# Energy band structure of spin-1 condensates in optical lattices*

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The energy band structure of spin-1 condensates with repulsive spin-independent and either ferromagnetic or antiferromagnetic spin-dependent interactions in one-dimensional (1D) periodic optical lattices is discussed. Within the two-mode approximation, Bloch bands of spin-1 condensates are presented. The results show that the Bloch bands exhibit a complex structure as the atom density of $m_{\rm F}=0$ hyperfine state increases: bands splitting, reversion, intersection and loop structure are excited subsequently. The complex band structure should be related to the tunneling and spin-mixing dynamics.

**Keywords:** spin-1 condensates, optical lattices, band structure

**PACC:** 0365, 0530, 0570

## 1. Introduction

The realization of spinor condensate of $^{23}$Na and $^{87}$Rb[1,2] in optical traps provides an active field for studying the many-body quantum system. The releasing of spin degree of freedom in spinor condensates results in many complex and novel spin-induced phenomena, such as spin-domains,[3−6] spin-texture,[7,8] spin-mixing[9−15] and spinor soliton.[16−19] Among them, great attention is paid to the spin-mixing dynamics inside a spin-1 condensate: two $|F=1,\ m_{\rm F}=0\rangle$ atoms are converted into one $|F=1,\ m_{\rm F}=1\rangle$ and one $|F=1,\ m_{\rm F}=-1\rangle$ upon an elastic collision and *vice versa*. More interestingly, because of controllable lattice parameters (such as lattice depth and spacing),[20−23] spinor condensates in optical lattices would reveal more interesting dynamical phenomena. Coherent spin-mixing oscillation in a Mott state of two atoms at a lattice site was observed.[24,25] Highly controllable magnetic solitons in spinor condensates confined in 1D optical lattices are also predicted.[26] Recently, hybrid localized states, i.e., spinor Bloch/gap waves and spinor gap solitons, in spin-1 condensates are revealed.[27]

In this paper, we focus on studying the energy band structure of spin-1 condensates trapped in 1D optical lattices. Within the two-mode approximation, the Bloch bands of spin-1 condensates are presented. The results show that the Bloch band structure is modified significantly by the atom density $n_0$ of the $m_{\rm F}=0$ hyperfine state. It indicates that, as $n_0$ increases, bands splitting, reversion and intersection occur subsequently, and then loop structures in Bloch bands at the first Brilliouin zone edge are excited. The complex and interesting band structure is related to the tunneling and spin-mixing dynamics.

## 2. Two-mode approximation and energy band structure

We focus our attention on the situation that $F=1$ spinor condensates with repulsive spin-independent and either ferromagnetic or antiferromagnetic spin-dependent interactions are loaded into 1D optical lattices in which the motion in the perpendicular directions is confined. In the absence of external magnetic field and at zero temperature, the dynamics of $F=1$ spinor condensates can be described by the following equations,[27]

$$\mathrm{i}\,\frac{\partial\psi_{\pm}}{\partial t}=-\frac{\partial^2\psi_{\pm}}{\partial x^2}+V_0\cos(2x)\psi_{\pm}$$

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$$
\begin{aligned}
&+\lambda_1(|\psi_\pm|^2+|\psi_0|^2+|\psi_\mp|^2)\psi_\pm\\
&+\lambda_2(|\psi_\pm|^2+|\psi_0|^2-|\psi_\mp|^2)\psi_\pm+\lambda_2\psi_0^2\psi_\mp^*,\\
\mathrm{i}\frac{\partial\psi_0}{\partial t} &= -\frac{\partial^2\psi_0}{\partial x^2}+V_0\cos(2x)\psi_0\\
&+\lambda_1(|\psi_+|^2+|\psi_0|^2+|\psi_-|^2)\psi_0\\
&+\lambda_2(|\psi_+|^2+|\psi_-|^2)\psi_0+2\lambda_2\psi_+\psi_-\psi_0^*, \quad (1)
\end{aligned}
$$

where $\psi_j$ is the 1D vector wave function, $j=\pm,0$ denotes atomic hyperfine states $|F=1,\ m_\mathrm{F}=\pm,0\rangle$, respectively. All the variables here are re-scaled to dimensionless as $t\sim t/\nu$, $x\sim xd/\pi$, $\psi_j\sim\sqrt{\nu/2a_0\omega_\perp}\psi_j$, where, $\omega_\perp$ is the trapping frequency in the direction perpendicular to the lattices, $\nu=E_R/\hbar$, and $E_R=\hbar^2\pi^2/2md^2$ is the recoil energy of the lattices. $V_0\cos(2x)$ is the external optical potential imposed on the system and $d$ is the period of the optical lattices. Terms with coefficients $\lambda_1$ and $\lambda_2$ are the effective spin-independent and spin-dependent interactions of spin-1 atoms expressed in terms of the scattering lengths $a_0$ and $a_2$ in the combined symmetric channel of total spin 0 and 2, $\lambda_1=(a_0+2a_2)/3a_0$, and $\lambda_2=(a_2-a_0)/3a_0$. The s-wave scattering lengths $a_0=101.8a_\mathrm{B}$, $a_2=100.4a_\mathrm{B}$ for $^{87}$Rb (ferromagnetic) and $a_0=50a_\mathrm{B}$, $a_2=55a_\mathrm{B}$ for $^{23}$Na (antiferromagnetic), $a_\mathrm{B}$ is the Bohr radius. Therefore, we obtain the dimensionless 1D coupling constants $\lambda_1\approx0.99,\lambda_2\approx-0.0046$ for $^{87}$Rb and $\lambda_1\approx1.067,\lambda_2\approx0.033$ for $^{23}$Na.

In optical lattice, the states of the condensates in the form of Bloch waves can be described by the energy, which is given by

$$
\begin{aligned}
\tilde{E} = \frac{1}{\pi}\int_{-\pi/2}^{\pi/2}\mathrm{d}x\Bigg[&\sum_{j=\pm,0}\left[\left(\left|\frac{\partial\psi_j}{\partial x}\right|^2+V_0\cos 2x|\psi_j|^2\right)\right]+\frac{\lambda_1}{2}(|\psi_+|^4+|\psi_0|^4+|\psi_-|^4)\\
&+\frac{\lambda_1}{2}(|\psi_+|^2|\psi_0|^2+|\psi_0|^2|\psi_-|^2+|\psi_-|^2|\psi_+|^2)+\frac{\lambda_2}{2}(|\psi_+|^4+|\psi_-|^4)\\
&+\frac{\lambda_2}{2}(|\psi_+|^2|\psi_0|^2+|\psi_0|^2|\psi_-|^2-|\psi_-|^2|\psi_+|^2)+\lambda_2(\psi_0^2\psi_+^*\psi_-^*+\psi_+\psi_-\psi_0^{*2})\Bigg]. \quad (2)
\end{aligned}
$$

In order to study the properties of the lowest energy band structure at the boundary of the first Brillouin zone when the spin-dependent interaction is considered, we employ a two-mode approximation with trial wave functions of the following form

$$
\begin{aligned}
\psi_\pm &= \sqrt{n_\pm}\,\mathrm{e}^{\mathrm{i}\,kx}(\cos\theta+\sin\theta\,\mathrm{e}^{-2\,\mathrm{i}\,x}),\\
\psi_0 &= \sqrt{n_0}\,\mathrm{e}^{\mathrm{i}\,kx}(\cos\theta_0+\sin\theta_0\,\mathrm{e}^{-2\,\mathrm{i}\,x}), \quad (3)
\end{aligned}
$$

where $\hbar k$ is the quasi-momentum and $n_j=\frac{1}{\pi}\int_{-\pi/2}^{\pi/2}\mathrm{d}x|\psi_j|^2$ is the average particle density of $\psi_j$, respectively. As shown in Refs. [28] and [29], the two-mode approximation (3) can give a good approximation in the neighbourhood of the zone boundary (in which we are especially interested). Introducing the above trial waves into Eq. (2), one can obtain the parameterized energy

$$
\tilde{E}=E_\mathrm{kin}+E_\mathrm{pot}+E_\mathrm{int1}+E_\mathrm{int2}, \quad (4)
$$

where $E_\mathrm{kin}=(n_++n_-)(k^2+4(1-k)\sin^2\theta)+n_0(k^2+4(1-k)\sin^2\theta_0)$ is the kinetic energy of the system, $E_\mathrm{pot}=0.5V_0[(n_++n_-)\sin2\theta+n_0\sin2\theta_0]$ is the potential energy,

$$
\begin{aligned}
E_\mathrm{int1} = &\lambda_1(n_++n_-)^2\left(\frac{1}{2}+\frac{1}{4}\sin^2 2\theta\right)\\
&+\lambda_1 n_0^2\left(\frac{1}{2}+\frac{1}{4}\sin^2 2\theta_0\right)\\
&+\lambda_1 n_0(n_++n_-)\left(1+\frac{1}{2}\sin2\theta\sin2\theta_0\right) \quad (5)
\end{aligned}
$$

and

$$
\begin{aligned}
E_\mathrm{int2} = &\lambda_2 n_0(n_++n_-)\left(1+\frac{1}{2}\sin2\theta\sin2\theta_0\right)\\
&+2\lambda_2 n_0\sqrt{n_+n_-}(\cos^2\theta\cos^2\theta_0\\
&+\sin2\theta\sin2\theta_0+\sin^2\theta\sin^2\theta_0) \quad (6)
\end{aligned}
$$

are the spin-independent and spin-dependent interaction energies, respectively. Assuming the system is near stationary configuration and spin-mixing is weak, the quasi-stationary configuration of the system can be obtained by a variational method requiring that the derivatives of the energy functional with respect to $\theta$ and $\theta_0$ vanish,

$$
\begin{aligned}
&4(1-k)\sin 2\theta + V_0\cos 2\theta + \frac{1}{2}\lambda_1(n_+ + n_-)\sin 4\theta + \lambda_1 n_0 \sin 2\theta_0 \cos 2\theta \\
&\quad + 2\lambda_2 \frac{n_0\sqrt{n_+ n_-}}{n_+ + n_-}(2\cos 2\theta \sin 2\theta_0 - \sin 2\theta \cos 2\theta_0) = 0, \\
&4(1-k)\sin 2\theta_0 + V_0\cos 2\theta_0 + \frac{1}{2}\lambda_1 n_0 \sin 4\theta_0 + \lambda_1(n_+ + n_-)\sin 2\theta \cos 2\theta_0 \\
&\quad + 2\lambda_2\sqrt{n_+ n_-}(2\cos 2\theta_0 \sin 2\theta - \sin 2\theta_0 \cos 2\theta) = 0.
\end{aligned} \tag{7}
$$

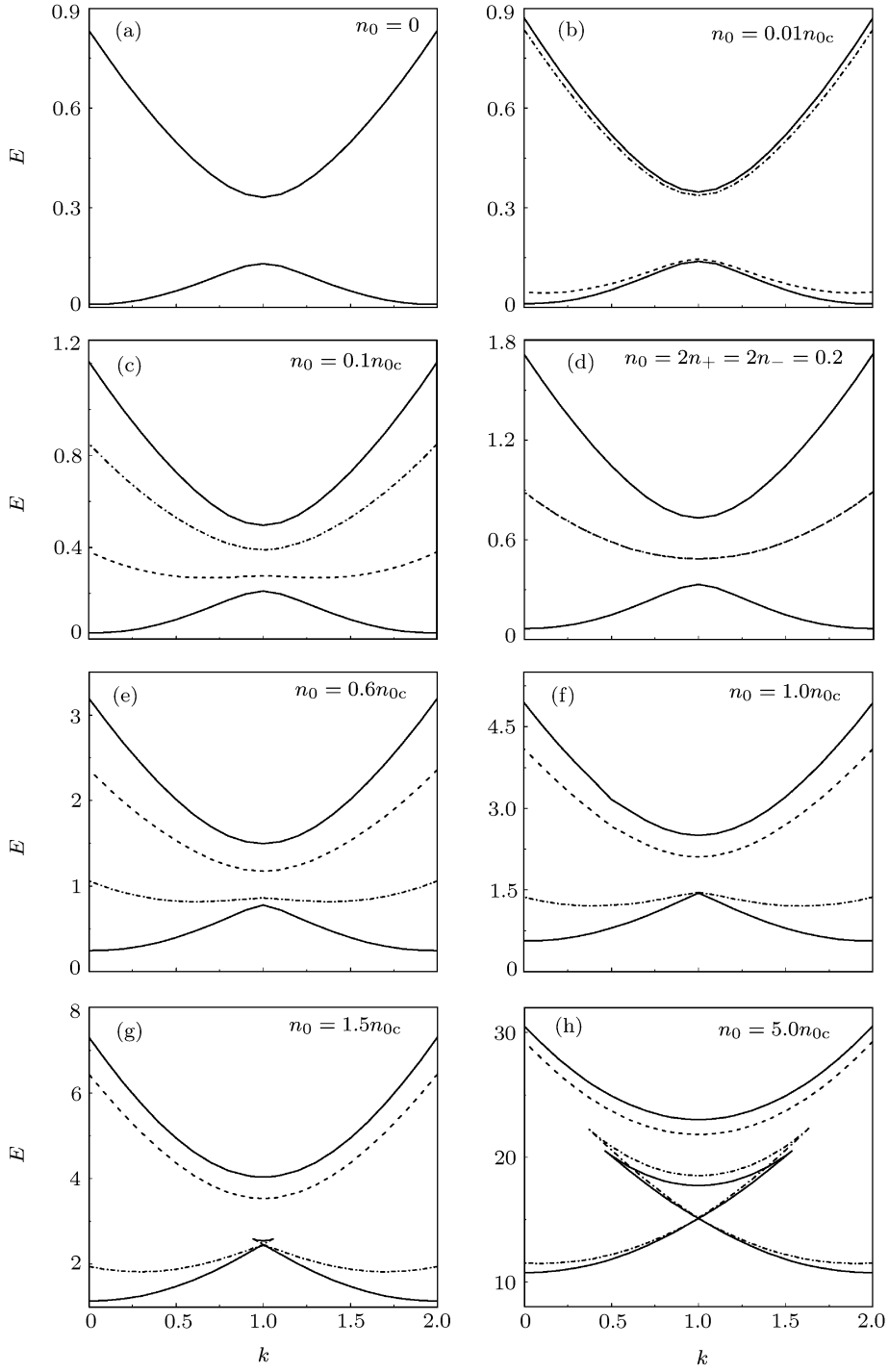



**Fig. 1.** Energy band structure at different $n_0$ for $^{23}$Na ($n_+ = n_- = 0.1$, $V_0 = 1$).

Then, from Eqs. (4)–(7), we can obtain the lowest energy bands of the system. Since the energy bands of $^{87}$Rb are similar to $^{23}$Na, so we just consider the energy bands of $^{23}$Na here. Fixing $n_+ = n_- = 0.1$ and varying the value of $n_0$, we discuss the effect of $n_0$ on energy bands. As shown in Fig. 1, complex band structure of spin-1 condensates with different $n_0$ is provided. Clearly, when $n_0 = 0$ (Fig. 1(a)), there only exist $\psi_\pm$ components. Because we have assumed $\psi_+ = \psi_-$, so the bands degenerate to the one-component case. When $n_0 > 0$, the two initial energy bands are split apart into four and two new bands are generated (the dash-dotted and dotted-lines in Fig. 1(b)). As $n_0$ increases, while all the four bands shift-upwards: the two new bands close together gradually (Figs. 1(b) and 1(c)); when $n_0 = 2n_+ = 2n_- = 0.2$, the two new bands degenerate to one (Fig. 1(d)); after that, the two new bands exchange their positions and bands reversion occurs, i.e., the energy of the upper new band becomes lower than that of the lower new band (Fig. 1(e)); when $n_0 = n_{0c}$ (Fig. 1(f)), the reversed upper new band (the dashed-line in Fig. 1(f)) intersects with the lowest band and a tip structure occurs at the boundary of the first Brillouin zone edge ($k = 1$); when $n_0 > n_{0c}$, two loop structures are developed at the zone edge ($k$=1); after that, two loops grow bigger and bigger as $n_0$ increases (Figs. 1(g) and 1(h)). It is clear that the $m_F = 0$ component provides significant effects on the energy band structure which shows very different characters from that in one-component Bose–Einstein condensation (BEC). The critical value $n_{0c}$ for appearance of loop structure is shown in Fig. 2. It is clear that $n_{0c}$ increases linearly with $V_0$.

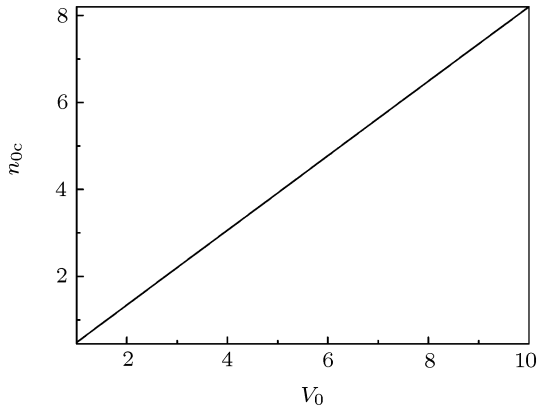
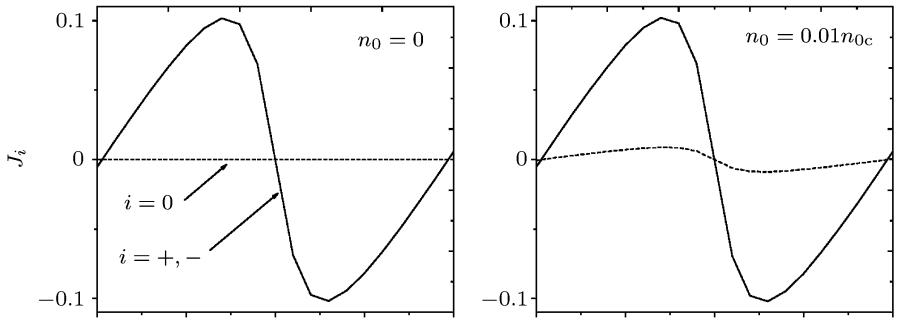



**Fig. 2.** Critical particle density $n_{0c}$ for developing the loop structure as a function of lattices depth $V_0$ ($n_+ = n_- = 0.1$).

The complex and interesting band structure in spin-1 condensates would be related to the spin-mixing dynamics: when $n_0 = 2n_+ = 2n_-$, the spin-1 condensates are prepared initially in a stationary configuration and spin-mixing is inhibited; when $0 < n_0 \neq 2n_\pm$, the condensates are prepared initially in a non-stationary configuration and spin-mixing takes place, the purely exchanged atoms originate from $m_F = \pm$ states when $0 < n_0 < 2n_\pm$ and from $m_F = 0$ state when $0 < n_0 < 2n_\pm$. The appearance of loop structure indicates the breakdown of Bloch oscillation due to the non-zero adiabatic tunnelling into the upper band. In Fig. 3 we show the current density $J_j(k,n) = \hbar/2mi(\psi_j^* \mathrm{d}\psi_j/\mathrm{d}x - \psi_j \mathrm{d}\psi_j^*/\mathrm{d}x)$ of the condensates for the same number densities as in Fig. 1. When $n_0 < n_{0c}$, the current goes to zero both at the zone centre ($k = 0$) and the zone boundary ($k = 1$). At the critical density ($n_0 = n_{0c}$), the current density $J_j(k, nc)$ goes to zero at the zone boundary but has an infinite derivative at this point. Consequently, the energy band develops a singularity at the zone boundary as shown in Fig. 2. When $n_0 > n_{0c}$, however, the current density has three solutions for a given $k$ near the zone boundary. It indicates the breakdown of Bloch oscillation due to the non-zero adiabatic tunnelling into the upper band.



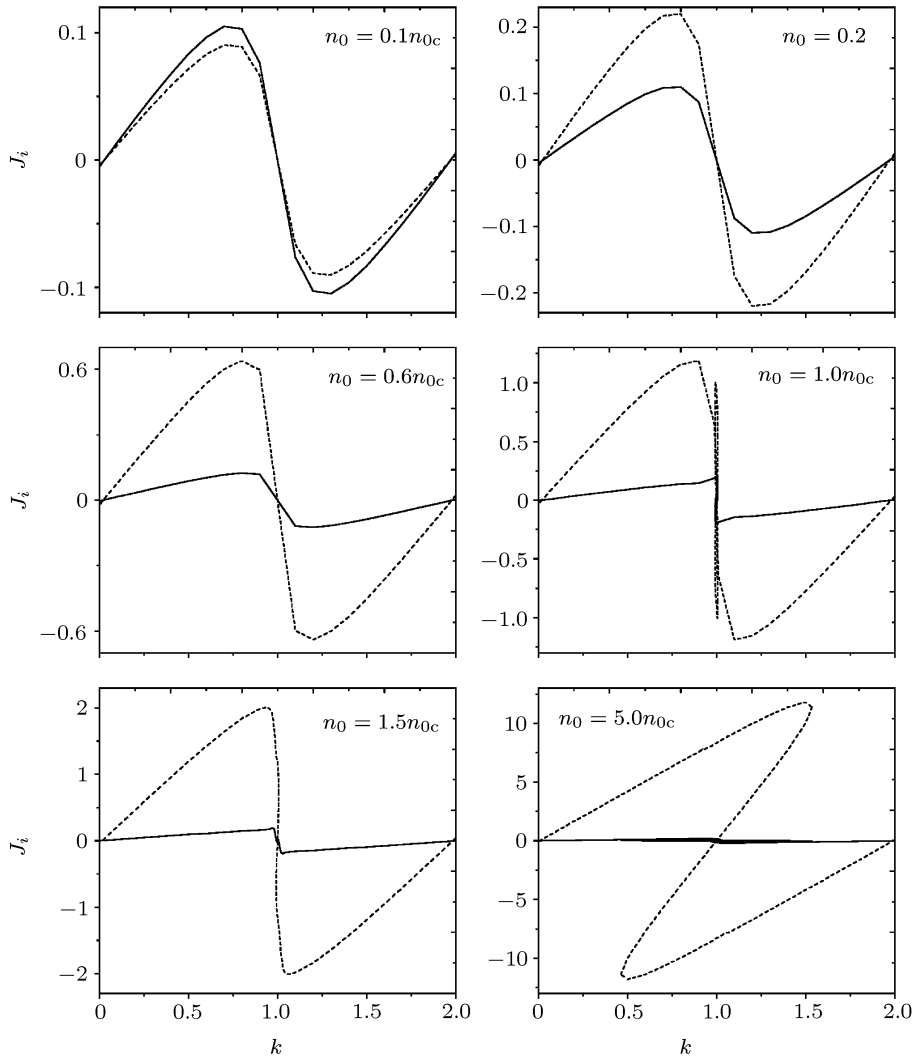



**Fig. 3.** Current density $J_j(k,n)$ as a function of quasimomentum at different densities $n$. $n_+ = n_- = 0.1, V_0 = 1$.

## 3. Conclusions

In summary, the energy band structure of spin-1 condensates in 1D optical lattices are discussed. We find that the Bloch bands of spin-1 condensates exhibit complex structure depending on the atom density of $m_{\rm F} = 0$ hyperfine state. The complex and interesting band structure is related to the spin-mixing and wave packets dynamics.

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