Unconventional Strongly Interacting Bose-Einstein Condensates in Optical Lattices

A. B. Kuklov

Department of Physics, CSI, CUNY - Staten Island, New York, New York 10314, USA

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Feschbach resonances in a non-s-wave channel of two-component bosonic mixtures can induce atomic Bose-Einstein condensates with a nonzero orbital momentum in the optical lattice, if one component is in the Mott insulator state and the other is not. Such non-s-wave condensates break the symmetry of the lattice and, in some cases, time-reversal symmetry. They can be revealed in specific absorption imaging patterns.

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Unprecedented advances in trapping and manipulating ultracold atoms in optical lattices (OLs) [1,2] have created a growing wave of interest in strongly correlated many-body phases and quantum phase transitions. The Mott insulator (MI) superfluid (SF) transition [3] realized in one-component lattice bosons [1] has inspired predictions of the variety of novel phases [4] in quantum mixtures. These phases are all described by the Hubbard-type Hamiltonian [3] in which the lowest single-particle band only is considered in the limit when a typical one-particle band gap exceeds considerably the on site interaction energy. Recently the opposite limit has been reached [5] in the s-wave channel. As pointed out by Diener and Ho in Ref. [6], the resulting effect of the interaction induced band mixing [5] can potentially be a source of yet novel quantum phases and phase transitions.

In this Letter, it is shown that the Feshbach resonance at some $L \neq 0$ angular momentum can induce an *atomic* Bose-Einstein condensate (BEC) which breaks crystal symmetries. Such non-s-wave BEC must be contrasted, on one hand, with the conventional (s-wave) BEC carrying no angular momentum in its ground state and, on the other hand, with the *paired* states found in the fermionic systems: ^{3}He and unconventional superconductors [7,8]. The p-wave resonances have been observed in one-component fermions [9,10]. Higher-L resonances have been detected in bosonic ^{87}Rb [11] and ^{133}Cs [12] systems as well. In the latter case spin-orbit coupling creates interference between different L channels. Here, however, the case of isolated resonance with $L > 0$ is considered for two *distinguishable* bosonic atoms in OLs in order to discuss novel phases and phase transitions in the simplest formulation.

The non-s-wave BECs are characterized by zeros and degeneracy. This apparently contradicts Feynman's argument that the bosonic many-body ground state must have no zeros [13]. In the case $L \neq 0$, however, the system is not in its absolute ground state due to the molecular component. Thus, a such BEC must be viewed in the context of metastable phases generic for atomic traps and OLs, with the stability insured by large difference between intramolecular and atomic center of mass energies.

For two *distinguishable and nonconvertible* bosons, e.g., A and B, in OLs, each site can be approximated by superimposed isotropic oscillator potentials characterized by respective frequencies ω_a, ω_b and masses m_a, m_b for the sorts A and B, respectively. For sake of clarity, however, it is reasonable to simplify further analysis by choosing $m_a = m_b = m$ and $\omega_a = \omega_b = \omega_0$ (the latter circumstance allows decoupling between center of mass and relative motions). The lowest energy one-particle states are classified according to the radial number and to the value of the angular momentum. The lowest states

$$1s, \qquad (1p), \qquad (1d, 2s) \tag{1}$$

are shown in order of increasing energy from left to right. The states $1s$, $2s$ carry no angular momentum L. The state $1p$ corresponds to $L = 1$. It is triple degenerate and transforms as a vector

$$\psi_{1p} \equiv \psi_i \sim x_i, \tag{2}$$

where $x_i = x, y, z$ stand for Cartesian coordinates. The state $1d$ with $L = 2$ is fivefold degenerate. It transforms as a tensor: $\psi_{1d} \equiv \psi_{ij} \sim x_i x_j - \frac{\mathbf{x}^2}{3}\delta_{ij}$.

Let us consider a situation of Feschbach resonance in the L-wave channel between the species. The corresponding closed channel molecular state $\Phi_\alpha(\mathbf{r})$ is characterized by some degeneracy index α (for $L = 1$, $\alpha = x, y, z$ [14]), with $\mathbf{r}$ standing for the relative coordinates of the A and B atoms. The analysis for one site closely follows the approach of Diener and Ho [6]. Its validity for the lattice is determined by smallness of a typical intersite tunneling amplitude t in comparison with the on site excitation energy ω_0. The size r_ϕ of the molecule is assumed to be much less than the oscillator length $r_0 = 1/\sqrt{m\omega_0}$ (units $\hbar = 1$ are employed here and below) [15]. Introducing the creation-annihilation operators for the molecule $c^\dagger_\alpha$, c_α and for the A and B bosons $a^\dagger_m$, a_m and $b^\dagger_n$, b_n, respectively, with m, n referring to the oscillator levels, the on site Hamiltonian can be written in the form

$$H = \sum_{\alpha} \bar{\nu}\, c_{\alpha}^{\dagger} c_{\alpha} + \sum_{m} [\varepsilon_{am} a_m^{\dagger} a_m + \varepsilon_{bm} b_m^{\dagger} b_m] - \sum_{m,n} \gamma_{\alpha,mn} (c_{\alpha}^{\dagger} a_m b_n + \text{H.c.}), \quad (3)$$

with $\bar{\nu}$ standing for the bare molecular energy and ε_{am}, ε_{bm} labeling the oscillator energy levels. Here particle interactions beyond the resonant one are not shown explicitly. The resonance-interaction matrix elements $\gamma_{\alpha,mn}$ are determined by the strength of the open-closed channels coupling and by the symmetry: for given α, it selects such states m, n so that the center of mass of the pair resides in the $1s$ oscillator state $\sim \exp(-m\omega_0 \mathbf{R}^2)$ and their relative motion is characterized by oscillator wave function $\psi_n(\mathbf{r})$ with given L. For example, for $L = 1$ the lowest energy term is the $1p$ state $\psi_{n=\alpha}(\mathbf{r}) \sim \exp(-m\omega_0 \mathbf{r}^2/4)(\mathbf{r})_{\alpha}$, $\alpha = x, y, z$. Here (for equal masses), $\mathbf{R} = (\mathbf{r_a} + \mathbf{r_b})/2$, $\mathbf{r} = \mathbf{r}_a - \mathbf{r}_b$, and $\mathbf{r}_a$ and $\mathbf{r}_b$ refer to the coordinates of the A and B particles, respectively.

For large enough $\gamma_{\alpha,mn}$ it is natural to expect that, upon proper tuning of $\bar{\nu}$, it is possible to make the lowest energy E_L of the AB pair with relative L to lie *below* the energy $E_0 = \varepsilon_{a0} + \varepsilon_{b0} = 3\omega_0$ of both atoms in the $1s$ state (in which they do not participate in the resonance). This is possible because no states with $L = 0$ are simply present in the expansion given by $\gamma_{\alpha,mn}$. The resulting ground state should be looked for in the form [6]:

$$|L, \alpha\rangle = B_{L\alpha}^{\dagger}|0\rangle, \qquad B_{L\alpha}^{\dagger} = \beta c^{\dagger} + \sum_{mn} \eta_{mn} a_m^{\dagger} b_n^{\dagger}, \quad (4)$$

with $\beta^2 + \sum_{mn} \eta_{mn}^2 = 1$, and the summation running over those oscillator states which are characterized by the selected α orbital of the given relative angular momentum L. The full procedure of finding β, η_{mn}, E_L requires proper renormalization of the detuning $\bar{\nu}$ [6]. Some complication also comes from the sensitivity of the eigenenergies to microscopic details of $\Phi_{\alpha}(\mathbf{r})$. One can, however, choose the variational approach in order to obtain the *upper bound* estimate for E_L in terms of the matrix elements $\gamma_{\alpha,mn}$ admixing the lowest oscillator levels only. Hence, if the condition $E_L < E_0$ holds for the upper bound of E_L, it will be satisfied within the exact scheme [6] for sure. This also helps establishing the symmetry and topological properties of the phase because these do not depend on the number of states involved in the expansion (4).

In the case $L = 1$, the lowest relevant oscillator states are $1s$ and $1p$ from the nomenclature (1). Then, the two-body wave function in the open channel $\Psi_{0\alpha}(\mathbf{r}_a, \mathbf{r}_b) \sim \exp(-m\omega_0 \mathbf{R}^2) \exp(-m\omega_0 \mathbf{r}^2/4)(\mathbf{r})_{\alpha}$ can be expanded as $\sim \exp(-m\omega_0 \mathbf{r}_a^2/2)(\mathbf{r}_a)_{\alpha} \exp(-m\omega_0 \mathbf{r}_b^2/2) - \exp(-m\omega_0 \mathbf{r}_b^2/2)(\mathbf{r}_b)_{\alpha} \exp(-m\omega_0 \mathbf{r}_a^2/2)$. This translates into truncating the expansion (4) by the lowest terms only: $|L = 1, \alpha\rangle = [\beta c^{\dagger} + \eta(a_0^{\dagger} b_{\alpha}^{\dagger} - b_0^{\dagger} a_{\alpha}^{\dagger})]|0\rangle$, with $\beta^2 + 2\eta^2 = 1$. Then, $E_L = \langle L = 1, \alpha | H | \alpha, L = 1\rangle$ selects only the terms with $\gamma_{\alpha,0\alpha} = -\gamma_{\alpha,\alpha 0} = \gamma$ in Eq. (3). The resulting *upper bound* estimate for the ground state energy is $E_L = (\bar{\nu} + 4\omega_0)/2 - \sqrt{(\bar{\nu} - 4\omega_0)^2/4 + \gamma^2}$, where $4\omega_0$ is the bare oscillator energy of the pair on $1p + 1s$ level. It must be compared with $E_0 = 3\omega_0$ of the state $1s + 1s$. Obviously, if $\bar{\nu}$ is tuned to $\approx 4\omega_0$, then $E_L \approx 4\omega_0 - |\gamma|$. Thus, for

$$|\gamma| \geq \omega_0, \quad (5)$$

the state $|L = 1, \alpha\rangle$ must become the ground state instead of $|L = 0\rangle$. Clearly, tuning $\bar{\nu}$ (or its renormalized value $\bar{\nu}^*$ [6]) to higher values will eventually raise the energy E_L above E_0. In contrast, if $|\gamma| < \omega_0$, no effect is most likely to be observed for any $\bar{\nu}$.

The matrix element γ is determined by exchange interaction V_{ex} on molecular distances further reduced by small overlap between the closed and open channels. Using $V_{\text{ex}} \sim 1$ eV on atomic distances $a_0 \sim 10^{-8}$ cm and taking $r_{\phi} \sim 1$ nm [15] and $r_0 \sim 10^{-4}$ cm, the estimate for arbitrary L gives $\gamma \sim V_{\text{ex}}(a_0/r_{\phi})(r_{\phi}/r_0)^{3/2+L}$, where it was taken into account that the wave function of the relative motion is $\sim r^L$ at the origin. For the p-wave case ($L = 1$) one finds $\gamma \approx 30\ \mu\text{K} \approx 3$ MHz. This shows plenty of room for satisfying the condition (5) for typical OL frequencies in the range of few kHz. Clearly, higher resonances with $L = 2, 3\ldots$ will be characterized by smaller γ. In terms of the typical exchange matrix element $\tilde{V}_{\text{ex}} = V_{\text{ex}} r_{\phi}/a_0$, the typical molecular kinetic energy $\epsilon_0 \approx 1/(m r_{\phi}^2)$ and r_{ϕ}/r_0 the estimate as a function of L becomes

$$\gamma/\omega_0 \approx (\tilde{V}_{\text{ex}}/\epsilon_0)(r_{\phi}/r_0)^{L-1/2}. \quad (6)$$

For chosen parameters, this gives $\gamma/\omega_0 \approx 10^5 (r_{\phi}/r_0)^{L-1/2}$, and the condition (5) can be satisfied by $L = 1, 2$. Choosing to work with smaller r_0, about $r_0 \approx 10^{-5}$ cm, will allow realization of the ground state with L as high as $L = 3$. For higher L, however, it becomes important that the one-particle band gap is $L\omega_0$, and the condition (5) must, actually, be $\gamma \geq L\omega_0$.

Non-s-wave Bose-Einstein condensate of the $A + B$ mixture.—Let us consider a situation when all N lattice sites are filled by A bosons in the deep MI regime, so that the vacuum state is $|\text{MI}\rangle = \prod_i^N a_0^{\dagger}(i)|0\rangle$. Adding a small number $N_B \ll N$ of B bosons to such vacuum in the regime of the L wave $A + B$ resonance will result in formation of the on site states (4). In the limit of weak tunneling such resonant complexes will delocalize over the lattice without changing their shape.

The state (4) is characterized by strong entanglement. Thus, it is important to verify that such entanglement is not in a conflict with the formation of the off-diagonal long range order (ODLRO). The operator $B_{L\alpha}^{\dagger}(i) a_0(i)$ creates one excitation on a site i from the vacuum $|\text{MI}\rangle$. Here and below the dependence on the site index i is shown explicitly. Since the limit of low density of the excitations is considered, it is enough to verify that one excitation forming a band wave

$$\tilde{B}^{\dagger}_{L\alpha} = \sum_i \frac{1}{\sqrt{N}} B^{\dagger}_{L\alpha}(i) a_0(i) \tag{7}$$

contributes constructively to the ODLRO density matrix $\rho^{(b)}_{mn}(i,j) = \langle \mathrm{MI}|\tilde{B}_{L\alpha} b^{\dagger}_m(i) b_n(j) \tilde{B}^{\dagger}_{L\alpha}|\mathrm{MI}\rangle$ in the limit $|\mathbf{x}_i - \mathbf{x}_j| \to \infty$. Direct calculation gives $\rho^{(b)}_{mn}(i,j) = \eta^*_{0n}\eta_{0m}/N$. For N_B bosons, with $1 \ll N_B \ll N$, the result becomes

$$\rho^{(b)}_{mn}(i,j) = \eta^*_{0n}\eta_{0m} n_B, \tag{8}$$

where $n_B = N_B/N$, with the index n referring to the on site oscillator states with the selected (by the resonance) angular momentum L of a B particle. It is worth noting quite significant quantum depletion of the condensate density even in the limit $n_B \ll 1$ due to $|\eta_{0n}| < 1$. Within the variational approach discussed above, η_{0n} is to be replaced by η, and the indices m, n must be set equal to a given α orbital of the, e.g., $1p$ oscillator state [16]. It is important to note that no other channel contains the ODLRO, that is, $\langle b^{\dagger}_0(i) b_0(j)\rangle = 0$, $\langle a^{\dagger}_m(i) a_n(j)\rangle = 0$ and $\langle c^{\dagger}_{\alpha}(i) c_{\alpha'}(j)\rangle = 0$ for $\mathbf{x}_i \neq \mathbf{x}_j$.

Macroscopic properties of the p-wave BEC.—Any $L > 0$-wave BEC have *zero* population of the zero-momentum state even in an infinite and uniform system. This follows from vanishing of the space integral of any non-s orbital function. In other words, $\int d\mathbf{x} W_{\alpha}(\mathbf{x} - \mathbf{x}_i) = 0$ where $W_{\alpha}(\mathbf{x} - \mathbf{x}_i)$ stands for a non-s-wave orbital Wannier function localized at the coordinates $\mathbf{x}_i$ of the ith site. This leads to quite unusual macroscopic properties.

Let us consider, first, two neighboring sites, say, i and j. Then, the tunneling part of the Hamiltonian can be constructed following the standard procedure [17]. The symmetry condition (2) immediately implies that no tunneling takes place between states with different $\alpha = x, y, z$. Furthermore, since $W_{\alpha}(\mathbf{x})$ is odd for the p wave, the tunneling amplitude $t^{(\alpha)}_{ij}$ is *negative* along the orientation of the α orbital and positive if perpendicular. The reason for that is that the symmetric combination $W_{\alpha}(\mathbf{x} - \mathbf{x}_i) + W_{\alpha}(\mathbf{x} - \mathbf{x}_j)$ for α being along the direction $\sim \mathbf{x}_i - \mathbf{x}_j$ has one extra zero in comparison with the antisymmetric one $W_{\alpha}(\mathbf{x} - \mathbf{x}_i) - W_{\alpha}(\mathbf{x} - \mathbf{x}_j)$. Thus, the lowest energy of the secular equation corresponds to the antisymmetric combination. In general, the sign of $t^{(\alpha)}_{ij}$ depends on mutual orientation of the vector $\mathbf{u} = (\mathbf{x}_i - \mathbf{x}_j)/|\mathbf{x}_i - \mathbf{x}_j|$ and of the orbital. If $u_x = 1$, $u_y = 0$, $u_z = 0$ and the orbital assignment is taken according to the x axis being along $\mathbf{u}$, then, there are two nonzero values in the set $t^{(\alpha)}_{ij}$. These are $t_{||} = t^{(x)}_{ij} < 0$ and $t_{\perp} = t^{(y)}_{ij} = t^{(z)}_{ij} > 0$.

The lattice Hamiltonian formulated in terms of the lowest $L = 1$-band operators $b^{\dagger}_{\alpha}(i)$, $b_{\alpha}(i)$ becomes

$$H_B = -\sum_{\alpha,\langle ij\rangle} t^{(\alpha)}_{ij} b^{\dagger}_{\alpha}(i) b_{\alpha}(j) - \sum_{i,\alpha\beta} \Omega \mathbf{L}_{\alpha\beta} b^{\dagger}_{\alpha}(i) b_{\beta}(i) \tag{9}$$

in the hard-core approximation $b_{\alpha}(i) b_{\beta}(i) = 0$. The last term in Eq. (9) describes the effect of external rotation of OLs at some angular frequency Ω, with $\mathbf{L}_{\alpha\beta}$ standing for the angular momentum operator $\hat{\mathbf{L}}$ built on the on site Wannier functions: $\mathbf{L}_{\alpha\beta} = \int d\mathbf{x} W^*_{\alpha}(\mathbf{x}) \hat{\mathbf{L}} W_{\beta}(\mathbf{x})$. Thus, in addition to the possibility of introducing vortices, external rotation induces mixing between the components. This effect of rotation is specific for the non-s-wave BEC.

In general, properties of the non-s-wave BEC depend strongly on the lattice symmetry and its structural defects and boundaries. In particular, the translational lattice symmetry is broken. Specifically for the p-wave BEC, the phase φ_r in $\langle b_{\alpha}(r)\rangle \sim e^{i\varphi_r}$ must oscillate as $\varphi_r = \pi(1 + (-1)^r)/2$ along the direction of the orbital in order to lower the tunneling energy. Such a tendency to form spatial superstructure of the phase can lead to *spontaneous* ground state currents in, e.g., the triangular lattice because of the sign frustration along the elementary plaquet.

In the tetragonal lattice the condensation proceeds into either $p = z$ or the $p = x, y$ states. If the z-axis lattice constant is the shortest one, the tunneling energy will be gained by forming the one-component z-BEC. In the opposite case, the two-component xy-BEC occurs with two options: (i) The order parameter (OP) is real of the type $x \pm y$; (ii) the OP is complex as $x \pm iy$ and, therefore, it breaks the time-reversal symmetry. What option is actually realized depends on the details of the interaction. On the mean field level, in the xy-BEC two components ψ_x and ψ_y must be considered [8]. The corresponding Landau expansion obeys the OL symmetry. Thus, the quadratic $|\psi_{x,y}|^2$ and the gradient terms do not distinguish between the options. Among the quartic terms, there is one $H_t = \int d^3x g_t(\psi^{*2}_x \psi^2_y + \text{c.c.})$ which determines the phase locking between the components similarly to the situation in the d-wave superconductor [18]. If $g_t < 0$, the option (i) takes place. Then, the phases φ_x and φ_y are equal to each other and the condensation proceeds into the state $\psi_x \pm \psi_y$ with $|\psi_y| = |\psi_x| = \sqrt{\rho_p}$. Accordingly, the line of zeros will be arranged along the plane $x = \mp y$. If, however, $g_t > 0$, the energy can be lowered if $\varphi_x - \varphi_y = \pm\pi/2$, so that there are no zeros in $\psi_{\pm} = \psi_x \pm i\psi_y$. Then, similarly to the case of the d-wave superconductor [18], the ground state can have spontaneous fractional vortices initiated close to the OL boundaries and structural defects.

The Josephson effect can also feature spontaneous currents [18] even though the time reversal is not broken. If the p-orbital BEC is surrounded by the s-wave BEC of the same particles, the tunneling current $J_c(\theta)$ between two BECs will strongly depend on the angle θ between the orientations of the orbital $\mathbf{u}$ and of the boundary $\mathbf{n}^{(s)}$. If $\mathbf{u} \cdot \mathbf{n}^{(s)} = 0$, no tunneling will take place because the current from the positive part of the lobe of the p orbital will be exactly compensated by the current from the negative part. In general, $J_c(\theta) \sim \cos\theta$. Thus, there will be a phase jump of π for a contour traversing both SFs so that θ changes by 180° along it. This implies that a spontaneous vortex, carrying 1/2 of the standard circulation, can form if the

system size R is macroscopic in comparison with the healing length and any length associated with the Josephson coupling.

L-wave Mott insulator.—At $N_B = N$ and for strong s-wave intraspecies repulsion the system becomes MI with broken lattice (including time-reversal) symmetries. Obviously, tuning away from the L-wave resonance will result in a phase transition into the two-component MI with no broken symmetries. The nature of the L-wave MI as well as of the phase transition requires separate analysis.

Detection.—Non-s-wave condensates should produce specific absorption imaging patterns due to condensation into the $\mathbf{k} \neq 0$ state. For example, considering the options (i) and (ii), the $\psi_{a=1,2}$ operator becomes

$$\psi_a(\mathbf{x}) = \sum_i W_a(\mathbf{x} - \mathbf{x}_i) b_a(i), \qquad a = 1, 2. \tag{10}$$

The Wannier function can be taken as $W_1(\mathbf{x}) \approx a_w^{-5/2} e^{-\mathbf{x}^2/2a_w^2}(x \pm y)$, with $a_w \approx r_0$, in the case of the time-invariant state (i) and as $W_2(\mathbf{x}) \approx a_w^{-5/2} e^{-\mathbf{x}^2/2a_w^2}(x \pm iy)$ in the case (ii) of the broken time-reversal symmetry. After atoms are released from the OLs, free expansion will transform the operator (10) so that $W_a(\mathbf{x})$ is replaced by the result of the application of the free-space propagator. Then, the cloud density $n_B(\mathbf{x}, t)$ of the B atoms in the far zone becomes [19]: $n_B(\mathbf{x}, t) \sim |\tilde{W}_a(\mathbf{q})|^2 \sum_{ij} \exp(i\mathbf{q}(\mathbf{x}_i - \mathbf{x}_j)) \times \langle b_a^\dagger(i) b_a(j) \rangle$, where $\tilde{W}_a(\mathbf{q})$ stands for the Fourier transform of $W_a(\mathbf{x})$ with the momentum $\mathbf{q} = \mathbf{x}/t$. These transforms $\tilde{W}_1(\mathbf{q}) \approx t^{-5/2}(x \pm y)$ and $\tilde{W}_2(\mathbf{q}) \approx t^{-5/2}(x \pm iy)$ should be contrasted with the one for the s-wave BEC, $\sim t^{-3/2}$. The expressions $\tilde{W}_{1,2}(\mathbf{q})$ feature modulation of the standard Bragg peaks [1] by the factors $(x \pm y)^2/t^2$ and $(x^2 + y^2)/t^2$ for the options (i) and (ii), respectively. In the first case, the peaks along the line (in the columnar image) $x = \mp y$ will be suppressed. In the second, the central Bragg spot only will be strongly suppressed. In general, the imaging pattern reflects the symmetry of the orbital and of the lattice. [Similar expression can be easily obtained for the p-wave BEC with the OP of the z-type]. The corresponding patterns are recognizable by the lines of zeros or by the suppression of the central Bragg peak. Higher L condensates will feature more complex patterns. It is worth noting that rotation of the lattice can produce switching between the patterns, e.g., from (i) to (ii) because finite Ω in Eq. (9) promotes ferromagnetic ordering of the on site angular momenta, that is, the state (ii): $\psi_\pm \sim x \pm iy$, with the sign chosen by the direction of Ω.

In conclusion, Feshbach resonance in a nonzero angular momentum channel favors formation of the non-s-wave BEC characterized by space-time symmetries lower than those of the OLs. The ground state contains lines of zeros and spontaneous currents induced by boundaries and structural defects. The absorption images exhibit additional strong modulational patterns reflecting the nontrivial symmetry of the ground state. Imposing non-s-wave Feschbach resonance on a lattice with double occupation in MI regime can induce insulating phases with broken lattice symmetry. Varying the detuning of non-s-wave resonance can lead to various quantum phase transitions between the phases: S-wave BEC, non-S-wave BEC, conventional MI and orbital MI (with broken lattice symmetries).

Similar conclusions about properties of the p-orbital BEC have been obtained in Refs. [20], where the case of a boson-fermion mixture in OLs was analyzed.

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