Spin-1 Bose Hubbard model with nearest neighbour extended interaction

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(Dated: August 29, 2018)

We have studied a spinor ($F = 1$) Bose gas in presence of the density-density interaction through the mean field approach and the perturbation theory for either sign of the spin dependent interaction, namely the antiferromagnetic (AF) and the ferromagnetic cases. In the AF case, the charge density wave (CDW) phase appears to be sandwiched between the Mott insulating (MI) and the supersolid phases for small values of the extended interaction strength. But the CDW phase completely occupies the MI lobe when the extended interaction strength is larger than a certain critical value related to the width of the MI lobes and hence opens up the possibilities of spin singlet and nematic CDW insulating phases. In the ferromagnetic case, the phase diagram shows similar features as that of the AF case and are in complete agreement with a spin-0 Bose gas. The perturbation expansion calculations nicely corroborate the mean field phase results in both these cases. Further, we extend our calculations in presence of a harmonic confinement and obtained the momentum distribution profile that is related to the absorption spectra in order to distinguish between different phases.

I. INTRODUCTION

The cooling and trapping of neutral alkali atoms in optical lattices, formed by two or more counter propagating laser beams make it possible to explore a plethora of quantum many body phenomena compared to its condensed matter counterpart due to adequate control over various experimental parameters. The general features of the cold atoms trapped in optical lattices were first theoretically described by the Bose Hubbard model (BHM) [1], where the superfluid (SF) to Mott insulator (MI) transition can be achieved by tuning a competition between the tunneling to the interatomic interaction potential. As a result of rapid technological improvement, the first experimental signature of the SF-MI transition was observed by Greiner et al. for a magnetically trapped scalar Bose gas in an optical lattice [2].

Despite success in magnetic trapping of a scalar or spin-0 Bose gas, efforts to study the spinor Bose gas have gained much more momentum after the MIT group successfully confined $^{23}$Na spin-1 condensate by using an optical dipole trap [3]. The optical trap which interacts via the electric fields of the laser beams with the dipole force of the neutral atoms helps in distinguishing all the hyperfine spin degrees of freedom and thus they are called as a gas of spinor bosons. Since then, several theoretical and experimental attention have been paid to study the spin-1 [4–8] as well as spin-2 [9–11] Bose gases which have rich ground state structures consisting of antiferromagnetic (or polar) and ferromagnetic for the former one [12, 13], while another additional cyclic phase [12–14] appears for the latter.

In this work, we primarily focus on the spin-1 ($F = 1$) Bose gas whose general properties were first theoretically analyzed by Ho [15] and Machida [16] to illustrate the spin textures and topological excitations where the spinor components transform to each other in the spin space via a spin-gauge rotational symmetry. Besides, different types of the MI phases, including the spin singlet, nematic as well as exotic fractionalized phase that break both the spin and charge symmetry and the SF phases were studied in Refs.[17, 18]. Later, possible ground state structures of the spin nematic and spin singlet MI phases and the transition between them were investigated in Refs.[18, 19]. Further the existence of the dimerized phase is explored using an effective spin Hamiltonian in Refs.[20, 21].

Apart from all these activities, a large number of review articles on the spinor Bose gas exist that emphasizes the studies in presence of disorder [22, 23], external magnetic field through the linear [24–26] and quadratic Zeeman strengths [24, 27–30], spin-orbit couplings (SOC) [31–35] and synthetic magnetic fields [36] etc. Among them, the inclusion of SOC after its recent experimental realization using Raman coupling between hyperfine levels [37] gives rise to more than one minima in the single particle dispersion relation which leads to different exotic ground state structures like plane and standing wave [31] and various striped ferromagnetic phases [32]. Also usages of the hyperfine spin states as short lattice dimension, known as the synthetic dimension [38], to create spatially varying SOC gives rise to multiple density ordered SF phases such as the charge density or the spin density wave phases [39].

Although the different density ordered SF phases have been proposed for a spin-1 system using SOC, a specific concern is the possibility to study also the charge density wave (CDW) Mott insulating phase by employing a spin-1 BHM with non local nearest neighbour extended interactions apart from the usual onsite interaction, that may help in realizing the CDW phase. We feel such an extended interaction is relevant in the present context. Although the issues are reasonably well studied in the context of scalar particles [40–44], however it has not been explored for systems with internal degrees of freedom. The CDW phase which breaks the crystal
translational symmetry and thus have different density modulation corresponding to different sublattices, forms a new crystalline phase which is also an incompressible phase like the MI phase defined by an integer occupancy at each lattice site. The extended interaction, which is long range in nature may be realized through the dipole-dipole interaction between the dipolar atoms, not only paves the way for the CDW phase, but also an additional compressible phase known as the supersolid (SS) phase which depicts a coexistence of both the crystalline and superfluid phases.

The experimental realization of $^{52}$Cr atoms, which have no nuclear spin but have hyperfine spin-3 [45, 46], has created much interest to study the extended BHM from a theoretical perspective. Also for small dipole interaction strengths, the ground state structure of spin-1 dipolar condensate has been studied through single mode approximation (SMA) in Ref.[47] and different spin textures like polar core vortices, chiral spin vortex in ferromagnetic case beyond SMA in Refs.[48, 49].

Motivated from such studies on magnetic dipole-dipole interaction which has quite a complicated form, in this work we study the spin-1 BHM in presence of the density-density interaction term via the mean field approach (MFA). Our plan is to obtain the phase diagrams for both the AF and the ferromagnetic interactions in presence of extended interaction strengths. We have also performed a perturbation expansion to provide support for the mean field phase diagrams. We extend our calculations in presence of an external harmonic confinement and calculate the momentum distribution corresponding to different phases.

This paper is organized as follows. In section II, we outline our theoretical model for a spinor Bose gas in presence of an extended interaction described by a BHM and study it via the familiar mean field technique. In section III, we discuss the phase diagrams of the system for both MFA and perturbative approach. Finally, conclusions are drawn in section IV to depict the key results obtained by us.

II. MODEL

The BHM for spin-1 ultracold atoms in presence of nearest neighbour extended interaction can be written as [15, 16, 40],

$$
\hat{H} = -t \sum_{<i,j>} \sum_\sigma (\hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma} + \text{h.c.}) + \frac{U_0}{2} \sum_i (\hat{n}_i - 1) \\
+ U_2 \sum_i (\hat{S}_i^z - 2\hat{n}_i) - \sum_i \mu_i \hat{n}_i + V \sum_{<i,j>} \hat{n}_i \hat{n}_j
$$

(1)

Here $<i,j>$ are the nearest neighbour sites, $t$ is the hopping amplitude, $\mu_i = \mu - V_{ho}$ is the chemical potential at site $i$ and $V_{ho}$ is the trapping potential for harmonic confinement which has the form $V_{ho} = V_T (x-x_i)^2$ [50] where $x = (x, y)$ and $x_i = (x_i, y_i)$ are the lattice coordinates at the center and $i$-site of the trap in a two dimensional square lattice, $V_T$ being the strength of such trap. $\hat{a}_{i\sigma}^\dagger (a_{i\sigma})$ is the boson creation (annihilation) operator at a site $i$ and the particle number operator is $n_i = \sum_\sigma \hat{n}_{i\sigma}$. $n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma}$. $U_0$ is the spin independent and $U_2$ is the spin dependent on-site interactions which are related to the scattering lengths, $a_{0,2}$ by $U_0 = \left(4\pi\hbar^2/M \right) (a_{0,2} + 2a_{2})/3$ and $U_2 = \left(4\pi\hbar^2/M \right) (a_{2} - a_{0})/3$ corresponding to $S=0$ and $S=2$ channels respectively [15, 16]. The spin dependent interaction, $U_2/U_0 > 0$ is known as the antiferromagnetic (AF) and $U_2/U_0 < 0$, is known as the ferromagnetic interaction. The total spin at a site $i$ is given by $S_i = a_{i\uparrow}^\dagger F_{\sigma\sigma'} a_{i\downarrow}$, where $F_{\sigma\sigma'}$ are the components of spin-$1$ matrices and $\sigma = \pm 1, 0, -1$. The last term includes nearest neighbour extended interaction with a repulsive strength $V$.

To decouple both the hopping and the density-density interaction terms, we use the mean field approximation as given by [51, 52],

$$
\hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma} \simeq \langle \hat{a}_{i\sigma}^\dagger \rangle \langle \hat{a}_{j\sigma} \rangle + \langle \hat{a}_{i\sigma}^\dagger \rangle \langle \hat{a}_{j\sigma} \rangle - \langle \hat{a}_{i\sigma}^\dagger \rangle \langle \hat{a}_{j\sigma} \rangle
$$

(2)

$$
\hat{n}_{i\sigma} \hat{n}_{j\sigma} \simeq \langle \hat{n}_{i\sigma} \hat{n}_{j\sigma} \rangle + \langle \hat{n}_{i\sigma} \hat{n}_{j\sigma} \rangle - \langle \hat{n}_{i\sigma} \hat{n}_{j\sigma} \rangle
$$

(3)

where $\langle \cdots \rangle$ denotes the equilibrium value of an operator. The superfluid order parameter and local density at site $i$ are defined as,

$$
\psi_{i\sigma} = \langle \hat{a}_{i\sigma} \rangle, \quad \rho_{i\sigma} = \langle \hat{n}_{i\sigma} \rangle
$$

(4)

where $\psi_i = \sqrt{\psi_{i\uparrow}^2 + \psi_{i\downarrow}^2 + \psi_{i0}^2}$ and $\rho_i = \sum_\sigma \rho_{i\sigma}$. Using Eqs.(2) and (3) in the Hamiltonian appearing in Eq.(1), its mean field form can be written as,

$$
\hat{H}_i^{MF} = -zt \sum_\sigma \langle \hat{\phi}_{i\sigma}^\dagger \hat{\phi}_{i\sigma} + \hat{\phi}_{i\sigma} \hat{\phi}_{i\sigma}^\dagger \rangle + zt \sum_\sigma \hat{\phi}_{i\sigma}^\dagger \hat{\phi}_{i\sigma}
$$

(5)

$$
+ \frac{U_0}{2} \langle \hat{n}_i \rangle (\hat{n}_i - 1) + \frac{U_2}{2} (\hat{S}_i^z - 2\hat{n}_i)
$$

$$
- \mu_i \hat{n}_i + zV \hat{n}_i (\hat{n}_i - \rho_i)
$$

$$
- \sum_j \langle \phi_{i\sigma} \phi_{j\sigma} \rangle + \sum_j \phi_{i\sigma} \phi_{j\sigma} - \sum_j \rho_{i\sigma} - \sum_j \rho_{j\sigma}
$$

Here $\phi_{i\sigma} = (1/z) \sum_j \phi_{i\sigma}$ and $\rho_{i\sigma} = (1/z) \sum_j \rho_{j\sigma}$ and the sum $j$ includes all the nearest neighbours of the site $i$ of a square lattice with the coordination number, $z = 4$. Here $H_i$ and $H_0$ are the perturbation term and the unperturbed Hamiltonian respectively.

The presence of an external trapping potential, $V_T$ makes the mean field Hamiltonian $H_i^{MF}$ inhomogenous across the lattice. Thus it necessitates diagonalization of Eq.(5) on a full lattice. Here we have considered a square lattice of size $L \times L$ and obtain the ground state energy and eigenfunctions of the system.

Since the extended interaction term gives an extra CDW phase which has density modulations as one tra-
verses from one lattice site to another, it is quite reasonable to break the entire lattice into two sublattices, such as the A and B sublattices. So the unit cell has two types of atoms, namely A and B, where an A atom has B atom as all its neighbours and vice versa. In the CDW phase, one type of sublattice has higher occupancy than the other, so without much loss of generality, we assume \( n_A > n_B \).

To begin with, let us consider \( V_T = 0 \). In the absence of trapping, we can diagonalize Eq.(5) over the unit cell consisting of two sites namely A and B. Thus for A type of sublattice, Eq.(5) can be written as,

\[
H^{MF}_A = -z t \sum_\sigma \langle \psi_{B\sigma} \hat{n}_{A\sigma} + h.c. \rangle + z t \sum_\sigma \psi_{B\sigma} \psi_{A\sigma} - \mu_A \hat{n}_A \frac{U_0}{2} \hat{n}_A (\hat{n}_A - 1) + \frac{U_2}{2} (S_A^2 - 2 \hat{n}_A) + z V \rho_B (\hat{n}_A - \rho_A)
\]  

(6)

Similarly one can easily obtain the \( H^{MF}_B \) by changing the indices from A to B (and B to A) and the total mean field Hamiltonian is just sum of two mean field Hamiltonians that is \( H^{MF} = H^{MF}_A + H^{MF}_B \). The self consistent ground state energy and the eigenfunctions are obtained by diagonalizing \( H^{MF}_i \) in the occupation basis \( |n_{i\sigma}⟩ \) with \( n_i = 7 \) starting with some guess values for \( \psi_{(A/B)\sigma} \) and \( \rho_{(A/B)\sigma} \) and continue the diagonalization process until self consistency conditions for the order parameter, \( \psi_i \) and occupation densities, \( \rho_i \) are reached.

III. RESULTS

It was experimentally found that for \(^{23}\)Na atoms, the spin dependent interaction values are \( U_2/U_0 = 0.031 \) while for \(^{87}\)Rb atoms, the same is -0.046 [15]. Thus here we present our numerical results for different strengths of the extended interaction, \( V \) corresponding to both the AF and ferromagnetic interactions. The phase diagrams are calculated based on the self consistent values of the SF order parameters, \( \psi^{eq}_{(A/B)} \) and the local densities, \( \rho^{eq}_{(A/B)} \) (we shall drop the superscript, \( eq \) from here)

FIG. 1. Phase diagrams in AF case with \( U_2/U_0 = 0.03 \) for different values of \( zV/U_0 \) are shown from (a)-(d). The dotted lines from the perturbation calculation and the circles represent the mean field phase diagrams. At \( zV/U_0 = 0.7 \) [Fig.(a)], phase diagram consists of various CDW phases and the even MI(2) and odd MI(1) phases. In Fig.(b), for \( zV/U_0 = 0.95 > 1 - 2U_2/U_0 \), the odd MI(1) lobes now gripped by the CDW(20) phase. In Fig.(c), the MI(2) phases now occupied by the CDW(40) phase since \( zV/U_0 = 1.15 > 1 + 2U_2/U_0 \). At strong interaction limit, \( zV/U_0 = 1.7 \), all insulating phase are now the CDW phases.
to characterize different phases.

Both the CDW and MI phases are incompressible phases with integer occupation densities and vanishing SF order parameters, however the CDW phase is characterized by unequal occupation densities in the $A$ and $B$ sublattices, that is, $\rho_A \neq \rho_B$, (the MI phase corresponds to $\rho_A = \rho_B$) where $\rho_{A/B}$ is an integer. Also the SF and SS phases are the compressible phases with non integer densities and finite values of the SF order parameters but in the SF phase, $\psi_A = \psi_B \neq 0$ and $\rho_A = \rho_B \neq \text{integer}$, while the SS phase is characterized by $\psi_A \neq \psi_B \neq 0$ and $\rho_A \neq \rho_B \neq \text{integer}$ respectively. We present our phase diagrams for four different values of $zV/U_0$ in Fig.1(a)-(d). The choice of different $zV/U_0$ is justified in the subsequent discussion as we move on and the effect of trapping is included at the end of this section.

In Fig.1(a), the phase diagram corresponding to AF case ($U_2/U_0 = 0.03$) presented for $zV/U_0 = 0.7$, shows that the CDW phase appears in between the MI lobes, and thus a direct transition from the CDW to the SF is interrupted due to the appearance of the SS phase. The symbol $DW(pAqB)$ implies the CDW phase having occupation densities, $\rho_A$ (corresponding to sublattice $A$) and $\rho_B$ (corresponding to sublattice $B$) with average occupation density, $\bar{\rho} = (1/2)[\rho_A + \rho_B]$. The SS phase, which not only appears along with the $DW(21)$ and $DW(32)$ phases, but also exists along with the $DW(10)$ phase for $\bar{\rho} < 1/2$, as was predicted earlier through quantum Monte Carlo (QMC) studies in Ref.[42]. The MI(1) and MI(2) are the Mott insulating phases with occupation densities $\rho_A = \rho_B = 1$ and $\rho_A = \rho_B = 2$ respectively. The odd and even MI phases which form the spin nematic and singlet phases are the distinguishing features of a spinor Bose gas compared to a spin-0 Bose gas and the stabilization of the singlet phase over the nematic phase has been studied extensively in Refs.[51, 53].

In Fig.1(b), we found that corresponding to $zV/U_0 = 0.95$, although the phase diagram consists of all the compressible and incompressible phases, however, interestingly, the MI(1) phase is now completely occupied by the $DW(20)$ phase and the chemical potential widths of the DW phases increase with $zV/U_0$, which is now 0.95 (Fig.1(b)) compared to 0.7 in Fig.1(a).

The disappearance of the MI(1) phase can be understood by considering the atomic limit, that is, $t = 0$ where the system only consists of the MI and CDW phases. In the atomic limit, the ground state energy $E_g(n_A n_B)$ from Eq.(1) in the CDW phase is given by,

$$E_g(n_A n_B) = \frac{U_0}{4} \sum_{i=A,B} [n_i(n_i - 1)] - \frac{\mu}{2} \sum_{i=A,B} n_i + \frac{U_2}{4} \sum_{i=A,B} [S_i(S_i + 1) - 2n_i] + \frac{zV}{2} n_A n_B \quad (7)$$

Following the calculations carried out in Ref.[22], we found that the chemical potential width for the odd MI lobes is $U_0 - 2U_2$, while for the even MI lobes, it is $U_0 + 2U_2$. Also we have checked that for the CDW phase, the chemical potential width is $zV$ using the same assumption that for the odd occupation densities, we shall consider the spin eigenvalues to be $S = 1$ and for even occupation densities, $S = 0$ will be considered. So for $zV/U_0 = 1 \pm 2U_3/U_0$, there are possibilities of coexistence of different CDW and MI phases because of the degeneracy in their ground state energies. As a result, at $U_2/U_0 = 0.03$, when $zV/U_0 > 0.94$, the MI(1) phase now gets absorbed by the $DW(20)$ phase and this applies for the other odd MI lobes as well for $U_2/U_0 < 0.5$.

At larger value of the extended interaction, that is for $zV/U_0 = 1 + 2U_3/U_0 = 1.06$, the MI(2) phase becomes degenerate with the $DW(40)$ phase and beyond this critical value, all insulating phases become CDW phases and the SS phase has now significantly expanded with increasing $zt/U_0$ [Fig.1(c)]. We have also obtained the phase diagrams at stronger values of the extended interaction strength, that is, $V/U_0 = 1.7$ in Fig.1(d), which indicates that the system is more likely to be in the SS phase compared to the CDW or the SF phases.

In Fig.2, we have plotted the phase diagrams for two different values of $zV/U_0$ corresponding to the ferromagnetic case and found that they show similar characteristics as that of a scalar Bose gas. In this case, there is no distinction between the odd and the even MI lobes and hence all the MI lobes have densities, $\rho_i$ with the maximum spin eigenvalue, that is, $S_i = \rho_i$ [22].

In the atomic limit, it turns out the the chemical potential width for each of the MI lobe is $U_0 + U_2$, while for the CDW phase, it is $zV$. The phase diagram with $zV/U_0 = 0.85$ for $U_2/U_0 = -0.04$ is shown in Fig.2(a) demonstrates all the MI and the CDW phases along with all the compressible phases, since the critical value at which both the MI and CDW phases become degenerate at $zV/U_0 = 0.96$. We have also considered a strong interaction limit, namely $zV/U_0 = 1.4$, which is larger than the critical value 1 for $U_2/U_0 = 0.0$ in Fig.2(b). Now all the CDW and the SS phases can be found, however there are no MI lobes. We have also checked for different values of $zV/U_0$ corresponding to $U_2/U_0 = 0.0$ and they
are in complete agreement with the results obtained via Gutzwiller approximation in Ref.[40].

Since the formation of spin singlet pairs corresponding to even occupation densities and their stabilization over the odd MI lobes has been studied in Refs.[19, 51, 53] without the extended interaction, one can ask, is it possible to have also the spin singlet phase corresponding to integer $\tilde{\rho}$ for the CDW phase. If we look at Fig.1(a)-(b), it can be concluded that although the critical tunneling strength, $zt_c/U_0$ for transition from the incompressible to the compressible phases still occurs at higher values of $zt/U_0$ for the MI(2) phase compared to that of the MI(1) phase, but $zt_c/U_0$ for the DW(20) phase is now enhanced with increasing $zV/U_0$ compared to the other insulating phases except for the DW(10) phase.

Interestingly, from Fig.1(c)-(d), we found that the $zt_c/U_0$ for a transition from the CDW to the SS phase corresponding to the DW(20) or DW(40) are higher than that of the DW(10) or DW(30), thereby indicating a possibility of spin singlet formation in these CDW phases which we shall confirm by calculating the local spin eigenvalue in the subsequent discussion.

It is also helpful to study the nature of phase transition for different phases in the AF case. Earlier studies indicate that the MI-SF phase transition is first order for the even MI phase and second order for the odd MI lobes without an extended interaction in Refs.[51, 53]. In Fig.3(a), we have shown the one dimensional behaviour of $\rho_{A/B}$ for $zV/U_0 = 0.7$ at $\mu/U_0 = 0.5$ and it shows a continuous transition from DW(10) to the SS and then to the SF phases, indicating a second order transition. The same holds true for other DW phases. However the transition from DW to SF phase is found to be first order in nature, and the SF-MI transition for the even and odd MI phases still show first and second order transition respectively for $zV/U_0 = 0.7$ and 0.95.

We have checked that for $zV/U_0 > 1.15$, the CDW phases indicate a first or second order transition depending upon the even or odd occupation densities respectively. There is a discontinuous transition from DW(20) or DW(40) with an average $\tilde{\rho}$ = integer to the SS phase [Fig.3(b)], while a continuous transition occurs for the DW(10) or DW(30) with an average $\tilde{\rho}$ $\neq$ integer to the SS phase. The SF order parameters, $\psi_{A/B}$ also show similar behaviour as that of $\rho_{A/B}$ for different phases with the extended interaction, $zV/U_0$.

In Fig.3(c) and (d), we have shown the variation of the total spin eigenvalue, $\langle S^2 \rangle$ with different values of $zV/U_0$ to verify our claims made in the previous discussion that the spin eigenvalue to be 0 for the even occupation densities and 1 for odd occupation densities to calculate the width of each of the CDW lobes and assess if there is any possibility of spin singlet formation for the CDW phase having integer $\tilde{\rho}$. At $zV/U_0 = 0.7$, we found that $\langle S_A^2 \rangle = 2$ and $\langle S_B^2 \rangle = 0$ for the DW(10) phase [Fig.3(c)] and $\langle S_A^2 \rangle = 0$ and $\langle S_B^2 \rangle = 2$ for the DW(21) phase (not shown here). This implies that $S_A = 1$ for $\rho_A = \text{odd}$ and $S_B = 0$ for $\rho_B = \text{even}$ and vice versa for the CDW phases, as $\langle S^2 \rangle = S_i(S_i + 1)$. We have checked that $\langle S_A^2 \rangle = 0$ for the even and $\langle S_B^2 \rangle = 2$ for the odd MI phases and the transition to the SF phase still remain first and second order respectively [51, 53]. At $zV/U_0 = 1.7$, both the $\langle S_A^2 \rangle = \langle S_B^2 \rangle = 0$ for DW(20) phase, then followed by a jump to the SS phase [Fig.3(d)] and we found an identical behaviour also for the DW(40) phase. While for DW(10) or DW(30) phases, $\langle S_A^2 \rangle = 2$. $\langle S_B^2 \rangle = 0$ in the CDW phase and show continuous transition to the SS and SF phases. So the DW(20) or DW(40) behave as the spin singlet while the DW(10) or DW(30) as spin nematic CDW insulator phases like the spin singlet and nematic phases corresponding to the even and the odd MI lobes.

Further we have plotted the relative spin eigenvalue that is $S_{rel}^2 = \langle S_A^2 \rangle - \langle S_B^2 \rangle$ with $zt/U_0$ for $zV/U_0 = 1.7$ in Fig.3(e). At this value, $S_{rel}^2$ shows that, for the CDW phases, $S_{A/B}$ oscillates between 0 and 1 depending upon...
the density variations of these particular phases, that is the blue and red lobes pertaining to the CDW phase having non integer and integer $\rho$ respectively. The yellow region is for the SS phase where $S^2_{rel} \neq 0$ and then the SF phase corresponds to the red region where $S^2_{rel} = 0$. Thus we found signatures of a spin density wave (SDW) pattern, where $S_i$ oscillates between 0 and 1 in a similar fashion as that of $\rho_i$ in different CDW phases.

We shall now turn our attention to the second order perturbation calculation to obtain the phase boundaries between different phases in order to compare them with the mean field results discussed above. The ground state energy, $E_0$, after incorporating the first order, $E^{(1)}$ and second order, $E^{(2)}$ corrections can be expressed in terms of $\psi$ and $\phi$ as,

$$ E_n(\psi, \phi) = E^{(0)} + E^{(1)} + E^{(2)} = E^{(0)} + C_2(U_0, U_2, \mu, n, V)f(\psi, \phi) $$ (8)

where $C_2$ is the coefficient arising from the perturbation correction, $f$ includes the order parameter and $E^{(0)}$ is the eigenvalue of $H^0$ which is given by (site indices are skipped for the time being),

$$ E^{(0)} = \frac{U_0}{2} n(n-1) - \mu n + \frac{U_2}{2} [S(S+1) - 2n] + V \bar{\rho}(n - \rho) $$ (9)

Since the order parameter vanishes in the insulating phase, and it remains finite in the compressible phases, the boundary between them can be obtained by putting $C_2 = 0$. The phase boundary between the SF-MI phase in the AF case was obtained earlier by using non degenerate and degenerate perturbation theory corresponding to the even and odd MI lobes respectively without $zV/U_0$ in Ref.[53]. Following similar calculations here, the above condition for the even MI lobes leads to the following equation,

$$ \left( \frac{1}{zt} \right)_{even} = \frac{(n_i + 3)/3}{\beta_i + zV \bar{\rho}_i} - \frac{n_i/3}{-\alpha_i - 2U_2 + zV \bar{\rho}_i} $$ (10)

while for the odd MI lobes, it is given by,

$$ \left( \frac{1}{zt} \right)_{odd} = \frac{(n_i + 2)/3}{\alpha_i - zV \bar{\rho}_i} + \frac{(n_i - 1)/15}{\alpha_i + 3U_2 - zV \bar{\rho}_i} + \frac{(n_i + 1)/3}{\beta_i - 2U_2 + zV \bar{\rho}_i} + \frac{4(n_i + 4)/15}{\beta_i + zV \bar{\rho}_i + U_2} $$ (11)

where $\alpha_i = \mu - (n_i - 1)U_0$ and $\beta_i = -\mu + n_i U_0$ respectively. Thus the phase boundary between the MI and SF phases in presence of $zV/U_0$ is obtained by using either of Eq.(10) or Eq.(11) separately, depending upon the even or odd MI lobes, with $\bar{\rho}_i = n_0$ for $i \in A, B$ since in MI phase, $\psi_A = \psi_B = 0$ and $\rho_A = \rho_B = n_0$, $n_0$ being the occupancy of that particular MI phase.

Now for the CDW-SS phase boundary, an immediate question arises, namely, which equation one should use for dealing with the different CDW phases, since it has both even and odd occupation densities. As we have seen before, the spin eigenvalue, $S_i = 0$ corresponding to $\rho_i = even$ and $S_i = 1$ for $\rho_i = odd$ in the CDW phases, we may use a combination of Eq.(10) and Eq.(11) depending upon the density to determine the phase boundary.
with $\psi_i = \psi_A$, $\rho_i = \rho_A$, $\bar{\rho}_i = \rho_B$ if $i \in A$ and vice versa for $i \in B$. For example, for the CDW(10) phase at $zV/U_0 = 0.7$, $n_A = 1$, $S_A = 1$ and $n_B = 0$, $S_B = 0$, thus the boundary equation is given by,

$$\frac{1}{z^2t^2} = \left( \frac{1}{0.7 - x} \right) \left( \frac{1}{x} + \frac{2}{3(0.97 - x)} + \frac{4}{3(1.03 - x)} \right) \quad (12)$$

FIG. 5. The variation of $\langle S_i^2 \rangle$ in the AF case with $zV/U_0 = 0.7$ and trapping potential, $V_T = 0.0002$ for the CDW-MI phase at $\mu/U_0 = 1.1$ and $zt/U_0 = 0.05$ in (a) and the SS-SF phase at $\mu/U_0 = 1.25$ and $zt/U_0 = 0.25$ in (b).

In a similar fashion, we have calculated the boundary between all the compressible and incompressible phases using Eq.(10) or Eq.(11) at different values of $zV/U_0$ corresponding to the AF case and are superimposed in Fig.2 (dotted line). It shows that both the MFA and the analytic phase diagrams are in accordance with each other for all the CDW and MI phases well inside the boundary region, small deviation is observed near the tip of the insulating phases. From Fig.1, we found that the deviation is particularly prominent for the even occupancies as compared to the odd ones corresponding to the CDW or the MI phases. This suggests that MFA fails to tackle the fluctuations properly and holds good only for small fluctuations, a fact that is very well known.

In the ferromagnetic case, we have done a similar perturbation calculation for the phase boundary for $U_2/U_0 \leq 0$ with maximum spin eigenvalue of $S_i$ that is $S_i = n_i$. We found that both the MFA and phase diagrams obtained via perturbed calculations are in complete agreement with each other in Fig.1. Moreover the resultant boundary equations for the MI-SF and CDW-SS phase are identical with those obtained for different values of $zV/U_0$ in Refs.[40, 54].

So far the results presented above do not include the trapping potential. Now we shall consider a two dimensional trapping potential as $V_{ho} = V_T[(x-x_i)^2+(y-y_i)^2]$, where the trap can be chosen at the center of the lattice $L \times L$ that is at $x = y = L/2$. Since the order parameter and the spin eigenvalues are now inhomogenous over the lattice sites, here we shall show their one dimensional behaviour along the $x$-axis as a function of the distance, $x_i$ from the center of the trap by choosing $y = L/2$. Thus we will be able to scan both types of sublattice simultaneously.

In Fig.4, we have shown density, $\rho_i$ and order parameter, $\psi_i$ profile in the AF case with a trapping potential, $V_T = 0.0002$ for a square lattice of size $L = 256$. A careful scrutiny reveals that $V_T \sim 10^{-4}$ for a square lattice of dimensions 256times256 will enable us to capture all the different phases and we choose $\mu/U_0$, $zt/U_0$ in such a way that the trap center is in the vicinity of the DW-MI and SS-SF phases respectively. The circles denote $A$ type and solid lines denote $B$ type sublattice.

From Fig.4(a), it is clear that they are symmetric about the center of $x_i$ and as one advances from the center in either direction, we find, $\psi_i = 0$ while $\rho_i = 1$ which signals the MI(1) phase. Further movement along the $x$ axis leads to a very narrow region where $\psi_i$ is finite and both $\psi_i$, $\rho_i$ are oscillatory in nature implying the presence of the SS phase. As we move with $x_i$, this narrow SS phase is now followed by a region where $\psi_i$ vanishes but $\rho_i$ oscillates between 0 and 1, thereby signifying the presence of the the DW(10) phase and finally lead to a vacuum with vanishing $\psi_i$ and $\rho_i$ at the edge of the trap.

In Fig.4(b), we found that around the trap center, $\psi_i$ and $\rho_i$ are finite and they are equal for both the sublattices, indicate the signature of the SF phase. Upon moving away from the SF phase, one encounters the SS phase with oscillating $\psi_i$ and $\rho_i$ values which enters into the SF phase and eventually to the vacuum phase. We have also obtained the density and order parameter dependencies with the lattice site, $x_i$ for different values of $zV/U_0$ and $V_T$ and they exhibit similar properties to those discussed above for different phases.

The variation of $\langle S_i^2 \rangle$ for different phases in the AF case with the trapping strength, $V_T = 0.0002$ are shown in Fig.5. It shows similar behaviour to that of $\psi_i$ and $\rho_i$.
and found that the MI(1) phase with \( \langle S^z \rangle = 2 \) is sandwiched between the DW(10) phases, where \( \langle S^z \rangle \) oscillates between 0 and 2 in Fig.5(a). Further an oscillatory behaviour of \( \langle S^z \rangle \) in the SS phase is observed which is in between the SF phases in Fig.5(b).

In the ferromagnetic case, the variations of \( \psi \) and \( \rho \) are in complete agreement with those in Refs.[52, 55]. We have also checked the spin eigenvalues and the order parameter profiles in presence of one dimensional trapping potential without \( zV/U_0 \) in both the AF and ferromagnetic cases are in agreement with the results obtained in Ref.[50].

Although the order parameter and the density modulation with lattice sites give an impression about the different phases but to experimentally realize their signature one has to record the interference pattern via a time-of-flight experiment. In a time-of-flight experiment, the trapped atoms in optical lattices are allowed to expand suddenly to register the interference patterns corresponding to a given Bloch state which is a superposition of plane waves with a spread in the momentum values.

In Fig.6, we have shown the Fourier transform amplitude of \( \rho \), \( \psi \) and \( S^2 \) with the momentum along the \( x \)-direction, namely \( k_x \) in the SF, SS and CDW phases. The variation of \( \rho_k \) [Fig.6(top)] shows the appearance of peaks at \( k_x = 0 \) and \( k_x = 2\pi \) for all the phases, while an additional peak appears at \( k_x = \pi \) for the CDW or the SS phase. The \( \psi_k \) [Fig.6(middle)] and \( S^2_k \) [Fig.6(bottom)] shows similar behaviour as that of the SF and the SS phases except for the CDW phase, no peak is observed in \( k_x \) while tiny peaks are due to the trapping potential.

We have also considered the scenario in two dimensions by including \( k_y \) and found that the peaks in \( \rho_k \) corresponds to \( (k_x, k_y) = (2\pi j, 2\pi m) \) for the SF or SS phases in addition to \( (k_x, k_y) = (\pi j, \pi m) \) for the SS or CDW phases where \( j, m \) are integers. The momentum profile of \( \psi_k \) and \( S^2_k \) shows similar peak positions as that of \( \rho_k \) in the SF and SS phases but no peak at \( (k_x, k_y) = (\pi j, \pi m) \) for CDW phase. In the ferromagnetic case, we have checked that the Fourier transform profiles are in agreement with those in Refs.[52, 55].

IV. CONCLUSION

In this work, we have studied the spin-1 BHM in presence of nearest neighbor extended interactions corresponding to both values of the spin dependent interactions using the mean field and the perturbation expansion approach. In the AF case, we have used different justifiable values of the extended interaction strength corresponding to the odd and even MI lobes. In the weak interaction limit, the phase diagram consists of the CDW phase, the MI phase along with the compressible SF and SS phases. In the strong interaction limit, when extended interaction is larger than the width of the odd and even MI lobes, all the MI phases get captured by the CDW phase, since at this critical value, both the CDW and MI phases become degenerate. Further increase of the interaction strength leads to the stability of the SS phase over the other phases.

We have also found that the DW-SF phase shows a first order transition due to a jump in the order parameter. While the DW-SS phase transition is second order in nature for the odd occupancies and of first order for the even occupation densities. The MI-SF phase transition still remain the first and second order respectively for the even and odd MI lobes. We have also calculated the local spin values to confirm the formation of the spin singlet and nematic CDW phases. In the CDW phase, the spin eigenvalues oscillate between 0 and 1 replicating a spin density wave (SDW) pattern.

Further, we have obtained the phase diagrams through the perturbation calculation and the boundary between the CDW-SS and MI-SF phases to compare them with the mean field results. Although the phase diagrams are in agreement with each other, however small discrepancy appears at the tip of the insulating phases and particularly it is prominent for the incompressible phases with even occupation densities.

Also we have studied the order parameter and spin profile in presence of the trapping potential to characterize different phases. In order to get a close resemblance with that of the experimental observations, we have computed the Fourier transform of the order parameter that demonstrates the appearance of peaks at different momenta values which can be experimentally observed via time-of-flight experiment. In the ferromagnetic case, the phase diagrams are similar to the spin-0 Bose gas and both the mean field and the analytic results are in excellent agreement with each other.

Finally, the extended interaction strength which is closely related with the long range dipole-dipole interaction can be of either electric or magnetic in nature having coupling constant \( C_{dd} = \mu^2/\varepsilon_0 \) or \( C_{dd} = \mu^2 \) respectively where \( \mu \) being the dipole moment. For a polarized molecules, the electric dipole moment is very prominent compared to the magnetic dipole moment. But for alkali atoms with spin degrees of freedom, magnetic dipole interaction is notable and very recently for spinor condensates, large magnetic dipole moment of the order of \( 1\mu_B \) for \( ^{87}\text{Rb} \) and \( 6\mu_B \) for \( ^{52}\text{Cr} \) are reported [56].

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