# Spin-1/2 fermions:

## Crossover from weak to strong attractive interaction

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## Spin-1/2 Fermions in an Optical Lattice

- optical lattice stabilizes molecules
- BCS state appears in the lattice
- Mott insulator appears in the lattice



#### **Attractive Interaction:** Molecules vs Cooper Pairs

Cooper pairs are global objects with U(1)-symmetry breaking

Molecules are local objects with broken translational symmetry

Molecules can BE condense  $\longrightarrow U(1)$ -symmetry breaking



Hamiltonian for short-range interaction:

$$H = -\bar{t} \sum_{\langle r,r' \rangle} \sum_{\sigma=\uparrow,\downarrow} c^{\dagger}_{r\sigma} c_{r'\sigma} - J \sum_{\langle r,r' \rangle} c^{\dagger}_{r\uparrow} c_{r'\uparrow} c^{\dagger}_{r\downarrow} c_{r'\downarrow}$$
$$-\mu \sum_{r} \sum_{\sigma=\uparrow,\downarrow} c^{\dagger}_{r\sigma} c_{r\sigma}$$

#### Variational States

BCS state:

$$|\Phi_{BCS}\rangle = \prod_{k} (u_k + v_k c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow})|0\rangle$$

molecular state:

$$|\Phi_m\rangle = \prod_r (u_r + v_r c_{r\uparrow}^{\dagger} c_{r\downarrow}^{\dagger})|0\rangle$$

$$|u_k|^2 + |v_k|^2 = |u_r|^2 + |v_r|^2 = 1$$

## **Mean-Field Theory**

$$\langle \Phi_{BCS} | H | \Phi_{BCS} \rangle = -\int_k (\epsilon_k + \mu) |v_k|^2 - J \Big| \int_k u_k v_k^* \Big|^2$$

minimum:

$$\Delta_k = J \int_p \frac{\Delta_p}{\epsilon_p^2 + \Delta_p^2}, \quad v_k^2 = \frac{\Delta_k}{\epsilon_k^2 + \Delta_k^2}$$

$$\langle \Phi_m | H | \Phi_m \rangle = -\mu \sum_r |v_r|^2 - 2J \sum_{\langle r, r' \rangle} (u_r v_r^*) (v_{r'} u_{r'}^*)$$

minimum:  $v_r = v$ 

$$v^2 = \frac{1}{2}(1 + \frac{\mu}{2J})$$

constant  $v_r, v_k$ 

$$\langle \Phi_{\dots} | H | \Phi_{\dots} \rangle = J v^4 - a v^2$$

#### **Molecular Gas**

 $\overline{t} = 0$ 

Hamiltonian:

$$H = -J \sum_{\langle r,r' \rangle} c^{\dagger}_{r\uparrow} c_{r'\uparrow} c^{\dagger}_{r\downarrow} c_{r'\downarrow} - \mu \sum_{r} \sum_{\sigma=\uparrow,\downarrow} c^{\dagger}_{r\sigma} c_{r\sigma}$$

Exactly solvable models:

1D hard-core Bose gas

*N*-component Bose gas:  $N \to \infty$ 

Theory of 1D Hard-Core Bose Gas:

Hard-core Bosons  $\longleftrightarrow$  Free Fermions



Density of a 1D Bose Gas in an optical lattice with harmonic potential





## **Density-Density Fluctuations**



#### Static Structure Factor

 $\xi_{ol} = 1/k^* \sim |\zeta - \zeta_c|^{-1/2}$ 

FT der Korrelationsfunktionen x\_0=0, mu\_0=0.3 , Omega=0 0.0014 w=0.3500 w=0.3502 w=0.3504 w=0.3506 0.0012 w=0.3508 w=0.3510 \_ . \_ . \_ . \_ 0.001 0.0008 0.0006 S(k) 0.0004 0.0002 0 -0.0002 0.4 0.2 0.6 0.8 0 1 0-10 <sup>k</sup>

#### Characteristic wavevector $k^*$

for J = 0.2 (solid), J = 0.5 (dashed), J = 0.8 (dotted)



Tonks-Girardeau gas:  $k^* = k_F = 2\pi n$ 

## N-component Bose Gas

$$H = -\sum_{\langle r,r'\rangle} \sum_{\sigma,\sigma'=1}^{N} J_{\sigma\sigma'} c_{r\sigma}^{\dagger} c_{r'\sigma} c_{r\sigma'}^{\dagger} c_{r'\sigma'}$$

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special cases:

$$J_{\sigma\sigma'} = J/N$$
$$J_{\sigma\sigma'} = J\delta_{\sigma\sigma'}$$

 $-N \rightarrow \infty$  can be solved exactly

-1/N-expansion is available

Total density & condensate density in the N-component Bose Gas





## **Atom-Molecule Mixture: Functional Integral**

partition function:

$$Z = Tre^{-\beta H} = \int e^{-S} \mathcal{D}[\psi]$$

action:

$$\begin{split} S &= \sum_{x} (\psi_{x,\uparrow} \bar{\psi}_{x,\uparrow} + \psi_{x,\downarrow} \bar{\psi}_{x,\downarrow}) - \sum_{r,r',t} (\zeta \delta_{r,r'} + \bar{t} w_{r,r'}) (\psi_{r,t,\uparrow} \bar{\psi}_{r',t+1,\uparrow} + \psi_{r,t,\downarrow} \bar{\psi}_{r',t+1,\downarrow}) \\ &- J \sum_{r,r',t} \psi_{r,t,\uparrow} \bar{\psi}_{r',t+1,\uparrow} \psi_{r,t,\downarrow} \bar{\psi}_{r',t+1,\downarrow} \\ \zeta &= e^{\mu} \end{split}$$

## Densities

averaging:

$$\langle ... \rangle = \frac{1}{Z} \int ... e^{-S} \mathcal{D}[\psi]$$

fermionic density

$$n_{f,x} = -\langle \psi_{x,\uparrow} \bar{\psi}_{x,\uparrow} + \psi_{x,\downarrow} \bar{\psi}_{x,\downarrow} + 2\psi_{x,\uparrow} \bar{\psi}_{x,\uparrow} \psi_{x,\downarrow} \bar{\psi}_{x,\downarrow} \rangle$$

molecular density

$$n_{m,x} = \langle 1 + \psi_{x,\uparrow} \bar{\psi}_{x,\uparrow} + \psi_{x,\downarrow} \bar{\psi}_{x,\downarrow} + \psi_{x,\uparrow} \bar{\psi}_{x,\uparrow} \psi_{x,\downarrow} \bar{\psi}_{x,\downarrow} \rangle$$

#### Conventional Form of the action

time shift

$$\bar{\psi}_{r,t,j} \to \bar{\psi}_{r,t-1,j} \quad (j=\uparrow,\downarrow)$$

action

$$S = \sum_{x} (\psi_{x,\uparrow} \partial_t^T \bar{\psi}_{x,\uparrow} + \psi_{x,\downarrow} \partial_t^T \bar{\psi}_{x,\downarrow})$$
$$- \sum_{r,r',t} (w_{\parallel} \delta_{r,r'} + w_{r,r'}) (\psi_{r,t,\uparrow} \bar{\psi}_{r',t,\uparrow} + \psi_{r,t,\downarrow} \bar{\psi}_{r',t,\downarrow})$$

$$-w_{\perp} \sum_{r,r',t} \psi_{r,t,\uparrow} \bar{\psi}_{r',t,\uparrow} \psi_{r,t,\downarrow} \bar{\psi}_{r',t,\downarrow}.$$

decoupling by a Hubbard-Stratonovich field:

 $(i\phi_x + \chi_x)\psi_{x,\uparrow}\psi_{x,\downarrow} + h.c.$ 

 $\phi, \chi$  are complex fields

#### **Effective Bosonic Action**

$$S_{eff} = (\phi, v^{-1}\phi) + \frac{1}{2J}(\chi, \chi) - \frac{1}{2}\log(\det A)$$

antisymmetric space-time matrix:

$$A = \begin{pmatrix} 0 & i\phi + \chi & \zeta + \bar{t}w - \partial_t^T & 0\\ -i\phi - \chi & 0 & 0 & \zeta + \bar{t}w - \partial_t^T\\ -\zeta - \bar{t}w + \partial_t & 0 & 0 & i\bar{\phi} + \bar{\chi}\\ 0 & -\zeta - \bar{t}w + \partial_t & -i\bar{\phi} - \bar{\chi} & 0 \end{pmatrix}$$
$$v^{-1} = (w + 2\mathbf{1})^{-1}/J.$$

Partition Function:

$$Z = \int e^{-S_{eff}} \mathcal{D}[\phi]$$

Dissociation of Atoms







density of individual fermions (dissociated atoms)





densities vs. interaction

#### Mixture of two Fermion Gases

Two types of fermionic atoms with different mass: e.g.  $^6\mathrm{Li}$  and  $^{40}\mathrm{K}$  Hamiltonian

$$H = -\bar{t}_c \sum_{\langle r,r'\rangle} c_r^{\dagger} c_{r'} - \bar{t}_f \sum_{\langle r,r'\rangle} f_r^{\dagger} f_{r'} + \sum_r \left[ -\mu(c_r^{\dagger} c_r + f_r^{\dagger} f_r) + U f_r^{\dagger} f_r c_r^{\dagger} c_r \right]$$

f atoms are heavy:  $\overline{t}_f \approx 0$ Realization as Correlated Disorder: Green's function (for  $\Delta \to 0$ )

$$G = \langle [-\partial_t + 1 - \Delta(\mu - \hat{t} + U\mathbf{I})]^{-1} \rangle_{\text{Ising}}$$

average  $\langle ... \rangle_{\text{Ising}}$  with respect to the distribution  $(\mathbf{I} = (1 - S)/2)$ 

$$P(\{S(r)\}) = \frac{e^{\mu\beta\sum_{r}\mathbf{I}(r)}\det[\mathbf{1} + \{1 - \Delta(\mu - \hat{t} + \mathbf{I})\}^{\beta/\Delta}]}{\sum_{\{S(r)=\pm 1\}} e^{\mu\beta\sum_{r}\mathbf{I}(r)}\det[\mathbf{1} + \{1 - \Delta(\mu - \hat{t} + U\mathbf{I})\}^{\beta/\Delta}]}$$

Typical Configurations of Heavy Atoms



Paramagnetic phase:  $t = 1, U = 3, \mu = U/2, \beta = 3$ 



 $t = 1, U = 3, \mu = U/2, \beta = 7$ 



 $t = 1, U = 3, \mu = U/2, \beta = 14$ 



Density of States for Light Atoms



DOS for U = 3,  $\mu = U/2$  (half filling) and decreasing temperatures.  $\beta = 3, 7, 10, 14$ 



DOS at  $\beta = 3$  for increasing interaction U and half-filling ( $\mu = U/2$ ). U = 1, 4, 6, 8

## Conclusions

BCS vs. molecular states:

Mean-field approach does not provide unique solution

Model for tunneling of fermions and molecules: Molecules and fermions compete in an optical lattice

#### Molecular Gas:

1D and  $N \to \infty$  can be treated exactly for BEC and Mott insulator

### Mixture of fermionic atoms and molecules:

Interaction favors formation of molecules at low density and dissociation at high densities

### Mixture of light and heavy atoms:

Heavy atoms represent correlated disorder for light atoms