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

3. Heavy solitary waves in a two-component Bose gas
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Takeru Nakayama
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Yasuyuki Kato
RIKEN → Univ. Tokyo

Daisuke Yamamoto
WIAS, Waseda Univ.
1.1. Schrödinger equation with cubic nonlinearity

Gross-Pitaevskii (GP) equation:

\[
\frac{i\hbar}{\partial t} \psi(r, t) = \left[ -\frac{\hbar^2 \nabla^2}{2m} + V(r, t) - \mu + \frac{4\pi\hbar^2 a_s}{m} |\psi(r, t)|^2 \right] \psi(r, t)
\]

Coupling constant for the two-body contact interaction:

\[ u = \frac{4\pi\hbar^2 a_s}{m} \]

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.


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

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

Increase the lattice depth \[ \frac{V_0}{E_R} = 0 \]  
Transition to the Mott insulator

Lattice depth:

Recoil energy:
\[ E_R = \frac{\hbar^2 \pi^2}{2md^2} \]

Shallow lattice → Superfluid
Particles are delocalized !!

Deep lattice → Mott insulator
Particles are localized !!

Atomic species: \(^{87}\text{Rb} \)
Lattice shape: Cubic

- 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:
     \[
     -\hbar^2 W \frac{\partial^2 \psi}{\partial t^2} = \left[ -\frac{\hbar^2}{2m_*} \nabla^2 - r + u|\psi|^2 \right] \psi
     \]
   - Notice the difference from the Gross-Pitaevskii eq. !!!
   - “Higgs” amplitude mode,
     Altman & Auerbach, PRL (2002)

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)
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

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

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

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

(more precisely, its two-component version)
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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, $\mu$: chemical potential

Near SF-MI transition

Time-dependent Ginzburg-Landau (TDGL) equation:

\[ iK \frac{\partial}{\partial t} \psi - W \frac{\partial^2}{\partial t^2} \psi = \left( -\frac{\nabla^2}{2m^*_\psi} + r + u |\psi|^2 \right) \psi \]

All the coefficients $K$, $W$, $m^*_\psi$, $r$, $u$ 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. $\psi \leftrightarrow \psi^\ast$. 
2.3. Collective modes in a homogeneous system

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

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

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

where \(S(x) = U(x) - V(x) \propto \delta \theta(x), T(x) = U(x) + V(x) \propto \delta n(x),\)

\[ |\psi_0|^2 = -r/u, \text{ and assume the plain wave solutions } S(x), T(x) \sim e^{ik \cdot x} \]

Dispersion of the NG mode: \(\omega^2 = (ck)^2\)
Dispersion of the Higgs mode: \(\omega^2 = (ck)^2 + \Delta^2\)
\[ c = \frac{1}{\sqrt{2m_* W}}, \Delta = \sqrt{-2r/W} \text{ Note } r = 0 \text{ at the Mott transition} \]
2.4. Beliaev decay of the Higgs mode into NG modes

Decay rate of the Higgs mode:
Altman & Auerbach, PRL (2002)

\[
\frac{\Gamma}{\Delta} \sim |\bar{U}_c - \bar{U}| \frac{D-3}{2}
\]

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

\[ T \approx 0.1J \]

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:

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

type (a)

type (b)
2.6. Dimensionless form

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

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

\[ \bar{v}_K = v_K/(-r_0W)^{1/2}, \quad \bar{v}_r = v_r/(-r_0), \quad \text{where } \xi = 1/(-m_*r_0)^{1/2} \]

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

Hereafter, we omit the bars for simplicity.

Note that in this unit

Sound speed: \( c = 1/\sqrt{2} \), \quad Higgs gap: \( \Delta = \sqrt{2} \)
2.7. Set of equations

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

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

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

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**:

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

**Higgs mode**:

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

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

We consider potential barriers of delta-function form:

\[ v_r(x) = V_r \delta(x), \quad v_K(x) = V_K \delta(x), \]

Solution of the static order parameter:

\[ \psi_0(x) = \tanh(|x| + x_0) \]

The constant \( x_0 \) is determined by the boundary condition:

\[ \psi_0'(-0) + 2V_r \psi_0(0) = \psi_0'(+0) \]

\[ \tanh(x_0) = \frac{-V_r + \sqrt{V_r^2 + 4}}{2} \approx \frac{1}{V_r} \text{ when } V_r \gg 1 \]
2.9. Higgs bound states

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

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

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

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

$A = B$ (even parity), $A = -B$ (odd parity)

Bound-state energy: $E_+, E_-$

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

The Higgs and NG modes are decoupled,
### 2.9. Higgs bound states

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

**NG mode:** 
\[
\left( -\frac{1}{2} \frac{d^2}{dx^2} - 1 + |\psi_0(x)|^2 + v_r(x) \right) S(x) = \omega^2 S(x) - \omega \psi_0(x)
\]

**Higgs mode:** 
\[
\left( -\frac{1}{2} \frac{d^2}{dx^2} - 1 + 3|\psi_0(x)|^2 + v_r(x) \right) T(x) = \omega^2 T(x) - \omega \psi_0(x)
\]

The Higgs and NG modes are decoupled,

\[
\psi_0(x) \qquad \Delta
\]

Lower energy than the bulk Higgs gap $\Delta$

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 $V_K \neq 0$, $V_r > 0$, and $\omega < \Delta$ breaks the p-h symmetry.

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

NG: $S(x) = \begin{cases} 
(\gamma(x) + ik_s)e^{ik_sx} + r_{ng}(\gamma(x) - ik_s)e^{-ik_sx}, & (x < 0), \\
\text{Incident} \\
\end{cases}$

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

Higgs: $T(x) = \begin{cases} 
(\gamma(x) + ik_s)e^{ik_sx} + r_{ng}(\gamma(x) - ik_s)e^{-ik_sx}, & (x < 0), \\
\text{Transmitted} \\
(\gamma(x) + ik_s)e^{ik_sx}, & (x > 0), \\
\end{cases}$

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

Boundary conditions:

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

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

All the coefficients, $r_{ng}$, $t_{ng}$, $A$, and $B$. 
2.11. Transmission probability

\[ T(E) = |t_{ng}|^2 = \frac{1}{1 + \frac{2E^2}{(2E^2 + 1)^2} V_{\text{eff}}(E)^2}, \quad (E < \Delta) \]

\[ V_{\text{eff}}(E) = (1 - V_K f(E)) V_r \]

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

\[ T(E) = |t_{ng}|^2 = \frac{1}{1 + \frac{2E^2}{(2E^2+1)^2} V_{\text{eff}}(E)^2}, \quad (E < \Delta) \]

\[ V_{\text{eff}}(E) = \left( 1 - V_K^2 f(E) \right) V_r \simeq V_r - \frac{\alpha V_K^2}{E - E_+} V_r. \quad \text{for } |E - E_+| \ll 1 \]

Direct scattering

Scattering through the even Higgs bound state.

\[(V_r, V_K) = (4, 4)\]

\[(4, 2)\]

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


**Outlook:**

- Response of the Higgs bound states to the lattice amplitude modulation.

- 2D

- Other condensed matter systems
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3.1. Bose-Bose mixture in optical lattices

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

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

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

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).

- First-order superfluid-Mott insulator transition

Altman et al., NJP (2003)
Mishra et al., PRA (2007)
Capogrosso-Sansone et al., PRA (2008)
etc.
3.2. Two-component Bose-Hubbard Model

\[ \hat{H} = \sum_{\alpha=A,B} \left[ -t_\alpha \sum_{\langle j,l \rangle} (\hat{b}_{j,\alpha}^\dagger \hat{b}_{l,\alpha} + \text{H.c.}) - \mu_\alpha \sum_{j} \hat{n}_{j,\alpha} + \frac{U_\alpha}{2} \sum_{j} \hat{n}_{j,\alpha}(\hat{n}_{j,\alpha} - 1) \right] + U_{AB} \sum_{j} \hat{n}_{j,A} \hat{n}_{j,B}, \]

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

This condition can be nearly satisfied in a gas of \(^{87}\text{Rb}\) 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 \( T=0 \)

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 !!!

Spin-1 case: T. Kimura et al., PRL (2005)

\( \rho = 1 \) MI

(\( \rho = 0 \) SCF order)

\( U_{AB}/U = 0.9 \)

\( \rho = 2 \) MI

(\( \rho = 3 \) MI \( \rho = 4 \) MI)

\( \rho = 0 \)

\( Z t/U \)

Is the 1st order transition real ??

SCF: Super-counter flow
Z: Coordination number

T. Ozaki et al., arXiv:1210.1370 (2012); D. Yamamoto et al., PRA 88, 033624 (2013)
3.4. QMC phase diagram at 2D and $U_{AB}/U=0.9$

MI: $n=2$

$Zt/U = 0.16$
$eta t = L$

$\mu/U$, $n_A + n_B$

Spinodal

Second order QPT

TCP

First order QPT

SF

L=12
L=16
TCP

$U_{AB}/U=0.9$
3.5. How to derive the effective action

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

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

\[
S_{AB} = \int \frac{\hbar}{2} d\tau \sum_j U_{AB} b_{A,j}^* b_{A,j} b_{B,j}^* b_{B,j}.
\]

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

- Stratonovich-Hubbard transformation to introduce \( \psi_\alpha \) fields
- Integrate out \( b_\alpha \) fields
- Cumulant expansion up to the sixth order w.r.t. the field \( \psi_\alpha \)
- Take the continuum limit

Effective action:

\[
S_{\text{eff}}[\psi_A, \psi_A^*, \psi_B, \psi_B^*] = \hbar \beta V f_0 + S_{\text{eff}}^A + S_{\text{eff}}^B + S_{\text{eff}}^{AB},
\]

where

\[
S_{\alpha}^\text{eff} = \int d\tau \int d^d x \left[ \hbar K_\alpha \psi_\alpha^* \frac{\partial \psi_\alpha}{\partial \tau} + \hbar^2 J_\alpha \left| \frac{\partial \psi_\alpha}{\partial \tau} \right|^2 + \frac{\hbar^2}{2m_\alpha} |\nabla \psi_\alpha|^2 \right.
\]

\[
- \left[ -r_\alpha |\psi_\alpha|^2 + \frac{u_\alpha}{2} |\psi_\alpha|^4 + \frac{w_\alpha}{3} |\psi_\alpha|^6 \right],
\]

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

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: $\psi_A(x, \tau) = \psi_B(x, \tau) = \phi$

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

assuming $w_+ > 0$

- $u_+ > 0$  \quad $r < 0$
  - Second order phase transition

- $r > 0$
  - Tricritical point

- $u_+ < 0$
  - First order phase transition
3.6. Mechanism for the first order transition

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

\[ u + u_{AB} = 0 \text{ @ TCP (} u_{AB} < 0 \text{)} \]

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

\[
u_{AB} = a^d Z^4 t_A^2 t_B^2 \left[ \left( \frac{g+1}{E_A^{(+)} - E_{g,g}} + \frac{g}{E_A^{(-)} - E_{g,g}} \right) \left( \frac{g+1}{(E_B^{(+)} - E_{g,g})^2} + \frac{g}{(E_B^{(-)} - E_{g,g})^2} \right) + \left( \frac{g+1}{E_B^{(+)} - E_{g,g}} + \frac{g}{E_B^{(-)} - E_{g,g}} \right) \left( \frac{g+1}{(E_A^{(+)} - E_{g,g})^2} + \frac{g}{(E_A^{(-)} - E_{g,g})^2} \right) \right.
\]

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

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

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

If \( U \sim U_{AB} \), these terms are strongly enhanced.
Why attractive?

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

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

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:
\[ \frac{\delta S^{\text{eff}}}{\delta \psi_\alpha} = 0, \quad \tau \rightarrow -i\tau \]

**Mean-field equation of motion:**

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


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

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

**Stationary solution:**
\[ \psi_\alpha(x, \tau) = \phi_\alpha(x) \]

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

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

\[ \phi_A = \phi_B \equiv \phi \]

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

We analytically solve this equation.
3.9. Stationary solution and first order transition

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

\[V(x) = 0, \; \phi(x) = \sqrt{n_0}\]
\[r = u_+n_0 + w_+n_0^2\]

We want to determine the first order transition point.

Free energy density:

\[f_{SF} = -2rn_0 + u_+n_0^2 + \frac{2}{3}w+n_0^3\]
\[f_{MI} = 0\]

\[f_{SF} = f_{MI}\]

\[\bar{u} = -\frac{4}{3}\]

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

Unstable | Metastability limit of SF | Metastable | 1st order transition point | Ground state \(\bar{u}\)
---|---|---|---|---
-2 | -4/3 | \(\bar{u}\)
3.10. Solution of a moving dark solitary wave

Problem:

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

\[
\phi(x) = \sqrt{n_0} A(x) e^{iS(x)}
\]

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

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

Boundary conditions:

\[
\lim_{x \to \pm \infty} A(x) = 1, \quad \lim_{x \to \pm \infty} S(x) = qx \pm \frac{\varphi}{2},
\]

Amplitude: 
\(A(x)\)

Phase: 
\(S(x)\)
3.10. Solution of a moving dark solitary wave

Solution: \[
\frac{\phi(x)}{\sqrt{n_0}} = Ae^{iS} = \frac{\sqrt{\alpha_+ + i \text{sgn}(q)\sqrt{\alpha_-}}} {\sqrt{\beta_+ - \beta_- [\eta(x)]^2}} e^{iq(x-x_s)}
\]

where \( \eta(x) \equiv \tanh(x/\xi) \),
\[
\xi \equiv \hbar/\sqrt{m(un + 2wn^2) - \hbar^2 q^2}
\]
\[
\alpha_\pm = \pm(-\gamma + 3\bar{q}^2) + \sqrt{\gamma^2 + 6\bar{q}^2}
\]
\[
\beta_\pm = 2 + \gamma \pm \sqrt{\gamma^2 + 6\bar{q}^2}
\]
\[
\gamma = 2 + 3\bar{u}/2,
\]
\[
\bar{q} = q\hbar/\sqrt{mw0^2}
\]

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

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

- $\bar{u} = -1.3$
- Dynamically stable in 1D

**GP Black soliton**

$$\phi(x) = \sqrt{n_0} \tanh(x/\xi)$$
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 $\gamma \equiv 2 + \frac{3}{2} \bar{u}, \eta(x) \equiv \tanh(x/\xi)$,

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

- No phase kink $\rightarrow$ 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: \( m_{\text{sol}} \equiv 2 \frac{\partial}{\partial (\psi^2)} \Delta E \) where \( \psi \) is the soliton velocity

\[ \Delta E \equiv E_{\text{sol}} - E_{\text{gs}} \]

and the soliton energy is given by

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

\( u \rightarrow u_c \)

\( m_{\text{sol}} \rightarrow (8\hbar m \xi_0) \)

\( \bar{u}_c = -4/3 \)

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: \( \frac{T_{sol}}{T_{trap}} \propto \sqrt{\frac{m_{sol}}{m N_{def}}} \)

Harmonic osc. period: \( \frac{T_{sol}}{T_{trap}} \)

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 $\pi$ phase kink and the bubble-like one.

- The soliton size and the soliton mass diverge at the first order transition point.

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

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


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