How much the single impurity atom problem can tell us about a many-body system?

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Seminar at KITP
“ Beyond Standard Optical Lattices ” program
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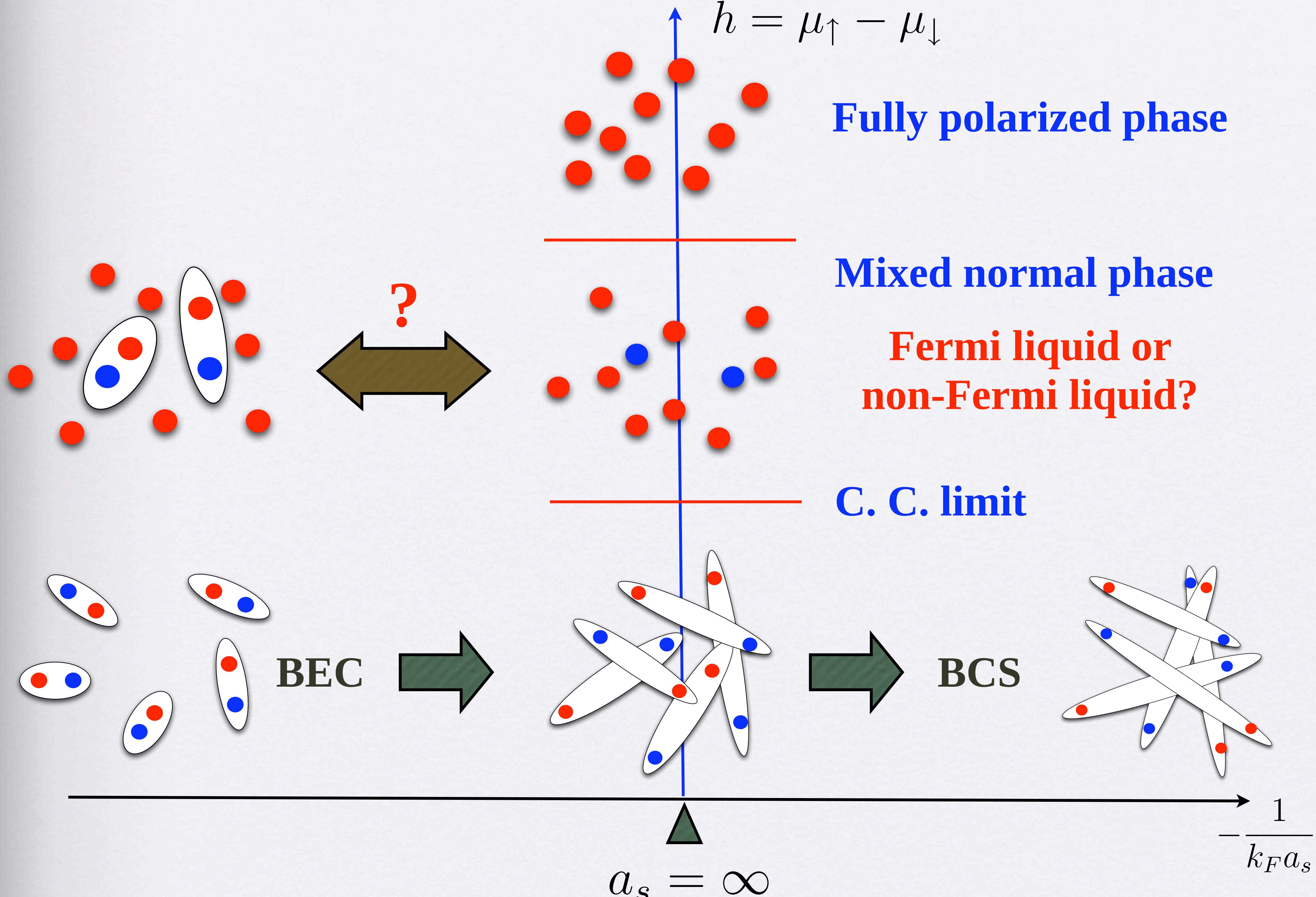
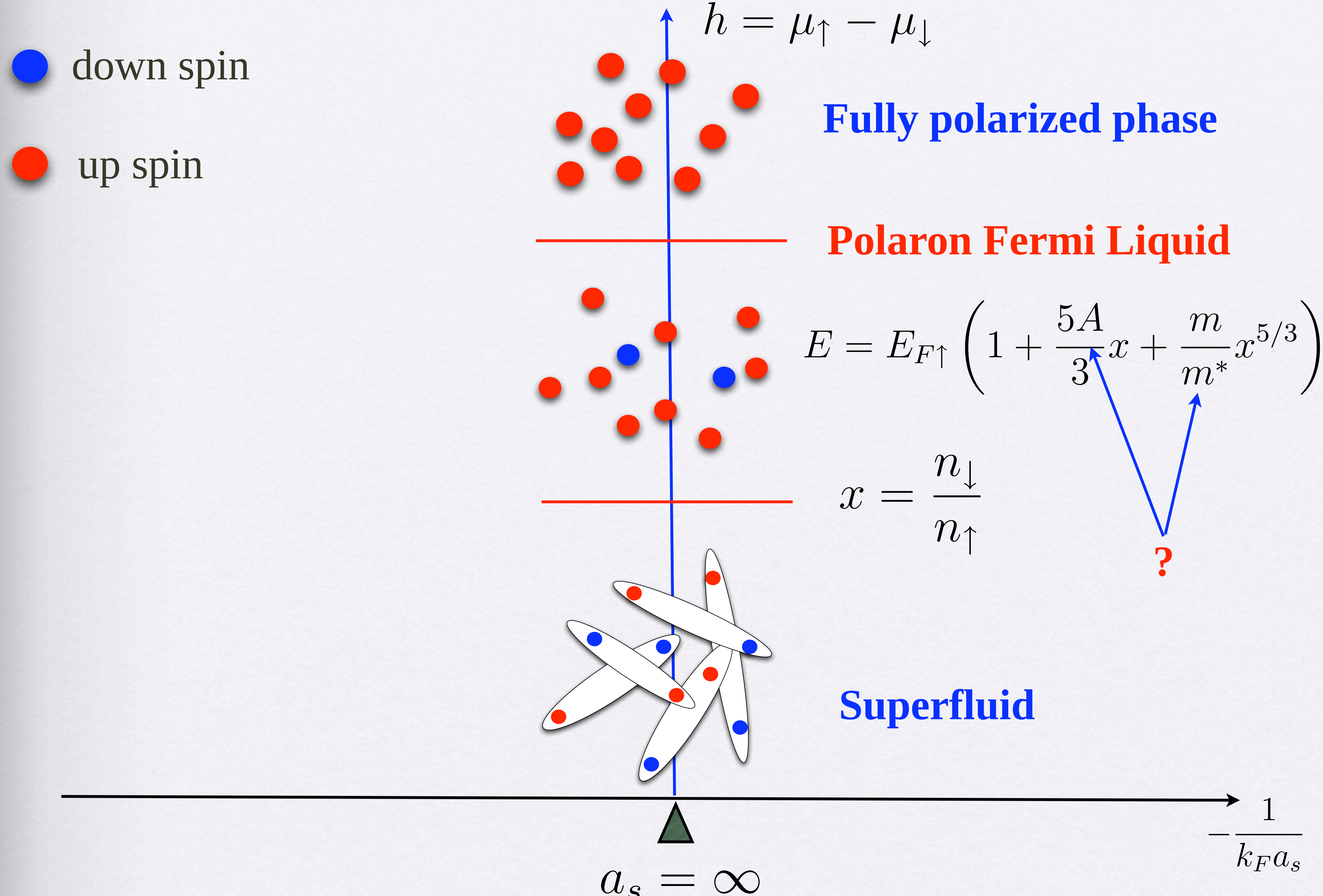
A brief history of polarons in cold atoms starts from imbalanced Fermi gases across a Feshbach resonance ---



This question is answered by numbers of theory work and later confirmed by experiments ---



The Fermi liquid parameter A, m* can be obtained from single impurity atom problem

Variational wave function approach:

$$|\Psi\rangle = \left(\phi_0 c^\dagger_{\mathbf{q_0}\downarrow} + \sum_{\mathbf{k}>\mathbf{k_F},\mathbf{q}<\mathbf{k_F}} \phi_{\mathbf{kq}} c^\dagger_{\mathbf{q_0}+\mathbf{q}-\mathbf{k}\downarrow} c^\dagger_{\mathbf{k}\uparrow} u_{\mathbf{q}\uparrow}\right)|N\rangle$$

$$A = -0.61 E_{F\uparrow} \qquad m^* = 1.17m$$

Chevy, PRA, 74, 063628 (2006)

Combescot, Recati, Lobo and Chevy, PRL, 98, 180402 (2007)

compared with MC results:

Fixed nodes MC: $A = -0.58 E_{F\uparrow}$

$m^* = 1.04m$

Lobo, Recati, Giorgini and Stringari, PRL, 97, 200403 (2006)

Diagrammatic MC: $A = -0.615 E_{F\uparrow}$

$m^* = 1.20m$

Prokofev and Svistunov, PRB, 77, 020408 (2008) and 77, 125101 (2008)

Experiments: $A = -0.64 E_{F\uparrow}$

MIT exp: PRL, 102, 230402 (2009)

$m^* = 1.17m$

ENS exp: PRL, 103, 170402 (2009)

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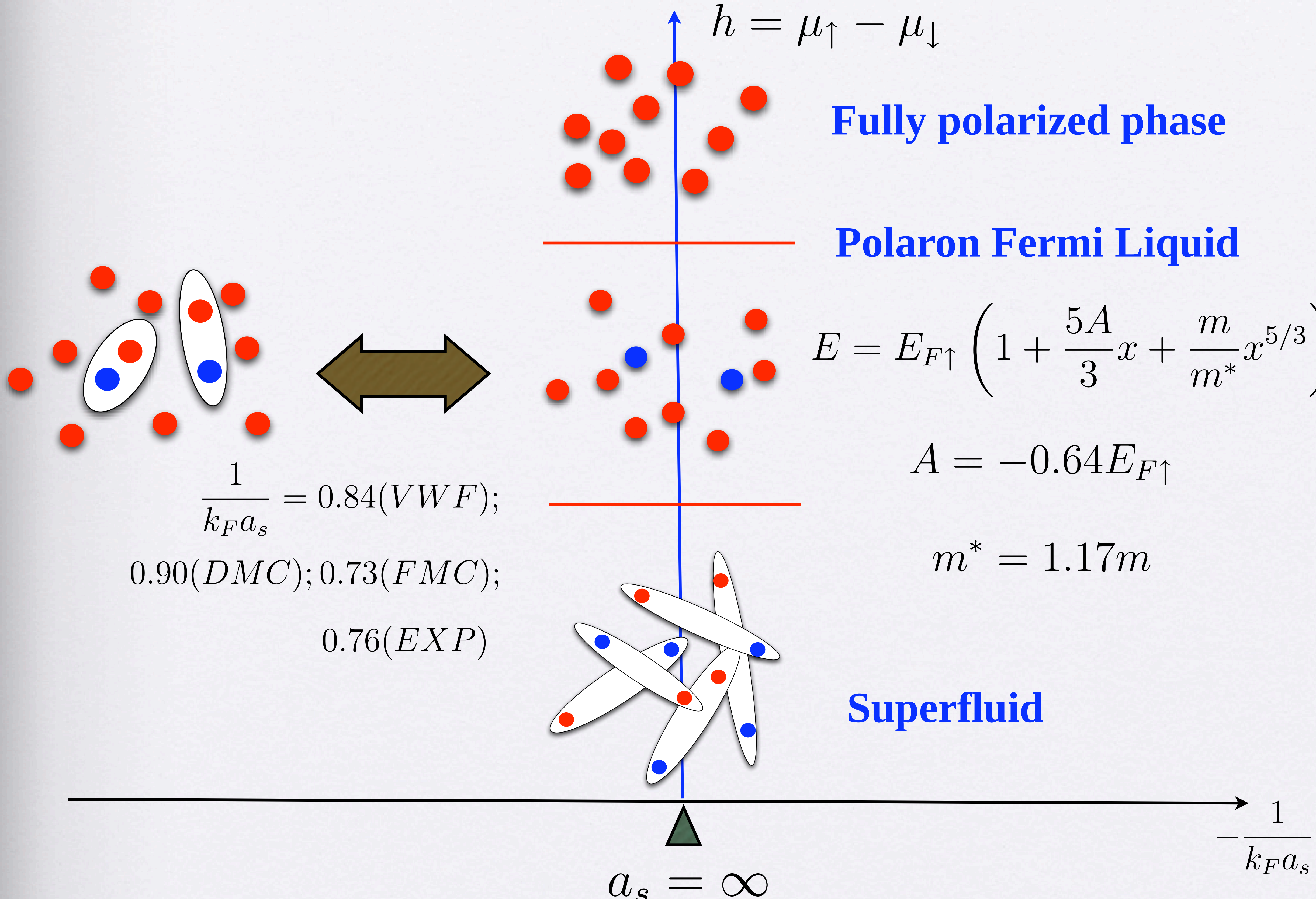


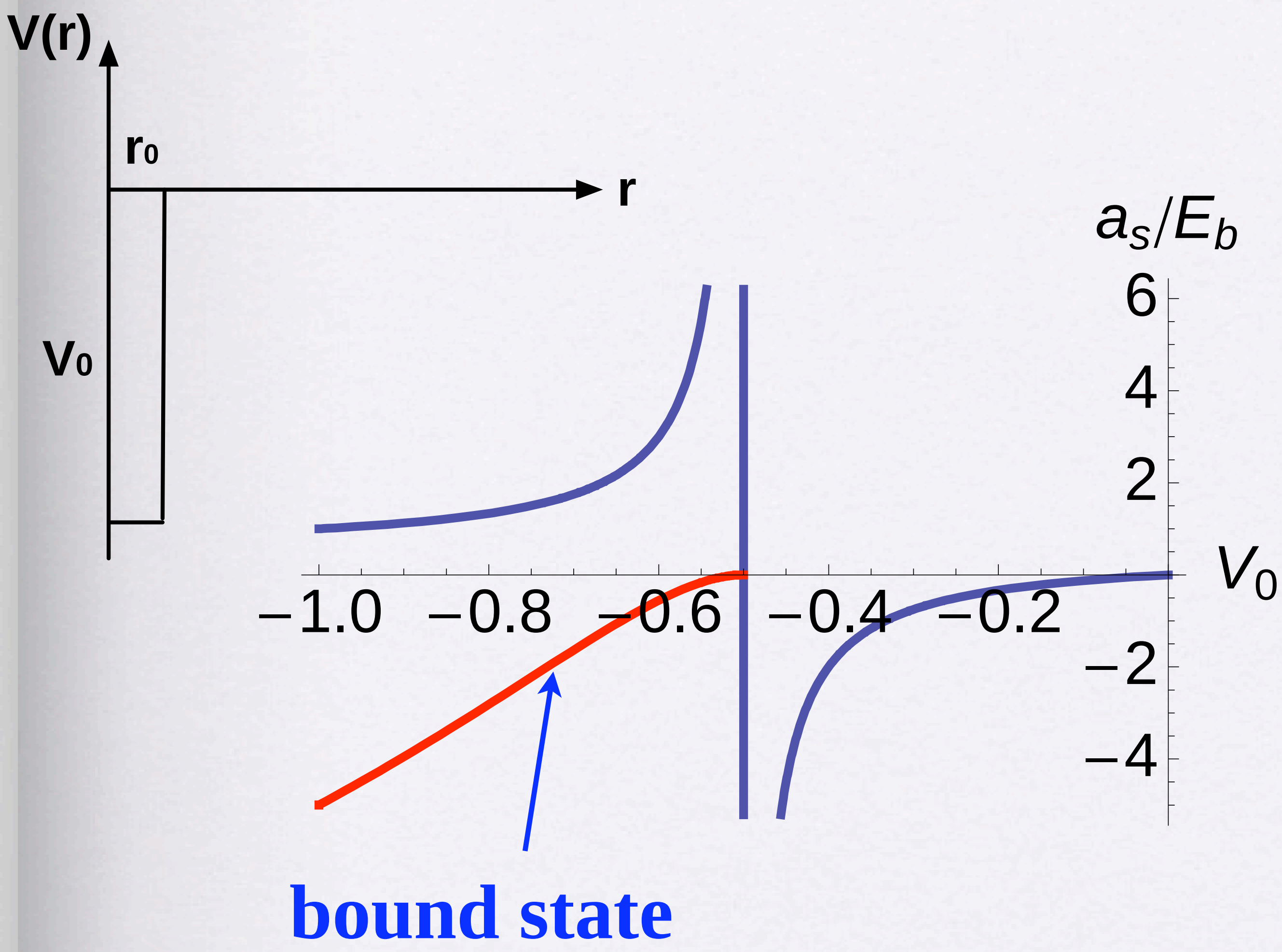
Two topics in this talk:

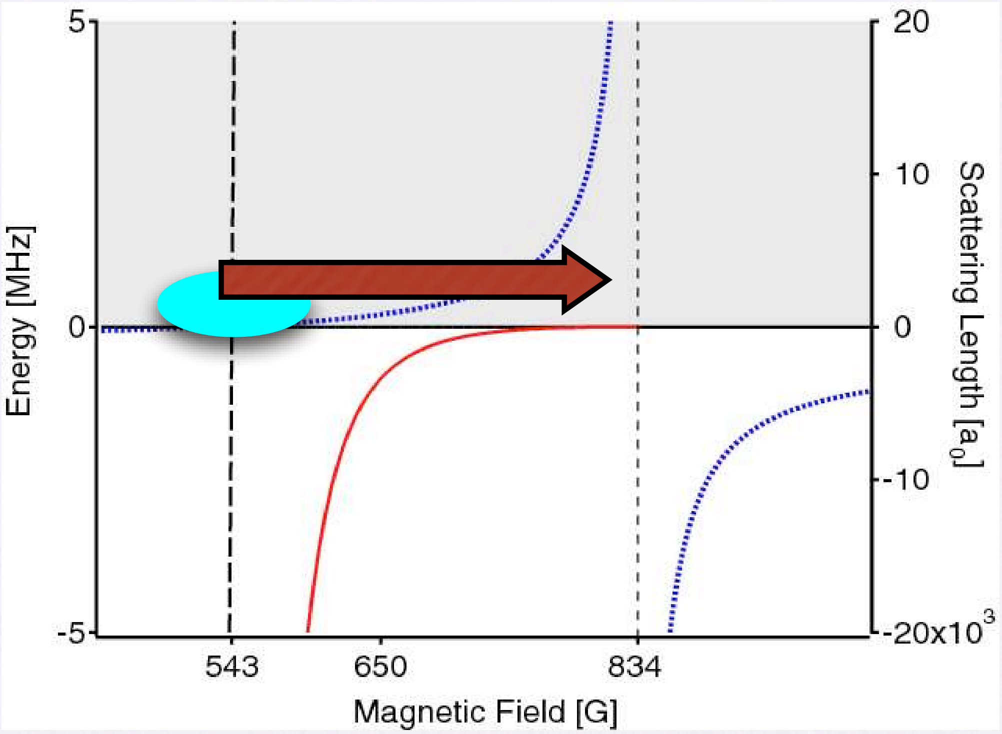
1. Whether a fully magnetized itinerant ferromagnetism is energetically favorable in a strongly repulsively interacting Fermi gas?

2. Whether a boson-fermion mixture is stable across an inter-species Feshbach resonance?

1. Whether a fully magnetized itinerant ferromagnetism is energetically favorable in a strongly repulsively interacting Fermi gas?

Repulsive interaction and “ upper branch ”





MIT experiment: Science (2009)

comment: HZ, PRA, 80, 051605 (2009)

upper branch --- atoms remain in the scattering state (with the molecular state excluded) with positive scattering length

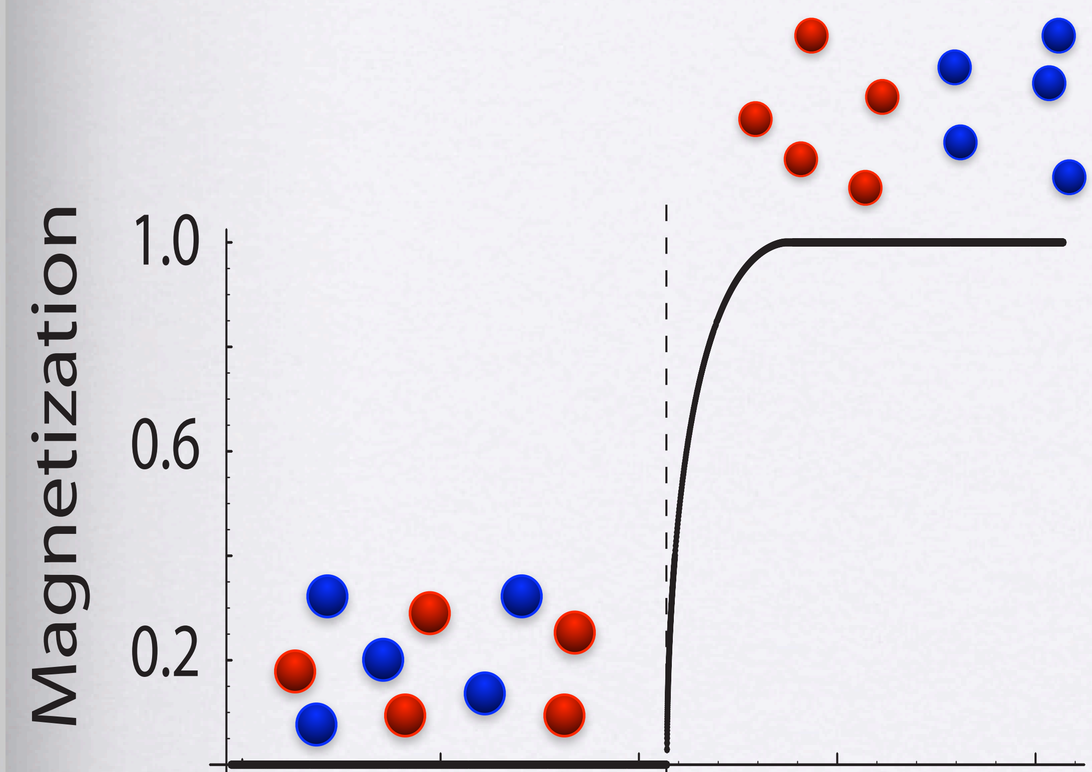
repulsive interaction --- the interaction energy of atoms in the upper branch is positive and increases with the increase of the scattering length

Whether the two-component Fermi gas will become ferromagnetic (phase separated) when repulsion is strong enough?

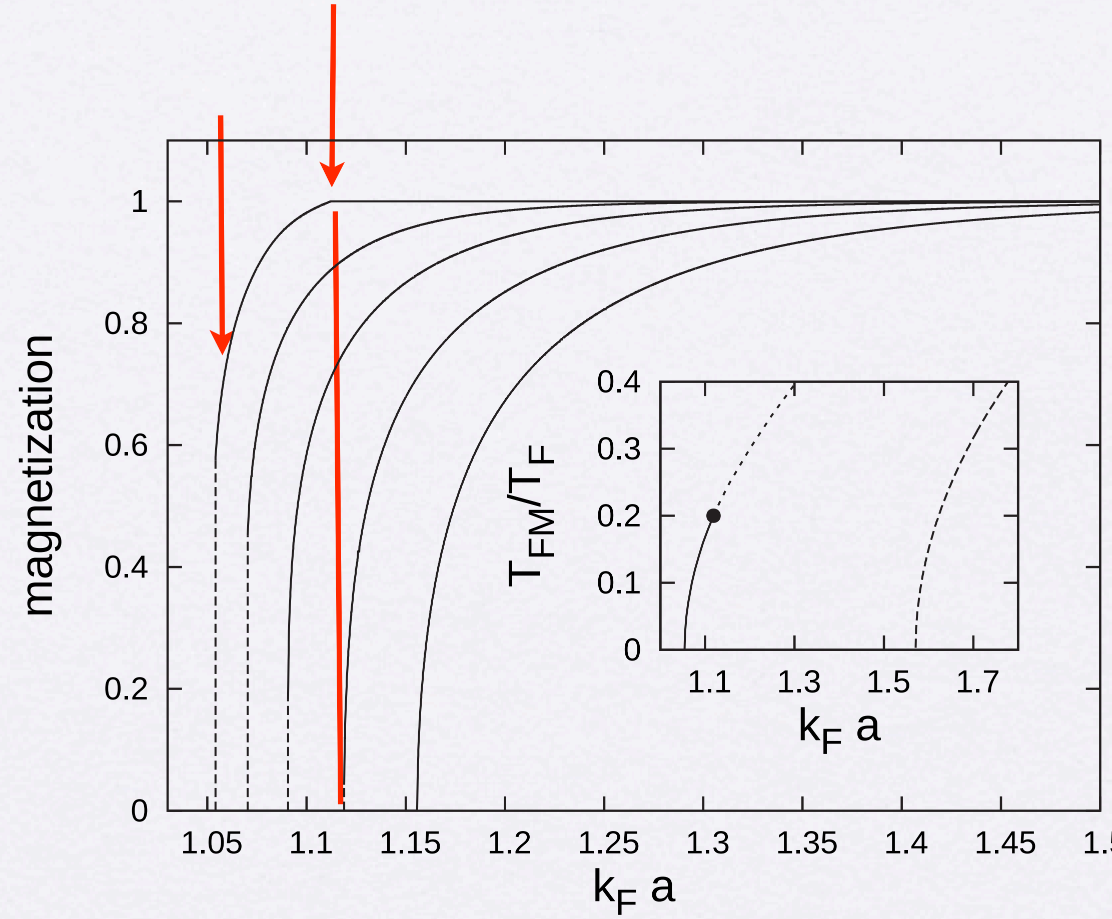
Mean field + Perturbation theory: Yes

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + g \sum_{\mathbf{r}} n_{\uparrow}(\mathbf{r}) n_{\downarrow}(\mathbf{r})$$

$$e^{(2)} = -\frac{2g^2}{V^3} {\sum}' \frac{N_{\mathbf{k}_1,+} N_{\mathbf{k}_2,-} (N_{\mathbf{k}_3,+} + N_{\mathbf{k}_4,-})}{\epsilon_{\mathbf{k}_1} + \epsilon_{\mathbf{k}_2} - \epsilon_{\mathbf{k}_3} - \epsilon_{\mathbf{k}_4}},$$



Stoner' MF theory



R. A. Duine and A. H. MacDonald, PRL, 95, 230404 (2005)

Whether the two-component Fermi gas will become ferromagnetic (phase separated) when repulsion is strong enough?

Strongly Correlated Approach : Maybe not

Effect of correlations on the ferromagnetism of transition metals

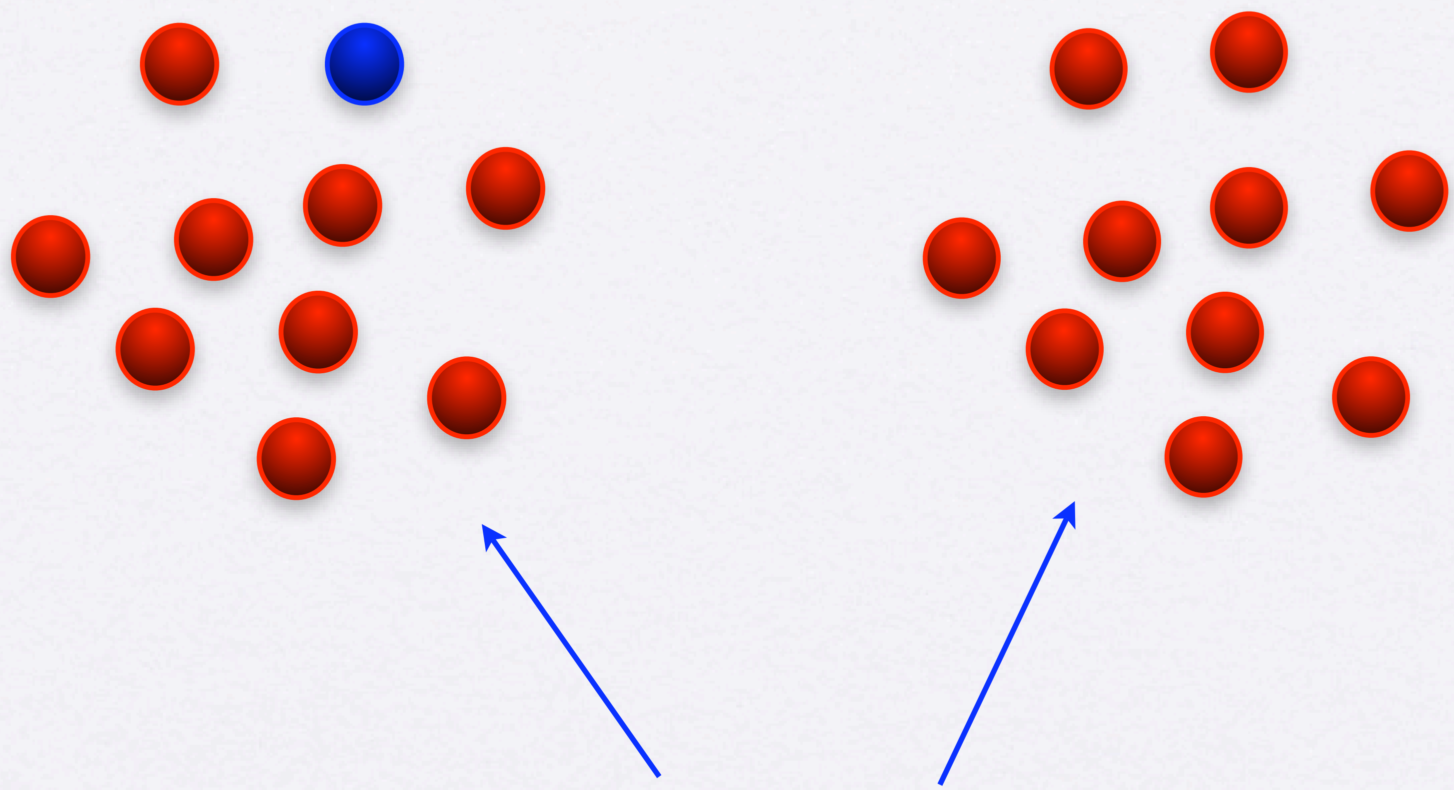
Martin C. Gutzwiller PRL 10, 159 (1963)

Projected wave function for Hubbard model

$$\prod_i (1 - \eta n_{i\uparrow} n_{i\downarrow}) |\Psi_0\rangle$$

Assuming a fully magnetized ferromagnetic state, and ask whether it is energetic stable

--- Single impurity atom problem can now help



$$\delta E = E_{N,1} - E_{N+1,0} < 0$$

==> A fully polarized state is unstable

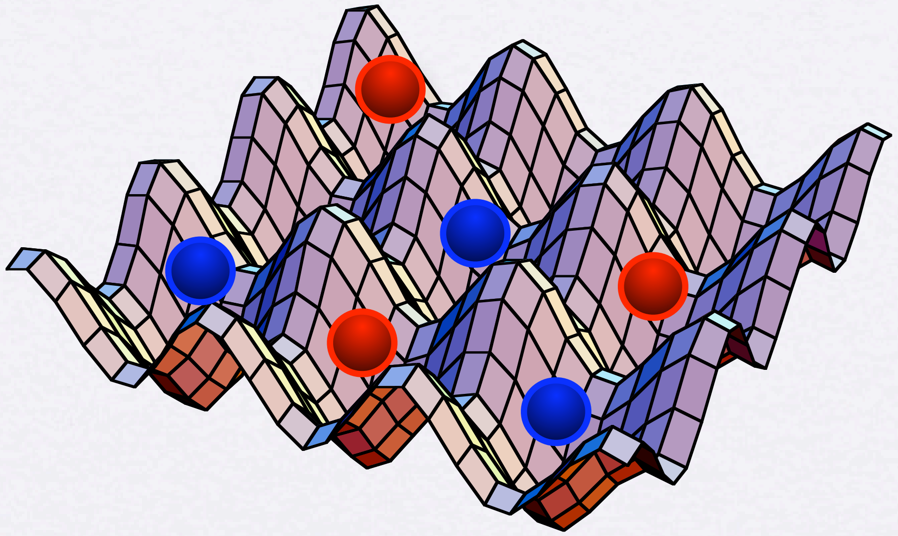
$$|\Psi\rangle = \left(\phi_0 c^\dagger_{\mathbf{q_0}\downarrow} + \sum_{\mathbf{k}>\mathbf{k_F},\mathbf{q}<\mathbf{k_F}} \phi_{\mathbf{kq}} c^\dagger_{\mathbf{q_0}+\mathbf{q}-\mathbf{k}\downarrow} c^\dagger_{\mathbf{k}\uparrow} u_{\mathbf{q}\uparrow} \right) |N\rangle$$

A upper bound of $E_{N,1}$

(I) Applying this method to Hubbard model

$$\hat{H} = \hat{H}_{\mathrm{t}} + \hat{H}_{\mathrm{int}}$$

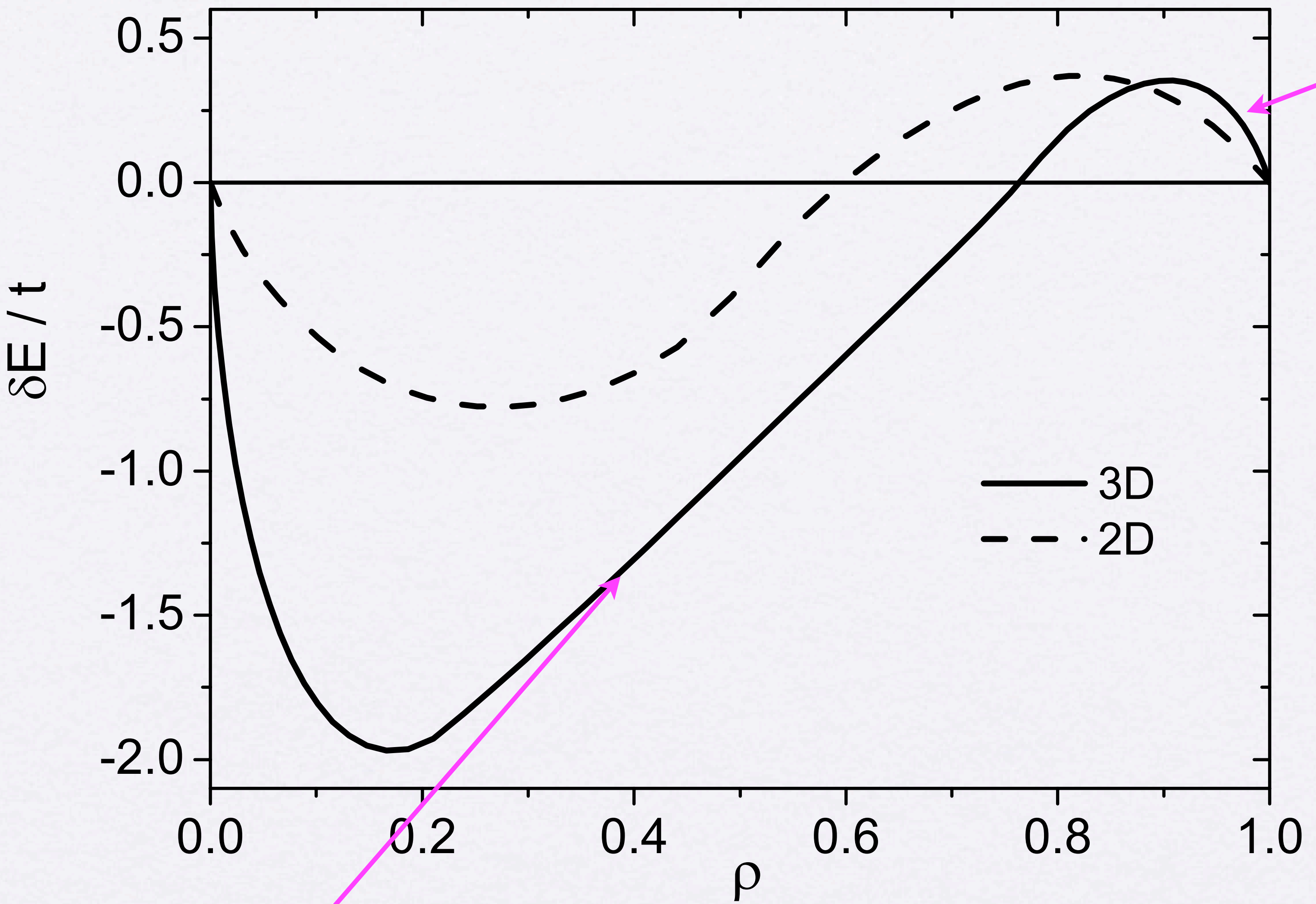
$$\hat{H}_{\mathrm{t}} = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + \mathrm{h.c.} \qquad H_{\mathrm{int}} = U \sum_i n_{i\uparrow} n_{i\downarrow}$$



To justify our approach

Applying this method to Hubbard model

Even at U=Infinity



FM is stable, rigorously proved by Nagaoka, PR, 147, 392 (1966)

$\rho = N/N_s$ fermion density

Fully magnetized FM is unstable even for infinite U

In sharp contrast to Stoner MF

Relation to Gutzwiller's wave function

$$|\Psi\rangle = \left(\phi_0 c^\dagger_{\mathbf{q_o}\downarrow} + \sum_{\mathbf{k}>\mathbf{k_F},\mathbf{q}<\mathbf{k_F}} \phi_{\mathbf{kq}} c^\dagger_{\mathbf{q_o}+\mathbf{q}-\mathbf{k}\downarrow} c^\dagger_{\mathbf{k}\uparrow} u_{\mathbf{q}\uparrow}\right)|N\rangle$$

$$\phi_{\mathbf{kq}} \equiv \phi_{\mathbf{k}}$$

$$\phi_0 = -\textstyle\sum_{\mathbf{k}>\mathbf{k_F}} \phi_{\mathbf{k}}$$

$$=$$

$$\left(\frac{\phi_0}{\sqrt{N_s}} \sum_{\mathbf{m}} c^\dagger_{\mathbf{m}\downarrow} \mathcal{P}_{\mathbf{m}} + \sum_{\mathbf{n}\neq\mathbf{m}} \phi_{\mathbf{mn}} c^\dagger_{\mathbf{m}\downarrow} c^\dagger_{\mathbf{n}\uparrow} c_{\mathbf{m}\uparrow}\right) e^{i\mathbf{q_o m}}|N\rangle.$$

$$\mathcal{P}_{\mathbf{m}} = 1 - c^\dagger_{\mathbf{m}\uparrow} c_{\mathbf{m}\uparrow}$$

Gutzwiller projection

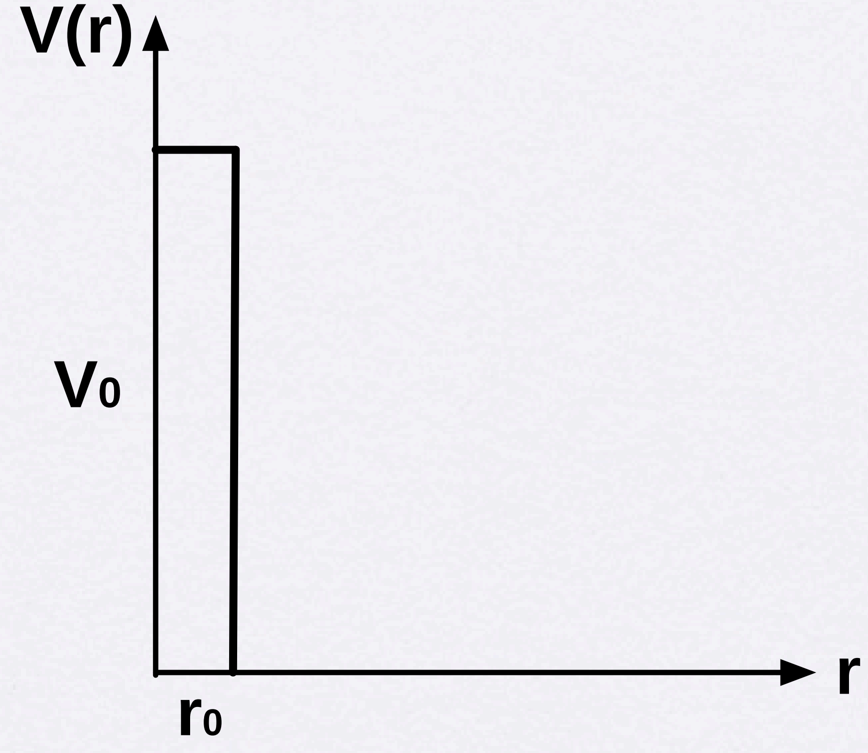
Back-flow correction

Shastry, Krishnamurthy
and Anderson, 41, 2375 (1990)

This variational wave function contains sufficient short-range correlations !!

(II) Applying this method to hard core gas in continuum

$$\hat{H} = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} n_{\mathbf{k}\sigma} + \int \Psi_\uparrow^\dagger(\mathbf{r})\Psi_\downarrow^\dagger(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\Psi(\mathbf{r}')_\downarrow\Psi_\uparrow(\mathbf{r})d\mathbf{r}d\mathbf{r}'$$

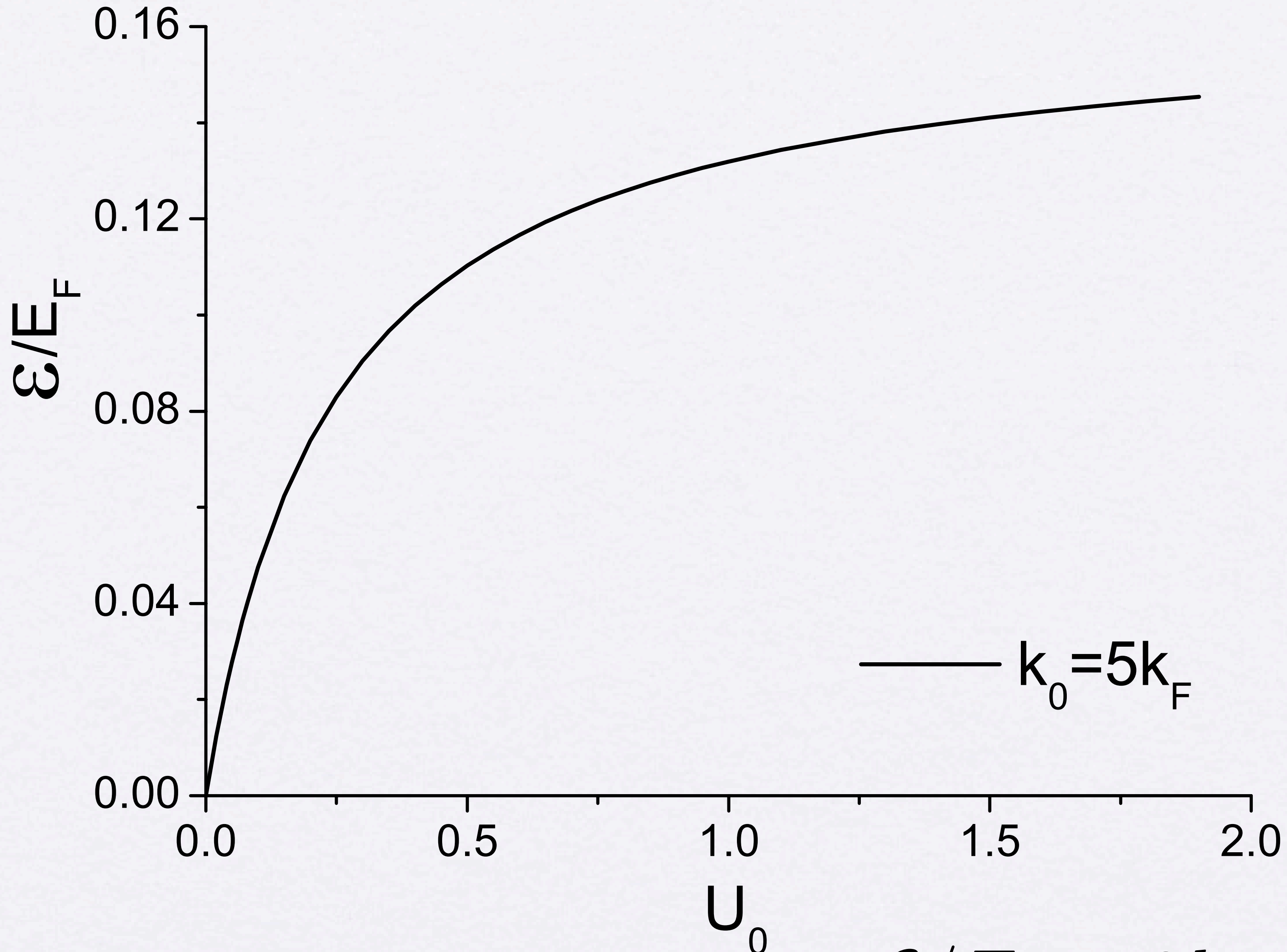


$$a_s < r_0 \ll 1/k_F$$

can never reach the regime $k_F a_s \gg 1$

Applying this method to hard core gas in continuum

$$\delta E = \mathcal{E} - E_{\rm F}$$



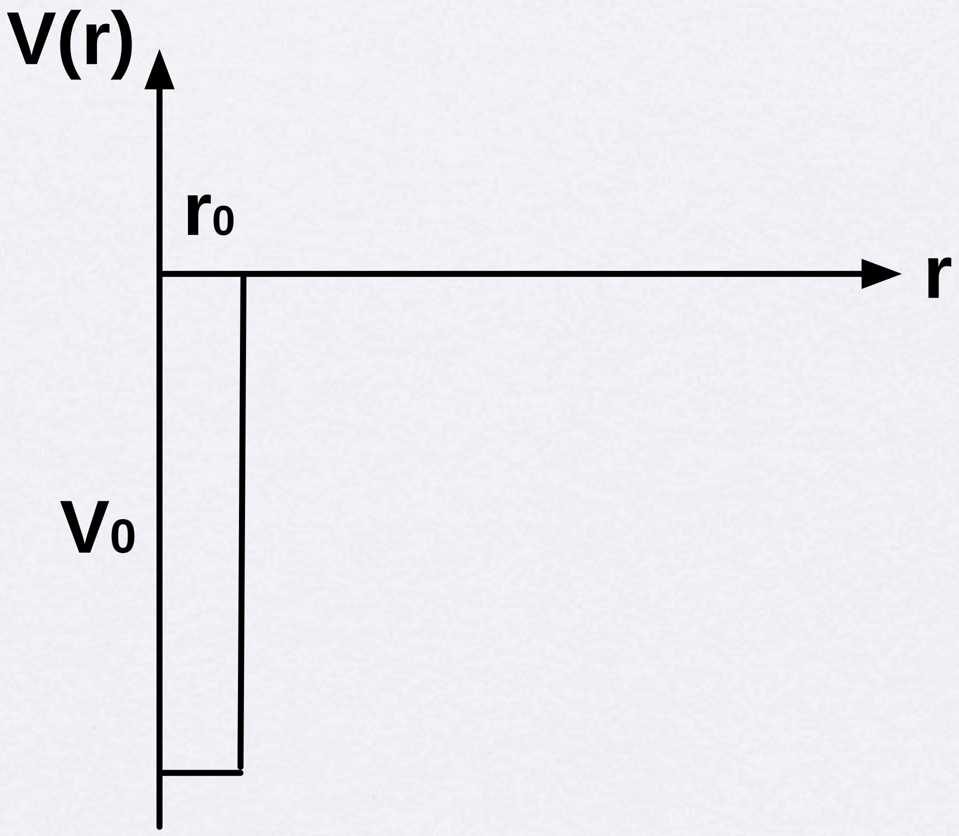
$$U \to +\infty, \qquad \mathcal{E}/E_{\rm F} = 2k_{\rm F}/(3k_0) < 1$$

$$k_0 = 1/r_0$$

no fully magnetized FM !

(III) Applying this method to resonant interacting gas in continuum

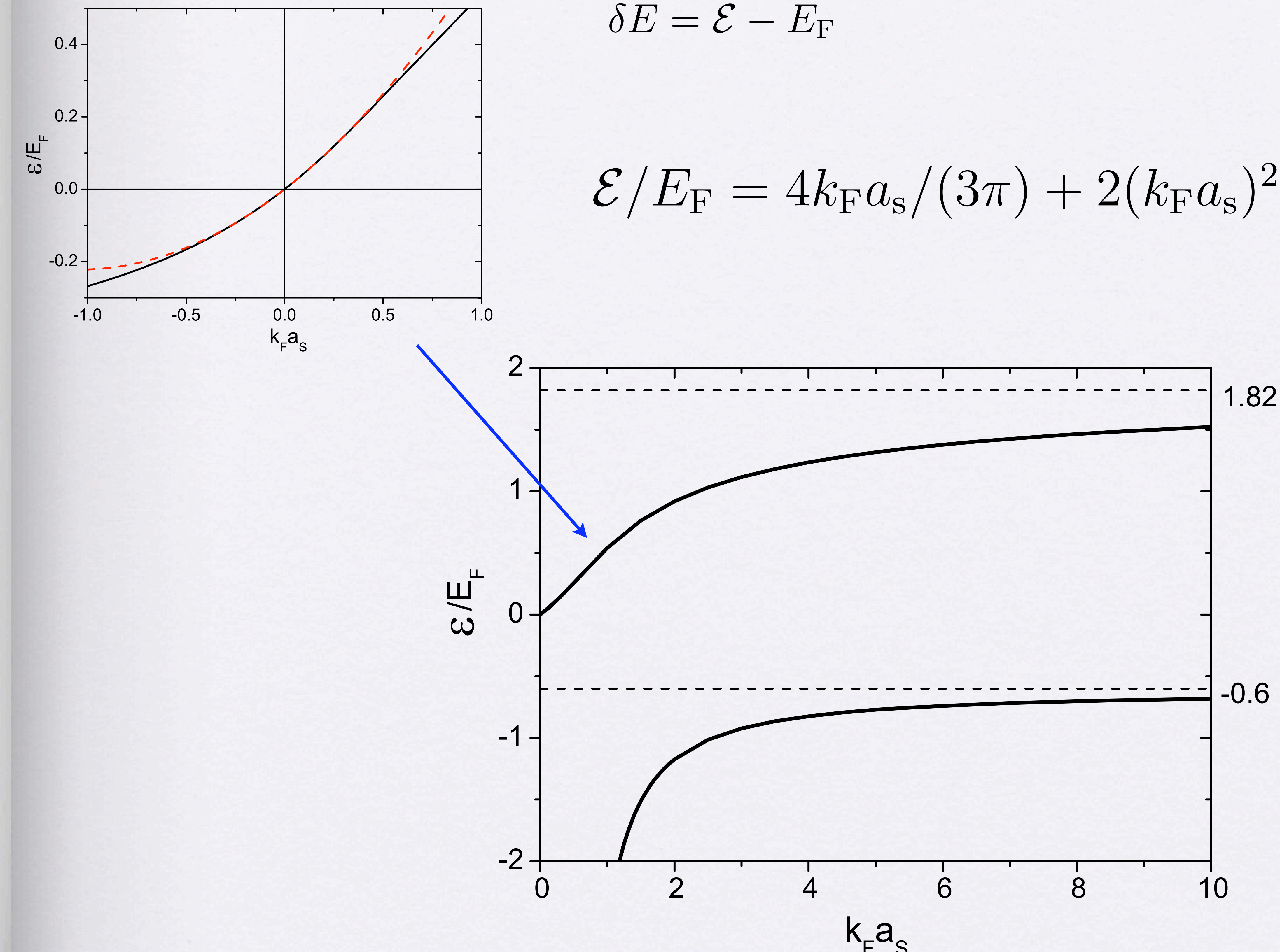
$$\hat{H} = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} n_{\mathbf{k}\sigma} + \int \Psi^{\dagger}_{\uparrow}(\mathbf{r})\Psi^{\dagger}_{\downarrow}(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\Psi(\mathbf{r}')_{\downarrow}\Psi_{\uparrow}(\mathbf{r})d\mathbf{r}d\mathbf{r}'$$



Applying this method to resonant interacting gas in continuum

$$\delta E = \mathcal{E} - E_{\rm F}$$

$$\mathcal{E}/E_{\rm F} = 4k_{\rm F}a_{\rm s}/(3\pi) + 2(k_{\rm F}a_{\rm s})^2/\pi^2$$



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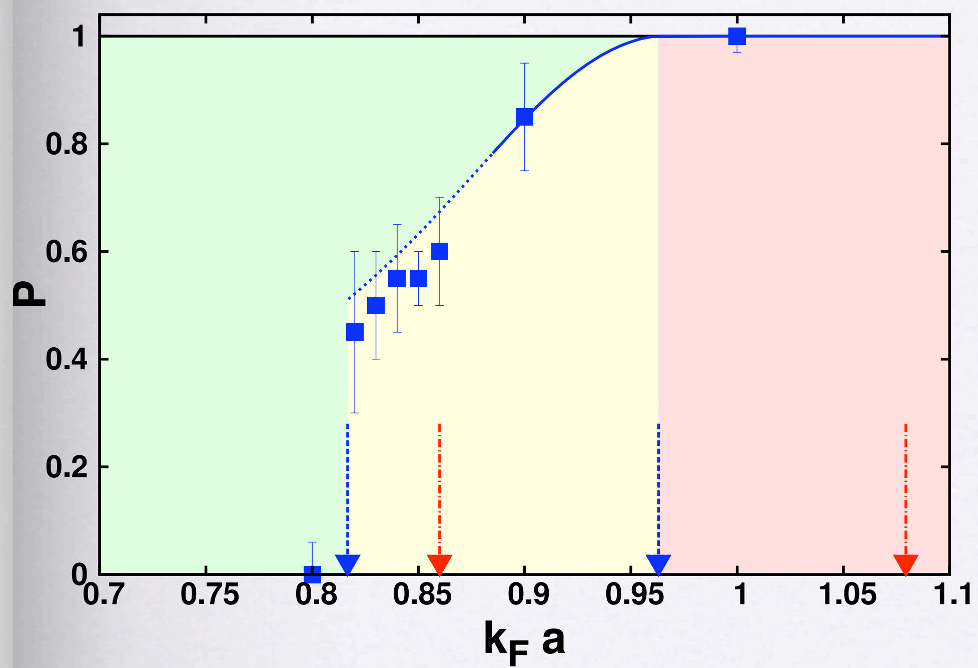
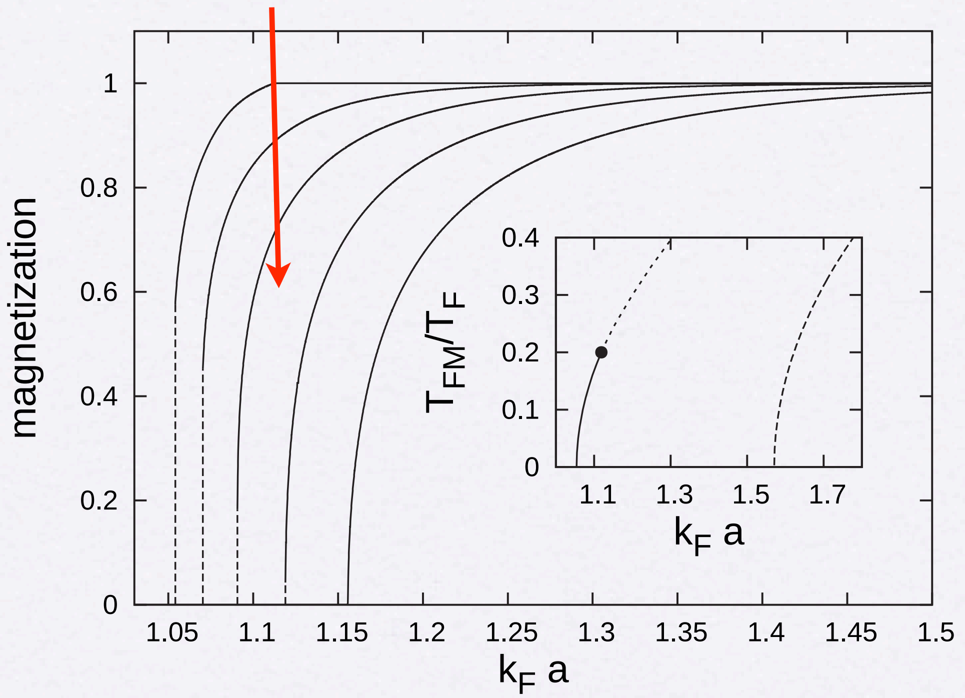


S. Pilati, et al. PRL, 105, 030405 (2010)

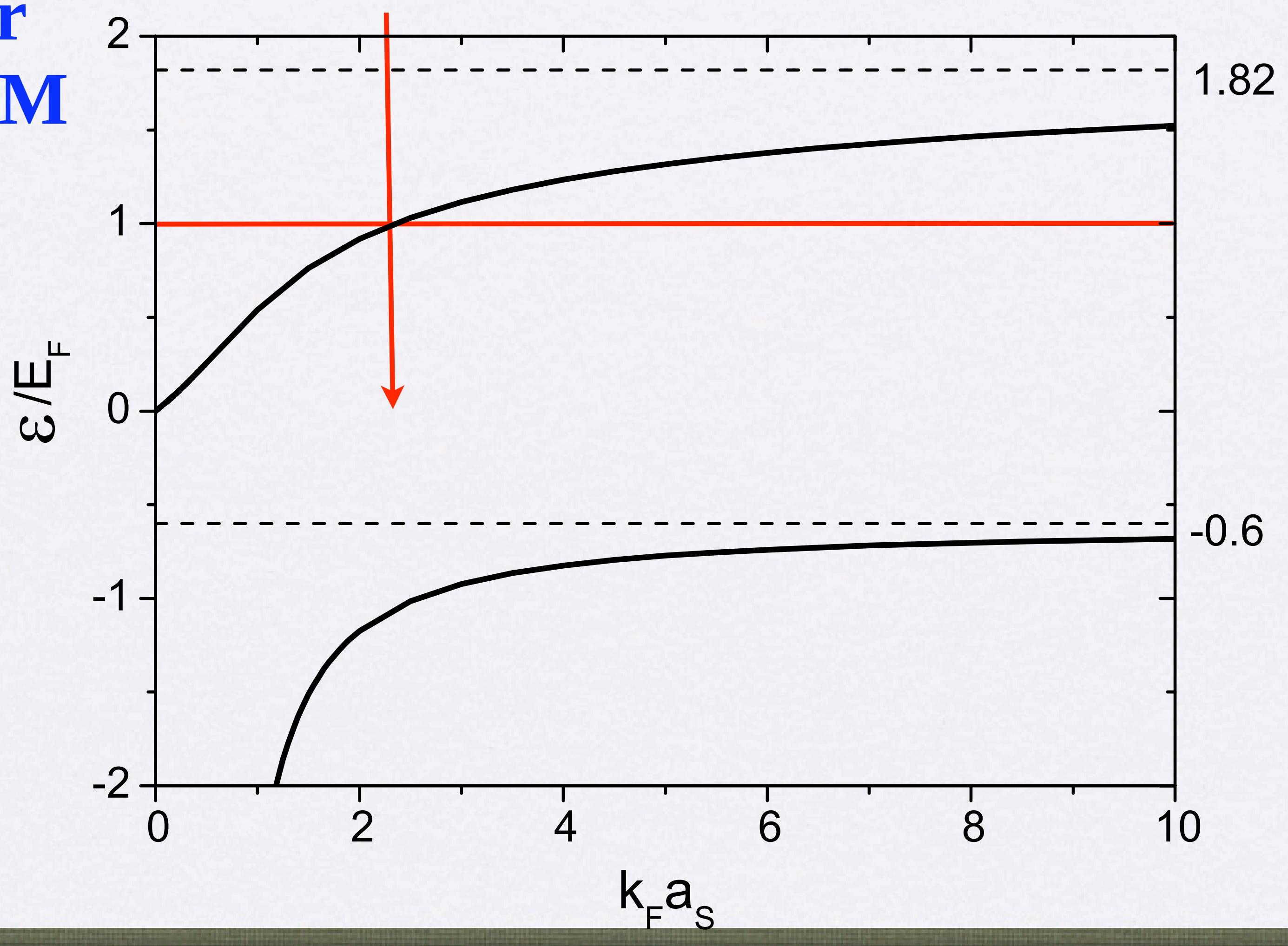
$$\delta E = \mathcal{E} - E_F$$



R.A. Duine and A. H. MacDonald, PRL, 95, 230403 (2005)

2.35 => 1.87

lower bound for fully polarized FM



Summary for this part

From the single impurity atom problem, we learn:

Conclusion 1: For a repulsive potential, both in lattice and in continuum, a fully polarized FM is not stable, in sharp contrast to Stoner’s mean-field results.
(Show important effect of correlation)

Conclusion 2: For a resonance model, in metastable scattering state, FM is possible, but the lower bound we obtained is larger than what obtained from mean-field+perturbation
(Also show substantial effect of correlation)

Ref: Xiao-Ling Cui and HZ, PRA, 81, 041602(R), 2010

Issues for this part :

1. The discrepancy between different approaches

2. Whether the metastability of “ upper branch ” is treated properly; effect of coupling (decay) to molecular branch to ferromagnetism ?

3. We can not rule out more stronger correlation effects can make the system non-ferromagnetic

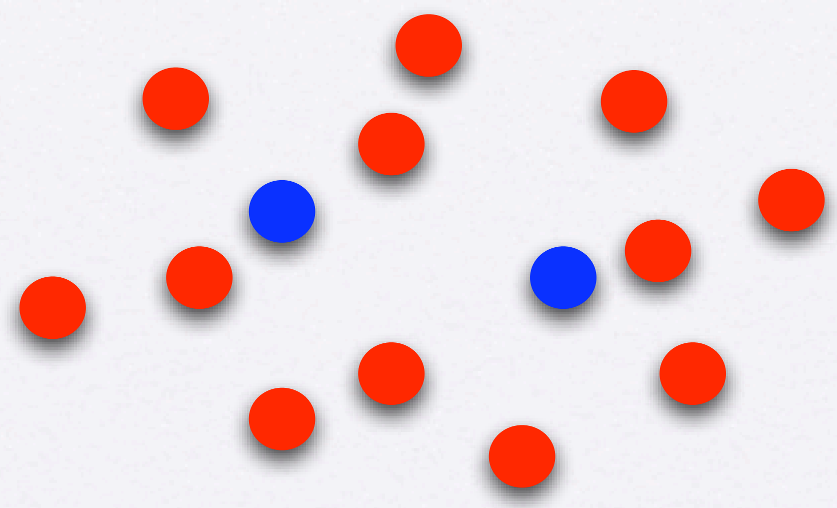
2. Whether a boson-fermion mixture is stable across an inter-species Feshbach resonance?

The requirement for a stable mixture at resonance ?

		small three-body loss rate ==> long enough life time	positive compressibility ==> stand against collapse
2-component Fermion		√	√
Bosons		×	×
Boson -fermion mixture	$n_B \gtrsim n_F$	×	?
	$n_B \ll n_F$	Very likely √	

Stability condition for a boson-fermion mixture:

- bosons
- fermions



new stable mixture at resonance !!

results from weak coupling mean-field theory:

$$k_{\rm F}a_{\rm BB} \geqslant \frac{1}{2\pi}(k_{\rm F}a_{\rm BF})^2\frac{(1+\gamma)^2}{\gamma}$$

$$\gamma = m_{\rm B}/m_{\rm F}$$

Ref: Veverit, Pethick and Smith, PRA, 61, 053605 (2000)

what if $a_{\rm BF} \to \pm\infty$ **?**

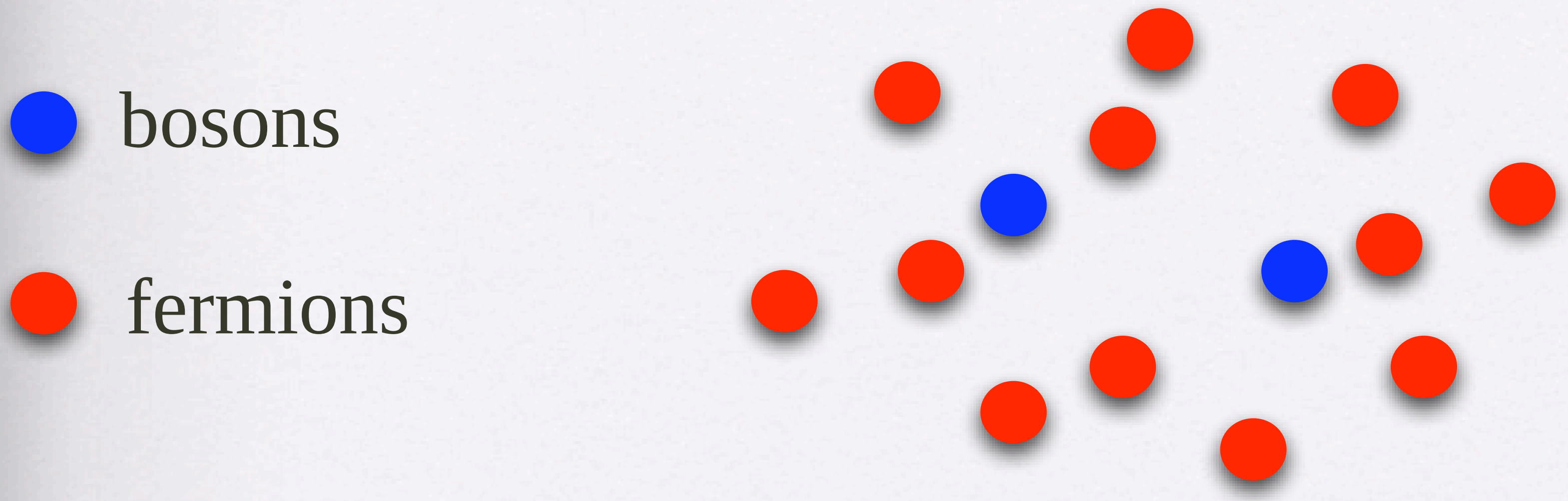
$$k_{\rm F}a_{\rm BB} \geqslant \zeta_{\rm c}$$

universal constant of the order of unity

$$n_{\rm B}/n_{\rm F} \ll 1 \;\Rightarrow\; n_{\rm B}^{1/3}a_{\rm BB} \ll 1 \;\Rightarrow$$

avoid significant loss due to boson-boson interactions

Universal Hypothesis for EoS of polaron condensate



new stable mixture at resonance !!

Boson ==> bosonic polarons ==> polaron condensate

dimensionless parameters in this problem:

$$x = \frac{n_B}{n_F} \qquad \eta = \frac{1}{k_F a_{BF}} \qquad \zeta = k_F a_{BB} \qquad \gamma = \frac{m_B}{m_F}$$

Expand EoS in terms of x:

$$E_{\rm p} = E_{\rm F}^0 \left[\frac{5}{3} A x + \frac{1}{2} F x^2 + \cdots \right]$$

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(i) A is independent of ζ $\qquad A(\eta, \gamma)$ is a universal function

(ii) F is a sum of two parts. $F_0 + F_1$

bare interaction between bosons (F_0) — induced interaction between bosons (F_1)

$F_1(\eta, \gamma)$ is another universal function

Estimation of A with the lowest order constrained variational method

$$|\Psi\rangle = \prod_{ij} f(\mathbf{r}_i^b - \mathbf{r}_j^f) \left(\frac{1}{\sqrt{V}}\right)^{N_B} |\Phi_{FS}\rangle$$

LOCV approximation:

to the first order of $h(r) \equiv f^2(r) - 1$

Pandharipande and Bethe, PRC, 7, 1212 (1973)

give an estimation of energy up to the first order of x

$$E_{\mathrm{p}} = n_{\mathrm{B}} n_{\mathrm{F}} \int \mathrm{d}^3\mathbf{r}\, f(\mathbf{r}) \left[-\frac{\nabla_{\mathbf{r}}^2}{2m_{\mathrm{r}}} + U_{\mathrm{BF}}(\mathbf{r}) \right] f(\mathbf{r})$$

$$(-\tfrac{1}{2m_{\mathrm{r}}} \tfrac{d^2}{dr^2} + U_{\mathrm{BF}}(r)) r f(r) = \lambda r f(r)$$

$$4\pi n_{\mathrm{F}} \textstyle\int_0^d \mathrm{d}r\, r^2 |f(r)|^2 = 1$$

$$\left.\frac{(rf)'}{rf}\right|_{r=0} = -\frac{1}{a_{\mathrm{BF}}} \quad f(d) = 1 \quad f(r)'|_{r=d} = 0$$

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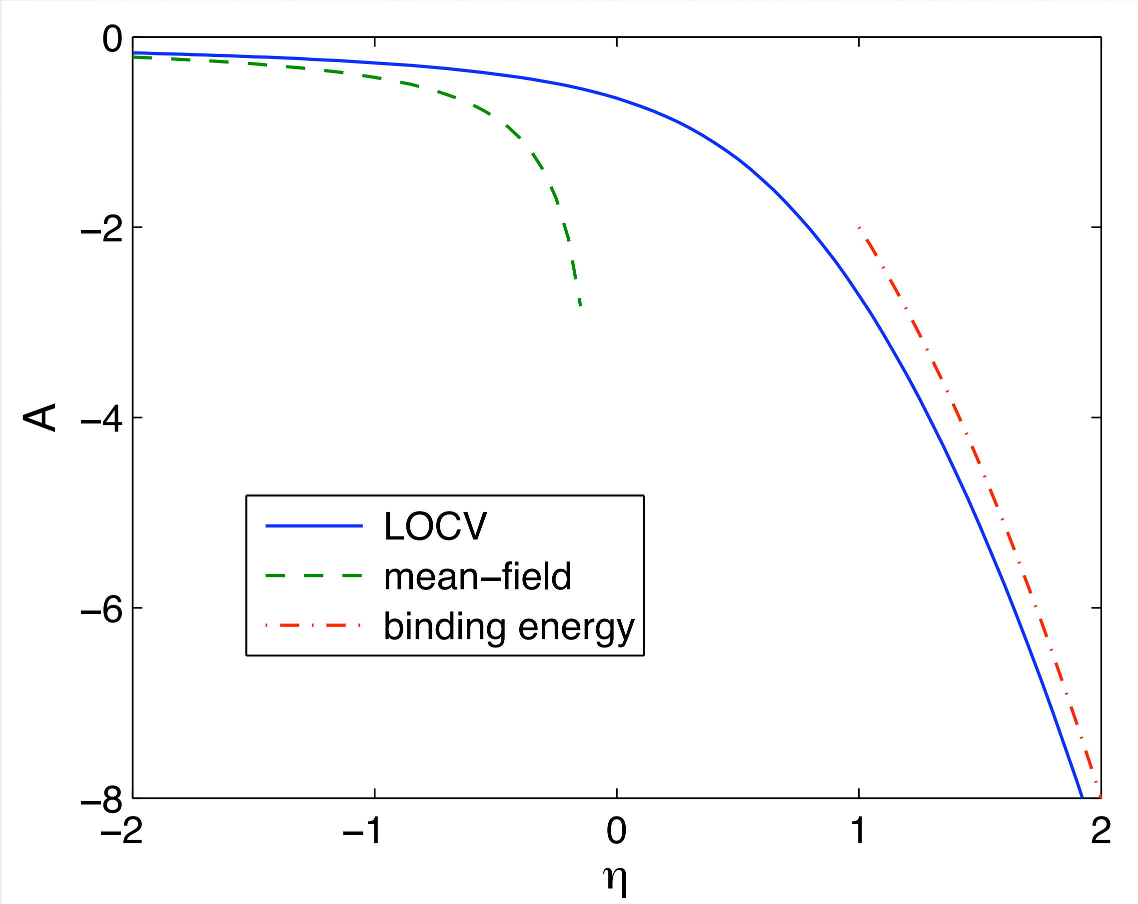

$$A(\eta, \gamma) = \frac{1+\gamma}{2\gamma} A(\eta, \gamma = 1)$$

At resonance:

$$A(\eta = 0, \gamma = 1) = -0.64$$

The Fermi liquid parameter A, m* can be obtained from single impurity atom problem

Variational wave function approach:

$$|\Psi\rangle = \left(\phi_0 c^\dagger_{\mathbf{q_0}\downarrow} + \sum_{\mathbf{k}>\mathbf{k_F},\mathbf{q}<\mathbf{k_F}} \phi_{\mathbf{kq}} c^\dagger_{\mathbf{q_0}+\mathbf{q}-\mathbf{k}\downarrow} c^\dagger_{\mathbf{k}\uparrow} u_{\mathbf{q}\uparrow}\right)|N\rangle$$

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Induced Interactions

$$\frac{1}{2}F_1 x^2 E_{\mathrm{F}}^0 = -\frac{1}{2}\left(\frac{\partial \mu_{\mathrm{B}}}{\partial n_{\mathrm{F}}}\right)^2 \left(\frac{\partial n_{\mathrm{F}}}{\partial \mu_{\mathrm{F}}}\right) n_{\mathrm{B}}^2.$$

$$\frac{\partial \mu_b}{\partial n_f} = \frac{2\pi^2}{m_f k_F}\left(A(\eta,\gamma) - \frac{1}{2}\eta \frac{\partial A(\eta,\gamma)}{\partial \eta}\right)$$

$$\frac{\partial n_f}{\partial \mu_f} = \frac{m_f k_F}{2\pi^2}$$

$$F_1(\eta,\gamma) = -\frac{5(1+\gamma)^2}{18\gamma^2}\left(A(\eta) - \frac{1}{2}\eta\frac{\partial A(\eta)}{\partial \eta}\right)^2$$

Stability

Reminder:

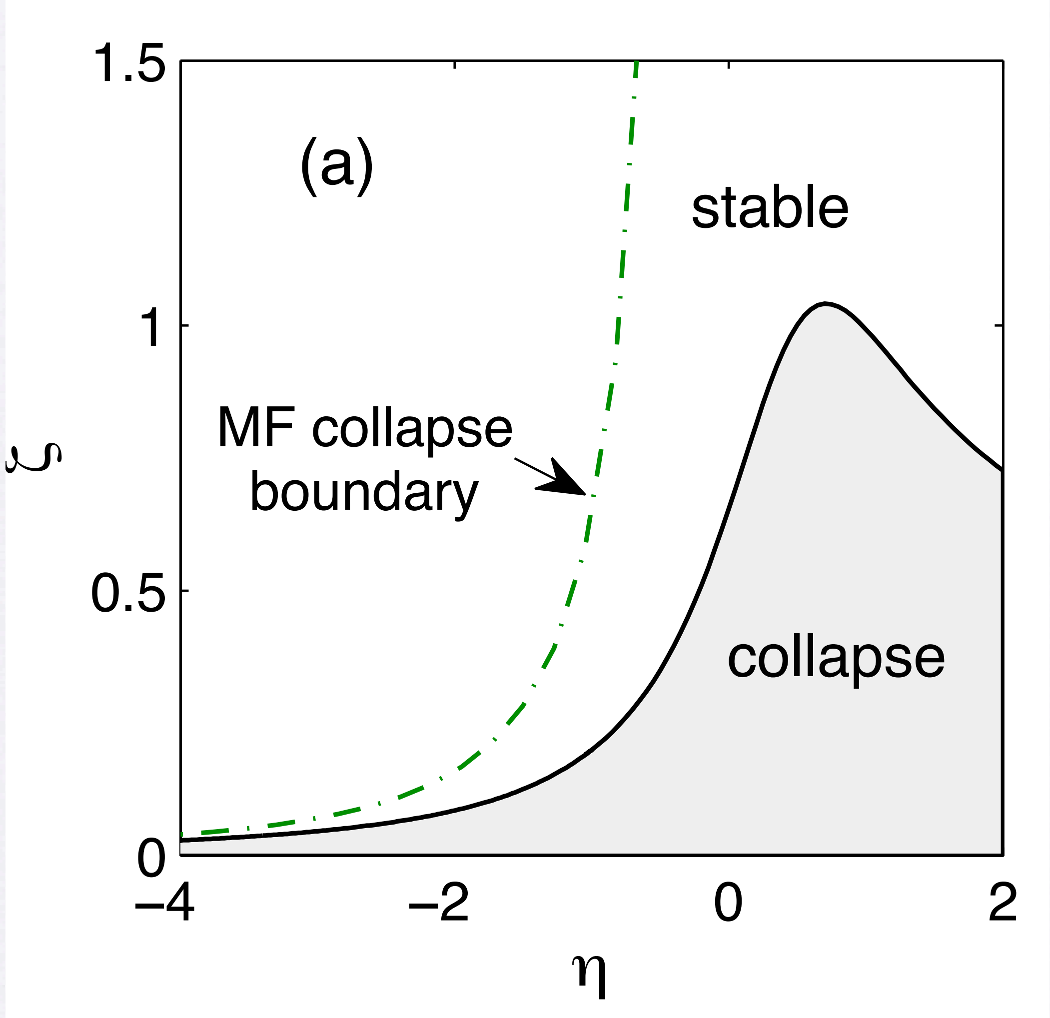
$$E_{\rm p} = E_{\rm F}^0 \left[\frac{5}{3} A x + \frac{1}{2} F x^2 + \cdots \right]$$

$$F_0 + F_1 \geqslant 0$$

$$\zeta \geqslant \zeta_c = -\frac{9\pi\gamma}{20} F_1(\eta, 1)$$

$$F_0 = \frac{20\zeta}{9\pi\gamma}$$

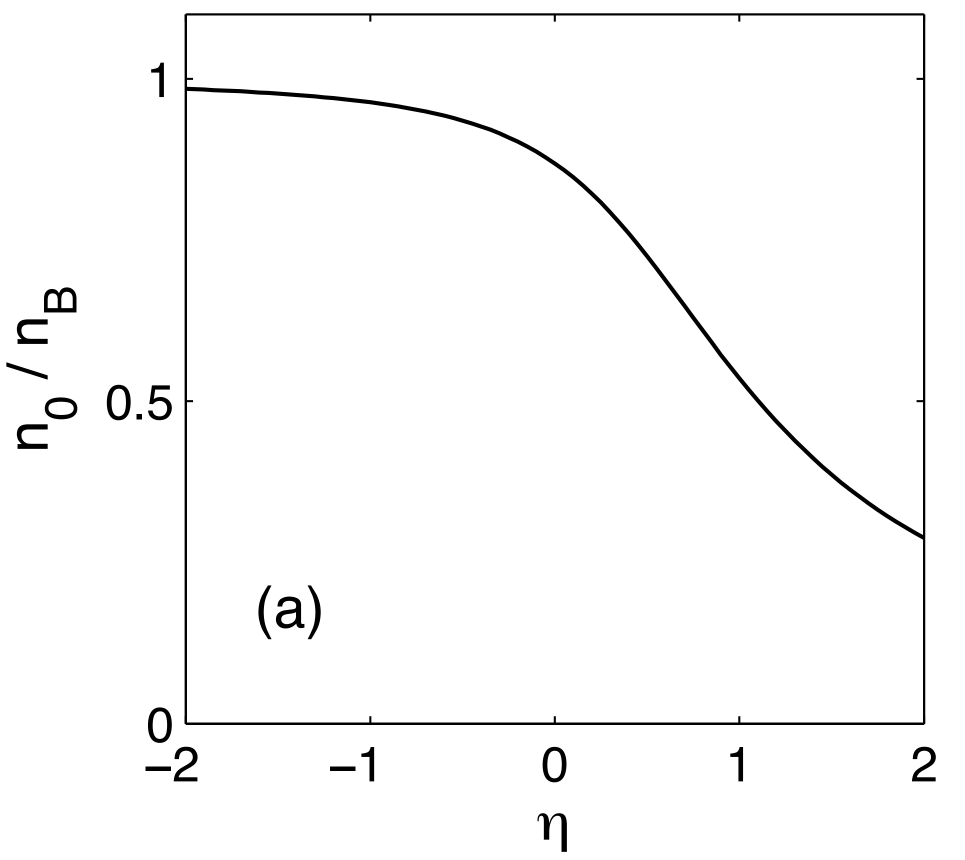
$$\zeta = k_F a_{BB}$$



Condensate Properties

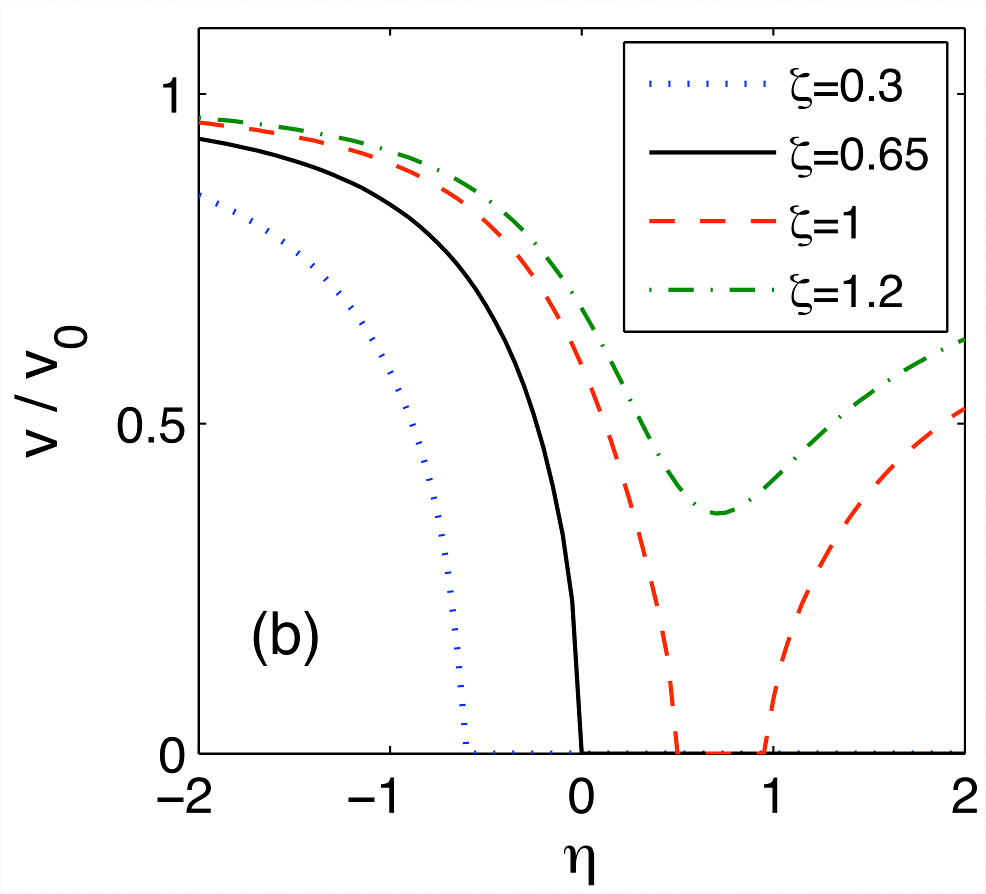
condensate fraction

$$\frac{n_0}{n_B} = 1 - n_F \int d^3\mathbf{r}\,[f(\mathbf{r}) - 1]^2$$



critical velocity

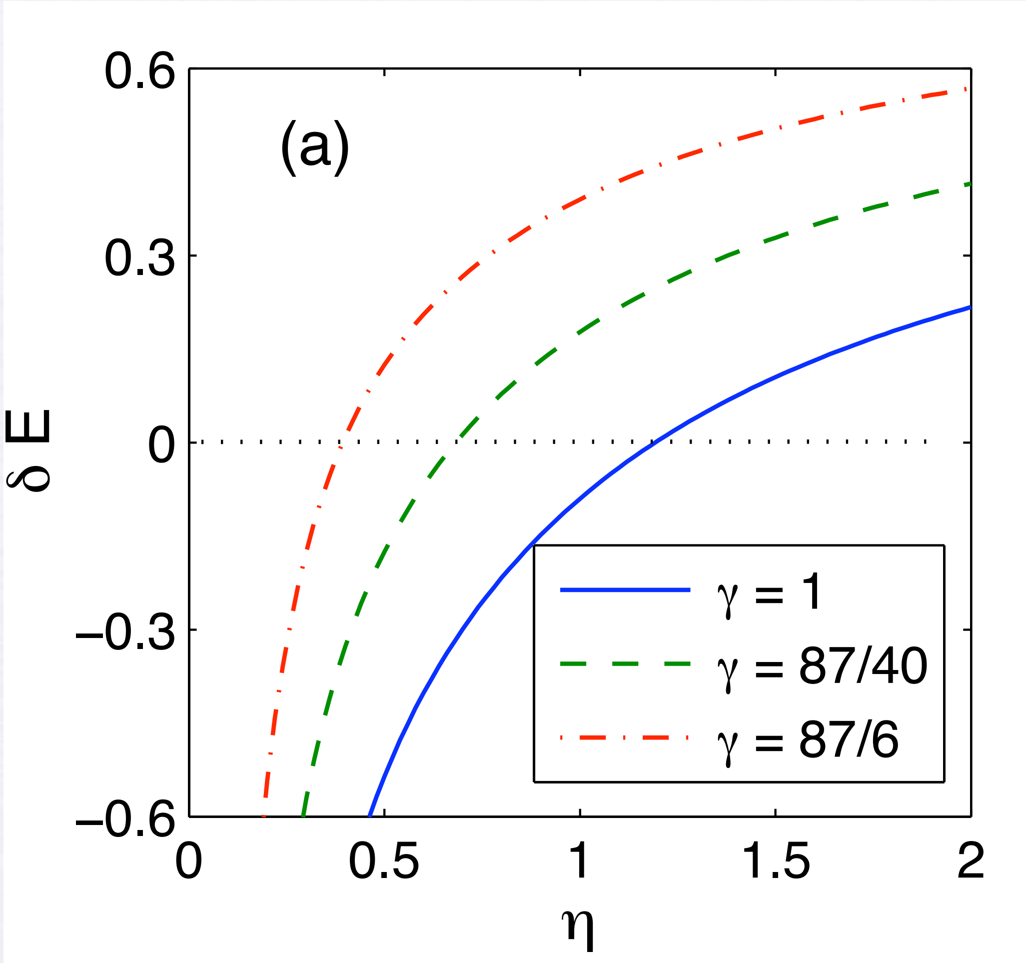
$$\frac{v}{v_0} = \sqrt{\frac{F_0 + F_1}{F_0}}$$



Polaron-to-molecule transition

$$\frac{E_m}{V} = E_F^0 \left[(1-x)^{5/3} + \frac{1}{1+\gamma} x^{5/3} - \frac{5(1+\gamma)\eta^2}{3\gamma} x + \frac{10(2+\gamma)}{9\pi(1+\gamma)\eta} \frac{a_{mf}}{a_{bf}} x(1-x) \right]$$

$$\frac{E_p}{V} = E_F^0 \left[1 + \frac{5}{3} A x + \frac{1}{2} F x^2 \right]$$



$$\delta E = \frac{E_p}{V} - \frac{E_m}{V}$$

Summary for this part

From the single impurity atom problem, we determine:

1. Stability condition for a boson-fermion mixture across a FR

2. Properties of a polaron condensate, such as condensate fraction and critical velocity

Ref: Zeng-Qiang Yu, Shizhong Zhang, HZ, to be submitted

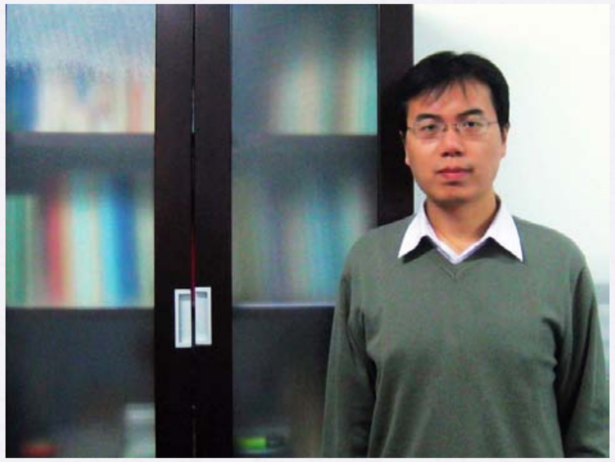
Issues for this part:

1. details of the phase transition:

condensate + 1 FS ==> no condensate + 2 FS

2. finite temperature part of the phase diagram

Thanks to my collaborates



Xiao-Ling Cui (Tsinghua)

Zeng-Qiang Yu (Tsinghua)

Shizhong Zhang (Ohio State)

Thank all of you for your attention !