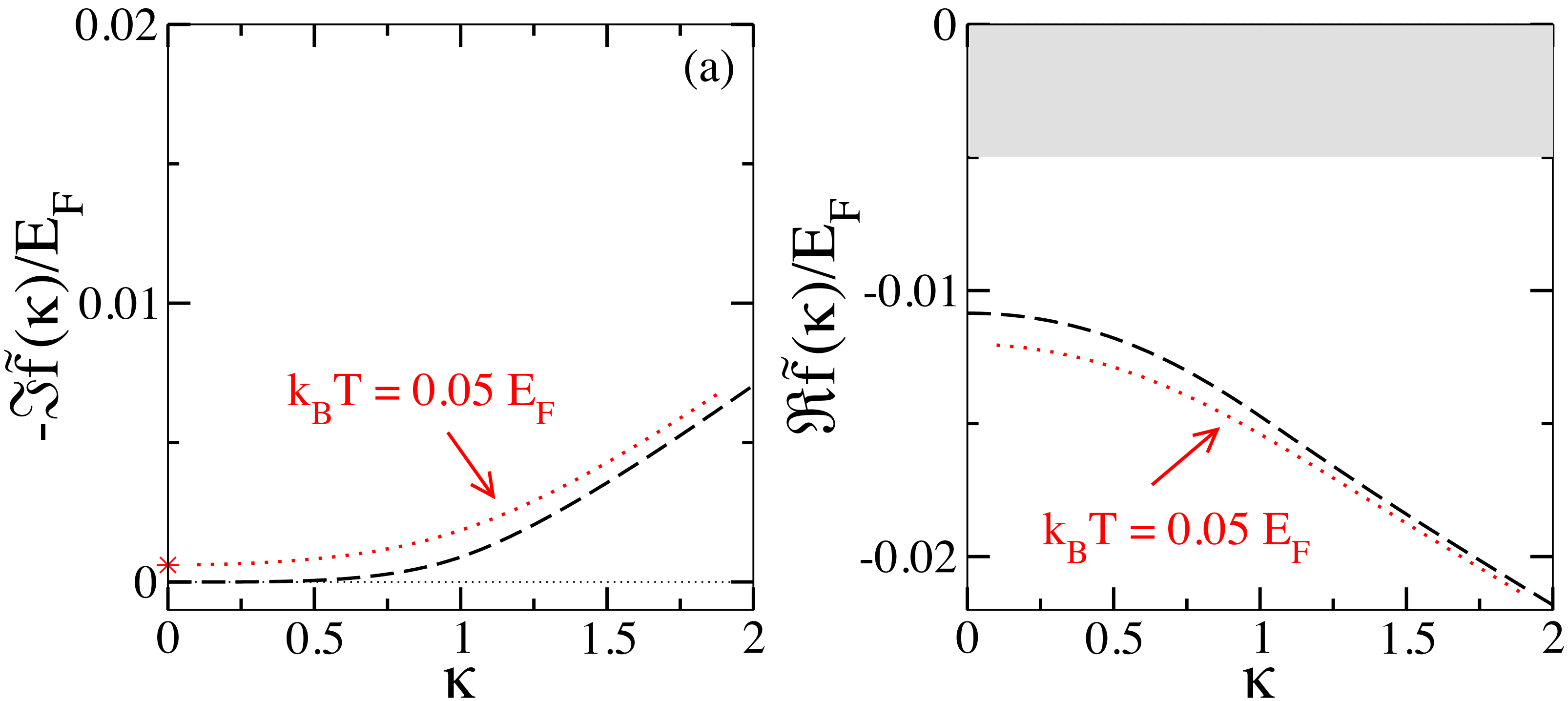
# Experiments? ($R_* \neq 0$)

$$\tilde{f}(\kappa) = f(\kappa) - (c_1 \kappa^2 + c_2) k_F R_*$$

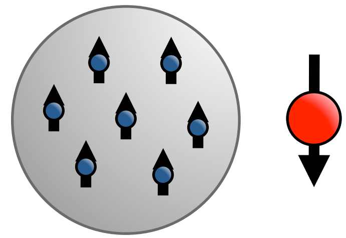
Measurable by RF-spectroscopy: Broadening and shift of the resonance

Innsbruck: C. Kohstall *et. al.*, Nature **485**, 615 (2012)

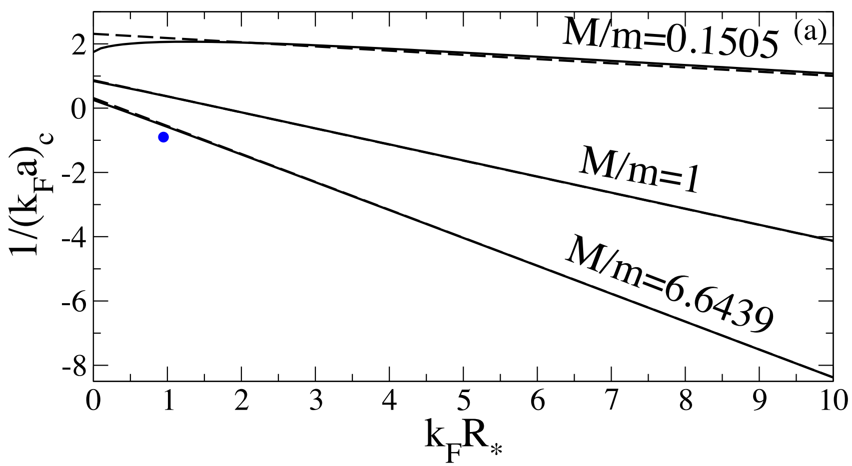
$$^{40}\mathrm{K}/^{6}\mathrm{Li} \qquad M/m = 6.6439 \qquad k_F R_* = 1 \qquad k_F a = -0.46$$



# Conclusions



s-wave narrow Feshbach resonance: $a, R_*$

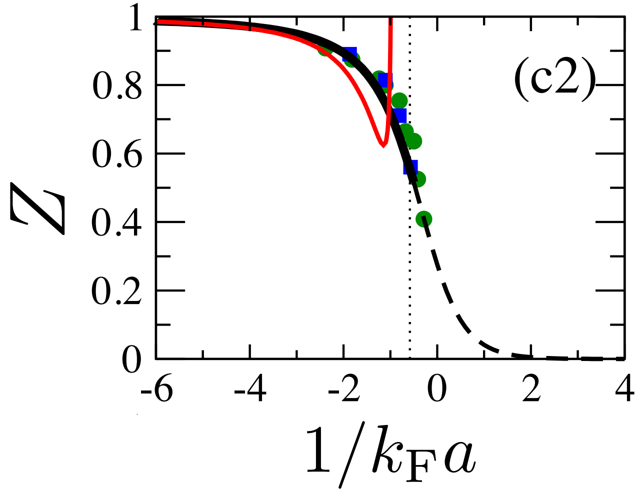


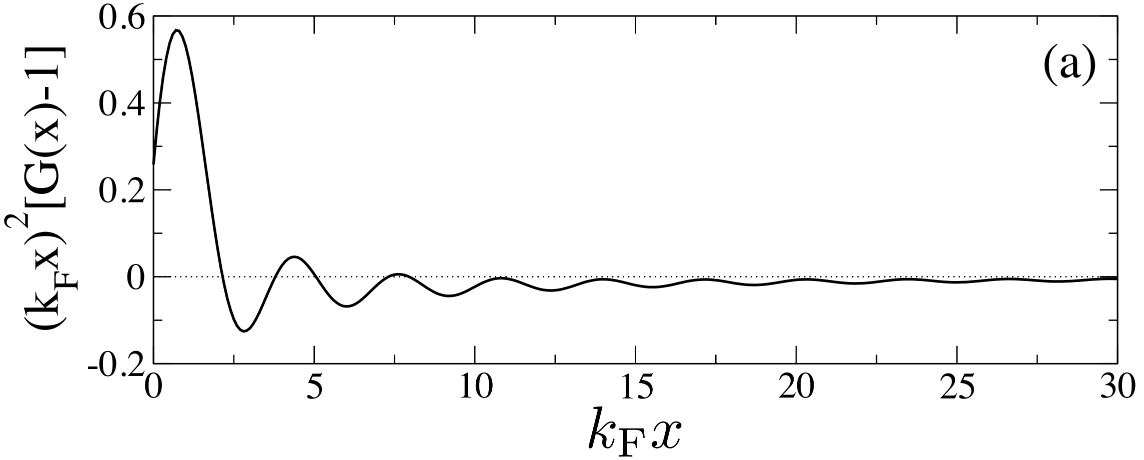

Ground state: polaron-to-dimeron crossing point

Physical interpretation in terms of the Lamb shift

# Conclusions

Polaronic ansatz: Good for the energy and the state




Moving polaron: experimentaly observable

$$\boxed{\Delta E(\mathbf{K}) \underset{g\to 0^-}{=} \frac{\hbar^2 K^2}{2M} + \rho g + \frac{(\rho g)^2}{E_F} f(K/k_F) + O(g^3)}$$

Yvan Castin

Laboratoire Kastler Brossel

Ecole normale supérieure

24 rue Lhomond, 75231 Paris, France

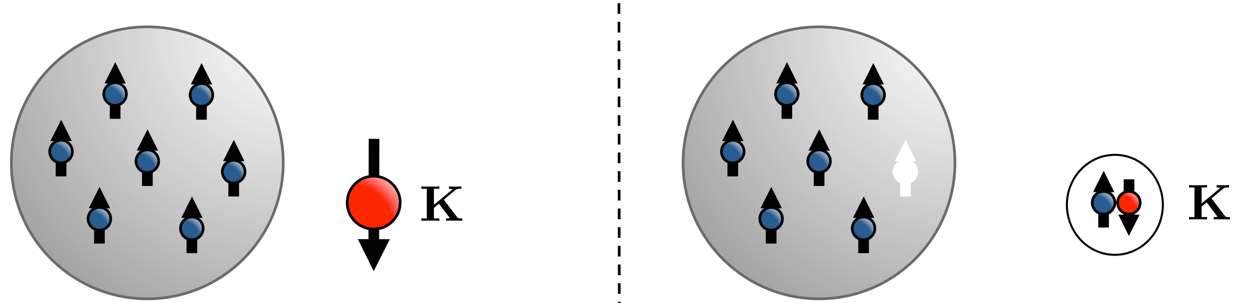
# Thank You!!

# (b) Effective mass

$$\boxed{\Delta E(\hbar \mathbf{K}) \underset{K\to 0}{=} \Delta E(0) + \frac{\hbar^2 K^2}{2m^*} + O(K^4)}$$

POLARON $\quad 1/(k_{\mathrm{F}} a)_{\mathrm{c}} \quad$ DIMERON

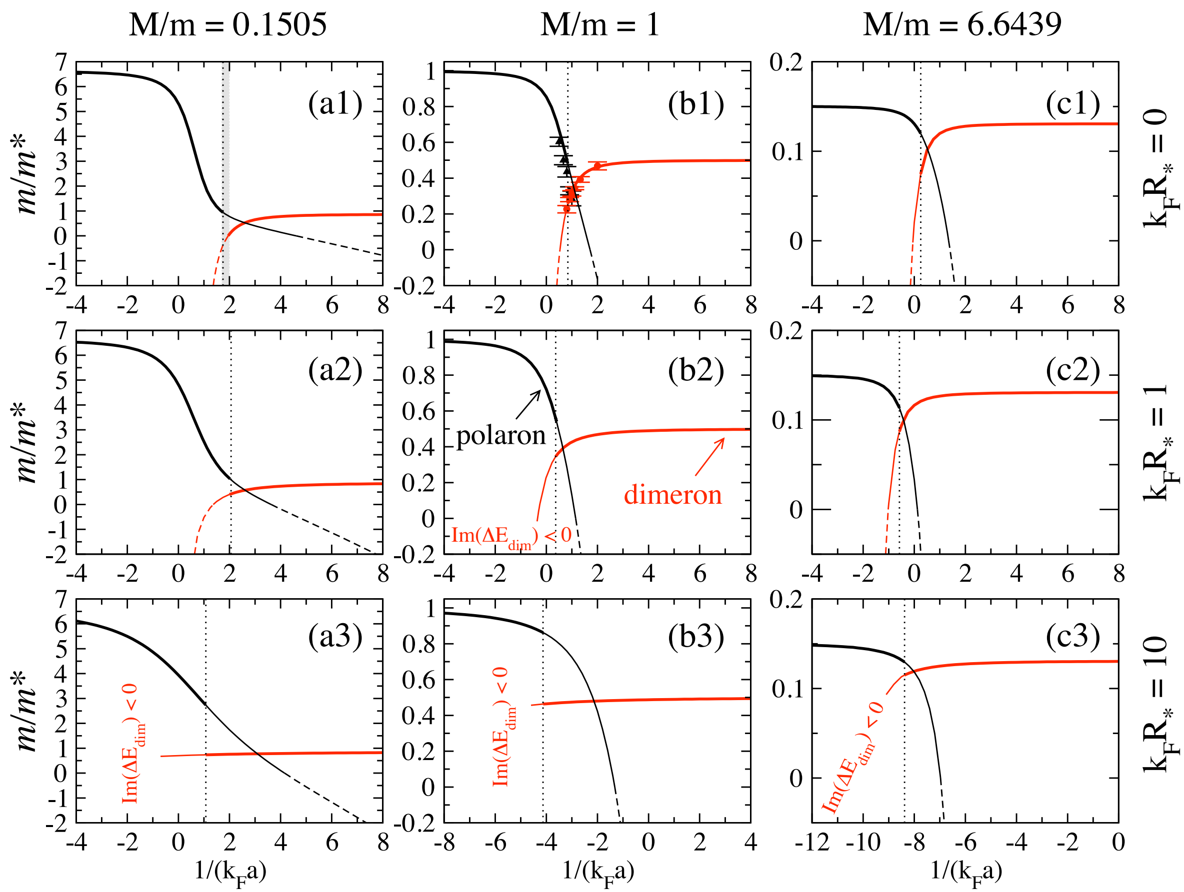
$\longrightarrow 1/k_{\mathrm{F}} a$




$m^*_{\mathrm{pol}} \overset{a\to 0^-}{\longrightarrow} M$

$m^*_{\mathrm{dim}} \overset{a\to 0^+}{\longrightarrow} m + M$

# (b) Effective mass




$$\frac{m}{m^*_{\mathrm{pol}}} \overset{a\to 0^-}{\longrightarrow} 6.6439 \qquad \frac{m}{m^*_{\mathrm{pol}}} \overset{a\to 0^-}{\longrightarrow} 1 \qquad \frac{m}{m^*_{\mathrm{pol}}} \overset{a\to 0^-}{\longrightarrow} 0.1505$$

$$\frac{m}{m^*_{\mathrm{dim}}} \overset{a\to 0^+}{\longrightarrow} 0.87 \qquad \frac{m}{m^*_{\mathrm{dim}}} \overset{a\to 0^+}{\longrightarrow} 0.5 \qquad \frac{m}{m^*_{\mathrm{dim}}} \overset{a\to 0^+}{\longrightarrow} 0.13$$

# (c) The closed-channel

Closed-channel-molecule population: $N_{\rm cc} = \sum_{\mathbf{k}} \langle \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} \rangle$

$$\hat{H} = \sum_{\mathbf{k}} E_{\rm mol} \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} + \ldots \quad \Rightarrow \quad \frac{\partial \hat{H}}{\partial E_{\rm mol}} = \sum_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}}$$

$$N_{\rm cc} = \frac{\partial \Delta E}{\partial E_{\rm mol}} \quad \Rightarrow \quad \boxed{N_{\rm cc} = -\frac{\partial \Delta E}{\partial (1/a)} \frac{2\mu R_*}{\hbar^2}}$$