Circulating Current States in Bilayer Fermionic and Bosonic Systems

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It is shown that fermionic polar molecules or atoms in a bilayer optical lattice can undergo the transition to a state with circulating currents, which spontaneously breaks the time reversal symmetry. Estimates of relevant temperature scales are given and experimental signatures of the circulating current phase are identified. Related phenomena in bosonic and spin systems with ring exchange are discussed.

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Introduction.— The technique of ultracold gases loaded into optical lattices [1,2] allows a direct experimental study of paradigmatic models of strongly correlated systems. The possibility of unprecedented control over the model parameters has opened wide perspectives for the study of quantum phase transitions. Detection of the Mott insulator to superfluid transition in bosonic atomic gases [3,4,5], of superfluidity [6,7] and Fermi liquid [8] in cold Fermi gases, realization of Fermi systems with low dimensionality [9,10] mark some of the recent achievements in this rapidly developing field [11]. While the atomic interactions can be treated as contact ones for most systems with low dimensionality [9,10] mark some of the recent advances. The nearest-neighbor dimers $t$, $t'$ respectively. A strong "on-dimer" nearest-neighbor repulsion $\gg V$ lar molecules [13, 14], or atoms with a large dipolar magnetic dipoles with respect to the bilayer plane. Let $\theta$, $\phi$ be the polar and azimuthal angles of the dipolar moment (the coordinate axes are along the basis vectors of the lattice, $z$ axis is perpendicular to the bilayer plane). Setting $\varphi = \pm \frac{\pi}{2}, \pm \frac{3\pi}{2}$ ensures the dipole-dipole interaction is the same along the $x$ and $y$ directions. The nearest neighbor interaction parameters in (1) take the following values: $V = (d_0^2/\ell_\perp^2)(1 - 3\cos^2 \theta)$, and $V_{12} = V_{21}' = (d_0^2/\ell_\parallel R^2)(1 - 3\sin^2 \varphi)$, where $d_0$ is the dipole moment of the particle, $\ell_\perp$ and $\ell_\parallel$ are the lattice spacings in the directions perpendicular and parallel to the layers, respectively, and $R^2 = \ell_\perp^2 + \ell_\parallel^2$. The strength and the sign of interactions $V$, $V'$ can be controlled by tuning the angles $\theta$, $\varphi$ and the lattice constants $\ell_\perp$, $\ell_\parallel$. Below we will see that the physics of the problem depends on the difference $V' = V_{11} - V_{12}'$, (2) with the most interesting regime corresponding to $V' < 0$.

Consider the model at half-filling. Since $V \gg t, t'$, we may restrict ourselves to the reduced Hilbert space containing only states with one fermion per dimer. Two states of each dimer can be identified with pseudospin-$\frac{1}{2}$ states $|\uparrow\rangle$ and $|\downarrow\rangle$. Second-order perturbation theory in $t'$ yields the effective Hamiltonian

$$\mathcal{H}_S = \sum_{\langle rr'\rangle} \left\{ J_1 S^x_{r'} S^x_r + S^y_{r'} S^y_r + J_2 S^z_{r'} S^z_r \right\} - H \sum_r S^z_r,$$

$$J = 4(t')^2/V, \quad J_1 = \Delta = J + |\mathbf{V}'|, \quad H = 2t,$$ (3)

describing a 2d anisotropic Heisenberg antiferromagnet in a magnetic field perpendicular to the anisotropy axis. The twofold degenerate ground state has the Néel antiferromagnetic (AF) order transverse to the field, with spins canted towards the field direction. The AF order is along the $y$ axis for $\Delta < 1$ (i.e., $\mathbf{V}' < 0$), and along the $z$ axis for $\Delta > 1$ ($\mathbf{V}' > 0$).

FIG. 1: Bilayer lattice model described by the Hamiltonian (1). The arrows denote particle flow in the circulating current phase.
The angle $\alpha$ between the spins and the field is classically given by $\cos \alpha = H/(2ZJS)$, where $S$ is the spin value and $Z = 4$ is the lattice coordination number. This classical ground state is exact at the special point $H = 2SJ\sqrt{2(1+\Delta)}$ [21]. The transversal AF order vanishes above a certain critical field $H_c$; classically $H_c = 2ZJS$, and the same result follows from the spin-wave analysis of [5] (one starts with the fully polarized spin state at large $H$ and looks when the magnon gap vanishes). This expression becomes exact at the isotropic point $\Delta = 1$ and is a good approximation for $\Delta$ close to 1.

The long-range AF order along the $y$ direction translates in the original fermionic language into the staggered arrangement of currents flowing from one layer to the other:

$$N_y = (-)^{C_y}(S_y^0) \mapsto (-)^C(-\frac{i}{2}(a^\dagger_{1,1},a_{2,1} - a^\dagger_{2,1},a_{1,1})).$$ (4)

In terms of the original model [1], the condition $H < H_c$ for the existence of such a staggered current order becomes

$$t < 8(t')^2/V.$$ (5)

The continuity equation for the current and the lattice symmetry dictate the current pattern shown in Fig. [1] This circulating current (CC) state has a spontaneously broken time reversal symmetry, and is realized only for attractive inter-dimer interaction $V' < 0$ (i.e., the easy-plane anisotropy $\Delta < 1$) [22]. If $\Delta = 1$, the direction of the AF order in the $xy$ plane is arbitrary, so there is no long-range order at any finite temperature. For $\Delta > 1$ (i.e., $V' > 0$) the AF order along the $z$ axis corresponds to the density wave (DW) phase with in-layer occupation numbers having a finite staggered component.

The phase diagram in the temperature-anisotropy plane is sketched in Fig. [2]. At the critical temperature $T_c = T_c$, the discrete $Z_2$ symmetry gets spontaneously broken, so the corresponding thermal phase transition belongs to the 2d Ising universality class (except the two lines $\Delta = 1$ and $H = 0$ where the symmetry is enlarged to U(1) and the transition becomes the Kosterlitz-Thouless one). Away from the phase boundaries the critical temperature $T_c \sim J$, but at the isotropic point $\Delta = 0$, $H = 0$ it vanishes due to divergent thermal fluctuations: for $1 - \Delta \ll 1$ and $H \ll J$, it can be estimated as

$$T_c \sim J/\ln[\min((1-\Delta)^{-1},J^2/H^2)].$$ (6)

The quantum phase transition at $T = 0$, $H = H_c$ is of the 3d Ising type (except at the U(1)-symmetric point $\Delta = 1$ where the universality class is that of the 2d dilute Bose gas [23]), so in its vicinity the CC order parameter $N_y \propto (H_c - H)^\beta$ with $\beta \approx 0.313$ [24], and $T_c \propto JN_y^2 H_c - H)^{2\beta}$. At $T > T_c$ or $H > H_c$, the only order parameter is the staggered correlator $\langle S_y \rangle$, corresponding to the Mott phase with one particle per dimer.

Bilayer lattice design and hierarchy of scales.— The bilayer can be realized, e.g., by employing three pairs of mutually perpendicular counter-propagating laser beams with the same polarization and adding another pair of beams with an orthogonal polarization and additional phase shift $\delta$, so that the resulting field intensity has the form $E_{\perp}(\cos kx + \cos ky) + E_z \cos k_z (\cos k_z(z \approx E_z (2E_{\perp} + \zeta E_z),$ with $\zeta = \pm 1$ for blue and red detuning, respectively, one obtains a three-dimensional stack of bilayers, separated by large potential barriers $U_{3d}$. Eq. (5) implies $V \gg t' \gg t,|V'|$, which can be achieved by making the $z$-direction potential barrier $U_{\perp}$ inside the bilayer sufficiently larger than the in-plane barrier $U_{\parallel}$, so that the condition $t \ll t'$ will be met; e.g., $E_{\parallel} / E_{\perp} \approx 20$, $E_{\parallel} / E_{\perp} \approx 15$ yields the barrier ratio $U_{3d} : U_{\perp} : U_{\parallel}$ of approximately $16 : 8 : 1$, and the lattice constants $t_{\perp} \approx 0.45 \lambda$, $t_{\parallel} \approx \lambda$, where $\lambda = 2\pi/k$ is the laser wave length. The parameter $V'$ has a zero as a function of the angle $\theta$, so it can be made as small as needed. Taking $\lambda = 0.400$, one obtains an estimate of $T_c = (0.1 \div 0.3) \mu K$ for cyanide molecules ClCN and HCN with the dipolar moment $d_0 \approx 3$ Debye, while the Fermi temperature for the same parameters is $T_F \approx (0.6 \div 1.3) \mu K$. This estimate corresponds to the maximum value of $T_c \sim J$ reached when $V' \sim -J$ and $t \lesssim J$. The hopping $t'$ was estimated assuming the in-plane potential barrier $U_{\parallel}$ is roughly equal to the recoil energy $E_r = (\hbar k)^2/2m$, where $m$ is the particle mass.

Experimental signatures.— Signatures of the ordered phases can be observed [25] in time-of-flight experiments by measuring the density noise correlator $\langle G(r, r') \rangle = \langle N_y \rangle$.
If the imaging axis is perpendicular to the bilayer, \( n(r) = \sum_{\sigma}(a_{r,\sigma}^d a_{r,\sigma}^\dagger) \) is the local net density of two layers. For large flight times \( t \) it is proportional to the momentum distribution \( U_\ell(r) \), where \( U_\ell(r) = m r / \hbar t \). In the Mott phase the response shows fermionic “Bragg dips” at reciprocal lattice vectors \( r = (2 \pi / \hbar t) \) and \( 2 \pi / \hbar t \).

In the DW phase the system is distributed along only one of the two in-plane directions. The unitary transformation \( \mathcal{A}(x) = \frac{1}{\hbar} (x + 1/2) \) makes hopping along the \( x \) axis imaginary, \( t' \to -i t' \). The unitary transformation \( S_{xy}^\pm \) maps the system onto a set of PM chains along the \( x \) axis, AF-coupled in the \( y \) direction and subject to a staggered field \( H = 2t \) along the \( x \) axis in the easy \((xy)\) plane. In the ground state these field moments are arranged in a staggered way along the \( y \) axis, so a current pattern similar to that of Fig. 1 emerges, now staggered along only one of the two in-plane directions.

A different type of CC states, with orbital currents localized at lattice sites, can be achieved with \( p \)-band bosons [28].

Yet another way to create a CC state in a bosonic bilayer is to introduce the ring exchange on interplactes:

\[
\mathcal{H}_{\text{ring}} = \frac{1}{2} K \sum_{(rr')} \left( b_{1,r}^d b_{2,r}^\dagger b_{2,r'} b_{1,r'} + \text{h.c.} \right),
\]

In pseudospin language, the ring interaction modifies the transverse exchange, \( J \leftrightarrow J + K \), so for \( K > 0 \) one can achieve the conditions \( J > 0, J > |J| \) necessary for the CC phase to exist. However, engineering a sizeable ring exchange in bosonic systems is difficult (see [29] for recent proposals).

Spin-\( \frac{1}{2} \) bilayer with four-spin ring exchange.– Consider the Hubbard model for spinful fermions on a bilayer shown in Fig. 1 with the on-site repulsion \( U \) and inter-and intra-layer hoppings \( t \) and \( t' \). At half filling (i.e., two fermions per dimer), one can effectively describe the system in terms of spin degrees of freedom represented by the operators \( S = \frac{1}{2} a_{\sigma}^d \sigma_{\alpha\beta} a_{\beta} \). The leading term in \( t / U \) yields the AF Heisenberg model with the nearest-neighbor exchange constants \( J_\perp = 4t^2 / U \) (inter-layer) and \( J_{\parallel} = 4(t')^2 / U \) (intra-layer), while the next term, with the interaction strength \( J_4 \approx 10t^2 (t')^2 / U^3 \), corresponds to the ring exchange [30, 31]:

\[
\mathcal{H}_4 = 2 J_4 \sum_{\sigma} \left\{ (S_{1,\sigma} S_{2,\sigma}) (S_{1,\sigma} S_{2,\sigma}) - (S_{1,\sigma} S_{2,\sigma})(S_{2,\sigma} S_{1,\sigma}) \right\} \tag{9}
\]

In the DW phase \( \langle S^x \rangle \neq 0, \langle S^y \rangle = 0 \), and so the density correlator depends only on \( r - r' \). In the CC phase \( \langle S^z \rangle = 0, \langle S^y \rangle \neq 0 \), and the relative strength of the two systems of dips varies periodically when one changes the initial point \( r \), see Fig. 1. This \( Q \)-dependent contribution stems from the inplane currents \( \langle a_{r,\sigma}^d a_{r',\sigma} \rangle = (-)^{\delta_{r,r'}} \delta(r-r') \langle i S^y / 4 \rangle \), where \( \frac{1}{4} \) comes from the fact that the inter-layer current splits into four equivalent inter-layer ones (see Fig. 1). \( \delta(r-r') \) means \( r \) and \( r' \) must be nearest neighbors, and \( (-)^{\delta_{r,r'}} \equiv e^{i Q_{r-r'} \cdot r} \) denotes an oscillating factor. If the correlator is averaged over the particle positions, the CC and DW phases become indistinguishable. A direct way to observe the CC phase could be to use the laser-induced fluorescence spectroscopy to detect the Doppler line splitting proportional to the current.

Bosonic models.– Consider the bosonic version of the model [1], with the additional on-site repulsion \( U \). The effective Hamiltonian has the form [3] with \( J = -4(t')^2 / V \) and \( J_2 = V' + 4(t')^2(1 / V - 1 / U) \). Due to fermionic (FM) transverse exchange, instead of spontaneous current one obtains the usual Mott phase. CC states can be induced by artificial gauge fields [27]. The vector potential \( A(x) = \frac{1}{\hbar} (x + 1/2) \) makes hopping along the \( x \) axis imaginary, \( t' \to -i t' \). The unitary transformation \( S_{xy}^\pm \) maps the system onto a set of PM chains along the \( x \) axis, AF-coupled in the \( y \) direction and subject to a staggered field \( H = 2t \) along the \( x \) axis in the easy \((xy)\) plane. In the ground state these field moments are arranged in a staggered way along the \( y \) axis, so a current pattern similar to that of Fig. 1 emerges, now staggered along only one of the two in-plane directions.

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Yet another way to create a CC state in a bosonic bilayer is to introduce the ring exchange on interplactes:
\( \chi = 0 \), strong ring exchange \( J_4 \) favors another solution with \( \varphi = 0, \chi \neq 0 \), describing the state with a staggered vector chirality. It wins over the AF one for \( J_4 > J_\parallel, J_4 > \frac{2}{2z} J_R \), which for the square lattice (\( Z = 4 \)) translates into

\[ J_4 > \max(J_\parallel, J_\perp/9). \tag{12} \]

On the line \( J_4 = J_\parallel \) the symmetry is enhanced from SU(2) to SU(2) \( \times \) U(1), and the AF and chiral orders can coexist: a rotation \( (\varphi + i\chi) \rightarrow (\varphi + i\chi)e^{i\alpha} \) leaves the action invariant.

The chiral state may be viewed as an analog of the circulating current state considered above: in terms of the original fermions of the Hubbard model, the \( z \)-component of the chirality \( (S_1 \times S_2)_z = \frac{1}{2}\{ (a_1^\dagger a_2^\dagger)(a_2 a_1) - (a_2^\dagger a_1^\dagger)(a_1 a_2^\dagger) \} \) corresponds to the spin current (particles with up and down spins moving in opposite directions).

**Summary.**—I have considered fermionic and bosonic models on a bilayer optical lattice which exhibit a phase transition into a circulating current state with spontaneously broken time reversal symmetry. The simplest of those models includes just nearest-neighbor interactions and hoppings, and can possibly be realized with the help of polar molecules.

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