Renormalization Group Approach from Ultra Cold Atoms to the Hot QGP Yukawa Institute for Theoretical Physics, Kyoto, Japan

One-dimensional Fermi gases: Density-matrix renormalization group study of ground state properties and dynamics

30 August 2011 Masaki TEZUKA (Kyoto University)

Plan of the talk

- Introduction
 - Low-dimensional cold atom systems
 - Density-matrix renormalization group
- <u>Harmonically trapped imbalanced system</u>
 - Larkin-Ovchinnikov state
- Optical lattice with disorder
 - Proving superfluidity by dynamics
- Collision dynamics
 - Non-classical reflectance
- Summary

PRL **100**, 110403 (2008) New J. Phys **12**, 055029 (2010) PRA **82**, 043613 (2010)

arXiv: 1107.0774



Collaborators

- Masahito Ueda (University of Tokyo)
 - Harmonically trapped imbalanced system

PRL **100**, 110403 (2008) New J. Phys **12**, 055029 (2010)

• Antonio M. García-García (Cambridge University)

- Optical lattice with disorder

PRA 82, 043613 (2010)

- Jun'ichi Ozaki (Kyoto University)
- Norio Kawakami (Kyoto University)
 Collision dynamics

arXiv: 1107.0774



Low-dimensional cold atom systems



→ Berezinskii-Kosterlitz-Thouless (BKT) transition is observed Hadzibabic *et al.*: Nature **441**, 1118 (2006)

WS Bakr et al.: Nature 462, 74 (2009)

Low-dimensional cold atom systems



- Low-dimensional but not necessarily solvable
- How to simulate numerically without uncontrollable approximations?

Density-Matrix Renormalization Group (DMRG) environment block System S = B + s + s' + B'

 $\left|\Psi_{ijj'i'}\right\rangle = c_{ijj'i'} \sum_{iii'i'} \left|\phi_{i}\right\rangle \left|\chi_{j}\right\rangle \left|\chi_{j'}\right\rangle \left|\phi_{i'}\right\rangle$



Partial density matrix for the left block L ($k \equiv (ij)$)

$$\rho_{kk'} = \sum_{i'j'} |\Psi_{kj'i'}\rangle \langle \Psi_{kj'i'}| = \sum_{i'j'} c_{kj'i'} c_{k'j'i'}^*$$





Has all information on L = B + s when S is in the **target state** $|\Psi>$

Diagonalize p : states with larger eigenvalues are more important

cf. In NRG (numerical renormalization group) the lowest energy states are kept

Reduce the dimension to *m* of the Hilbert space for L

= "renormalization"

S. R. White: PRL (1992) PRB (1993) **Reviews**: Schollwöck: Ann. Phys. **326**, 96 (2011), RMP 77, 259 (2005) Hallberg: Adv. Phys. 55, 477 (2006)



Iterate until the desired system size is reached

Finite system DMRG



One of the blocks can be made longer iteratively

Finite system DMRG



Iterate until physical quantities (e.g. energy) converge

Application of DMRG: Low-dimensional quantum systems

DMRG: variational method Error in ground state energy is positive, and decrease as # of states *m* is increased 1D Heisenberg model (White: PRB **48**, 10345 (1993))

DMRG publications from 1994 to 2009

Annual number of

(a) published papers on the topic "density-matrix-renormalization" and
 (b) citations to Steve White's original paper [PRL 69, 2863-2866 (1992)].
 Data from the ISI Web of Science database at http://apps.isiknowledge.com/

Eric Jeckelmann, April 16, 2010

http://www.itp.uni-hannover.de/~jeckelm/ dmrg/paper_stat5.pdf

Application of DMRG: Low-dimensional quantum systems

Mixtures of bosons and fermions Fractional Quantum Hall systems Spin-polarized half-filled fermions + bosons (Landau levels: effectively 1D) Mering and 0.7 O DMRG (c) $L_{\alpha}/L_{y}=2.3$ Fleischhauser: (a) $L_{\alpha}/L_{y}=1.3$ (b) $L_x/L_y=1.8$ ED 2nd order -9.26-10.90-12.32PRA 81, 011603 -4.63-(R) (2010) -5.45 0 -6.168 x 0 X 0 X 0 4.63 0.55 Phase separation 5.45 $(0_{-}=0)$ 9.26 6.16 between CDW and 0.5<u></u> 0 10.900.07 0.05 0.06 0.09 0.1 0.01 0.02 0.03 0.04 0.08 Mott insulator 8 8 12.32 bosonic hopping J (a) v = 8/271.2 0.8 0.4 (b) v = 2/9(C) -12.70-10.09* fermions o bosons -6.35-5.04^λ↑ CDW/SC Correlated electrons + phonons X 0 X 0 5.04 6.35 $\mathbb{C}($ 10.09 12.70 8.41 SD Phase diagram of Hubbard-Holstein model Shibata and Yoshioka: PRL 86, 5755 (2001) U Tezuka, Arita and Aoki: PRB 76, 155114 (2007)

Also, quantum chemistry, 2D & 3D classical systems, ...

Two-component Fermi gas

Neutral atoms: bosons or fermions depending on parity of A + Z (nucleon number + electron number)

Atom: fine structure, hyper fine structure electron spin *S*, orbital degrees of freedom, nuclear spin *I*

Fermions in two hyperfine states:

Loss due to three-body collisions is rare - Pauli principle (pseudo-) spin population preserved

→ Fermi gas with fixed spin imbalance can be realized

Feshbach resonance

A (highly excited) molecular state close to $E_{\rm B}$ =0 can modify the scattering length

When the open and close channels differ in magnetic moment, we can utilize Rapid change of scattering length as function of magnetic field *B*

→ interaction (including sign) can be controlled

For equal number of atoms,

BEC-BCS crossover

BEC : Bosons might break into fermions at energy Δ , but Δ is not correlated with T_c BCS-type condensate : Pairing gap Δ is in proportion to T_c (density determines T_c)

BEC of diatomic molecules : smoothly connected with BCS condensate? Theory: Eagles (1969), Leggett (1980), Nozières and Schmidt-Rink (1985), ...

Experiment for the same number of Fermi atoms in two of the hyperfine states:

1) Harmonically trapped imbalanced system

Motivation: condensation of population imbalanced fermions in elongated traps

Zwierlein *et al.*(MIT): Science **311**, 492 (2006) Partridge *et al.*(Rice): Science **311**, 503 (2006)

More recent experiment:

- Nascimbène et al. (ENS): Nature 463, 1057 (2010)
- → Discrepancy in cloud shape and maximum imbalance *P* for condensate

 $P = (N_{\uparrow} - N_{\downarrow}) / (N_{\uparrow} + N_{\downarrow})$

Q. What happens when the atom trap is essentially 1D?

s-wave scatt. length ($\propto g^{-1}$)

$$a_{\rm 1D} = -\frac{a_{\perp}^2}{2a} \left(1 - C \ \frac{a}{a_{\perp}}\right)$$

Kinetic energy << level separation of the radial trap

Olshanii: PRL 1998 2D optical lattice \rightarrow array of 1D traps realized

(Esslinger group, ETH Zürich; Hulet group, Rice) I. Bloch: Nature Phys. (2005)

(Situation in 2006-2008) 3D: Controversy over experiments

→ What happens in 1D?

DMRG simulation of continuous system with the lattice introduced

Smaller lattice spacing \rightarrow continuum limit approached

Density difference: shows oscillation incommensurate with lattice

Pair correlation

$$\left\langle \Psi_{0}^{(N)} \left| \hat{c}_{i,\downarrow}^{\dagger} \hat{c}_{j,\uparrow}^{\dagger} \hat{c}_{j,\downarrow} \hat{c}_{j,\downarrow} \right| \Psi_{0}^{(N)} \right\rangle \approx \Delta (z_{i})^{*} \Delta (z_{j})$$

Pair correlation

$$\left\langle \Psi_{0}^{(N)} \left| \hat{c}_{i,\downarrow}^{\dagger} \hat{c}_{j,\uparrow}^{\dagger} \hat{c}_{j,\downarrow} \hat{c}_{j,\downarrow} \right| \Psi_{0}^{(N)} \right\rangle \approx \Delta (z_{i})^{*} \Delta (z_{j})$$

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Condensate? – two-body density matrix

N Fermions in *M* states:

Maximum possible eigenvalue = $N(M-N+2)/M \sim N$

(C.N. Yang, RMP 1962)

→ Measure of pair condensation

$$\rho_{ii',jj'}^{(2)} \equiv \langle \psi_0 | \hat{c}_{i',\downarrow}^{\dagger} \hat{c}_{i,\uparrow}^{\dagger} \hat{c}_{j,\uparrow} \hat{c}_{j',\downarrow} | \psi_0 \rangle$$

L⁴ matrix elements for *L*-site chain

Diagonalize to obtain eigenvalue distribution

Eigenfunction: state occupied by (\uparrow, \downarrow) pairs

cf. Condensate fraction for Bose gas - one-body DM

Eigenvalue distribution

Most of minority atoms contribute to quasi-condensate

LO condensate at trap center (())

Pair correlation: periodic sign change

P=0.1

P = 0.3

1D: LDA (local density approximation) results Exact solution for system without trap

(Yang's generalied Bethe ansatz → Gaudin's integral equation)

Orso, PRL 98, 070402 (2007)

Hu, Liu and Drummond, PRL 98, 070403 (2007)

→ Consistent with our DMRG results

1D Experiment (Rice group)

Conclusion: (1)

0.6

Imbalance parameter P 0.10.2 0.4

a=2∆k

Population imbalance + harmonic trap

- Pairing? → LO (quasi-) condensate
- Phase separation? \rightarrow Yes (LO at center)
- Upper limit in imbalance *P* for condensation?

 not observed

M. Tezuka and M. Ueda:

80

PRL 100, 110403 (2008); NJP 12, 055029 (2010)

see also:

Feiguin and Heidrich-Meisner: PRB 76, 220508R (2007); PRL 102, 076403 (2009) (Ladder); Lüscher, Noack, and Läuchli: PRA 78, 013637 (2008); Batrouni et al.: PRL 100, 116405 (2008) (QMC) Machida, Yamada, Okumura, Ohashi, and Matsumoto: PRA 77, 053614 (2008); Rizzi et al.: PRB 77, 245105 (2008); Machida et al.: PRB 78, 235117 (2008)

2) Optical lattice with disorder

Now widely controllable in cold Fermi atomic gases

- Optical lattice laser standing wave
 - Bichromatic lattice [Roati *et al.*: Nature **453**, 895 (2008)]
- Holographic potential imprinting in 2D
 - M. Greiner's group [Gillen *et al.*: PRA 2009; Bakr *et al.*: Nature 2009]

Experimental realization

- Optical lattice ← laser standing wave
 - Bichromatic lattice
 - G. Roati *et al.*, Nature 453, 895 (2008) (Firenze-Rome Trento)
- Another possibility: holographic potential imprinting in 2D
 - M. Greiner's group
 - J. I. Gillen et al., PRA 80, 021602(R) (2009)
 - W.S. Bakr *et al.*, Nature 462, 74 (2009)

Our motivation: what happens in 1D?

- Quantum fluctuation suppresses true long range order (even for T=0)
- Finite system : can have condensate (superfluid)
- Is coherence length O(system size)?

Can be studied with numerically exact low-energy methods (Here we use DMRG)

Existing results

- Speckle potential (Gaussian random)
 - All eigenstates exponentially localized
 - L. Sanchez-Palencia *et al.*: PRL 98, 210401(2007)
 - A.M. García-García and E. Cuevas: PRB 79, 073104 (2009)
- Fibonacci potential ABAABABA ...
 - J. Vidal et al.: PRL 83, 3908 (1999), PRB 65, 014201 (2001); K. Hida: PRL 86, 1331 (2001)
 - Critical irrespective of the strength of λ
- Bichromatic potential

"Aubry-Andre model"

$$V(n) \equiv \lambda \cos(2\pi\omega n + \theta)$$

- non-interacting : metal-insulator transition at $\lambda = 2J$ (J: hopping)
- Numerical studies of interacting systems
 - Bose Hubbard (DMRG): Deng *et al.*: PRA 78, 013625 (2008); Roux *et al.*: PRA 78, 023628 (2008)
 - Spinless Fermions : Chaves and Satija (ED, PRB 55, 14076 (1997)); Schuster et al. (PBC DMRG, PRB 65, 115114 (2002))

Quasiperiodic potential

Modeled by a single-band Hubbard model with site level modification

Formulation: Hubbard model + quasiperiodic potential

- Ratio of consective Fibonacci numbers → golden ratio (=irrational number) as k→∞
- $(N_{\sigma}, L) = (10,90), (26, 234), (42, 378) : v=2/9$
- Non-interacting case: all eigenstates become critial at $\lambda = 2J$

One-electron level scheme (non-interacting)

Interaction strength

Negative U: |interaction energy| linearly increase as |U| is increased Positive U: it has a peak because double occupancy is suppressed as $U \rightarrow$ large

How to detect pairing and delocalization?

<u>Pairing</u>

<u>On-site pair correlation function</u>: easy to calculate with DMRG Depends on the site potentials of the site pair <u>Averaged equal-time pair structure factor</u>

Sum of pair correlation for all lengths

➔ average over sites

cf. Hurt *et al.*: PRB 72, 144513 (2005); Mondaini *et al.*: PRB 78, 174519 (2008)

$$\Gamma(i,r) \equiv \left\langle \hat{c}_{i+r,\downarrow}^{\dagger} \hat{c}_{i+r,\uparrow}^{\dagger} \hat{c}_{i,\uparrow} \hat{c}_{i,\downarrow} \right\rangle$$
$$P_{s} \equiv \left\langle \sum_{r} \Gamma(i,r) \right\rangle_{i}$$

Increasing function of *L* if decay of correlation is slow

Delocalization

<u>Phase sensitivity</u>: requires (anti-)periodic condition [see *e.g.* Schuster *et al.*: PRB 65, 115114 (2002)] Hard to calculate within DMRG (not open BC) in large systems (OK for small systems)

Inverse participation ratio (IPR)

 $I_{E} \equiv \left(\sum_{i} \left(\left\langle \hat{n}_{i} \right\rangle_{N+1,N+1} - \left\langle \hat{n}_{i} \right\rangle_{N,N} \right)^{2} \right)^{-1}$

Add 2 atoms - How uniformly is the population increase distributed?

Compare between different system sizes

The case without disorder (λ =0)

Pair structure factor indicator of global (quasi long-range) superfluidity Inverse participation ratio indicator of atom delocalization

Both increase with |U|, and system size L

λ

Spin gap

Minimum energy to break a pair by spin flipping

Schematic phase diagram

- Effect of coexisting disorder (bichromatic potential) and short-range attractive interaction
 - Studied for 1D fermionic atoms on optical lattice

What about dynamics?

• Many experiments observe the dynamics of the atomic clouds after release from a trap

Bosons: E. Lucioni et al. (LENS, Florence): PRL 106, 230403 (2011)

Subdiffusion observed in bichromatic lattice (3D)

 $V(x) = V_1 \cos^2(k_1 x) + V_2 \cos^2(k_2 x), k_1 = 2\pi/(1064.4 \text{nm}), k_2 = 2\pi/(859.6 \text{nm})$ 50 thousand ³⁹K atoms, almost spherical trap switched off at *t*=0

Initially $a=280a_0$ (repulsive), $\lambda \sim 3J$ (localized) \rightarrow tuned to final value within 10 ms

Does the phase depend on filling? What do we see?

If the phase diagram is sensitive to the filling

Density decrease after release may induce (de)localization

Intuitively,

The density is decreased as the atoms flow to the outer side of the system; density of states at the Fermi surface changes (not monotonously) But we checked

The ground state phase diagram: does not depend strongly up to filling ~ 0.31 (per spin per site)

Gap at ~31% filling

One parameter scaling theory

Abrahams *et al.*: PRL 42, 673 (1979) see also Garcia-Garcia and Wang: PRL 100, 070603 (2008)

L : system size, δ : (one-particle) mean level spacing

Dimensionless conductance (d>2)D Normal metal : g(L) $\propto L^{d-2} \rightarrow \infty$ $E_{\tau} \propto L^{-2}, \delta \propto L^{-d}$ $g(L) = E_{T} / \delta$ E_{τ} : Thouless energy γ - Metal-insulator transition : $g(L) = g_c$ ---(related to typical time for particle to travel L_{\perp} Insulator : $g(L) \propto \exp(-L/\xi) \rightarrow 0$ $\langle x^2(t) \rangle \propto t^{\alpha}$ Motion slowed down, Multifractal spectrum with ~ $L^{2/\alpha}$ time to propagate L, Hausdorff dimension $d_{\rm H}$ $\rightarrow \delta \propto I^{-d/d_{\rm H}}$ $E_{\tau}^{-1} \propto t^{-2/\alpha}, \alpha < 1$ Localization length ξ : MIT should occur at $\alpha = 2d_{\rm H}/d = 2d_{\rm H}$

MIT should occur at $\alpha = 2d_H/d = 2d_H$ (has been checked for the non-interacting case; Artuso et al.: PRL 68, 3826 (1992); Piechon et al.: PRL 76, 4372 (1996)) Localization length ξ : should diverge as $|\lambda - \lambda_c|^{-\nu}$ (v=1 at *U*=0)

Near metal—insulator transition

Disordered 1D system, U < 0

→ Let us numerically check by studying the dynamics

similar to Cayley tree

Setup (1)

- Optical lattice + incommensurate potential (Aubry-André model)
- On-site attractive interaction
- Initially trapped in a harmonic potential

- Remove the harmonic potential but keep the incommensurate potential on: what happens?
- Study by time-dependent DMRG

Finite system DMRG wavefunction constructed from the previous step

Iterate until physical quantities (e.g. energy) converge

Time-dependent DMRG

White and Feiguin: PRL 93, 076401 (2004)

Application of $exp(-i\tau H_{i,j})$ is almost exact if $H_{i,j}$ only affects neighboring sites *i*, *j*

 T/τ finite system iterations to reach time T

$$\begin{split} \hat{H} &= \hat{H}_{1,2} + \hat{H}_{2,3} + \dots + \hat{H}_{L-2,L-1} + \hat{H}_{L-1,L} \\ \exp(-i\tau\hat{H}) & \text{Suzuki-Trotter decompotision} \\ &= \exp(-i\tau\hat{H}_{L/2,L/2+1}/2) \cdots \exp(-i\tau\hat{H}_{2,3}/2) \exp(-i\tau\hat{H}_{1,2}) \\ \exp(-i\tau\hat{H}_{2,3}/2) \cdots \exp(-i\tau\hat{H}_{L-2,L-1}/2) \exp(-i\tau\hat{H}_{L-1,L}) \\ \exp(-i\tau\hat{H}_{L-2,L-1}/2) \exp(-i\tau\hat{H}_{L/2,L/2+1}/2) + O(\tau^3) \end{split}$$

Time-dependent DMRG: other schemes

Cazalilla and Marston: PRL 88, 256403 (2002) Luo et al.: PRL 91, 049701 (2003) Vidal: PRL 93, 040502 (2004) Feiguin and White: PRB 72, 020404 (2005) Dutta and Ramasesha: PRB 82, 035115 (2010)

Time-evolving block decimation (TEBD) has also been applied to cold atom systems *e.g.* Macroscopic quantum tunneling between different supercurrent states in a ring Danshita and Polkovnikov: PRB 82, 094304 (2010)

Applications of time-dependent DMRG on cold atom systems

Propagating 1D density waves of bosons in optical lattice Kollath *et al.*: PRA 71, 053606 (2005)

> 0.4 0.2 0 -0.2 0 0.8 0 0 8 16 24 32 (c) 8 16 24 32

n_e - 1.

Applications of time-dependent DMRG on cold atom systems

Andreev-like reflection in bosons Daley *et al.*: PRL 100, 110404 (2008)

Setup (1)

- Optical lattice + incommensurate potential (Aubry-André model)
- On-site attractive interaction
- Initially trapped in a harmonic potential

- Remove the harmonic potential but keep the incommensurate potential on: what happens?
- → Study by time-dep. DMRG for Hubbard model

Non-interacting case

Smooth diffusion until bouncing back at (artificial) system boundary

 $\lambda = 0.5 < \lambda_c (U = -1)$

Atoms quickly flow to both sides

 $\lambda = 1.0 \sim \lambda_c(U = -1)$

Significantly slower diffusion

 $\lambda = 1.5 > \lambda_c(U = -1)$

Atoms move only locally

Setup (2)

- Optical lattice + incommensurate potential (Aubry-André model)
- On-site attractive interaction
- Initially trapped in a box potential

- Remove the box potential but keep the incommensurate potential on: what happens?
- → Study by time-dep. DMRG for Hubbard model

Check: energy is nearly preserved

160 sites, 12+12 fermions, $\Delta t = 0.01$

Suppressed motion for $\lambda > \lambda_c$

200 sites, 18 up and 18 down fermions, U=-1

J. Ozaki, M. Tezuka, and N. Kawakami: arXiv: 1107.0774

3) Collision dynamics

Elongated two-component Fermi gas: up and down spins released from separate traps to collide ("Little Fermi Collider") cf. 1D Bosons: absence of thermalization Kinoshita et al.:

Motivation

What kind of many-body effects are observed during a single collision between two one-dimensional fermion clusters?

- A spin-dependent harmonic trap
- Quenched to a shared potential
- The fermions collide at the trap center

Model: Hubbard model Method: time-dependent DMRG

Example U/J = 0.80 (7+7 atoms, ~55% reflectance)

Weak interaction: most of atoms are not reflected

particle reflectance for n + n atoms R_n : $R_1 \propto u^2$ ($u \rightarrow 0$)

Quasi-classical model

Quasi-classical model: a series of one-to-one collisions between two types of *independent* classical particles

(i) $u \rightarrow 0$: n^2 times of independent spin-up and spin-down collisions $\Rightarrow R^{qc}_n = n^2 R_1/n = nR_1$

Consistent with the simulation

Strong interaction: most of atoms are reflected back

Transmittance for n + n atoms $T_n : T_1 \propto u^{-2}$ ($u \rightarrow \infty$), $R_n + T_n = 1$

Quasi-classical model

Quasi-classical model: a series of one-to-one collisions between two types of *independent* classical particles

(ii) $u \rightarrow \infty$: *n* atoms collide successively against *n* atoms $\Rightarrow T^{qc_n} = nT_1/n = T_1$

Inconsistent with the simulation!

What is going on? The work is in progress.

Summary

- Application of DMRG for static and dynamic behavior of Fermi cold atom gases in 1D
 - Population-imbalanced gas in harmonic trap: FFLO-like
 condensate
 PRL 100, 110403 (2008); New J. Phys 12, 055029 (2010)
 - Quasiperiodic disorder
 - Can enhance condensation for weak attraction PRA 82, 043613 (2010)
 - Trap-release dynamics close to metal-insulator transition: anomalous diffusion observed
 - arXiv: 1107.0774 — Collision of spin clusters: more atoms pass through than quasi-classically expected = emergent many-body behavior
- There is much more to explore with powerful numerical methods!