Higgs bound states and heavy solitons of Bose gases in optical lattices

— Designing different kinds of superfluid —

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Outline:

1. Introduction:
   Strongly correlated superfluids in optical lattices

2. Higgs bound states in a single-component Bose gas

T. Nakayama, I. Danshita, T. Nikuni, & S. Tsuchiya, arXiv:1503.01516 (2015)

3. Heavy solitary waves in a two-component Bose gas

Y. Kato, D. Yamamoto, & I. Danshita, Phys. Rev. Lett. 112, 055301 (2014)
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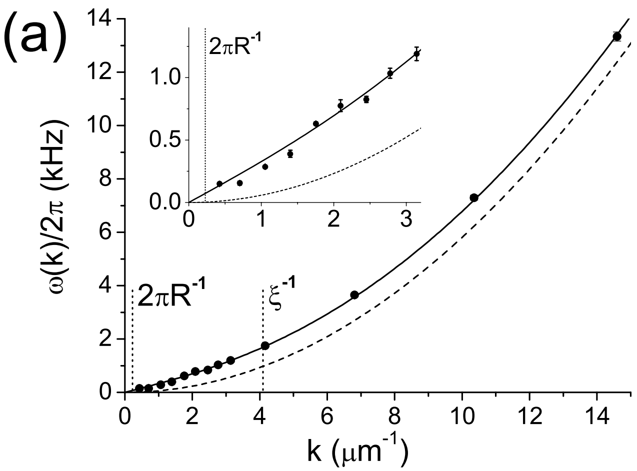
1.1. Schrödinger equation with cubic nonlinearity

Gross-Pitaevskii (GP) equation:

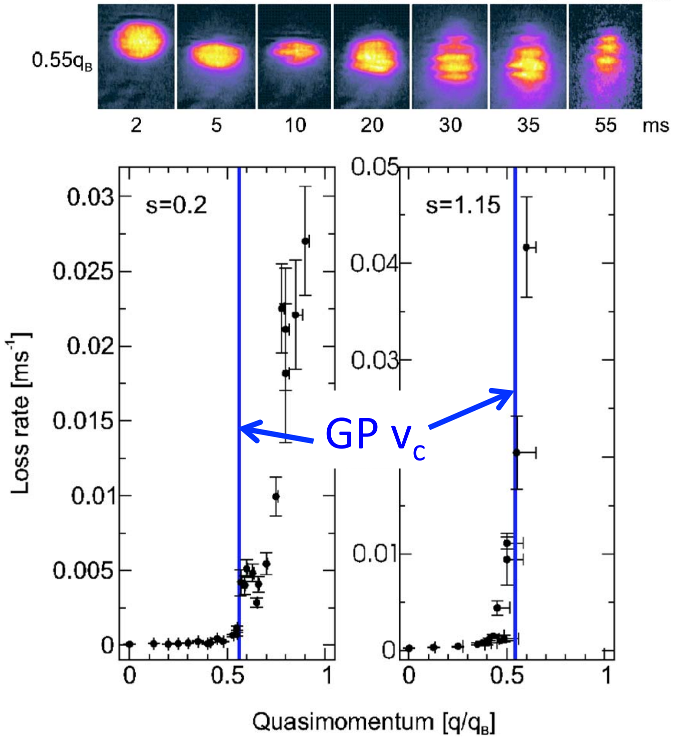
$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[-\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{r},t) - \mu + \boxed{u}|\psi(\mathbf{r},t)|^2\right]\psi(\mathbf{r},t)$$

Coupling constant for the two body contact interaction: $u = \frac{4\pi\hbar^2 \underline{\underline{a_s}}}{m}$ s-wave scattering length

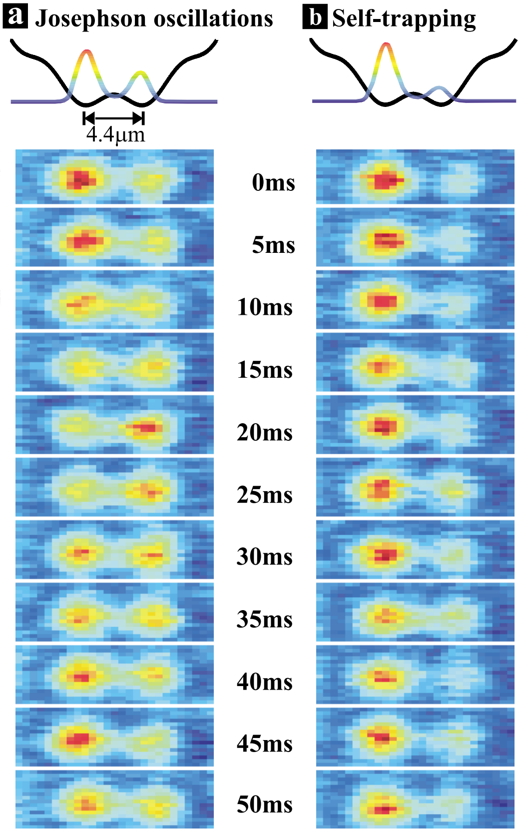
The system of atomic **weakly-interacting** BECs at T<<Tc is well described by this simple equation of motion, such as ground states, excited states, and non-equilibrium dynamics.



Bogoliubov spectrum. Rehovot: Steinhauer et al., PRL (2002)



Critical velocity in an optical lattice. Florence: De Sarlo et al., PRA (2005)

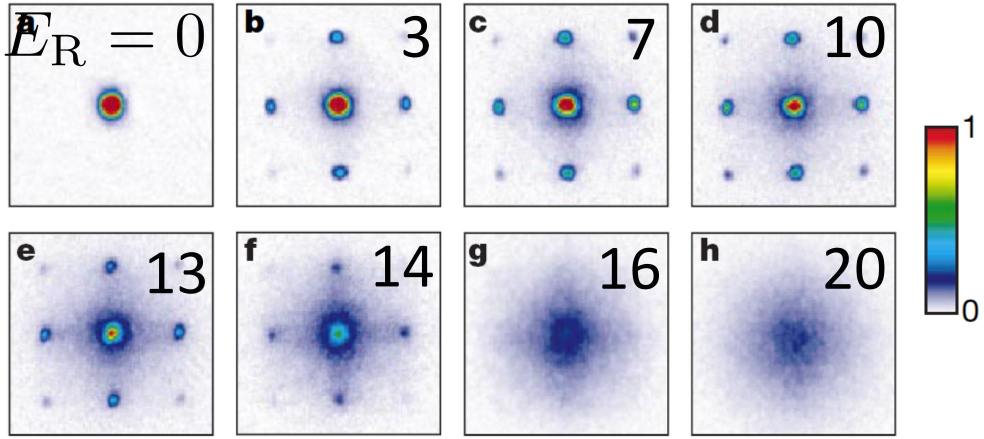


Josephson effects. Heidelberg: Albiez et al., PRL (2005)

1.2. Superfluid (SF)-Mott insulator (MI) transition of Bose gases in optical lattices

Increase the lattice depth → Transition to the Mott insulator

Lattice depth: $V_0/E_R = 0$



Greiner et al., Nature (2002)

Recoil energy:

$$E_R = \frac{\hbar^2\pi^2}{2md^2}$$

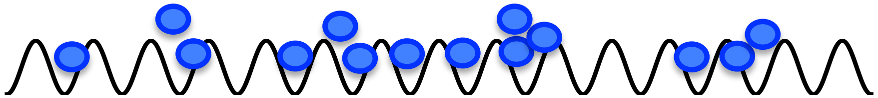
Atomic species:

^{87}Rb

Lattice shape:
Cubic

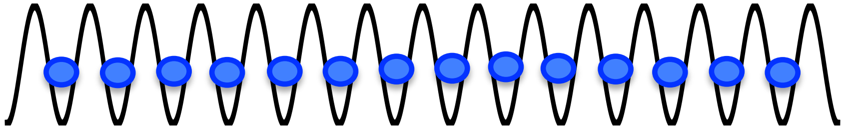
Shallow lattice → Superfluid

Particles are delocalized !!



Deep lattice → Mott insulator

Particles are localized !!



- Quantum phase transitions
- ***Superfluidity in a strongly interacting regime***

1.3. Designing SF equations of motion with optical lattices

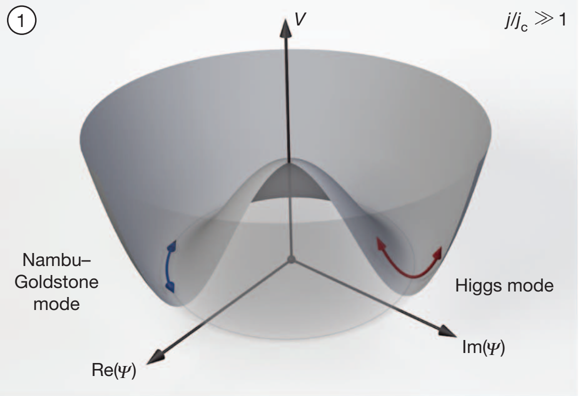
① Near the tips of the Mott lobes ●

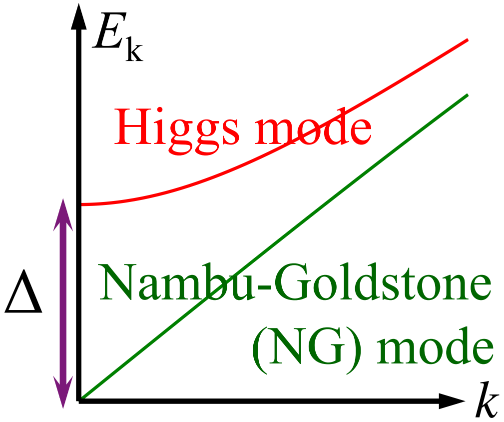
Klein-Gordon equation with cubic-nonlinearity:

$$\underline{-\hbar^2 W \frac{\partial^2}{\partial t^2}}\psi = \left[-\frac{\hbar^2}{2m_*}\nabla^2 - r + u|\psi|^2\right]\psi$$

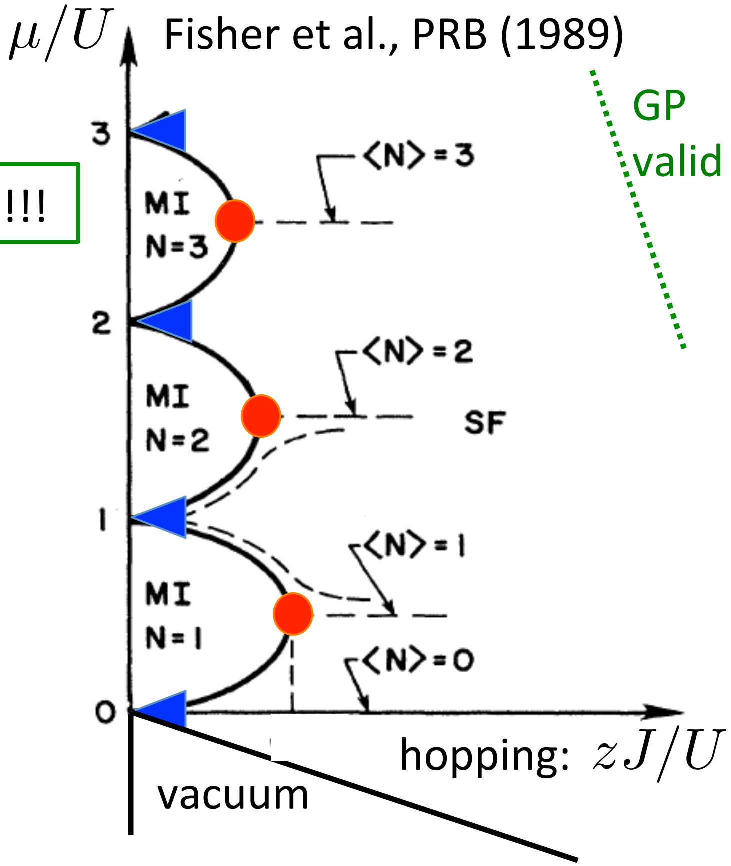
Notice the difference from the Gross-Pitaevskii eq. !!!

“Higgs” amplitude mode,
Altman & Auerbach, PRL (2002)





Ground-state phase diagram
of the Bose-Hubbard model
Fisher et al., PRB (1989)



② Hardcore boson region ◀

Discrete Landau-Lifshitz equation with no damping:

$$i\hbar\frac{d}{dt}\psi_j = -2J\left(\frac{1}{2} - n_j\right)\sum_{\langle l\rangle_j}\psi_l - \mu_0\psi_j$$

Different solitary waves
Barakrishnan et al., PRL (2009)
Demler & Maltsev, Ann. Phys. (2011)

1.4. What we do here

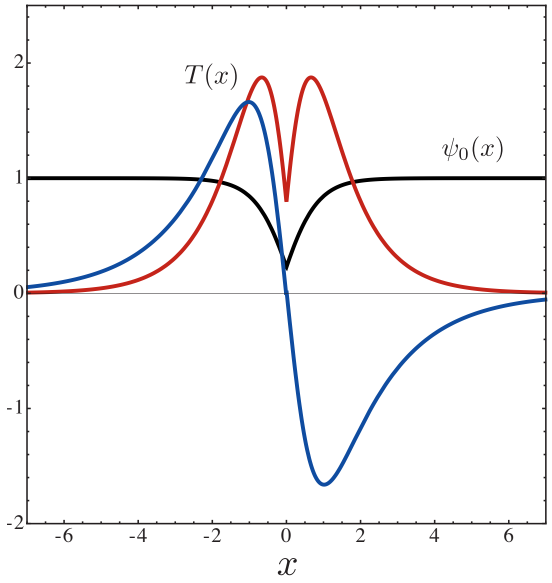
The strong correlations in optical-lattice systems can be useful for designing SF equations of motion in various forms.

Specifically, we study

◇ Effects of potential barriers on the relativistic SF, especially the Higgs modes

$$i\hbar \underline{v_K(\mathbf{x})} \frac{\partial\psi}{\partial t} - \hbar^2 W_0 \frac{\partial^2\psi}{\partial t^2} = \left(-\frac{\hbar^2\nabla^2}{2m_*} + r_0 + \underline{v_r(\mathbf{x})} + u_0|\psi|^2\right)\psi$$

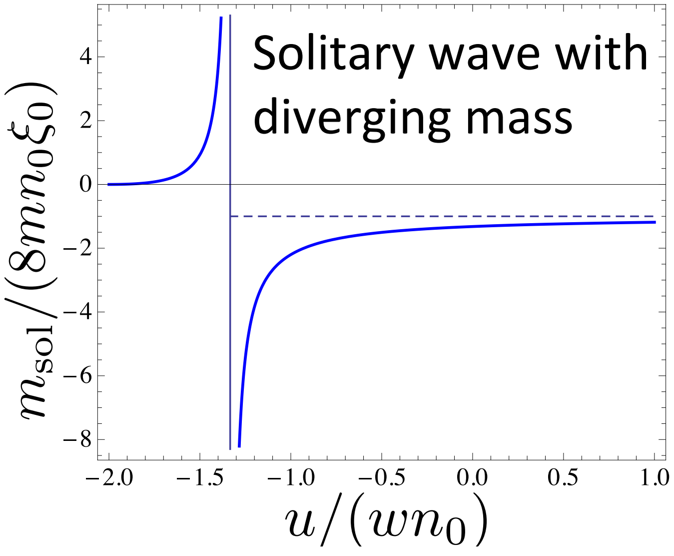
Higgs bound states



◇ Solitary waves of SF obeying NLSE with cubic and quintic nonlinearity

$$i\hbar\frac{\partial}{\partial t}\psi = \left[-\frac{\hbar^2\nabla^2}{2m_*} + V - \mu + u|\psi|^2 + \boxed{w|\psi|^4}\right]\psi$$

(more precisely, its two-component version)


Solitary wave with diverging mass

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2.1. Higgs modes in condensed matter physics

Experiments on Higgs modes:

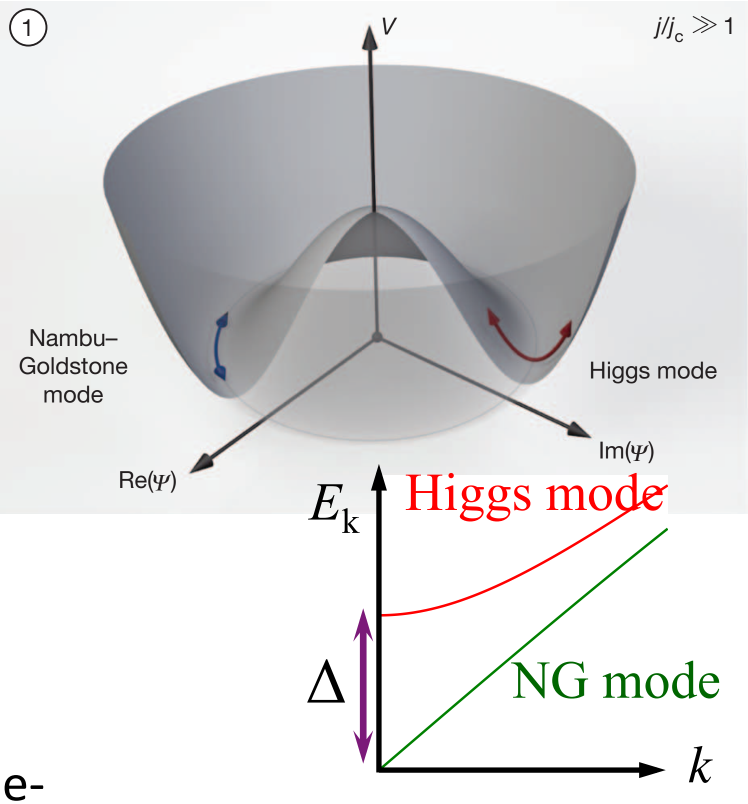
◇ Quantum magnets; Rüegg *et al.*, PRL (2008)

◇ Superconductors; Matsunaga *et al.*, PRL (2013).

◇ Charge density wave materials;
Yusupov *et al.*, Nat. Phys. (2010).

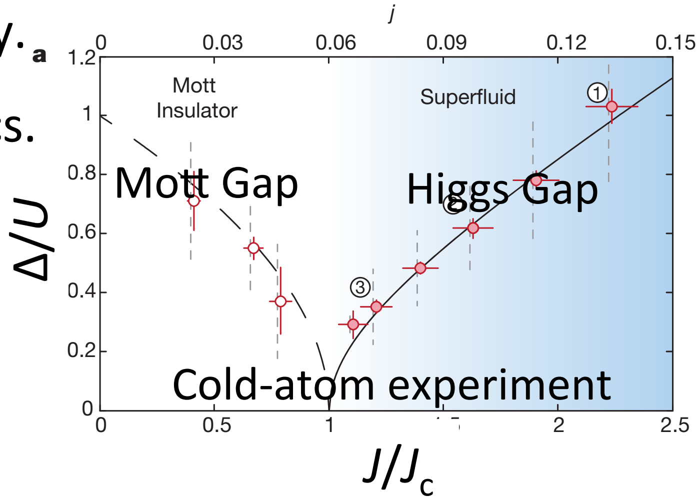
◇ Superfluid ^{3}He-*B*; Collett *et al.*, JLTP (2013)

◇ Superfluid Bose gases in optical lattices;
Endres *et al.*, Nature (2012).



Higgs modes are interesting because …

- Ubiquitous collective mode in systems with particle-hole symmetry and breaking of continuous symmetry.
- Analogous to the Higgs particle in high energy physics.
- Low-energy mode playing a crucial role in the vicinity of quantum phase transitions.
- Smoking gun of the “relativistic” SF.



2.2. Bose gases in optical lattices

Bose-Hubbard model:

$$\hat{H} = -J \sum_{\langle j,l \rangle} (\hat{b}_j^\dagger \hat{b}_l + \hat{b}_l^\dagger \hat{b}_j) + \frac{U}{2} \sum_j \hat{n}_j (\hat{n}_j - 1) - \mu \sum_j \hat{n}_j$$

J: hopping, *U*: onsite interaction, μ: chemical potential

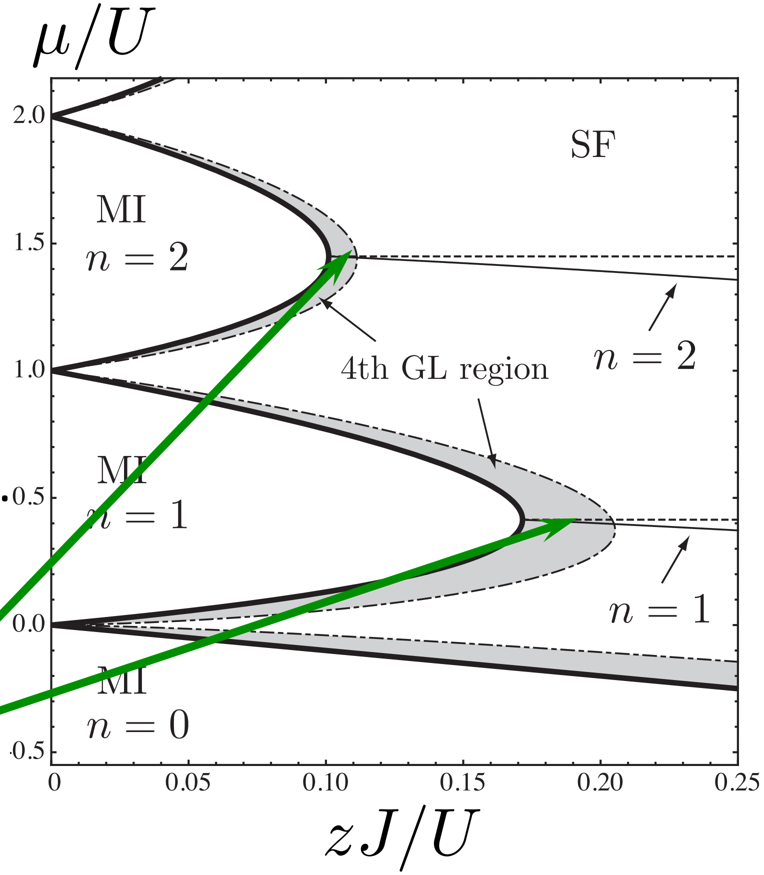
Near
SF-MI
transition

Time-dependent Ginzburg-Landau (TDGL) equation:
(See, e.g. Sachdev "Quantum Phase Transitions")

$$iK \frac{\partial}{\partial t} \psi - W \frac{\partial^2}{\partial t^2} \psi = \left[-\frac{\nabla^2}{2m_*} + r + u|\psi|^2 \right] \psi$$

All the coefficients *K*, *W*, m_*, *r*, u can be explicitly expressed by the original Bose-Hubbard parameters.

We set $\hbar = 1$.



When *K*=0 (dashed line), TDGL eq. is particle-hole (p-h) symmetric, i.e. symmetric w.r.t. $\psi \leftrightarrow \psi^*$.

2.3. Collective modes in a homogeneous system

Varma, JLTP (2002)

When *K*=0, $i\cancel{K\frac{\partial}{\partial t}}\psi - W\frac{\partial^2}{\partial t^2}\psi = \left[-\frac{\nabla^2}{2m_*} + r + u|\psi|^2\right]\psi$

$$\psi(\mathbf{x},t) = \underline{\psi_0} + \underline{\mathcal{U}(\mathbf{x})e^{-i\omega t} + \mathcal{V}^*(\mathbf{x})e^{i\omega^* t}}$$

Static value

Small fluctuations

Linearize the TDGL eq. w.r.t. the fluctuations.

Eq. for the static order parameter: $(r + u|\psi_0|^2)\psi_0 = 0$

Eq. for the NG phase mode: $\left(-\frac{\nabla^2}{2m_*} + r + u|\psi_0|^2\right)S(\mathbf{x}) = W\omega^2 S(\mathbf{x})$

Eq. for the Higgs amplitude mode: $\left(-\frac{\nabla^2}{2m_*} + r + 3u|\psi_0|^2\right)T(\mathbf{x}) = W\omega^2 T(\mathbf{x})$

where $S(\mathbf{x}) = \mathcal{U}(\mathbf{x}) - \mathcal{V}(\mathbf{x}) \propto \delta\theta(\mathbf{x}),\ T(\mathbf{x}) = \mathcal{U}(\mathbf{x}) + \mathcal{V}(\mathbf{x}) \propto \delta n(\mathbf{x}),$

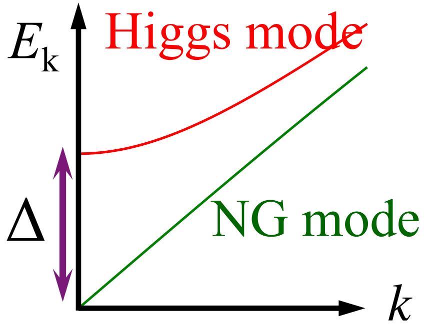
$|\psi_0|^2 = -r/u,$ and assume the plain wave solutions $S(\mathbf{x}), T(\mathbf{x}) \sim e^{i\mathbf{k}\cdot\mathbf{x}}$

Dispersion of the NG mode: $\omega^2 = (ck)^2$

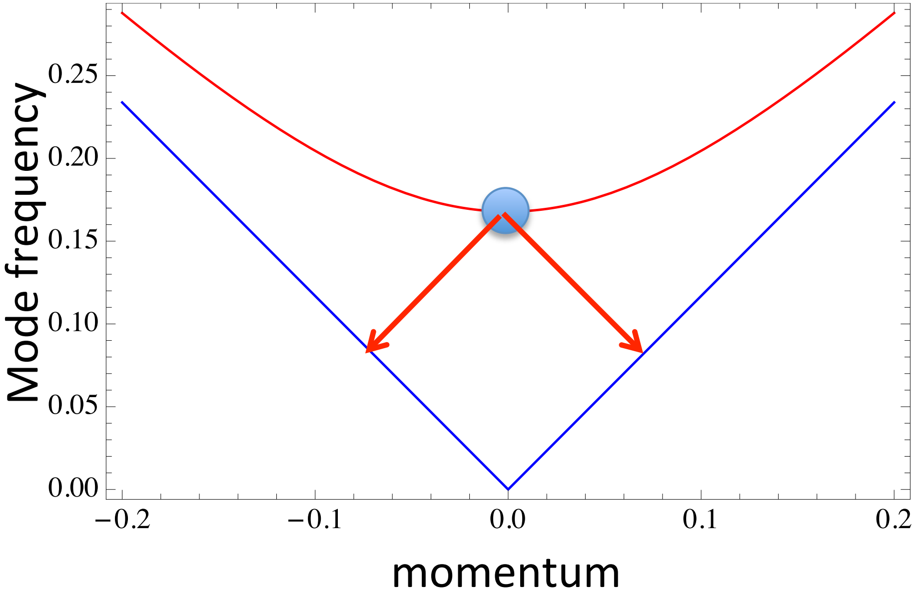
Dispersion of the Higgs mode: $\omega^2 = (ck)^2 + \Delta^2$

$c = \sqrt{1/(2m_* W)},\ \Delta = \sqrt{-2r/W}$

Note $r = 0$ at the Mott transition



2.4. Beliaev decay of the Higgs mode into NG modes



Decay rate of the Higgs mode:

Altman & Auerbach, PRL (2002)

$$\frac{\Gamma}{\Delta} \sim |\bar{U}_{\mathrm{c}} - \bar{U}|^{\frac{D-3}{2}}$$

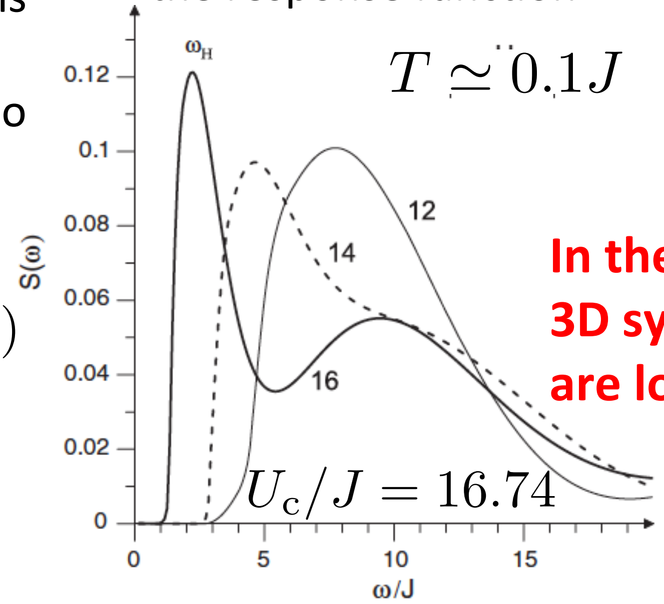
When D<3, the Higgs mode is overdamped near the critical point. Thus, it is naively expected that long-lived Higgs modes are not present in **2D**.

However, recent QMC simulations found the peak corresponding to the Higgs mode in the response to the hopping vibration:

$$\hat{V}(t) = -A_J \cos(\omega t) \sum_{\langle j,l \rangle} (\hat{b}_j^{\dagger} \hat{b}_l + \hat{b}_l^{\dagger} \hat{b}_j)$$

Pollet & Prokof’ev, PRL (2012)

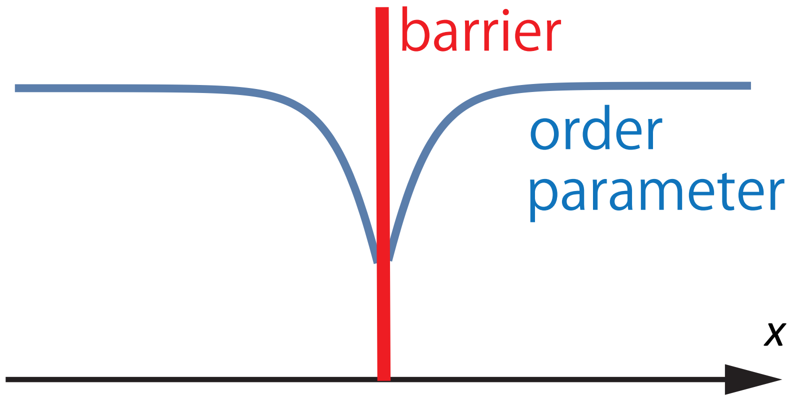
Imaginary part of the response function



See also,
Podolsky et al., PRB (2011)
Gazit et al., PRL (2013)
Chen et al., PRL (2013)
Rancon & Dupuis, PRA (2014)

In the following, we assume 3D system, where Higgs modes are long-lived.

2.5. Effects of potential barriers



- Materials are much dirtier than the universe.

- A single potential barrier is one of the simplest disorder.

- It can be created in cold-atom experiments in a well-controlled manner.

2.5. Effects of potential barriers

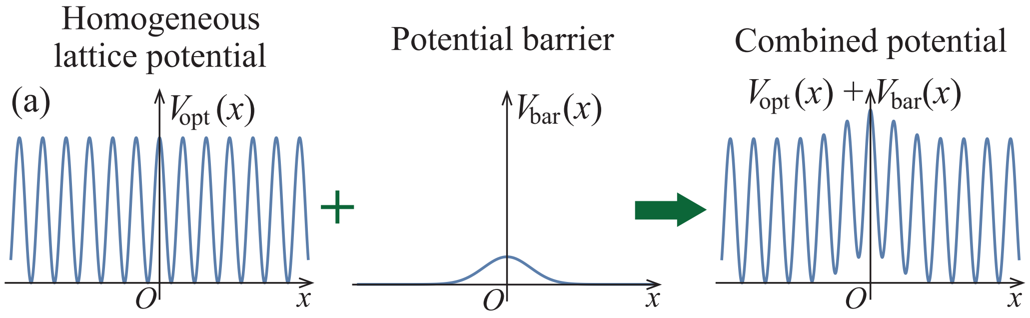
We consider potential barriers that are present only in the x direction.
We assume that *K*=0 far from potential barriers.

(a) Local modulation of the chemical potential:

$$\mu_{i_x} = \mu_0 - V_{i_x}$$

$$K(x) \simeq -2WV(x) \equiv v_K(x)$$

which breaks the p-h symmetry.

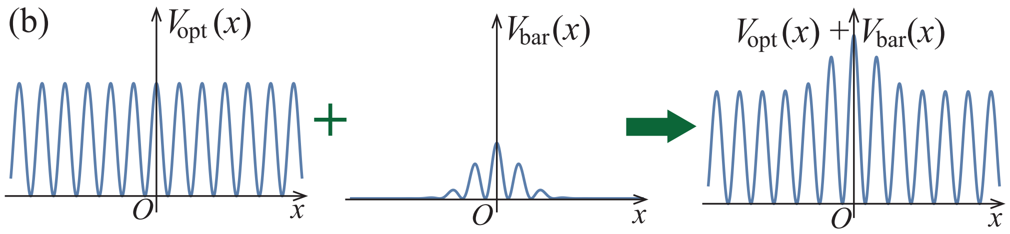


(b) Local modulation of the hopping amplitude:

$$J_{i_x} = J + J'_{i_x}$$

$$r(x) \simeq r_0 - 2J'(x) \equiv r_0 + v_r(x)$$

which keeps the p-h symmetry.



TDGL eq. with the effects of the potential barriers:

$$\underbrace{iv_K(x)}_{\text{type (a)}}\frac{\partial}{\partial t}\psi - W\frac{\partial^2}{\partial t^2}\psi = \left[-\frac{\nabla^2}{2m_*} + r_0 + \underbrace{v_r(x)}_{\text{type (b)}} + u|\psi|^2\right]\psi$$

2.6. Dimensionless form

$$iv_K(x)\frac{\partial}{\partial t}\psi - W\frac{\partial^2}{\partial t^2}\psi = \left[-\frac{\nabla^2}{2m_*} + r_0 + v_r(x) + u|\psi|^2\right]\psi$$

$$\bar{t} = t(-r_0/W)^{1/2},\ \bar{x} = x/\xi,\ \bar{\psi} = \psi(-u/r_0)^{1/2},$$

$\bar{v}_K = v_K/(-r_0 W)^{1/2},\ \bar{v}_r = v_r/(-r_0),$ where $\xi = 1/(-m_* r_0)^{1/2}$

$$i\bar{v}_K(x)\frac{\partial}{\partial \bar{t}}\bar{\psi} - \frac{\partial^2}{\partial \bar{t}^2}\bar{\psi} = \left[-\frac{\bar{\nabla}^2}{2} - 1 + \bar{v}_r(x) + |\bar{\psi}|^2\right]\bar{\psi}$$

Hereafter, we omit the bars for simplicity.

Note that in this unit

Sound speed: $c = 1/\sqrt{2},$ Higgs gap: $\Delta = \sqrt{2}$

2.7. Set of equations

We assume that the order parameter is homogeneous in the y and z directions.

$$iv_K(x)\frac{\partial}{\partial t}\psi - \frac{\partial^2}{\partial t^2}\psi = \left[-\frac{1}{2}\frac{\partial^2}{\partial x^2} - 1 + v_r(x) + |\psi|^2\right]\psi$$

$$\psi(x,t) = \underline{\underline{\psi_0(x)}} + \underline{\underline{\mathcal{U}(x)e^{-i\omega t} + \mathcal{V}^*(x)e^{i\omega^* t}}}$$

Static order parameter

Small fluctuations

Linearize the TDGL eq. w.r.t. the fluctuations.

Static GP-like eq.: $\left(-\frac{1}{2}\frac{d^2}{dx^2} - 1 + |\psi_0(x)|^2 + v_r(x)\right)\psi_0(x) = 0$

No effect of $v_K(x)$ term

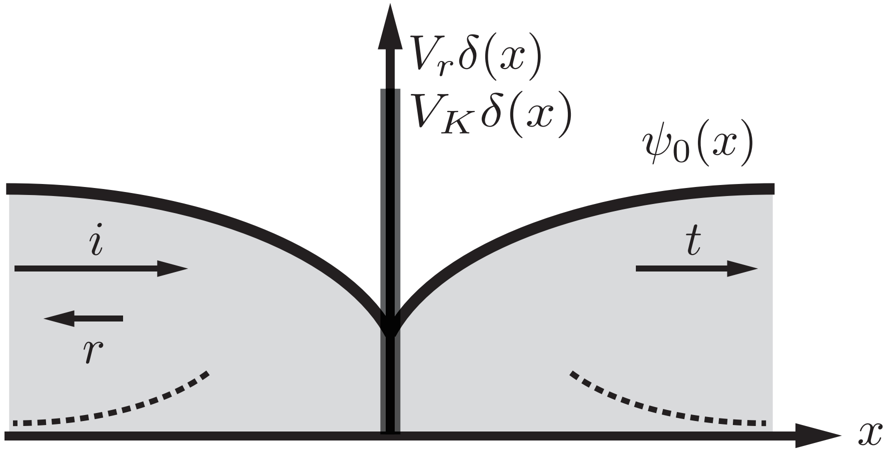
NG mode: $\left(-\frac{1}{2}\frac{d^2}{dx^2} - 1 + |\psi_0(x)|^2 + v_r(x)\right)S(x) = \omega^2 S(x) - \underline{\omega v_K(x)T(x)}$

Higgs mode: $\left(-\frac{1}{2}\frac{d^2}{dx^2} - 1 + 3|\psi_0(x)|^2 + v_r(x)\right)T(x) = \omega^2 T(x) - \underline{\omega v_K(x)S(x)}$

The Higgs and NG modes are coupled via the potential barrier $v_K(x)$.

2.8. Static order parameter

Kovrizhin Phys. Lett. A (2001)



We consider potential barriers of delta-function form:

$$v_r(x) = V_r\delta(x),\ \ v_K(x) = V_K\delta(x),$$

Solution of the static order parameter:

$$\psi_0(x) = \tanh(|x| + x_0)$$

The constant x_0 is determined by the boundary condition:

$$\psi_0'(-0) + 2V_r\psi_0(0) = \psi_0'(+0)$$

$$\Downarrow$$

$$\tanh(x_0) = \frac{-V_r + \sqrt{V_r^2 + 4}}{2} \simeq \frac{1}{V_r} \text{ when } V_r \gg 1$$

2.9. Higgs bound states

Let us consider the case that $V_K = 0, V_r > 0.$

The Higgs and NG modes are decoupled,

NG mode: $\left(-\frac{1}{2}\frac{d^2}{dx^2} - 1 + |\psi_0(x)|^2 + v_r(x)\right) S(x) = \omega^2 S(x) - \cancel{\omega v_K(x) T(x)}$

Higgs mode: $\left(-\frac{1}{2}\frac{d^2}{dx^2} - 1 + 3|\psi_0(x)|^2 + v_r(x)\right) T(x) = \omega^2 T(x) - \cancel{\omega v_K(x) S(x)}$

There are two bound state solutions of the Higgs mode:

$$T(x) = \begin{cases} A\left(3[\gamma(x)]^2 + 3\kappa_t\gamma(x) + \kappa_t^2 - 1\right) e^{\kappa_t x}, & x < 0 \\ B\left(3[\gamma(x)]^2 + 3\kappa_t\gamma(x) + \kappa_t^2 - 1\right) e^{-\kappa_t x}, & x > 0 \end{cases}$$

where $\gamma(x) = \tanh(|x| + x_0),\ \kappa_t = \sqrt{4 - 2\omega^2}$

Boundary conditions: $T(+0) = T(-0),\ T'(+0) = T'(-0) + 2V_r T(0)$

➡ one bound-state solution respectively for

$A = B\,(\text{even parity}),\ \ A = -B\,(\text{odd parity})$

Bound-state energy: E_+, E_-

Note: There is no bound state of the NG mode.

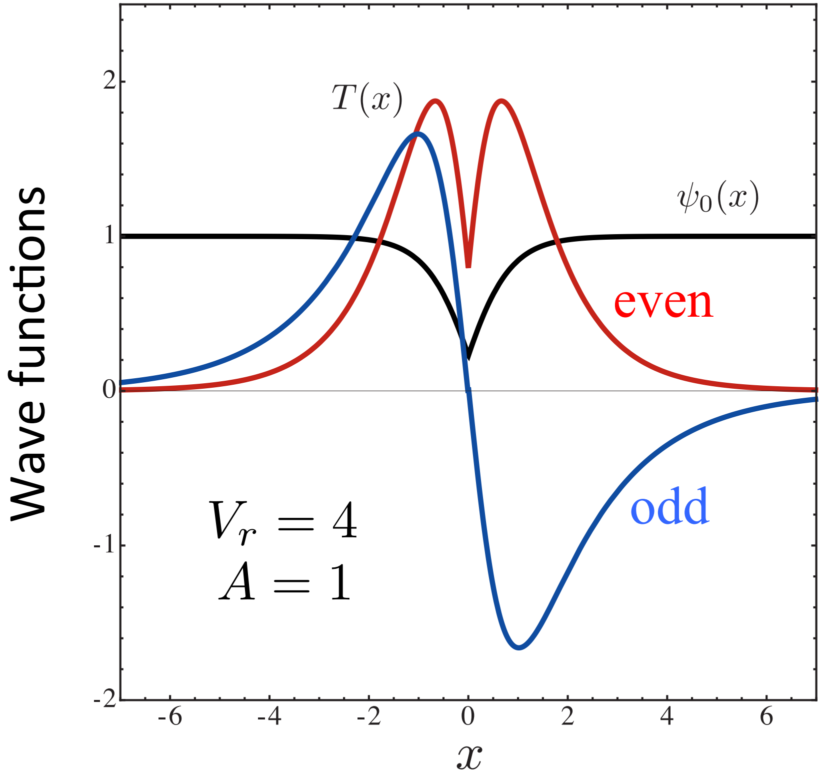
2.9. Higgs bound states

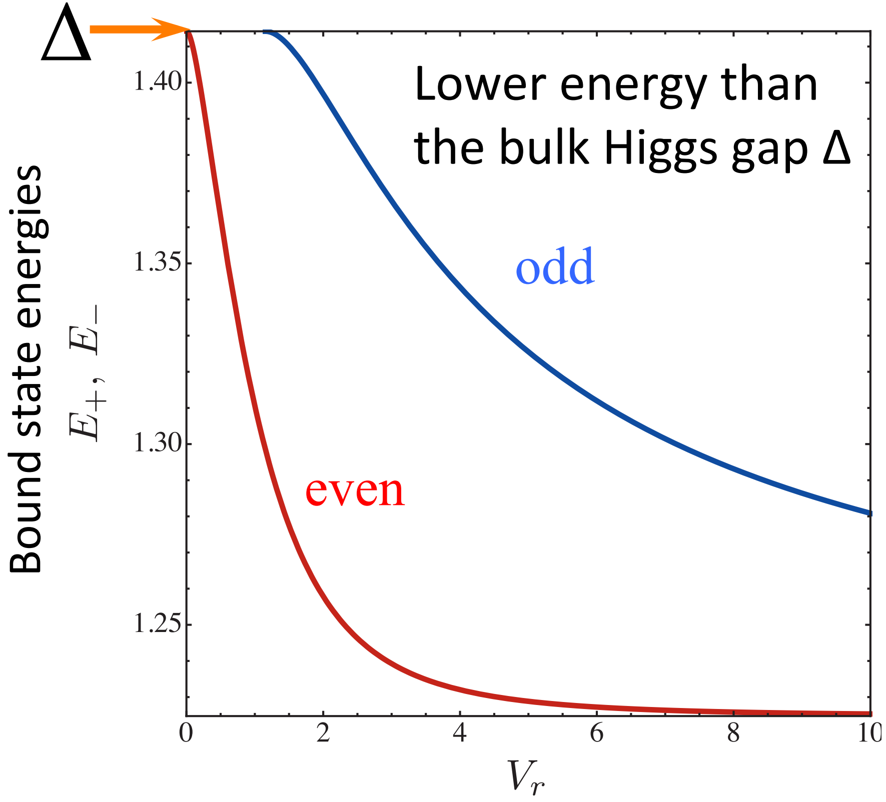
Let us consider the case that $V_K = 0, V_r > 0.$

The Higgs and NG modes are decoupled,

NG mode: $$\left(-\frac{1}{2}\frac{d^2}{dx^2} - 1 + |\psi_0(x)|^2 + v_r(x)\right) S(x) = \omega^2 S(x) - \omega \cancel{v_K(x)T}(x)$$

Higgs mode: $$\left(-\frac{1}{2}\frac{d^2}{dx^2} - 1 + \boxed{3}|\psi_0(x)|^2 + v_r(x)\right) T(x) = \omega^2 T(x) - \omega \cancel{v_K(x)S}(x)$$





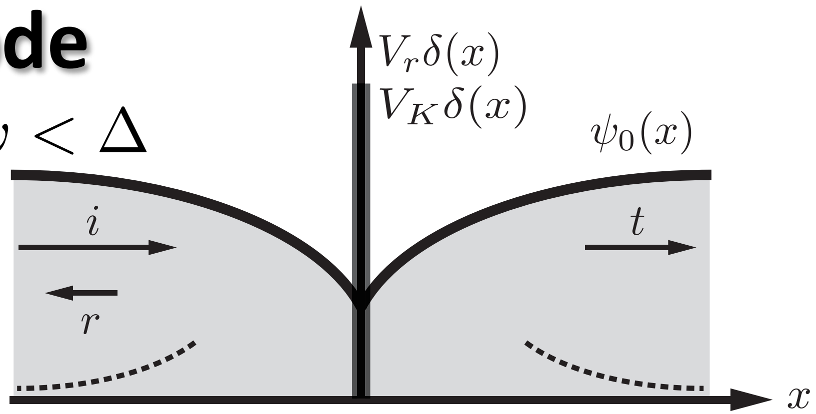
Lower energy than the bulk Higgs gap Δ

The diminishing order parameter combined with the potential barrier constitutes a **double well potential** for collective modes. It allows for formation of **bound states of the Higgs mode**.

2.10. Tunneling of the NG mode

Let us assume that $\underbrace{V_K \neq 0}_{\text{breaks the p-h symmetry}},\ V_r > 0,\ \text{and}\ \omega < \Delta$

We consider the scattering problem of
a NG mode incident to the potential barriers.



$$\text{NG:}\quad S(x) = \begin{cases} \underbrace{(\gamma(x) + ik_s)e^{ik_s x}}_{\text{Incident}} + \underbrace{r_{\rm ng}(\gamma(x) - ik_s)e^{-ik_s x}}_{\text{Reflected}}, & (x < 0), \\ \underbrace{t_{\rm ng}(\gamma(x) - ik_s)e^{ik_s x}}_{\text{Transmitted}}, & (x > 0), \end{cases}$$

where $k_s = \sqrt{2\omega^2 - 4}$

$$\text{Higgs:}\quad T(x) = \begin{cases} A\left(3[\gamma(x)]^2 + 3\kappa_t\gamma(x) + \kappa_t^2 - 1\right)e^{\kappa_t x}, & x < 0 \\ B\left(3[\gamma(x)]^2 + 3\kappa_t\gamma(x) + \kappa_t^2 - 1\right)e^{-\kappa_t x}, & x > 0 \end{cases}$$

Boundary conditions:

$$S(+0) = S(-0),\ \ S'(-0) + 2V_r S(0) + 2EV_K T(0) = S'(+0)$$
$$T(+0) = T(-0), T'(-0) + 2V_r T(0) + 2EV_K S(0) = T'(+0)$$

➡ All the coefficients, $r_{\rm ng}$, $t_{\rm ng}$, A, and B.

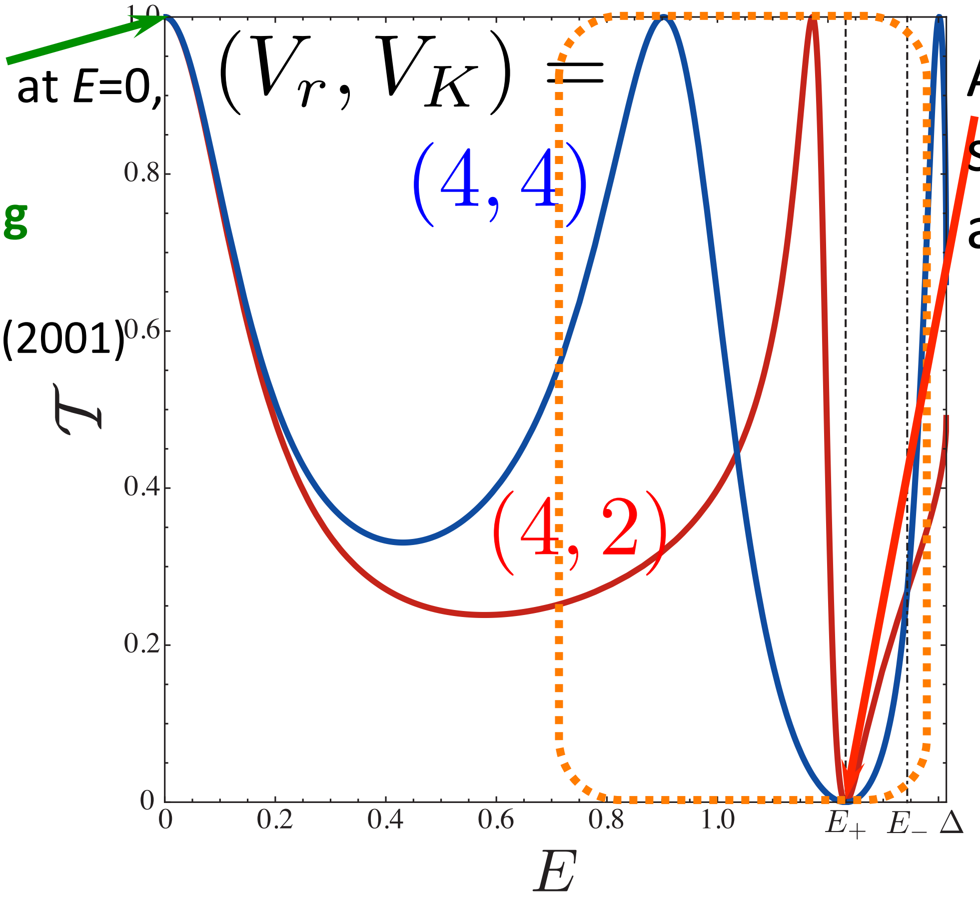
2.11. Transmission probability

$$\mathcal{T}(E) = |t_{\rm ng}|^2 = \frac{1}{1 + \frac{2E^2}{(2E^2+1)^2} V_{\rm eff}(E)^2}, \quad (E < \Delta)$$

$$V_{\rm eff}(E) = \left(1 - V_K^2 f(E)\right) V_r$$

Perfect transmission at *E*=0, which is known as **anomalous tunneling** of the NG mode

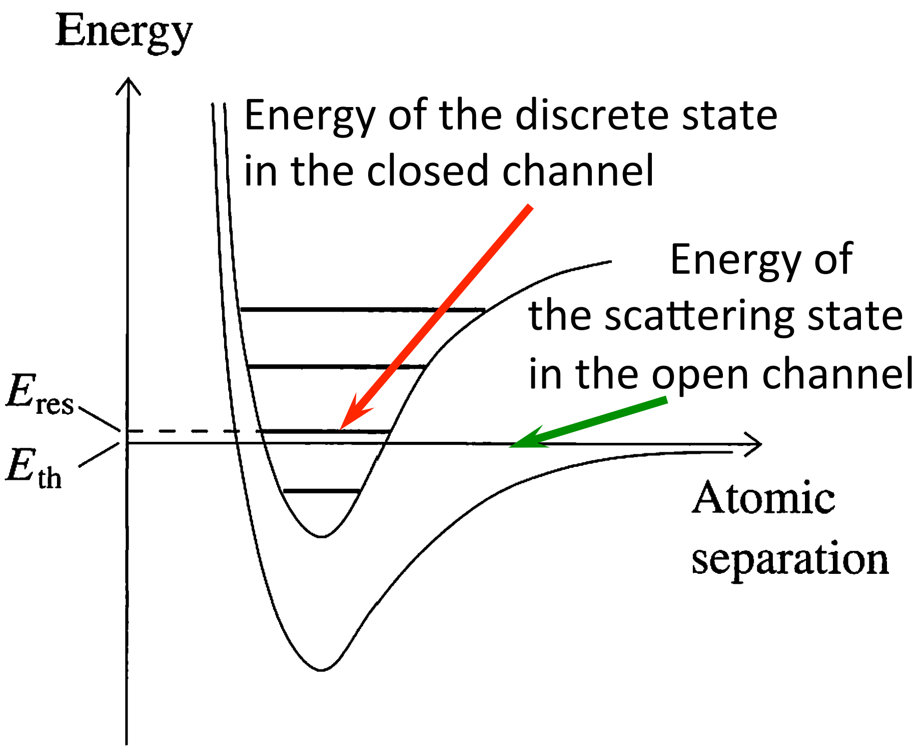
Kovrizhin, Phys. Lett A (2001)



Asymmetric peak structure emerges around E_+ !!!

Fano resonance

2.12. Remember Feshbach resonance



Energy of the discrete state in the closed channel

Energy of the scattering state in the open channel

Figure is from the Pethick-Smith textbook.

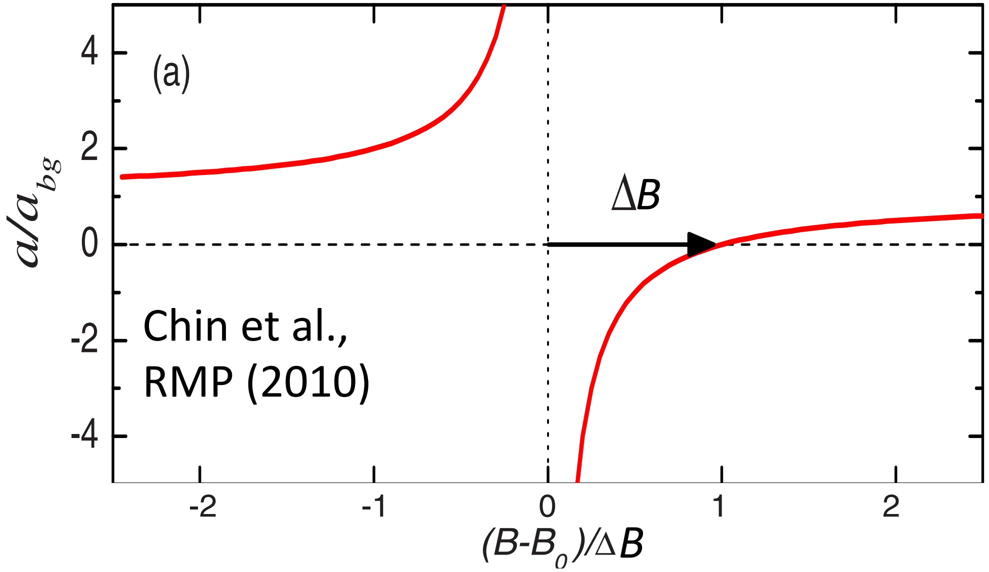
Scattering length:

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

Direct scattering

Scattering through the discrete state

The interference with the scattering process through the discrete state leads to the dramatic change of the scattering length, namely the **Feshbach resonance**.



Chin et al., RMP (2010)

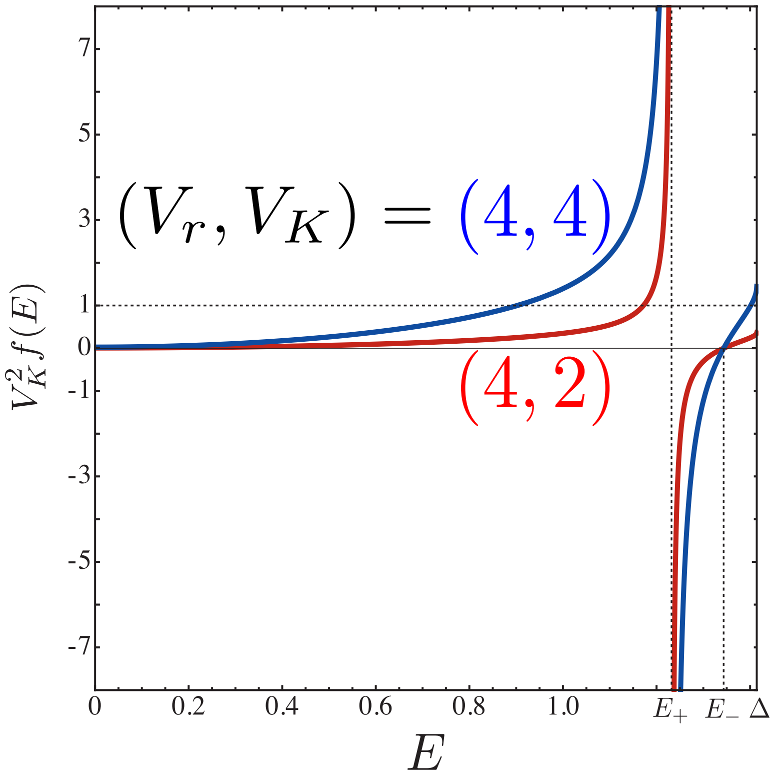
2.13. Fano resonance

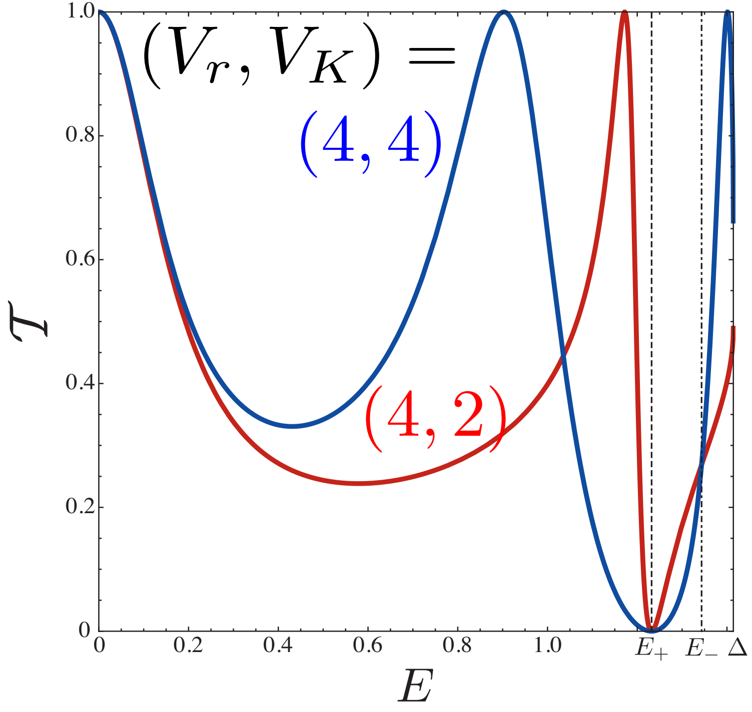
$$\mathcal{T}(E) = |t_{\rm ng}|^2 = \frac{1}{1+\frac{2E^2}{(2E^2+1)^2}V_{\rm eff}(E)^2}, \quad (E<\Delta)$$

$$V_{\rm eff}(E) = \left(1 - V_K^2 f(E)\right) V_r \simeq \underline{V_r} - \underline{\frac{\alpha V_K^2}{E-E_+}V_r}.$$ for $|E-E_+| \ll 1$

Direct scattering

Scattering through the even Higgs bound state.





The asymmetric peak is manifestation of the Fano resonance of the **NG mode (open channel)** mediated by **the even Higgs bound state (closed channel)**.

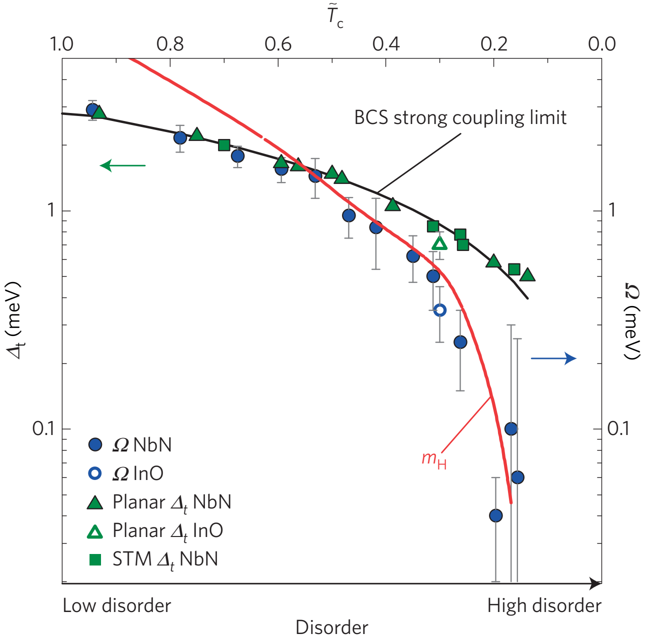
2.14. Summary of this part

- We derived the time-dependent Ginzburg-Landau equation including effects of potential barriers.
- Higgs bound states are present under the barrier potential that does not break the particle-hole symmetry.
- Fano resonance of the NG mode mediated by the Higgs bound state

T. Nakayama, I. Danshita, T. Nikuni, & S. Tsuchiya, arXiv:1503.01516 (2015)

Outlook:

- Response of the Higgs bound states to the lattice amplitude modulation.
- 2D
- Other condensed matter systems
  Especially disordered superconductors,
  Sherman et al., Nat. Phys. (2015).



Outline:

1. Introduction:
   Strongly correlated superfluids in optical lattices

2. Higgs bound states in a single-component Bose gas
T. Nakayama, I. Danshita, T. Nikuni, & S. Tsuchiya, arXiv:1503.01516 (2015)

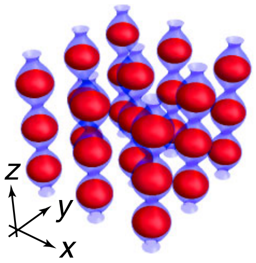
3. Heavy solitary waves in a two-component Bose gas
Y. Kato, D. Yamamoto, & I. Danshita, Phys. Rev. Lett. 112, 055301 (2014)
I. Danshita, D. Yamamoto, & Y. Kato, Phys. Rev. A 91, 013630 (2015)

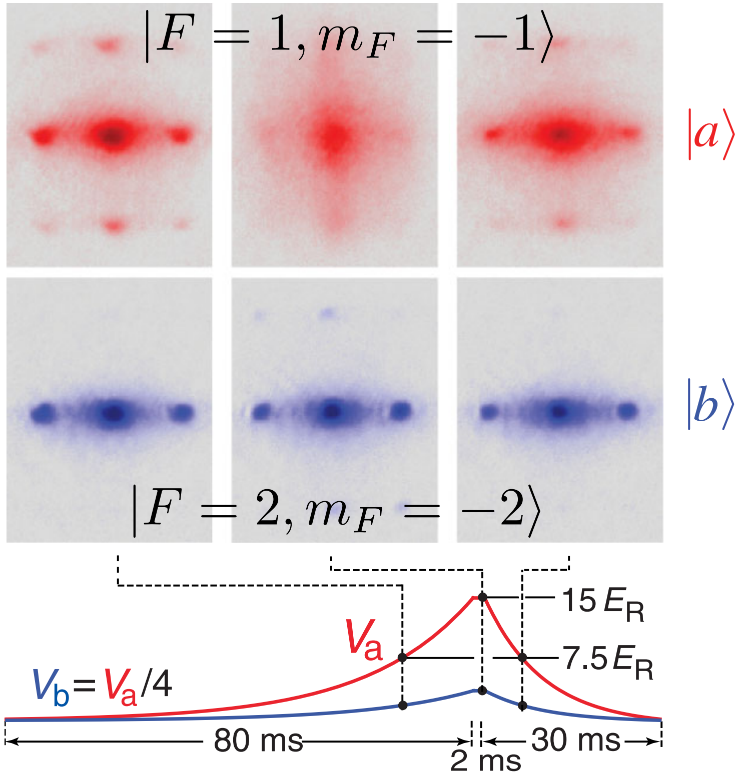
Yasuyuki Kato
RIKEN → Univ. Tokyo

Daisuke Yamamoto
WIAS, Waseda Univ.

3.1. Bose-Bose mixture in optical lattices

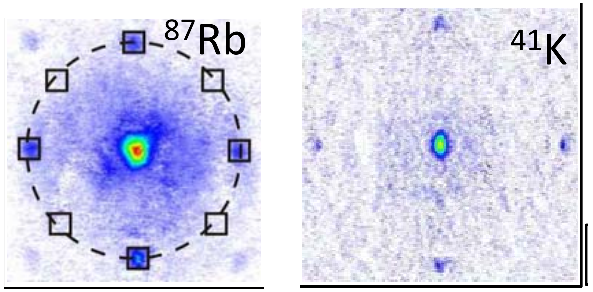
Stony Brook: B. Gadway et al., PRL (2010)





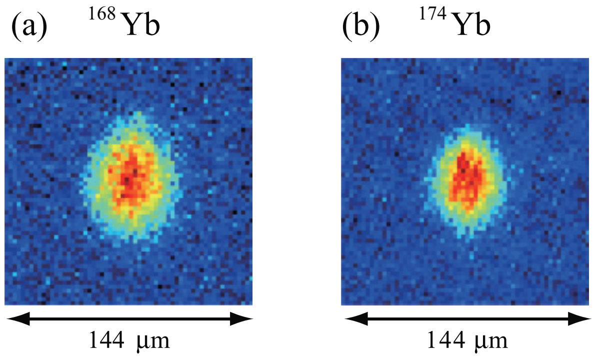
Atomic species: ^{87}Rb

Florence: J. Catani et al., PRA (2008)



^{87}Rb-^{41}K

Kyoto: S. Sugawa et al., PRA (2011)



^{168}Yb-^{174}Yb

A simple extension, but rich physics

- New quantum phases have been predicted, such as phase separation, pair- and counterflow- superfluids, checkerboard solid, supersolid (checkerboard + superfluid).

Kuklov & Svistunov, PRL (2003)
Altman et al., NJP (2003)
Paredes & Cirac, PRL (2003)
Mishra et al., PRA (2007)
Capogrosso-Sansone et al., PRA (2008)
etc.

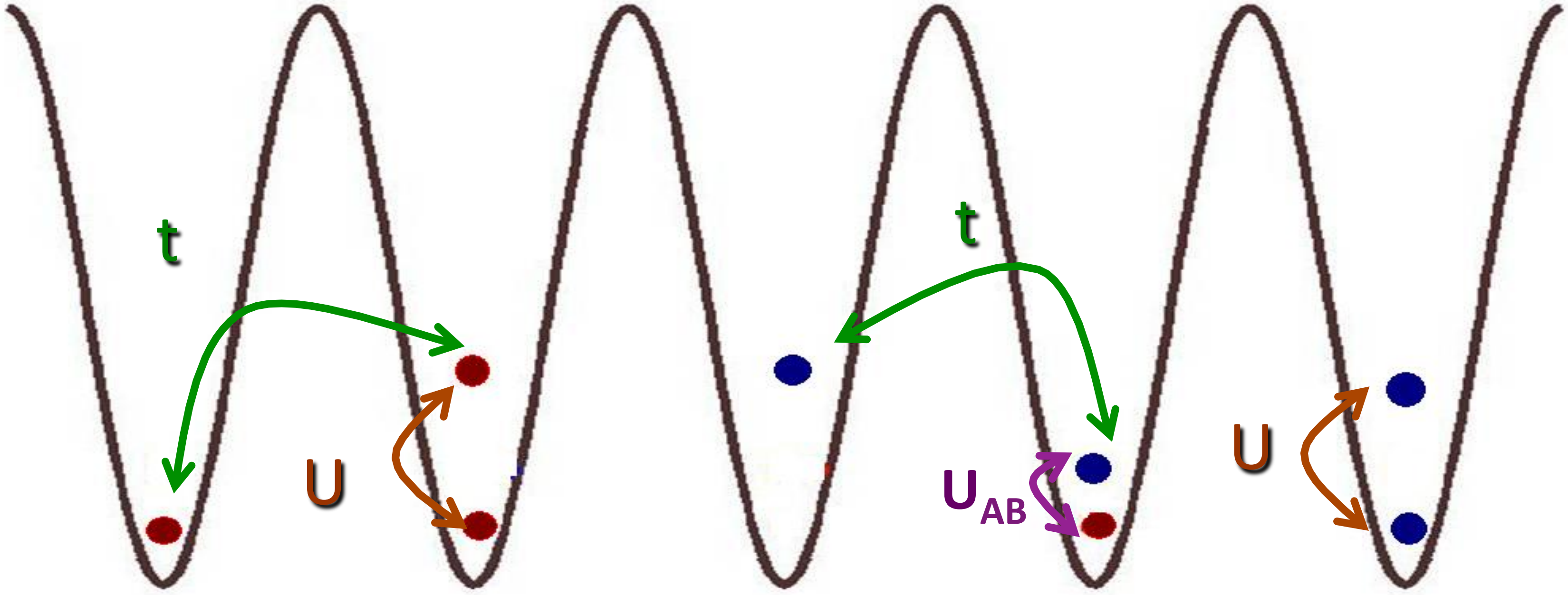
- First-order superfluid-Mott insulator transition

3.2. Two-component Bose-Hubbard Model

$$\hat{H} = \sum_{\alpha=A,B} \left[\underbrace{-t_\alpha \sum_{\langle j,l\rangle} (\hat{b}^\dagger_{j,\alpha}\hat{b}_{l,\alpha} + \text{H.c.})}_{\text{Hopping}} \underbrace{- \mu_\alpha \sum_j \hat{n}_{j,\alpha}}_{\text{Chemical potential}} + \underbrace{\frac{U_\alpha}{2}\sum_j \hat{n}_{j,\alpha}(\hat{n}_{j,\alpha}-1)}_{\text{Intra-component repulsion}} \right] + \underbrace{U_{AB}\sum_j \hat{n}_{j,A}\hat{n}_{j,B}}_{\text{Inter-component Repulsion } (U_{AB}>0)},$$

Hereafter, we assume $t_A=t_B\equiv t$, $U_A=U_B\equiv U>0$, and $\mu_A=\mu_B\equiv\mu$.

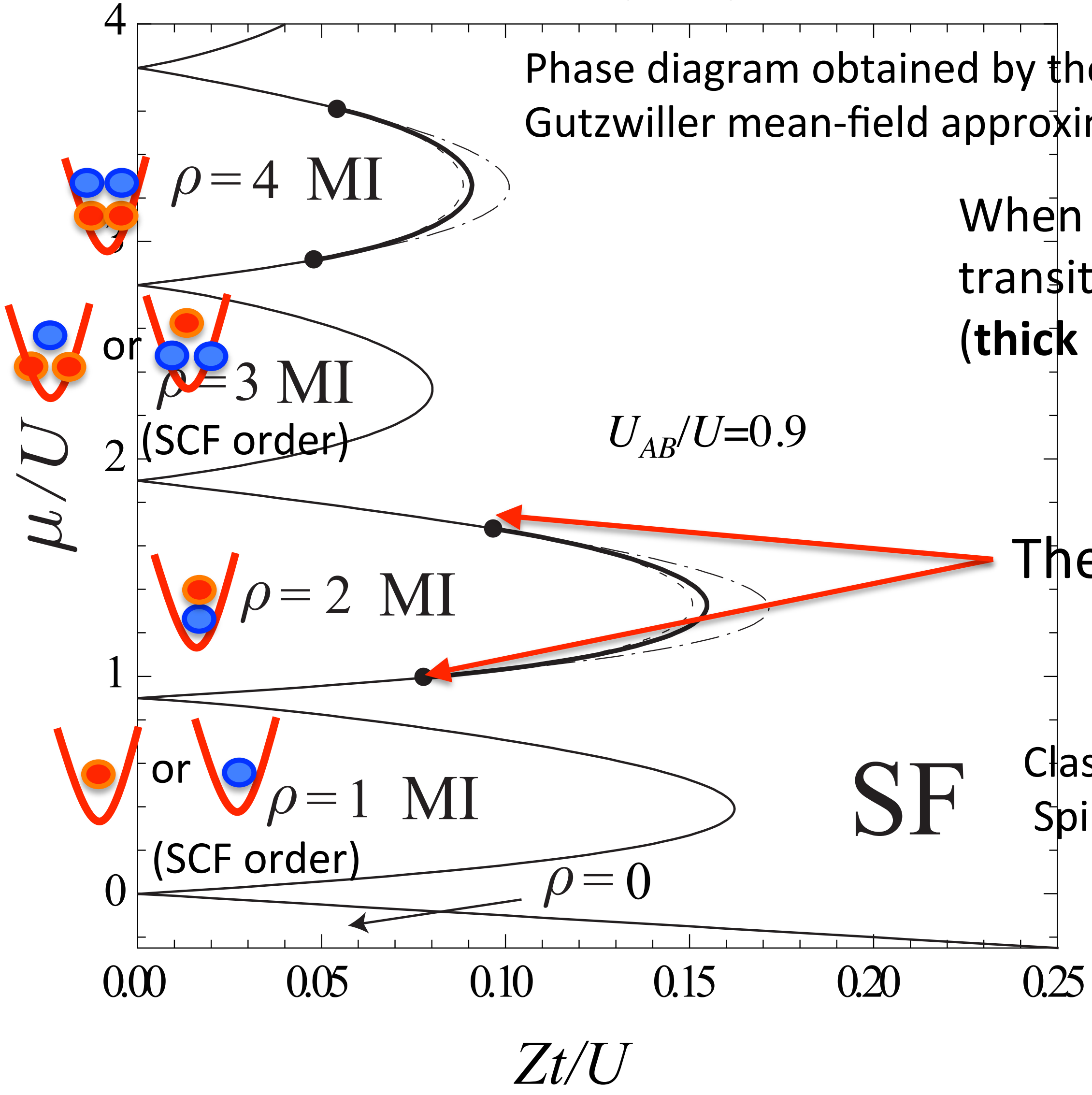
This condition can be nearly satisfied in a gas of ^{87}Rb binary mixtures with $|F=2,m_F=-1>$ and $|F=1,m_F=1>$ (or |2,-2> & |1,-1>) states, which are confined in optical lattices by many groups, such as Max Planck, Stony Brook, MIT, NIST.



See e.g. Jaksch et al., PRL (1998)

3.3. Mean-field phase diagram at *T*=0

T. Ozaki et al., arXiv:1210.1370 (2012); D. Yamamoto et al., PRA 88, 033624 (2013)



Phase diagram obtained by the Gutzwiller mean-field approximation

When $U_{AB} < U$ but $\sim U$, the SF-MI transition at even filling is first order (**thick lines**) near the tip of the Mott lobe.

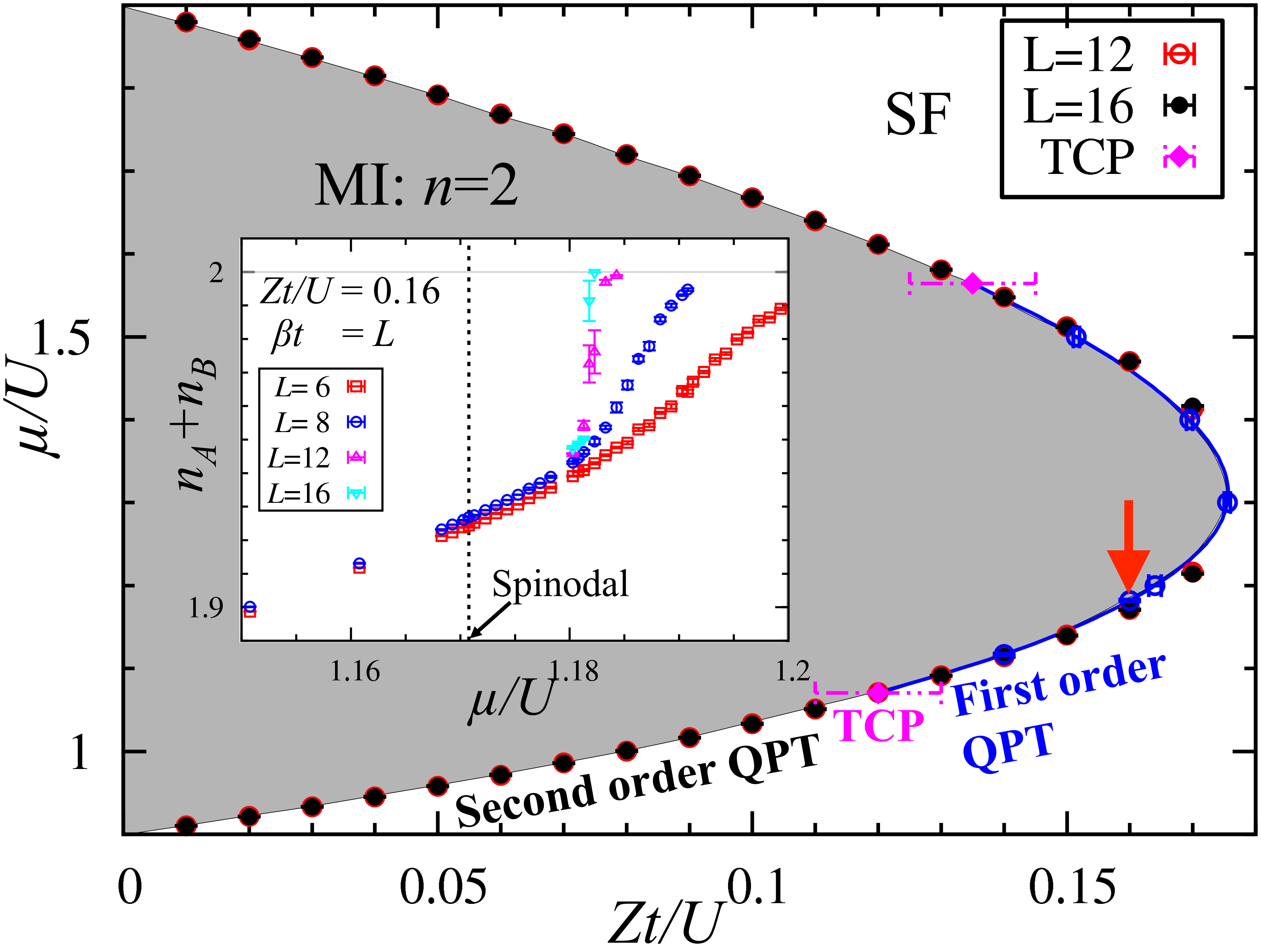
The associated quantum TCPs !!!

Classical analog: A. Kuklov et al., PRL (2004)
Spin-1 case: T. Kimura et al., PRL (2005)

Is the 1st order transition real ??

SCF: Super-counter flow
Z: Coordination number

3.4. QMC phase diagram at 2D and U_{AB}/U=0.9



3.5. How to derive the effective action

Euclidian action for the two-comp. BHM: $S[b_A, b_A^*, b_B, b_B^*] = S_A + S_B + S_{AB},$

$$S_\alpha = \int_{-\frac{\hbar\beta}{2}}^{\frac{\hbar\beta}{2}} d\tau \left[\sum_j b^*_{\alpha,j} \left(\hbar \frac{\partial}{\partial \tau} - \mu_\alpha + \frac{U_{\alpha\alpha}}{2} b^*_{\alpha,j} b_{\alpha,j} \right) b_{\alpha,j} - \sum_{\langle j,l \rangle} t_\alpha \; (b^*_{\alpha,j} b_{\alpha,l} + c.c.) \right],$$

$$S_{AB} = \int_{-\frac{\hbar\beta}{2}}^{\frac{\hbar\beta}{2}} d\tau \sum_j U_{AB} \, b^*_{A,j} b_{A,j} b^*_{B,j} b_{B,j}.$$

M. P. A. Fisher et al.,
PRB (1989) for the
single-component
BHM

- Stratonovich-Hubbard transformation to introduce $\underline{\underline{\psi_\alpha}}$ fields
- Integrate out b_α fields

Superfluid order parameter

- Cumulant expansion up to the **sixth** order w.r.t. the field ψ_α
- Take the continuum limit

Effective action: $S^{\text{eff}}[\psi_A, \psi_A^*, \psi_B, \psi_B^*] = \hbar\beta V f_0 + S_A^{\text{eff}} + S_B^{\text{eff}} + S_{AB}^{\text{eff}},$

where $$S_\alpha^{\text{eff}} = \int d\tau \int d^d x \left[\hbar K_\alpha \psi_\alpha^* \frac{\partial \psi_\alpha}{\partial \tau} + \hbar^2 J_\alpha \left| \frac{\partial \psi_\alpha}{\partial \tau} \right|^2 + \frac{\hbar^2}{2 m_\alpha} |\nabla \psi_\alpha|^2 \right.$$
$$\left. - r_\alpha |\psi_\alpha|^2 + \frac{u_\alpha}{2} |\psi_\alpha|^4 + \frac{w_\alpha}{3} |\psi_\alpha|^6 \right],$$

$$S_{AB}^{\text{eff}} = \int d\tau \int d^d x \left[u_{AB} |\psi_A|^2 |\psi_B|^2 + w_{AB} |\psi_A|^4 |\psi_B|^2 + w_{BA} |\psi_A|^2 |\psi_B|^4 \right].$$

All the coefficients $K_\alpha, J_\alpha, m_\alpha, r_\alpha, u_\alpha, u_{AB}, w_\alpha, w_{AB(BA)}$ can be explicitly expressed as functions of the original Hubbard parameters.

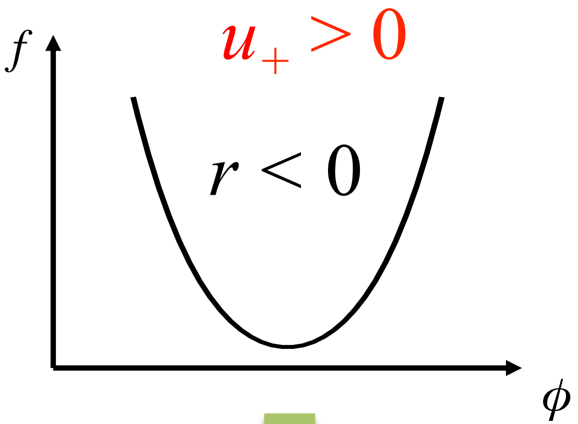
$\psi_\alpha \propto \langle \hat{b}_j \rangle$ such that it plays a role of the superfluid order parameter.

3.6. Mechanism for the first order transition

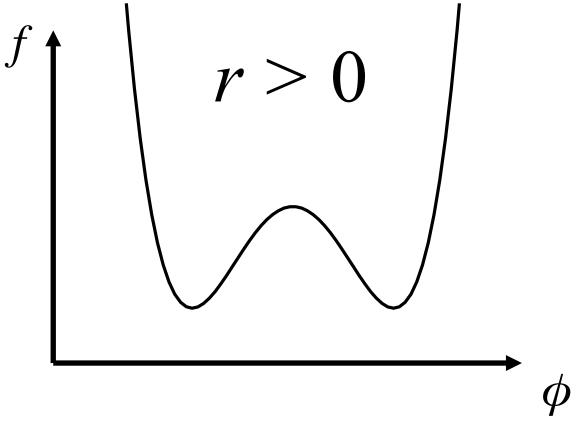
Mean-field approximation: $\psi_A(\mathbf{x},\tau) = \psi_B(\mathbf{x},\tau) = \phi$

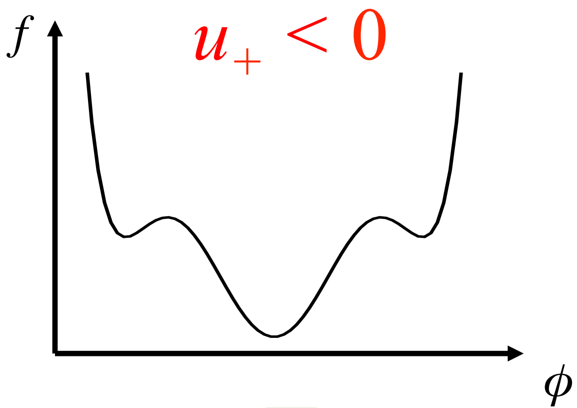
$$S^{\text{eff}} = \hbar\beta V f \quad \text{with} \quad f = f_0 - 2r\phi^2 + \underset{\equiv u_+}{\underline{(u+u_{AB})}}\phi^4 + \frac{2}{3}\underset{\equiv w_+}{\underline{\underline{(w+3w_{AB})}}}\phi^6,$$

Assuming $w_+ > 0$

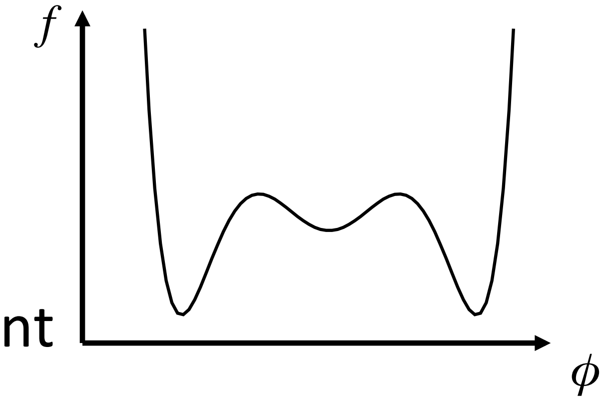


Second order phase transition





First order phase transition

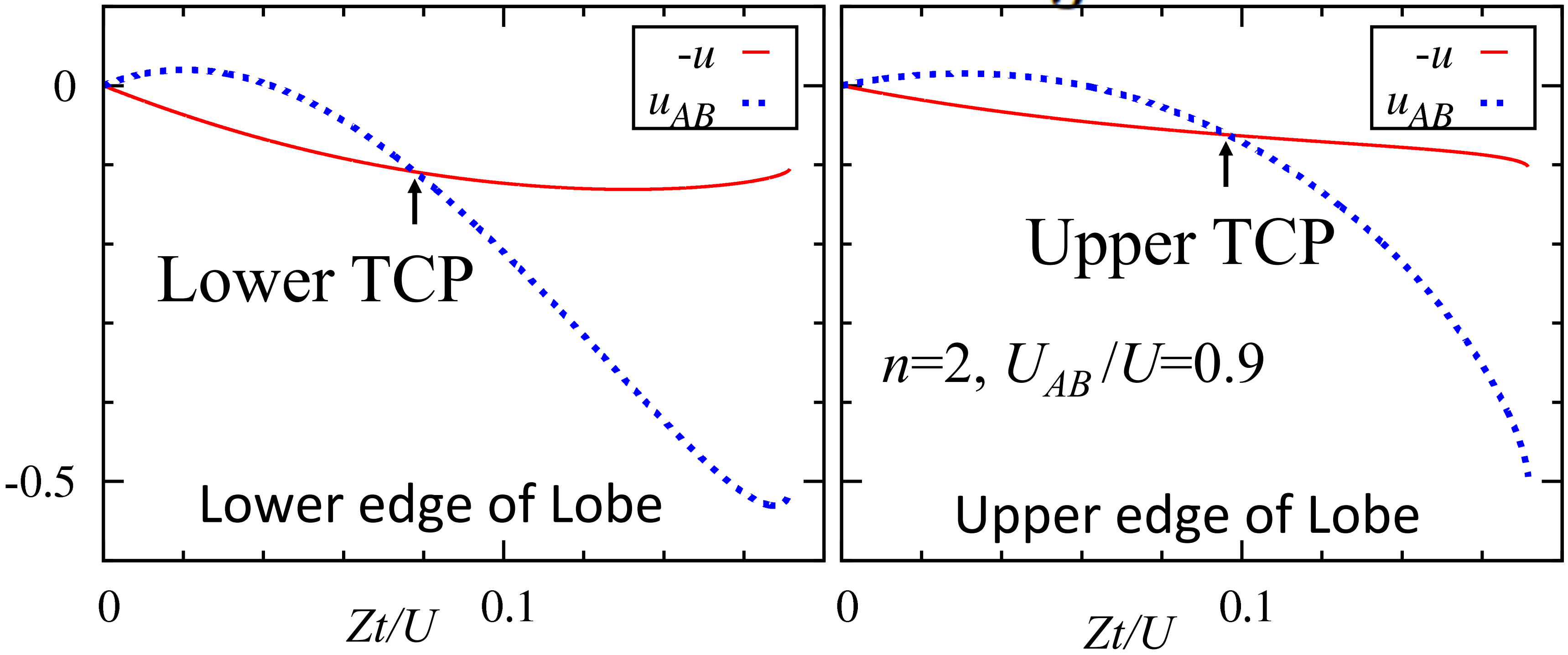


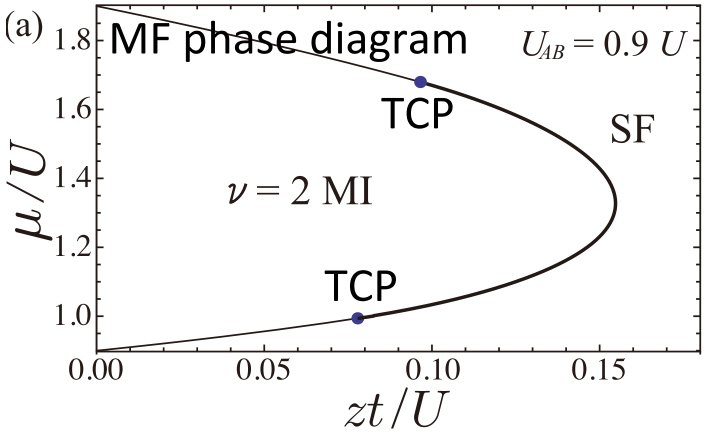
$u_+ = 0$

Tricritical point

3.6. Mechanism for the first order transition

$$f = f_0 - 2r\phi^2 + (u + u_{AB})\phi^4 + \frac{2}{3}(w + 3w_{AB})\phi^6,$$





$u+u_{AB}$=0 @ TCP (u_{AB}<0)

Effective attraction

between $|\psi_A|^2$ and $|\psi_B|^2$

3.7. Why attractive?

Assuming the Mott insulating state is described as $|n_A, n_B\rangle = |g, g\rangle$, we obtain

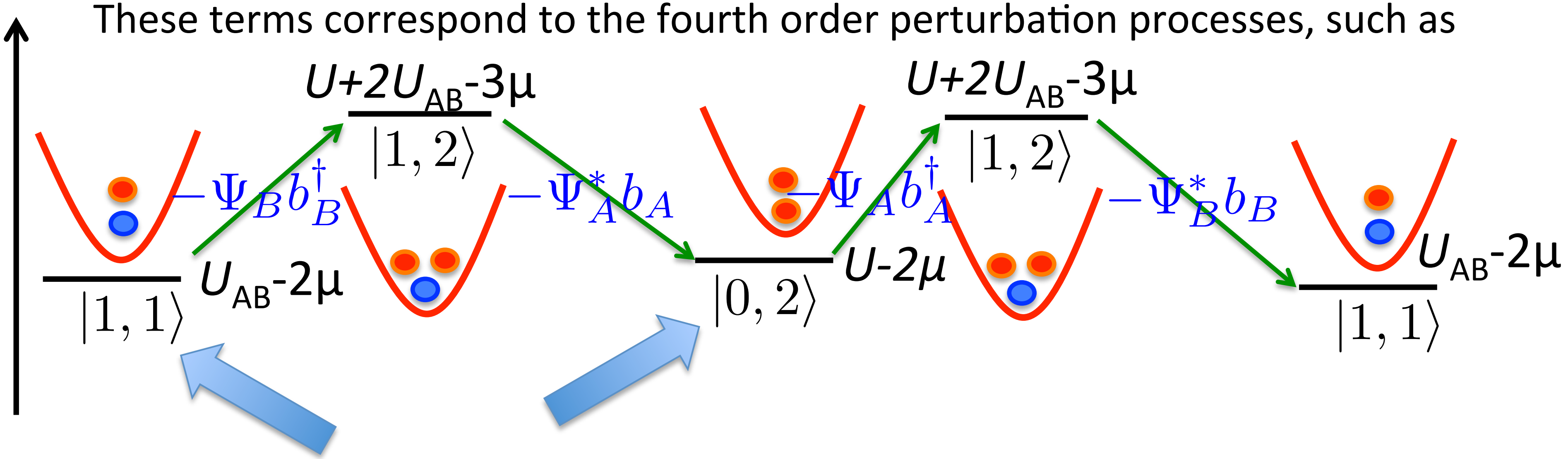
$$
\begin{aligned}
u_{AB} = \quad a^d Z^4 t_A^2 t_B^2 \Bigg[& \left(\frac{g+1}{E_A^{(+)} - E_{g,g}} + \frac{g}{E_A^{(-)} - E_{g,g}} \right) \left(\frac{g+1}{(E_B^{(+)} - E_{g,g})^2} + \frac{g}{(E_B^{(-)} - E_{g,g})^2} \right) \\
& + \left(\frac{g+1}{E_B^{(+)} - E_{g,g}} + \frac{g}{E_B^{(-)} - E_{g,g}} \right) \left(\frac{g+1}{(E_A^{(+)} - E_{g,g})^2} + \frac{g}{(E_A^{(-)} - E_{g,g})^2} \right) \\
& - \left(\frac{1}{E_A^{(+)} - E_{g,g}} + \frac{1}{E_B^{(+)} - E_{g,g}} \right)^2 \frac{(g+1)^2}{E_{AB}^{(++)} - E_{g,g}} \\
& \boxed{\begin{aligned} & - \left(\frac{1}{E_A^{(+)} - E_{g,g}} + \frac{1}{E_B^{(-)} - E_{g,g}} \right)^2 \frac{g(g+1)}{E_{AB}^{(+-)} - E_{g,g}} \\ & - \left(\frac{1}{E_A^{(-)} - E_{g,g}} + \frac{1}{E_B^{(+)} - E_{g,g}} \right)^2 \frac{g(g+1)}{E_{AB}^{(-+)} - E_{g,g}} \end{aligned}} \\
& - \left(\frac{1}{E_A^{(-)} - E_{g,g}} + \frac{1}{E_B^{(-)} - E_{g,g}} \right)^2 \frac{g^2}{E_{AB}^{(--)} - E_{g,g}} \Bigg],
\end{aligned}
$$

If $U \sim U_{AB}$, these terms are strongly enhanced.

3.7. Why attractive?

$$-\left(\frac{1}{E_A^{(+)}-E_{g,g}}+\frac{1}{E_B^{(-)}-E_{g,g}}\right)^2\frac{g(g+1)}{E_{AB}^{(+-)}-E_{g,g}}-\left(\frac{1}{E_A^{(-)}-E_{g,g}}+\frac{1}{E_B^{(+)}-E_{g,g}}\right)^2\frac{g(g+1)}{E_{AB}^{(-+)}-E_{g,g}}$$

These terms correspond to the fourth order perturbation processes, such as



Since these two states have nearly equal energy when $U \sim U_{AB}$, this process gives a large negative contribution to u_{AB}.

Reminiscent of the Feshbach resonance

Such processes do not exist in the single-component case.

Indeed, the first-order transition emerges only when $U \sim U_{AB}$
(more precisely, when $0.68 < U/U_{AB} < 1$ according to the Gutzwiller analysis)

3.8. Superfluid equation of motion

Minimize the action by the condition: $\frac{\delta S^{\rm eff}}{\delta \psi_\alpha} = 0$,

Im time Re time

$\tau \to -i\tau$

Two-comp. NLSE with cubic-quintic nonlinearity !!!

Mean-field equation of motion:

Maimistov et al., Phys. Lett.A (1999)

$$i\hbar \frac{\partial \psi_A}{\partial \tau} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) - r + u|\psi_A|^2 + u_{AB}|\psi_B|^2 + w|\psi_A|^4 + w_{AB}(2|\psi_A|^2|\psi_B|^2 + |\psi_B|^4) \right] \psi_A$$

$$i\hbar \frac{\partial \psi_B}{\partial \tau} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) - r + u|\psi_B|^2 + u_{AB}|\psi_A|^2 + w|\psi_B|^4 + w_{AB}(2|\psi_A|^2|\psi_B|^2 + |\psi_A|^4) \right] \psi_B$$

Stationary solution: $\psi_\alpha(\mathbf{x}, \tau) = \phi_\alpha(\mathbf{x})$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) - r + u|\phi_A|^2 + u_{AB}|\phi_B|^2 + w|\phi_A|^4 + w_{AB}(2|\phi_A|^2|\phi_B|^2 + |\phi_B|^4) \right] \phi_A = 0$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) - r + u|\phi_B|^2 + u_{AB}|\phi_A|^2 + w|\phi_B|^4 + w_{AB}(2|\phi_A|^2|\phi_B|^2 + |\phi_A|^4) \right] \phi_B = 0$$

$$\phi_A = \phi_B \equiv \phi$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) - r + u_+|\phi|^2 + w_+|\phi|^4 \right] \phi = 0 \quad \text{where} \quad \begin{array}{l} u_+ \equiv u + u_{AB} \\ w_+ \equiv w + 3w_{AB} \end{array}$$

We analytically solve this equation.

3.9. Stationary solution and first order transition

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) - r + u_+|\phi|^2 + w_+|\phi|^4\right]\phi = 0$$

⇓ $V(\mathbf{x}) = 0,\ \phi(\mathbf{x}) = \sqrt{n_0}$

$$r = u_+ n_0 + w_+ n_0^2$$

We want to determine the first order transition point.

Free energy density:

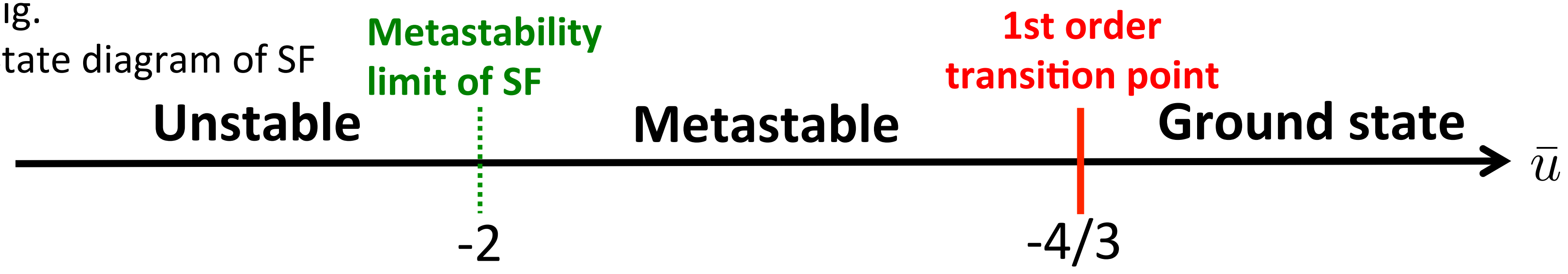
$$f_{\mathrm{SF}} = -2rn_0 + u_+ n_0^2 + \frac{2}{3}w_+ n_0^3$$

$$f_{\mathrm{MI}} = 0$$

$f_{\mathrm{SF}} = f_{\mathrm{MI}}$ ⇒ $\underline{\underline{\bar{u} = -\frac{4}{3}}}$ **1st order transition point !!!** where $\bar{u} \equiv \frac{u_+}{w_+ n_0}$

In a similar way, one can determine the metastability limits of SF $\bar{u} = -2$

Fig.
State diagram of SF



Metastability limit of SF

1st order transition point

Unstable

Metastable

Ground state

$\bar{u}$

-2

-4/3

3.10. Solution of a moving dark solitary wave

Problem:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-r+u_+\phi^2+w_+\phi^4\right]\phi=0\ ,$$

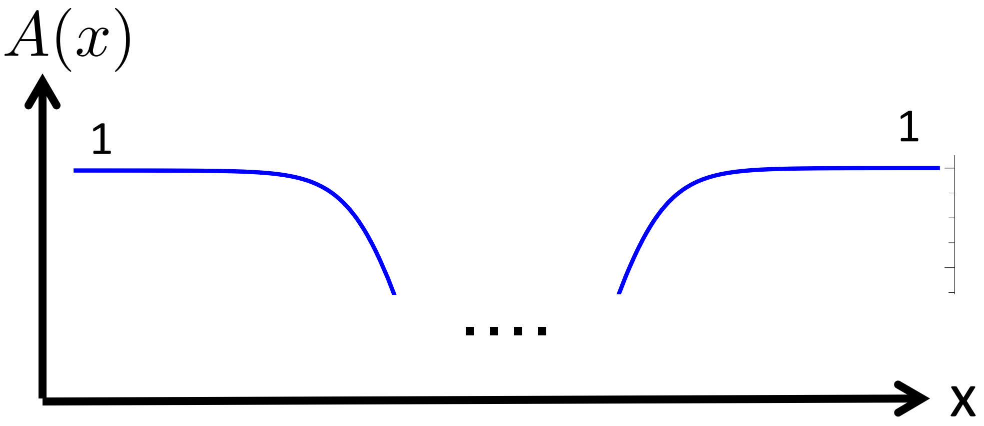
$$\phi(x)=\sqrt{n_0}A(x)\mathrm{e}^{iS(x)}$$

Separate the amplitude A(x)
and the phase S(x)

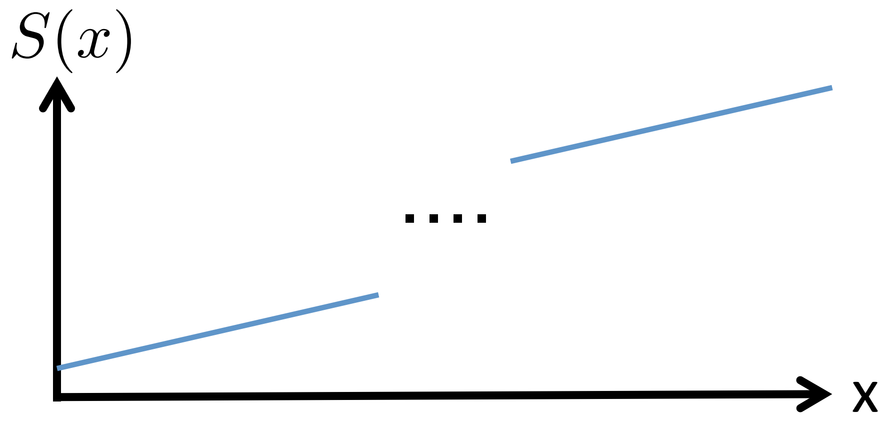
$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{\hbar^2q^2}{2m}A^{-4}-r+u_+n_0A^2+w_+n_0^2A^4\right)A=0,\quad A^2\frac{dS}{dx}=q$$

Boundary conditions: $\lim\limits_{x\to\pm\infty}A(x)=1,\quad \lim\limits_{x\to\pm\infty}S(x)=qx\pm\frac{\varphi}{2},$

Amplitude:



Phase:



3.10. Solution of a moving dark solitary wave

Barashenkov &
Makhankov,
Phys. Lett. A (1988)

Solution:
$$\frac{\phi(x)}{\sqrt{n_0}} = Ae^{iS} = \frac{\sqrt{\alpha_+} + i\,\mathrm{sgn}(q)\sqrt{\alpha_-}\eta(x)}{\sqrt{\beta_+ - \beta_-\left[\eta(x)\right]^2}} e^{iq(x-x_\mathrm{s})}$$

where
$$\eta(x) \equiv \tanh(x/\xi),$$

$$\xi \equiv \hbar/\sqrt{m(un+2wn^2)-\hbar^2q^2}$$

$$\alpha_\pm = \pm(-\gamma+3\bar{q}^2)+\sqrt{\gamma^2+6\bar{q}^2}$$

$$\beta_\pm = 2+\gamma\pm\sqrt{\gamma^2+6\bar{q}^2}$$

$$\gamma = 2+3\bar{u}/2,$$

$$\bar{q} = q\hbar/\sqrt{mwn_0^2}$$

Standing solitary wave in a flowing condensate as background

Galilean transformation

Moving solitary wave in a static condensate

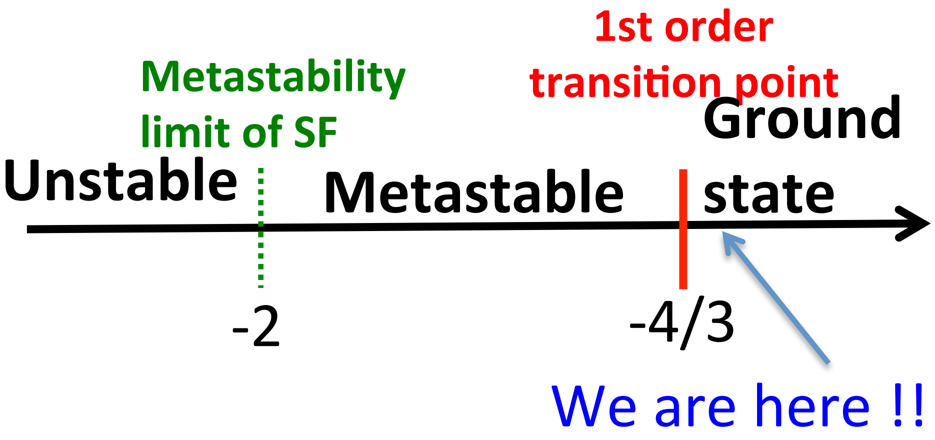
3.11. Case of u_+> -4/3 (SF state is the ground state)

Standing solitary wave (*q*=0):

$$\phi(x) = \sqrt{n_0} \times \frac{\sqrt{\gamma}\eta(x)}{\sqrt{1+\gamma-[\eta(x)]^2}}$$

where $\gamma \equiv 2 + \frac{3}{2}\bar{u}$, $\eta(x) \equiv \tanh(x/\xi)$,

$$\xi \equiv \hbar/\sqrt{m(u_+ n_0 + 2w_+ n_0^2)}$$



1st order transition point

Metastability limit of SF

Unstable

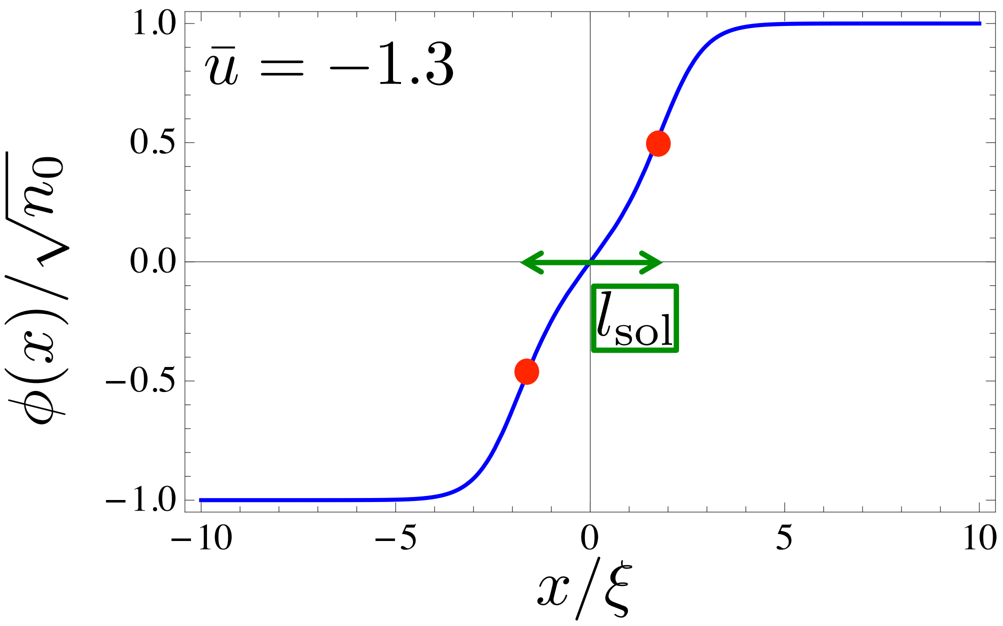
Metastable

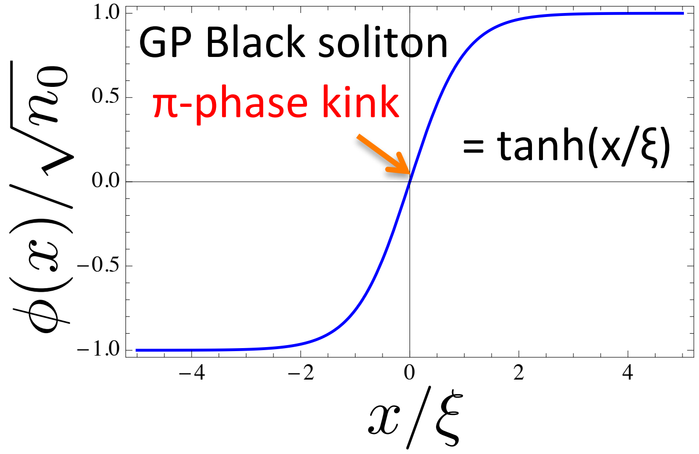
Ground state

-2

-4/3

We are here !!





- π-phase kink
- Dynamically stable in 1D

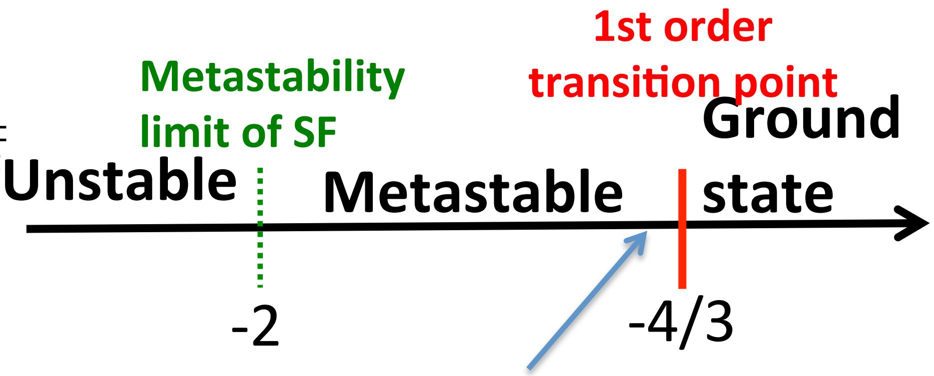
3.12. Case of -2< u_+<-4/3 (SF state is metastable)

Standing solitary wave (q=0):

$$\phi(x) = \sqrt{n_0} \times \frac{\sqrt{-\gamma}}{\sqrt{1-(1+\gamma)[\eta(x)]^2}}$$

where $\gamma \equiv 2 + \frac{3}{2}\bar{u}, \eta(x) \equiv \tanh(x/\xi),$

$\xi \equiv \hbar/\sqrt{m(u_+ n_0 + 2w_+ n_0^2)}$



1st order transition point

Metastability limit of SF

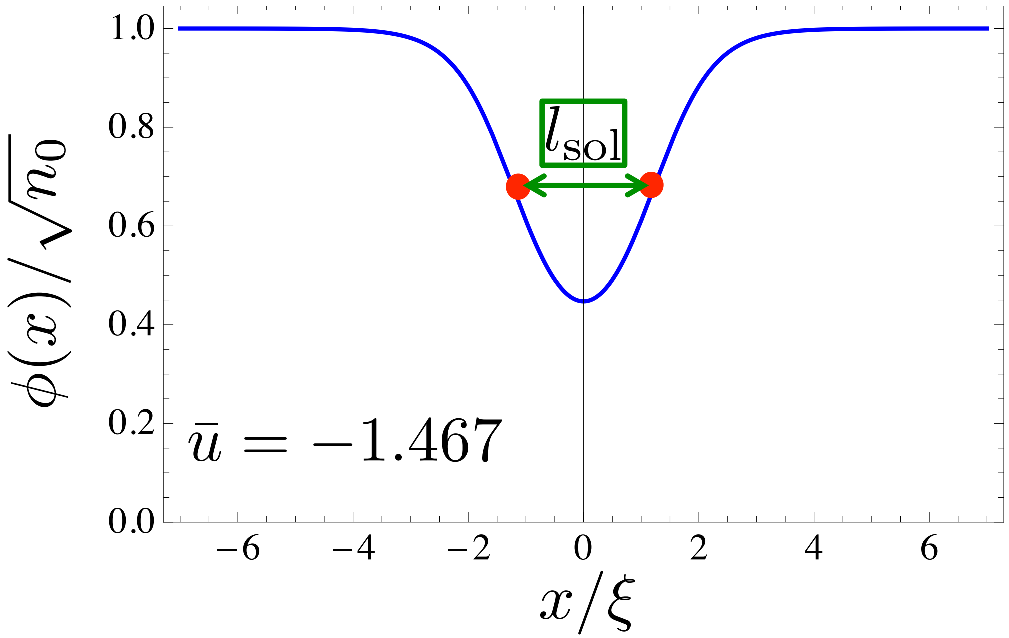
Unstable

Metastable

Ground state

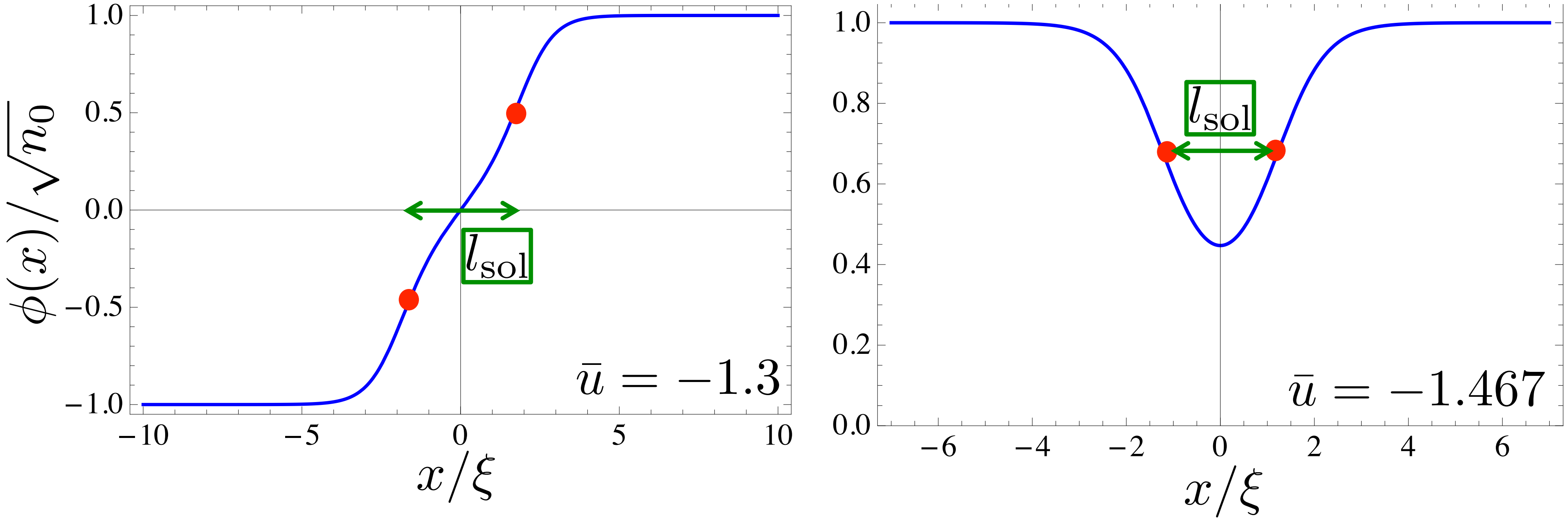
-2

-4/3

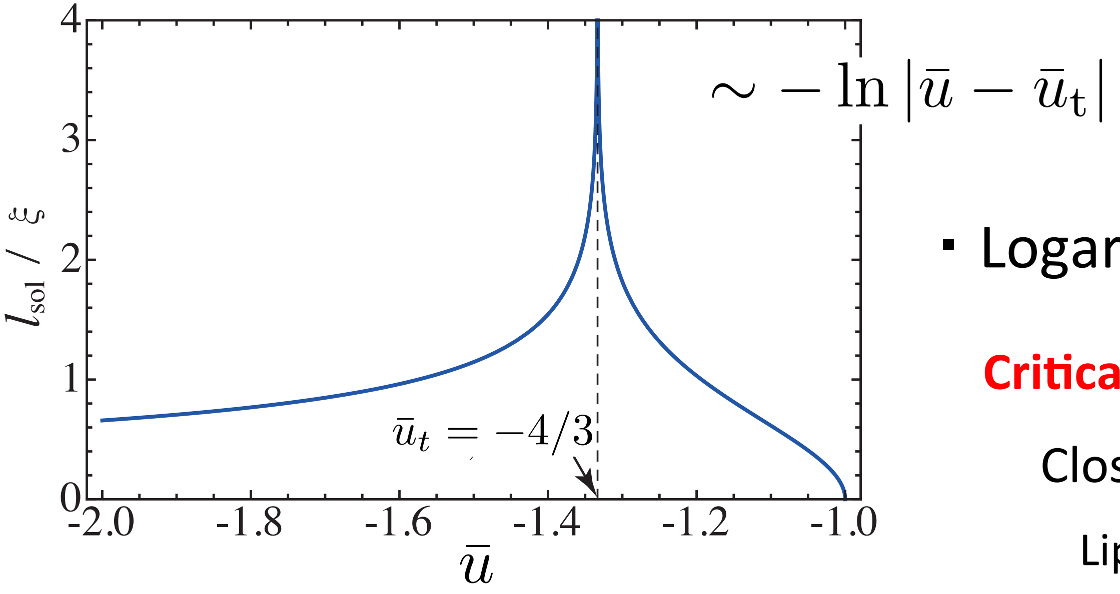


- No phase kink → **Bubble-like dark soliton !!!**

3.13. Divergence of the soliton size



- New inflection points when $\bar{u} < -1$



- Logarithmic divergence at $\bar{u} = \bar{u}_t$

Criticality at the first order transition !!

Closely related to surface criticality

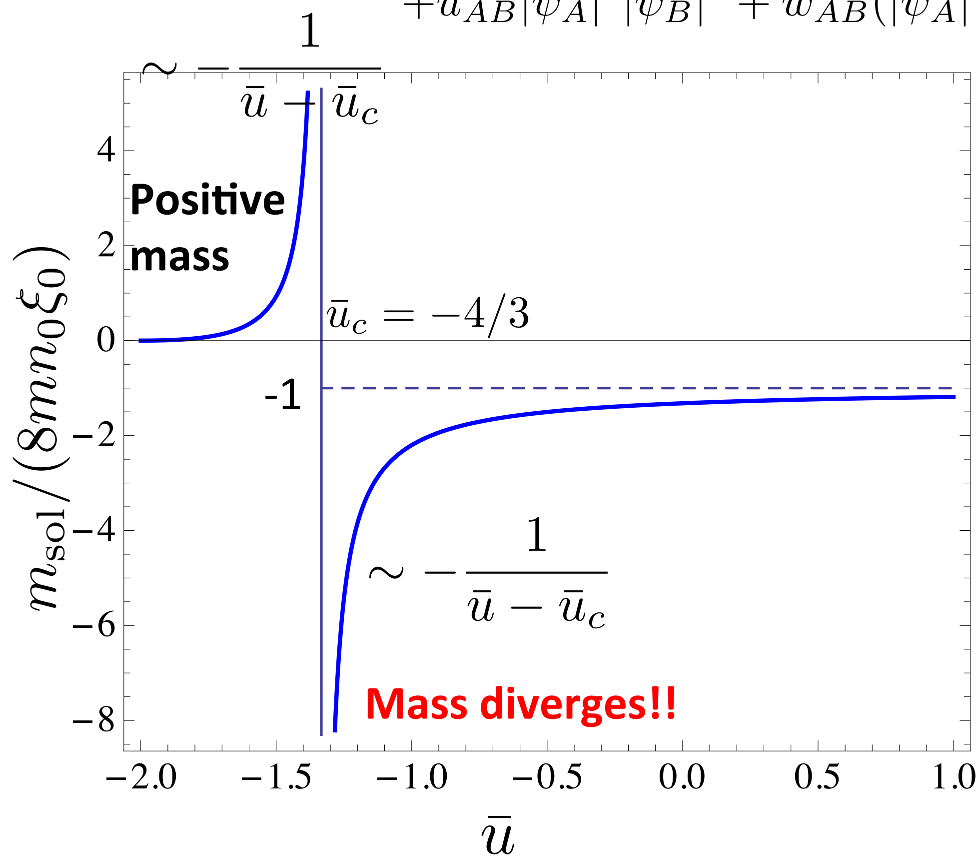
Lipowsky and Gompper, PRB (1984)

3.14. Soliton mass across the first order transition

Effective mass: $m_{\rm sol} \equiv 2\frac{\partial}{\partial(v^2)}\Delta E$ where v is the soliton velocity

$\Delta E \equiv E_{\rm sol} - E_{\rm gs}$ and the soliton energy is given by

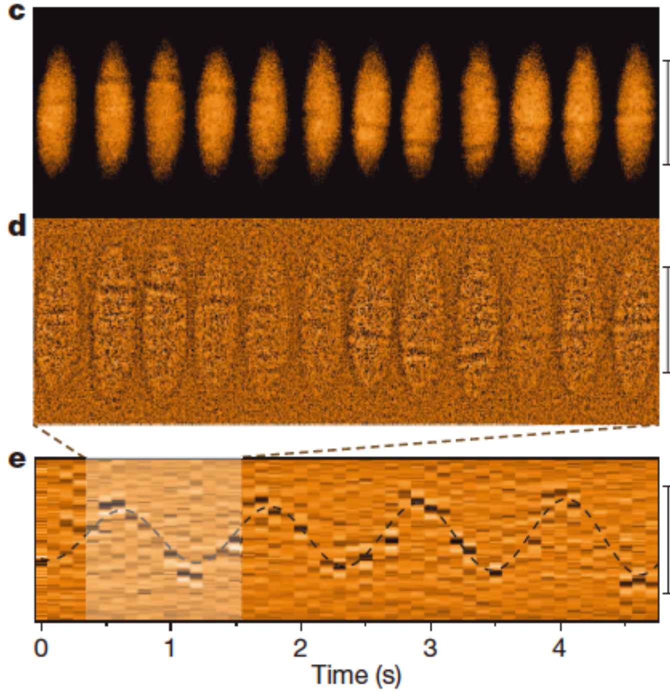
$$E = \int dx \left[\sum_\alpha \psi_\alpha^* \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - r + \frac{u}{2}|\psi_\alpha|^2 + \frac{w}{3}|\psi_\alpha|^4 \right) \psi_\alpha \right.$$
$$\left. + u_{AB}|\psi_A|^2|\psi_B|^2 + w_{AB}(|\psi_A|^2|\psi_B|^4 + |\psi_A|^4|\psi_B|^2) \right]$$

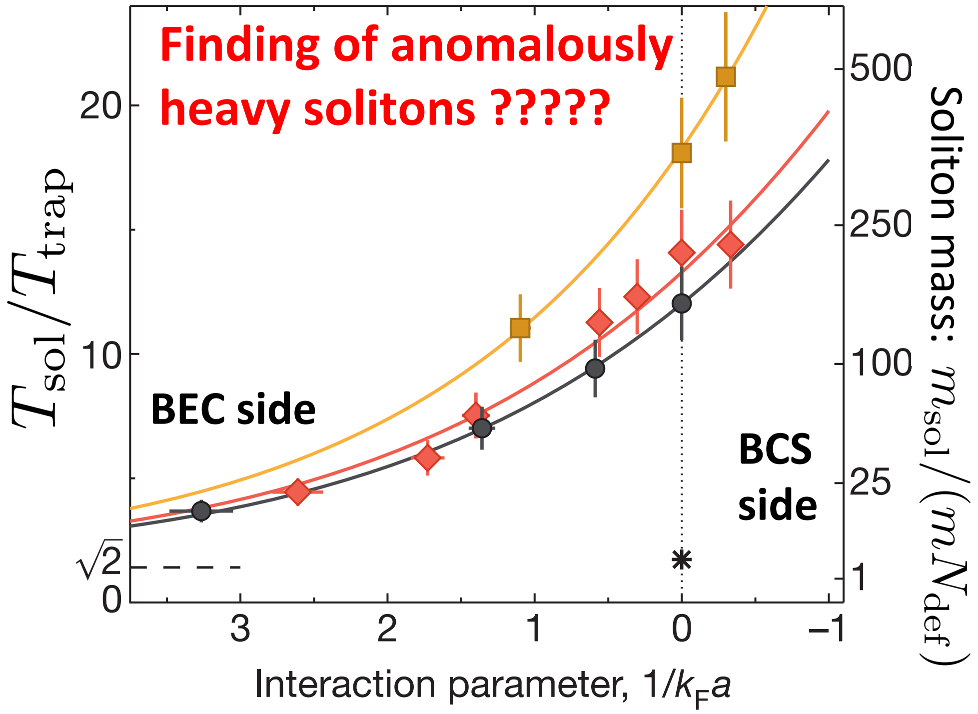


Divergence of the mass is stronger !!!

3.15. Heavy soliton ?? in unitary Fermi gases @ MIT

Yefsah et al., Nature (2013)





Finding of anomalously heavy solitons ?????

Soliton osc. period:

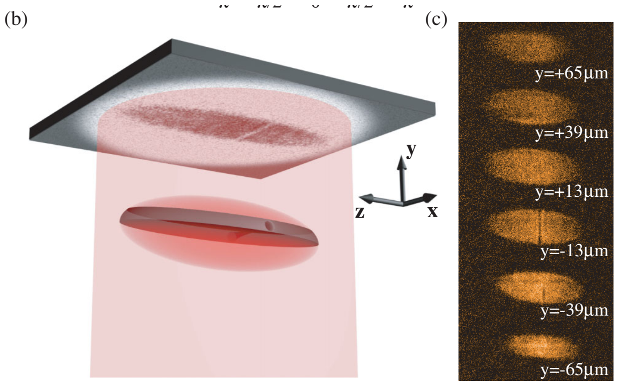
Harmonic osc. period:

$$\frac{T_{\rm sol}}{T_{\rm trap}} \propto \sqrt{\frac{m_{\rm sol}}{mN_{\rm def}}}$$

: Soliton mass

Eventually, it has been concluded that it is not a soliton but a vortex line !!!!!

Ku et al., PRL (2014)



Can there be such a heavy soliton??

Our solitary wave serves as the first example of such a heavy soliton !!!

3.16. Conclusions of part 2

- The first order Mott transition of a binary Bose mixture in 2D was confirmed by the quantum Monte Carlo simulations.
- Binary Bose mixtures in optical lattices near the first order Mott transition are described by the NLSE with cubic-quintic nonlinearity.
- There are two types of single solitary wave in the cubic-quintic NLSE: the standard one with π phase kink and the bubble-like one
- The soliton size and the soliton mass diverge at the first order transition point.

$$l_{\rm sol} \sim -\ln|\bar{u}-\bar{u}_c|, \;\; m_{\rm sol} \sim -\frac{1}{\bar{u}-\bar{u}_c}$$

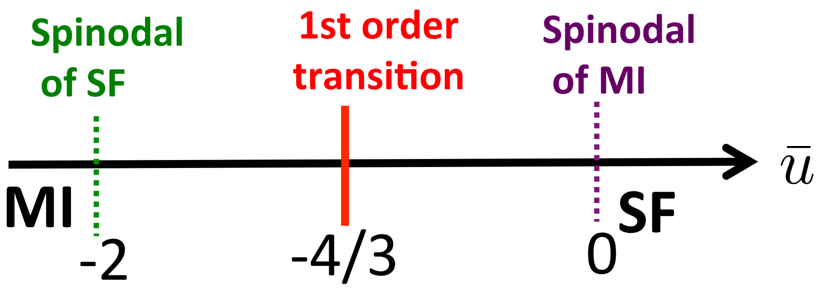
A sort of criticality in the first order transition !!!

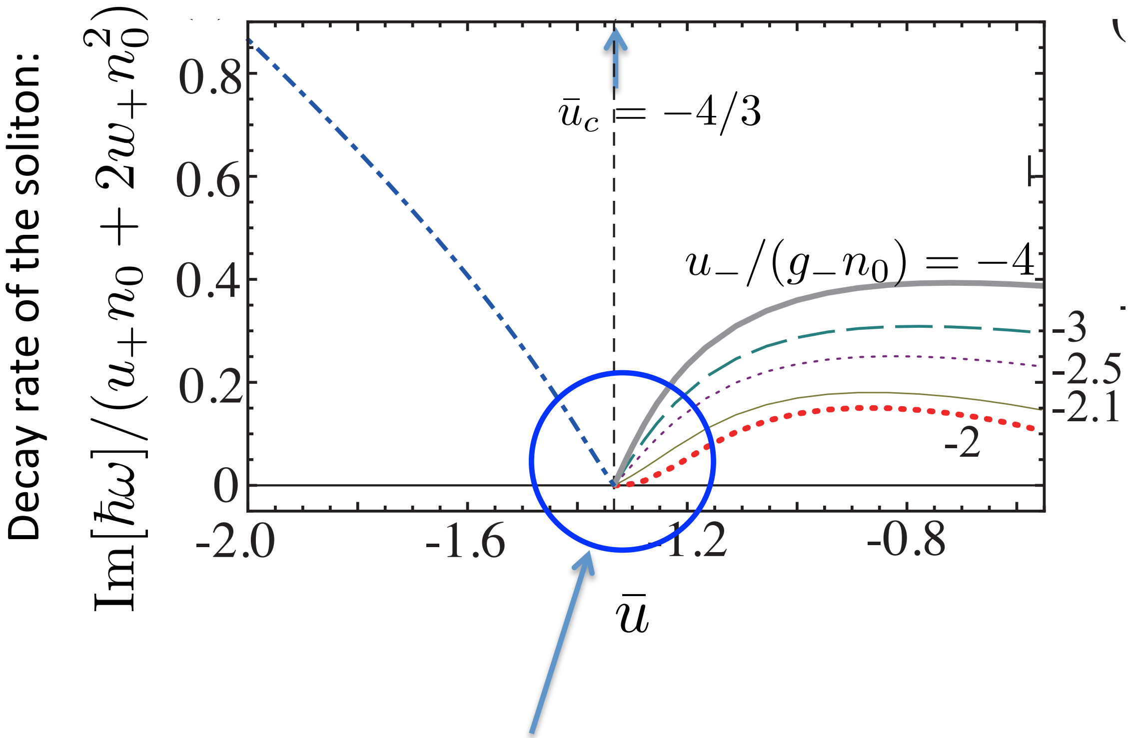
Y. Kato, D. Yamamoto, & I. Danshita, Phys. Rev. Lett. 112, 055301 (2014)
I. Danshita, D. Yamamoto, & Y. Kato, Phys. Rev. A 91, 013630 (2015)

Outlook:

There are many other interesting properties in the cubic-quintic NLSE, which are qualitatively different from the GP equation.

- **Stability of solitary waves**





- Dynamically unstable even in 1D (but lifetime can be long enough)

Appendix: Max-Planck Experiment

Endres *et al.*, Nature (2012).