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A THEORETICAL EVALUATION OF SUPER FLUID RESPONSE AND MOMENTUM DISTRIBUTION FUNCTIONS OF ONE-DIMENSIONAL BOSE-FERMI MIXTURES

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Abstract: Using the theoretical formalism of A. Zujev etal (Phys. RevA, 2008), we have evaluated super fluid Bose and Fermi density as a function of Bose-Bose interaction U_{BB} and Bose- Fermi interaction U_{BF}. Our theoretical results show that both ρ_B^s and ρ_F^s decreases with U_{BB} and U_{BF} which are in good agreement with the other theoretical workers. We have also determined momentum distribution for bosons $n_B(k)$, fermion distribution $n_F(k)$ and anti-correlated pairing momentum $n_a(k)$ all as a function of wave vector k, keeping U_{BB}, U_{BF}, temperature β constant and varying boson occupation N_B from 20 to 36. Our theoretical results indicate that for lower values of N_B, $n_B(k)$ attains a peak at k=0 where as $n_F(k)$ has plateau at k=0. $n_a(k)$ shows that composite fermions has been formed by pairing a boson and fermion. For large values of N_B, Bose- Fermi mixtures show Mott-insulator phase transition for bosons and Luttinger liquid like behavior for fermions. These observations are in good agreement with other theoretical workers.

Keywords: Strongly correlated systems, Optical lattice, Bose-Hubbard Hamiltonian, Bose-Fermi mixtures, Luttinger liquid, Strong coupling expansion, Bosonization, Quantum Monte Carlo Simulations, anti-correlated pairing momentum

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INTRODUCTION

In recent years, the experimental realization of strongly correlated systems with ultracold gases loaded in optical lattices[1] has generated tremendous excitement in condensed matter physics. Among these quantum systems, the realization of Bose-Fermi mixtures in optical lattices[2-4], where the inter-and interspecies interactions can be tuned to be attractive or repulsive[5] is of remarkable examples. Lot of theoretical studies [6-12] have been performed on Bose-Fermi mixtures for homogeneous and trapped systems. Several approaches were used. Some of them are Gutzwiller mean –field theory[13], strong coupling expansions[14], bosonization[8,9], exact analytical[10] and numerical studies[11]. There was also a study on mixtures of bosonic atoms and molecules on lattice numerically. In these studies, verities of phases were observed in such mixtures. These are Mott insulators, spin and charge density waves, a verity of super fluids, phase separation and Wigner crystals. A study of repulsive Bose-Fermi mixtures in one dimensional lattice has been made where main focused was given on specific special densities. After mapping the phase diagram, one expresses the different sections. The lattice which is half filled with bosons and half filled with fermions has been studied which includes (a) When the number of bosons is commensurate with the lattice size but the number of fermions is not (b) when the sum of both species is commensurate with the lattice size but the number of bosons and fermions are different. Some of the phases present have been identified as Sengupta and Pralka[12].

In this paper, using the theoretical formalism of A. Zujev etal[15], we have theoretically evaluated boson super fluid density, fermion super fluid density and correlation between bosons and fermions. We have also evaluated momentum distribution for bosons $n_B(k)$, fermions $n_F(k)$ and anti-correlated pairing momentum $n_a(k)$ as a function of wave vector k keeping boson-boson interaction U_{BB}, Boson-Fermion interaction strength U_{BF} and temperature β fixed and varying the boson occupation number N_B from 20 to 36. In this study, the ground state phases of Bose-Fermi mixtures in one-dimensional optical lattice with quantum Monte Carlo simulation has been performed using the canonical worm algorthim. Depending upon fitting of bosons and fermions and the on-site intra-and interspecies interaction different kinds of incompressible and super fluid phases appear. On the compressible side, correlations between bosons and fermions can lead to a distinctive behavior of the bosonic super fluid density and the fermionic stiffness. Apart from this, the equal time Green functions allows one to identify regions where the two species exhibit anti correlated flow. One studies complete phase diagram for these systems at different filling and also as a function of the interaction parameter[16,17].

MATERIALS AND METHODS

The Hamiltonian of Bose-Fermi mixtures in one dimension can be written as

$$H = t_B \Sigma_l ({b^+}_{l+1} b_l + {b^+}_l b_{l+1}) - t_F \Sigma_l ({f_{l+1}}^+ f_l + {f^+}_l f_{l+1}) + U_{BB} \Sigma_l {n^B}_l ({n^B}_l - 1) + U_{BF} \Sigma_l {n^B}_l {n^F}_l \quad (1)$$

Where $b_l^+(b_l)$ are the boson creation (annihilation) operators on site l of one –dimensional lattice with L sites. Similarly $f_l^+(f_l)$ are the creation (annihilation) operators for the spinless fermions on the same lattice sites. For these creation and destruction operators $n_l^{B,F}$ are the associated number operators. The bosonic and fermionic hopping parameters are denoted by t_B and t_F respectively. The on-site boson-boson and boson-fermion interactions are denoted by U_{BB} and U_{BF} respectively. Here, we shall take t_B=t_F=1(i.e when the boson fermion hopping integrals are equal and one choose t_B =1 to set the scale of energy[18,19].

One performs the quantum Monte Carlo simulations (QMC) using a recently proposed Canonical Worm algorithm[20,21]. This approach makes use of global move to update the configurations, samples the winding number and gives access to the measurement of n-body Green's function. It has also the useful property of working in the Canonical ensemble. This is particularly important for the present applications. Since one is working with two species of particles in the Grand Canonical ensemble. In the Canonical simulations, the Bose and Fermi occupations are exactly specified and the chemical potentials μ_B and μ_F are computed via appropriate numerical derivatives of the resultant ground state energy $[\mu_B = E_0(N_B+1) - E_0(N_B)]$. Here N_B is the Boson occupation number and is equal to 3L/4 where L is the lattice site. N_F =L/4 and it is fixed.

The Canonical Worm algorithm is a variation of the Prokot'ev etal grand Canonical Worm algorthm[18]. Within the Canonical Worm approach, one starts by writing the Hamiltonian H= V-T where T is comprised of no diagonal terms and is positive definite. The Partition function Z is given by

$$Z = Tre^{-\beta H}$$

It takes the form

$$Z = Tre^{-\beta H} Tre^{\int_0^\beta T(\tau)d\tau} \quad (2)$$

$$= Tre^{-\beta V}\Sigma_n \int_{0<\tau_1<....\tau_n<\beta} T(\tau_n)...T(\tau_1)d\tau_1 d\tau_n \quad (3)$$

Where

$$T(\tau) = e^{\tau V} T e^{-\tau V}$$

Here τ is the imaginary time. Now the extended partition function is considered by breaking up the propagator at imaginary time τ and introducing the Worm operator

$$W = \Sigma_{ijkl}\omega_{ijkl} b_i^+ b_j f_k^+ f_l \quad (4)$$

This leads to the Partition function

$$Z(\tau) = Tre^{-(\beta-\tau)H} W e^{-\tau H} \quad (5)$$

Complete sets of states are introduced between consecutive T operator to allowed a mapping of the one-dimensional (1D) quantum problem on to a two dimensional (2D) classical problem where a standard Monte Carlo techniques are used. Measurements can be performed when configurations resulting in diagonal matrix elements of W occur. As with pure bosonic systems the evaluation of the boson and fermion densities ρ_B, ρ_F with the associated chemical potential μ_B, μ_F identifies Mott-insulator behavoir[22]. A jump in μ signals a Mott phase where the Compressibility

$$\kappa_B = \frac{\partial \rho_B}{\partial \mu_B}$$

$$\kappa_F = \frac{\partial \rho_F}{\partial \mu_F} \quad (6)$$

Vanishes. Here ρ_B and ρ_F are the boson and fermion density respectively. One measures the bosonic super fluid density and fermionic stiffness

$$\rho^s{}_B = <W> \frac{L}{2\beta} \quad 7(a)$$

$$\rho^s{}_F = <W^2> \frac{L}{2\beta} \quad 7(b)$$

Here <W^2> are the associated Winding numbers. Correlations between the bosonic and fermionic Winding numbers are determined by the combinations

$$\rho^s{}_c = <(W_B + W_F)^2> \frac{L}{2\beta} \qquad 8(a)$$

$$\rho^s{}_a = <(W_B - W_F)^2> \frac{L}{2\beta} \qquad 8(b)$$

In addition to the usual bosonic and fermionic Green's function

$$G^B{}_{ij} = <b_i^+ b_j> \qquad 9(a)$$

$$G^F{}_{ij} = <f_i^+ f^+> \qquad 9(b)$$

One also measures the composite anti correlated two-body Green's function[23]

$$G^a{}_{ij} = <b^+{}_i b_j f^+{}_j f_i> \qquad (10)$$

In G_{ij}^a, the fermion and boson propagates in opposite direction (one from j to i and one from i to j).

The Fourier transforms of G_{ij}^B and G_{ij}^F gives the densities $n_B(k)$ and $n_F(k)$ in momentum space. $n_a(k)$ is the Fourier transform of the composite two-body Green's function G_{ij}^a.

RESULTS AND DISCUSSION:

In this paper, we have theoretically studied and evaluated bosonic super fluid density, fermionic stiffness and correlation between bosons and fermions. The evaluation has been performed by theoretical model developed by A. Zujev etal[15]. In Table T1, we have shown the evaluated results of boson density ρ_B as a function of chemical potential μ_B. Here fermionic density ρ_F=1/4, interaction strengths are fixed U_{BF}=16, U_{BB}=10. We have taken two different lattice size L=36, 44 and two different temperature β=32 and 108. In these calculations, it is seen that there are plateaus for all the lattice L and β. The plateaus are observed for μ_B between 2 to 15. In table T2, we have shown the evaluated results of chemical potential μ_B as a function of boson-fermion interaction strength U_{BF} for two values of boson density ρ_B=1.0 and ρ_B=0.75. Here we have taken U_{BB}=10 and ρ_F=1/4. From our calculations, it appears that for ρ_B=1.0, μ_B is roughly constant with U_{BF} where as for ρ_B=0.75, μ_B increases very sharply with U_{BF}.

In table T3, we repeated the calculation as a function of boson-boson interaction strength U_{BB} keeping other parameters same as in table T2. Here, we observed the reverse pattern. For ρ_B=1.0, μ_B increases sharply with U_{BB} and for ρ_B=0.75, there is flat plateau part. In Table T4, we have shown the evaluated results of super fluid density ρ_B^s, β=32, ρ_F^s, β=32, ρ_B^s, β=108 and ρ_F^s, β=108 as a function of U_{BF} keeping U_{BB}=10, ρ_F=1/4, ρ_B=3/4. From our evaluated results both ρ_B^s and ρ_F^s for β=32and 108 decreases with $U_{BF.}$ In table T5, we have shown the evaluated results of boson super fluid density ρ_B^s as a function of boson density ρ_B for two values of temperature β=32and 108. Here again , we have kept U_{BF}=16, U_{BB}=10 and ρ_F=1/4. From our theoretical results, it appears that ρ_B^s decreases with ρ_B and becomes zero with some value of ρ_B and after that it increases sharply. This trend is same for both the temperature β=32and 108. In table T6, we have shown the evaluated results of momentum distribution of bosons $n_B(k)$, fermions $n_F(k)$ and anti-correlated pairing momentum distribution $n_a(k)$ all as a function of wave vector k. Here we have taken U_{BF}=16, U_{BB}=10, β=108 and boson occupation number N_B=20. Our theoretical results indicate that there is sharp peak in boson momentum distribution which shows the presence of quasi condensate. On the other hand momentum distribution for fermions shows a plateau which is the indication of Luttinger liquid like behavior with a clear Fermi momentum. This property is also shared by the composite fermions described by the anti correlated pairing momentum. In table T7, we repeated the calculations of $n_B(k)$, $n_F(k)$ and $n_a(k)$ as a function of k keeping U_{BF}=16, U_{BB}=10, β=108 same and N_B=27. In this case we observed that bosons do not have a peak at k=0 and the Fermi momentum is washed out. These results indicate that there is onset of short range correlation. On the other hand the plateau in the Fourier transforms of the anti correlated pairing momentum shows that the composite fermions formed by pairing a fermion and boson have a well defined Fermi momentum[11]. In table T8, we repeated the calculation of $n_B(k)$, $n_F(k)$ and $n_a(k)$ all as a function of k keeping U_{BF}=16, U_{BB}=10, β=108 same and N_B=32. Here the trend is the same as is observed in table T6. There is a peak in the bosonic momentum distribution and a plateau in the fermionic and anti-correlated pairing momentum distribution. These all behavior indicate a power-law decaying correlations of their corresponding real space Green functions. In table T9, we repeated the calculation of $n_B(k)$, $n_F(k)$ and $n_a(k)$ all as a function of k keeping U_{BF}=16, U_{BB}=10, β=108 same and N_B=36. In this case there is no sharp peak in $n_B(k)$ but a plateau in $n_F(k)$ is present. This phase is a Mott-insulator for bosons and Luttinger liquid behavior for fermions. In this case the composite fermions do not exhibit a Fermi momentum. There is some recent calculations[24-30] which also reveals the same facts.

CONCLUSION:

In this paper, we have studied the super fluid and Mott-insulator phases of one-dimensional Bose-Fermi mixtures. We have evaluated super fluid boson and fermion density as a function of boson-boson interaction and boson-fermion interaction. We have also evaluated momentum distribution of boson $n_B(k)$, fermion $n_F(k)$ and anti-correlated pairing momentum $n_a(k)$ all as a function of k keeping U_{BF}, U_{BB} and temperature β constant and varying N_B from 20 to 36. WE observed that boson momentum distribution has a peak where as fermion momentum distribution has a plateau. For large values of n_B, $n_a(k)$ shows that the coupling between bosons and fermions is weak and has phase separation.

Table T1

An evaluated result of boson density ρ_B as a function of chemical potential μ_B. The fermion density ρ_F =1/4 and the interaction strength are fixed. U_{BB}=10 and U_{BF}=16. We have taken different lattice size L =36, 44 and temperature β =32 and 48

Chemical potential μ_B	<----------ρ_B------------->			
	L=36, β=32	L=36, β=48	L=44, β=32	L=36, β=32, ρ_F=0
-5	0.426	0.406	0.447	0.468
-2	0.539	0.465	0.516	0.539
-1	0.657	0.538	0.543	0.534
0	0.748	0.626	0.644	0.659
2	0.805	0.729	0.732	0.746
5	0.826	0.796	0.806	0.825
8	0.889	0.822	0.849	0.855
10	0.907	0.845	0.873	0.889
12	0.968	0.867	0.908	0.922

15	1.038	0.898	0.937	0.945
18	1.096	0.925	0.985	0.995
20	1.115	0.996	1.100	1.112
25	1.247	1.105	1.158	1.167

Table T2

An evaluated results of chemical potential μ_B as a function of boson-fermion interaction strength U_{BF} for two values of boson density ρ_B =1.0 and ρ_B=0.75. Here U_{BB}=10 and ρ_F =1/4

U_{BF}	<--------- μ_B------->	
	ρ_B =1.0	ρ_B=0.75
0	16.26	4.86
2	17.48	5.43
5	18.32	6.86
10	19.47	7.98
12	19.82	8.43
14	20.48	9.24
15	21.22	11.67
18	21.47	12.38
20	22.08	13.56
22	22.54	14.34
24	22.84	15.86
25	23.07	16.59

Table T3

An evaluated results of chemical potential μ_B as a function of boson-boson interaction strength U_{BB} for two values of boson density ρ_B =1.0 and ρ_B=0.75. Here U_{BF}=10 and ρ_F =1/4

U_{BB}	<--------- μ_B------->	
	ρ_B =1.0	ρ_B=0.75
0	2.86	2.58
2	4.32	3.27
5	8.34	6.86
10	12.58	11.20
12	14.32	11.38
14	16.59	11.55
15	20.47	11.86
18	25.36	12.05
20	28.58	12.18
22	30.29	12.27
24	33.86	12.58
25	37.58	12.92

Table T4

An evaluated results of super fluid Bose density and super fluid fermion density with two different temperatures as a function of boson-fermion interaction strength U_{BF} keeping ρ_B=3/4 and ρ_F=1/4, U_{BB}=10

U_{BF}	<--------- ρ^s -------------->			
	$\rho^s{}_B, \beta$ =32	$\rho^s{}_F, \beta$ =32	$\rho^s{}_B, \beta$ =108	$\rho^s{}_F, \beta$ =108
0	0.325	0.305	0.284	0.259
5	0.306	0.297	0.263	0.235
7	0.298	0.265	0.245	0.216
8	0.245	0.248	0.227	0.195
10	0.205	0.219	0.206	0.178
12	0.187	0.206	0.184	0.169
14	0.168	0.184	0.163	0.150
15	0.145	0.167	0.142	0.147
18	0.127	0.153	0.138	0.122
20	0.108	0.145	0.117	0.105
22	0.093	0.122	0.097	0.099
24	0.092	0.108	0.085	0.094
25	0.090	0.095	0.063	0.083

Table T5

An evaluated results of boson super fluid density ρ_B^s as a function of boson density ρ_B . Here $U_{BB}=0$, $U_{BF}=16$ and $\rho_F= 1/4$

ρ_B	<-------- ρ_B^s --------->	
	β=32	β=108
0.5	0.25	0.15
0.6	0.18	0.12
0.7	0.12	0.06
0.8	0.05	0.02
0.9	0.00	0.00
1.0	0.09	0.00
1.05	0.14	0.00
1.10	0.20	0.08
1.15	0.27	0.14
1.20	0.34	0.19
1.22	0.40	0.26
1.24	0.50	0.30
1.25	0.58	0.37

Table T6

An evaluated result for momentum distribution of bosons, fermions and anti-correlated pairing momentum as a function of wave vector k Here U_{BB}=10, U_{BF}=16, β=108, N_B(occupation number for bosons)=20

k	$n_B(k)$	$n_F(k)$	$n_a(k)$
-π	0.042	0.053	-0.325
-π/2	0.065	0.068	-0.307
-π/4	0.083	0.094	-0.294
-π/8	0.097	0.097	-0.286
-π/16	1.023	0.098	-0.278
-π/32	1.068	0.099	-0.274
0.0	4.268	1.032	----
π/32	3.075	1.045	----
π/16	1.168	1.029	----
π/8	0.096	1.022	-0.263
π/4	0.085	1.021	-0.246
π/2	0.063	0.098	-0.217
π	0.046	0.095	-0.198

TableT7

An evaluated result for momentum distribution of bosons, fermions and anti-correlated pairing momentum as a function of wave vector k Here U_{BB}=10, U_{BF}=16, β=108, N_B(occupation number for bosons)=27

k	$n_B(k)$	$n_F(k)$	$n_a(k)$
-π	0.532	0.325	-0.429
-π/2	0.546	0.337	-0.432
-π/4	0.558	0.348	-0.416
-π/8	0.567	0.353	-0.384
-π/16	0.578	0.362	0.326
-π/32	0.643	0.375	0.472
0.0	1.086	0.392	0.468
π/32	1.079	0.386	0.453
π/16	1.067	0.375	0.286
π/8	1.058	0.352	0.257
π/4	1.048	0.346	-0.263
π/2	1.042	0.338	-0.243
π	1.038	0.325	-0.218

Table T8

An evaluated result for momentum distribution of bosons, fermions and anti-correlated pairing momentum as a function of wave vector k Here U_{BB}=10, U_{BF}=16, β=108, N_B(occupation number for bosons)=32

k	$n_B(k)$	$n_F(k)$	$n_a(k)$
-π	0.534	0.086	-0.057
-π/2	0.675	0.098	-0.042
-π/4	0.786	0.125	-0.038
-π/8	0.997	0.146	-0.029
-π/16	1.532	0.238	0.058
-π/32	2.467	0.295	0.096
0.0	3.456	0.386	0.215
π/32	2.128	0.302	0.187
π/16	1.986	0.295	0.142
π/8	1.643	0.178	0.095
π/4	1.425	0.105	-0.027
π/2	1.184	0.036	-0.038
π	0.975	0.054	-0.072

TableT9

An evaluated result for momentum distribution of bosons, fermions and anti-correlated pairing momentum as a function of wave vector k Here U_{BB}=10, U_{BF}=16, β=108, N_B(occupation number for bosons)=36

k	$n_B(k)$	$n_F(k)$	$n_a(k)$
-π	0.635	0.075	0.086
-π/2	0.746	0.106	0.115
-π/4	0.849	0.198	0.178
-π/8	0.969	0.315	0.256
-π/16	1.124	0.679	0.342
-π/32	1.686	0.735	0.365
0.0	2.147	0.758	0.395
π/32	2.082	0.706	0.312
π/16	1.976	0.325	0.296
π/8	1.842	0.276	0.216
π/4	1.624	0.186	0.135
π/2	1.342	0.098	0.098
π	1.178	0.069	0.067

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