Effective orbital ordering in multiwell optical lattices with fermionic atoms

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We consider the behavior of Fermi atoms on optical superlattices with two-well structure for each node. Fermions on such lattices serve as an analog simulator of the Fermi-type Hamiltonian. We derive a mapping between fermion quantum ordering in the optical superlattices and the spin-orbital physics developed for degenerate d-electron compounds. The appropriate effective spin-orbital model appears to be a modification of the Kugel-Khomskii Hamiltonian. We show how different ground states of this Hamiltonian correspond to particular spin-pseudospin arrangement patterns of fermions on the lattice. The dependence of the fermion arrangement on phases of complex hopping amplitudes is illustrated.

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I. INTRODUCTION

Experimental investigations of ultracold atoms in optical lattices, apart from their own intrinsic value, have opened up a unique flexibly tunable simulator for the study of quantum many-body physics [1–4]. In this regard ultracold atoms form a major part of the rapidly developing field of analog quantum simulation (AQS), which includes also trapped ions, polar molecules, quantum dots, and cavity arrays (see Ref. [5] for a recent review). Analog quantum simulation allows one to manipulate the parameters in a regime that had been hardly possible or even impossible to achieve in the natural physics of the initial problem [5–9].

For the case of an optical lattice the atom temperature can be made extremely low. This allows one to experimentally investigate in detail the ground-state structure and the low-lying many-body states of atoms [10,11]. On the other hand, it enables AQS for different solid-state (and not only solid state) models [5].

One of the most interesting regimes corresponds to strong atom-atom quantum correlations. Interactions between lattice atoms have a different nature. Atoms can jump (tunnel) from site to site on the optical lattice with the hopping energy t. There is typically repulsion U between atoms within the site and exchange interaction between the spins of neighboring atoms. The lattice atoms' quantum state also strongly depends on the statistics: Atoms are either bosons or fermions [12]. In what follows we shall focus on the fermion case.

Typically atoms on the lattice are well described by modifications of the Hubbard model due to the short-range character of the U interaction [7]. The problems of the ground state and the low-lying many-body states of atoms on the lattice have been successfully investigated within the mean-field theory; see, e.g., Ref. [12]. Progress have also been made beyond the mean field in particular with numerical simulations of the Hubbard-type models.

For bosons on the lattice the parameter range at which one could expect Bose condensation or Mott insulator behavior has been thoroughly investigated [12,13]. For fermions on the optical lattice experimental realization of a Mott insulator regime [14] offered a unique possibility to simulate various ground states and spin orderings of fermions, complying with theoretical predictions for the repulsive Fermi-Hubbard model.

Recently, optical lattices with complicated structure of the node have attracted attention. In particular, these are superlattices with two-well structure [15–18]. The mean-field ground-state phase diagram of spinor bosons in a two-well superlattice was derived from the Bose-Hubbard Hamiltonian in Ref. [18]. It was shown that the system supports Mott insulating and superfluid phases like in one-well latices; however, the quadratic Zeeman effect lifts the degeneracy between different polar superfluid phases leading to additional metastable phases and first-order phase transitions.

Here we focus on spinor fermions on optical superlattices with multiwell structure of each node. Specifically, we consider two-well nodes in the strong correlation regime (large U/t). We show how the ground-state many-body atom can be understood from the well-known results of the machinery developed long ago for degenerate d-electron compounds [19,20]. We show that there is a mapping between fermion quantum ordering in the optical superlattices and the spin-orbital physics of degenerate d-electron compounds. This means that fermions on the two-well optical superlattices afford AQS for spin-orbital compounds where direct experimentation remains hard and debatable [21].

We derive the effective spin-orbital model and show that it appears to be the generalization of the Kugel-Khomskii Hamiltonian [19]. Different ground states of this Hamiltonian correspond to a particular nontrivial fermion arrangement on the lattice.

The paper is organized as follows. In Sec. II A we write the Hubbard-type Hamiltonian for fermions on a multiwell lattice. Section II B enumerates more or less standard steps to reduce the model to the effective spin-orbital Hamiltonian. Cumbersome technical details of the reduction are put in the Appendix. In Sec. III we give examples of the possible ground states of the many-body atom on the lattice that can be obtained from the mapping to spin-orbital physics.

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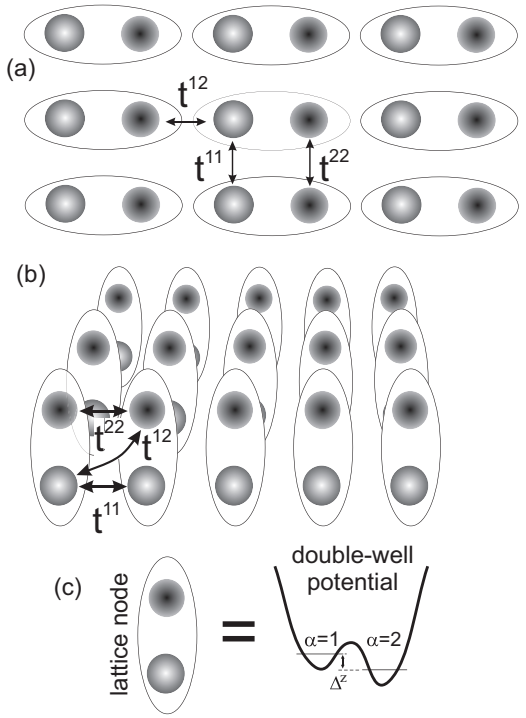

FIG. 1. (a) and (b) Sketch of possible optical lattices with two-well structure where spin-orbital effects may appear. Here $t^{\alpha\beta}$ are hopping amplitudes between wells on nearest nodes. Indices $\alpha,\beta = 1,2$ numerate the two wells at a given lattice node (two quantum pseudospin states). (c) Structure of the lattice node. Here Δ^z is the energy offset between the two wells.

II. MICROSCOPIC MODEL FOR FERMIONS IN THE DOUBLE-WELL OPTICAL LATTICE

A. Tunnel Hamiltonian model

We consider the d-dimensional hypercubic optical lattice where each node is a double well, as illustrated for the two-dimensional lattice in Fig. 1. The Hamiltonian describing the quantum states of fermions on the lattice can be written as

$$H = H_\Delta + H_\mathrm{T} + H_\mathrm{U} + H_\mathrm{J}\,. \tag{1}$$

The term H_Δ describes the level structure of each node

$$H_\Delta = \sum_{i,\sigma,\alpha,\beta} \frac{1}{2}\left(\Delta_i^z \sigma_{\alpha\beta}^z + \Delta_i^x \sigma_{\alpha\beta}^x\right) c_{i\alpha\sigma}^\dagger c_{i\beta\sigma}\,, \tag{2}$$

where the index i labels the nodes, $\alpha = 1,2$ is the well number at a given node, Δ_i^z is the difference of the ground-state energies between the two wells, Δ_i^x takes into account possible tunneling between the wells in a node, and σ^z and σ^x are Pauli matrices. The operator $c_{i\alpha\sigma}^\dagger$ ($c_{i\alpha\sigma}$) is the fermion creation (annihilation) operator for the fermion atom residing at a node i in a well α with spin projection σ.

Tunneling between the nodes specifies

$$H_\mathrm{T} = -\sum_{i\neq j,\sigma,\alpha,\beta} t_{ij}^{\alpha\beta} c_{i\alpha\sigma}^\dagger c_{j\beta\sigma}\,, \tag{3}$$

where $t_{ij}^{\alpha\beta}$ is the tunnel matrix element. The structure of the tunnel matrix elements is schematically depicted in Figs. 1(a) and 1(b). The hopping amplitudes $t_{ij}^{\alpha\beta}$ can be arranged into complex-valued amplitude matrix in the well space:

$$t_{ij}^{\alpha\beta} = t^{\alpha\beta} = \begin{pmatrix} t^{11} & t^{12} \\ t^{21} & t^{22} \end{pmatrix}. \tag{4}$$

We shall omit for brevity the lattice indices in hopping amplitudes. Below the notation $t^\dagger = t_{ij}^\dagger$ will be used for the Hermitian conjugation in the well subspace. Note that, in general, $t \neq t^\dagger$. Due to the Hermitian character of H_T there is a standard symmetry $t_{ij}^{\alpha\beta} = (t_{ji}^{\beta\alpha})^*$. It follows that $t^\dagger$ corresponds to the hopping amplitude matrix with interchanged lattice indices, i.e., $(t^\dagger)^{\alpha\beta} = (t_{ij}^{\beta\alpha})^* = t_{ji}^{\alpha\beta}$.

Since each node has a fine structure related to the wells it is convenient to split the interaction Hamiltonian into two parts $H_\mathrm{U} + H_\mathrm{J}$. The first term has a trivial structure in the well index space and describes the Coulomb repulsion ($U_i > 0$) of fermions at one node:

$$H_\mathrm{U} = \sum_{i,\sigma,\sigma',\alpha,\alpha'} U_i n_{i\alpha\sigma} n_{i,\alpha',\sigma'} (1 - \delta_{\alpha\alpha'}\delta_{\sigma\sigma'}), \tag{5}$$

where $n_{i\alpha\sigma} = c_{i\alpha\sigma}^\dagger c_{i\alpha\sigma}$. The second term describes the ferromagnetic Hund's coupling [20] ($J_\mathrm{H}{}^{(i)} > 0$) between fermions in wells $\alpha = 1$ and 2 at a given lattice node

$$H_\mathrm{J} = -\sum_{i,\sigma,\sigma'} J_\mathrm{H}{}^{(i)}\, c_{i,1,\sigma}^\dagger c_{i,1,\sigma'} c_{i,2,\sigma'}^\dagger c_{i,2,\sigma}\,. \tag{6}$$

This term comes into effect if the average fermion density at a node $\langle n_i\rangle = \sum_\sigma (\langle n_{i1\sigma}\rangle + \langle n_{i2\sigma}\rangle)$ is equal to $\langle n_i\rangle = 2$.

B. The effective Hamiltonian for single-atom filling of the nodes

We shall focus on the case when U_i is the largest energy scale, in particular when U_i is much larger than the hopping amplitudes $t_{ij}^{\alpha\beta}$. Then each node, on average, is occupied by one fermion and the Hamiltonian (1) can be simplified. To proceed, we introduce a standard presentation [22] of the spin $S = \frac{1}{2}$ and the pseudospin $\tau = \frac{1}{2}$ operators through the fermion creation and annihilation operators (see, e.g., Ref. [23]):

$$S_i^a = \tfrac{1}{2} c_{i\alpha\sigma}^\dagger \sigma_{\sigma\sigma'}^a c_{i\alpha\sigma'}, \tag{7}$$

$$\tau_i^a = \tfrac{1}{2} c_{i\alpha\sigma}^\dagger \sigma_{\alpha\beta}^a c_{i\beta\sigma}\,. \tag{8}$$

The index $a = x,y,z$ or sometimes it is convenient to use $a = 1,2,3$. Summation over recurring spin and pseudospin indices is implied. We recall that the representation in (7) and (8) is valid only at the single-atom filling of each node.

Below we focus on the case when the interactions U and J_H do not depend on the site index. Using (7) and (8) we can present the term H_Δ in the form $H_\Delta = \sum_i (\Delta_i^z \tau_i^z + \Delta_i^x \tau_i^x)$. The term $H_\mathrm{TUJ} = H_\mathrm{T} + H_\mathrm{U} + H_\mathrm{J}$ after the standard perturbation procedure in hopping amplitudes [19,20,23–29] can be transformed into the general form (the derivation details are in the Appendix)

$$H_\mathrm{TUJ} = \sum_{\langle i,j\rangle} \Bigg[\frac{1}{4} A_{ij} + A_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + B_{ij}^{ab} \tau_i^a \tau_j^b - \frac{1}{2} K_{ij}^a \left(\tau_i^a + \tau_j^a\right) + 4\mathbf{S}_i \cdot \mathbf{S}_j \left\{ D_{ij}^{ab} \tau_i^a \tau_j^b + \frac{1}{2} K_{ij}^a \left(\tau_i^a + \tau_j^a\right) \right\} \Bigg], \tag{9}$$

where the summation runs over bonds $\langle i,j\rangle$ between nearest neighbors. The coefficients A_{ij} B_{ij}^{ab}, K_{ij}^{a}, and D_{ij}^{ab} are quadratic in the tunnel amplitudes $t_{ij}^{\alpha\beta}$ and can be considered as generalized exchange coupling constants of the resulting spin-spin, spin-pseudospin, and pseudospin-pseudospin interactions between fermions. The vectors K_{ij}^{a} introduce as well an effective magnetic field into the pseudospin space, resulting from nondiagonal structure of the hopping matrix $t^{\alpha\beta}$.

For the particular case of real hopping amplitudes, $t^{11} = t^{22} = t$, $t^{12} = t^{21} = 0$, and zero Hund's coupling $J_H = 0$, the model (9) is equivalent to the Hamiltonian of the SU(4) model [23]

$$H_{\mathrm{TUJ}} \to \frac{2t^2}{U}\sum_{\langle i,j\rangle}\left(\frac{1}{2}+2\mathbf{S}_i\cdot\mathbf{S}_j\right)\left(\frac{1}{2}+2\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j\right). \quad (10)$$

If we identify the space of well indices with the orbital space then the Hamiltonian (9) for real $t_{ij}^{\alpha\beta}$ becomes similar to the Kugel-Homsky Hamiltonian [19] developed for degenerate d-electron compounds [20,23–27].

Equation (9) has been derived assuming $J_{\mathrm{H}}/U \ll 1$. However, in d-electron compounds it is quite often that $J_{\mathrm{H}} \sim U$. In a similar way it may take place for atoms on the optical lattice. The conjecture has been made in Ref. [20] that the form of interaction terms in the Kugel-Khomskii Hamiltonian remains the same for $J_{\mathrm{H}} \sim U$ and tensor coefficients A, K, B, and D would preserve their symmetry structure in the orbital space. For the case of a diagonal hopping amplitude matrix $t^{\alpha\beta} \sim \delta^{\alpha\beta}$ this conjecture has been confirmed in Ref. [20] by direct calculation of the Kugel-Khomskii Hamiltonian coefficients in all orders in J_{H}/U. The same conclusion applies for atoms on the lattice described by the effective Hamiltonian (9).

III. DISCUSSION

A. Symmetrical Hamiltonian

Now we focus on the symmetrical case when the nearest-neighbor hopping matrix $t^{\alpha\beta}$ is diagonal in the orbital space. This case could be realized in the optical lattice sketched in Fig. 1(b). Then K_{ij}^{a} is equal to zero while B_{ij}^{ab} and D_{ij}^{ab} are diagonal matrices in the orbital space. For this case the symmetrical model Hamiltonian follows from Eq. (9) (see the Appendix),

$$H_{\mathrm{TUJ}} \to H_{\mathrm{sym}} = \sum_{\langle ij\rangle}\{J_1\mathbf{S}_i\cdot\mathbf{S}_j + J_2\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j + 4J_3(\mathbf{S}_i\cdot\mathbf{S}_j)(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j)\}, \quad (11)$$

where we consider exchange constants J_1, J_2, and J_3 as independent input parameters.

Let us consider the most interesting case $\Delta^{x,z} \ll J_{1,2,3}$; we can neglect the term H_Δ comparing with H_{TUJ}. Then the isolated minima of the double-well potential are the same. The spin-pseudospin interaction resulting from virtual hoppings between neighboring notches gives rise to the occupancy of that subwell, which is preferable.

The properties of the Kugel-Khomskii symmetrical Hamiltonian (11) have been well investigated (see, e.g., Refs. [19,20]). In Fig. 2 we present the result of the analysis of the model (11) in the mean-field approximation for $J_3 > 0$

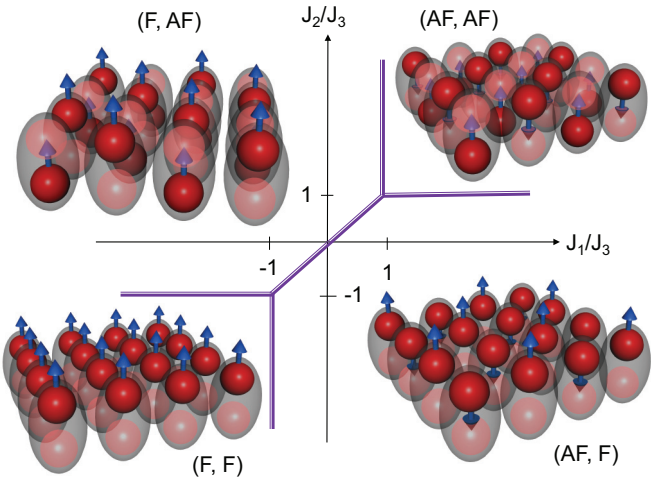

FIG. 2. (Color online) Mean-field phase diagram of the symmetrical model (11) for $J_3 > 0$ (see, e.g., Refs. [30,31] for d-electron compounds). Here F stands for ferromagnetic ordering and AF is for antiferromagnetic ordering. The first and second abbreviations in the designations of phases are for the spin and pseudospin subsystems, respectively. The ordering patterns of atoms on the optical lattice are shown in the insets. For ferromagnetic orbital arrangement atoms are localized in one particular type of subwell (for example, in the upper subwells). For antiferromagnetic orbital arrangement atoms alternate between the lower and upper subwells. Red spheres show the lattice site with the maximum probability of occupation by an atom, while transparent spheres show nearly empty sites. Arrows indicate spin directions.

(which would look like the figure for $J_3 < 0$ [32]). The figure shows possible phases of spin-pseudospin arrangements for various values of exchange parameters. For example, the case $J_1 > J_3 > J_2 > 0$ corresponds to the ground state of H_{sym}, which is antiferromagnetic in the spin space and ferromagnetic in the pseudospin space [the (AF,F) phase in Fig. 2]. The effective orbital exchange can be estimated as $J_\tau^{\mathrm{eff}} = J_2 + 4J_3\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle$. Similarly, the effective spin exchange is approximately equal to $J_s^{\mathrm{eff}} = J_1 + 4J_3\langle\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j\rangle$. When spins are antiferromagnetically ordered $J_\tau^{\mathrm{eff}} = J_2 - J_3 < 0$ and one obtains orbital ferromagnetism. If we turn on the external effective magnetic field we can change the orbital ferromagnetism to orbital antiferromagnetism when the field is sufficiently strong that $\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle > J_2/4J_3$. Finite Δ^x and Δ^z play the role of the built-in effective magnetic field in the pseudospin space. Large enough Δ^z would also drive the system into the ferromagnetic orbital state (in such a case one of the two minima of the double well is much lower than the other).

To illustrate the possible arrangement patterns of atoms in real space let us consider the pseudospin (orbital) state in the mean-field approximation. It can be presented as a product of one-site orbital states $|\psi_{\mathrm{MF}}\rangle = \prod_i |\theta_i\varphi_i\rangle$. The orbital one-site state $|\theta_i\varphi_i\rangle$ can be chosen as

$$|\theta_i\varphi_i\rangle = \cos\frac{\theta_i}{2}|1\rangle + e^{i\varphi_i}\sin\frac{\theta_i}{2}|2\rangle. \quad (12)$$

The direction (in pseudospin space) of the averaged pseudospin $\langle\boldsymbol{\tau}_i\rangle$ is defined in terms of the polar and azimuth angles

$$\langle\theta_i\varphi_i|\boldsymbol{\tau}_i|\theta_i\varphi_i\rangle = \tfrac{1}{2}(\sin\theta_i\cos\varphi_i, \sin\theta_i\sin\varphi_i, \cos\theta_i). \quad (13)$$

The orbital state

$$|\pi-\theta_i,\pi+\varphi_i\rangle = \sin\frac{\theta_i}{2}|1\rangle - e^{i\varphi_i}\cos\frac{\theta_i}{2}|2\rangle \qquad (14)$$

is orthogonal to $|\theta_i\varphi_i\rangle$ and sets $\langle\boldsymbol{\tau}_i\rangle$ in the opposite direction. The ferromagnetic orbital arrangement corresponds to identical orbital states $|\theta_i\varphi_i\rangle = |\theta\varphi\rangle$ at different sites. The antiferromagnetic orbital state corresponds to $|\theta_i\varphi_i\rangle = |\theta\varphi\rangle$ at sublattice $i \in A$ and $|\theta_j\varphi_j\rangle = |\pi-\theta,\pi+\varphi\rangle$ at sublattice $i \in B$. The average pseudospin vectors alternate at the sublattices A and B, $\langle\boldsymbol{\tau}_i\rangle = -\langle\boldsymbol{\tau}_j\rangle$.

The simplest illustration of the orbital arrangement of atoms can be given for the case of $\theta = 0$ or $\theta = \pi$. Then atoms with probability equal to one occupy either well $\alpha = 1$ or well $\alpha = 2$, respectively. The illustrative example of phase diagrams for this case is sketched in Fig. 2, where we adapted the results of Refs. [25,30–32] on the Kugel-Khomskii model to our problem of atom arrangements on the optical lattice. The sketch shows the ordering patterns of atoms on the optical lattice of the type presented in Fig. 1(b). For the ferromagnetic orbital arrangement atoms are localized in one of the subwells, for example, in upper subwells. For the antiferromagnetic arrangement atoms alternate between $\alpha = 1$ and $\alpha = 2$ wells (upper and lower wells in the figure). If we consider the antiferromagnetic orbital arrangement beyond the mean-field approximation then atoms are spread between two subwells with some probability due to quantum fluctuation. Red spheres in Fig. 2 show lattice sites with the maximum probability of occupation by an atom, while white spheres show nearly empty sites. Arrows indicate spin directions. The phase boundaries in Fig. 2 actually do not exactly match coordinate axes in (J_1, J_2) space: The absolute value and sign of J_3 specify the position of the phase boundaries [25,30–32], as illustrated.

B. Complex hopping amplitudes

One of the unique properties of optical lattices is the possibility to tune the complex tunnel amplitudes by manipulating the laser field [33]. This includes also the possibility to manipulate the Hamiltonian by changing the phases of the hopping amplitudes t_{ij} and leaving their absolute values fixed (i.e., no geometric distortion of the optical lattice).

Toy model. To illustrate the importance of the complex phases of the hopping amplitudes t_{ij} we consider the following toy model. We suppose that $J_{\rm H} = 0$ and we account for those hoppings that go through different orbitals (wells):

$$t^{11} = 0, \quad t^{22} = 0, \quad t^{12} = t', \quad t^{21} = t'e^{i\chi}. \qquad (15)$$

The constant phase χ accounts for the phase difference in the nondiagonal hopping amplitudes. Then the effective Hamiltonian (9) can be written as (see the Appendix)

$$H_\chi = J\sum_{\langle ij\rangle}\left(\frac{1}{2}+2\mathbf{S}_i\cdot\mathbf{S}_j\right)\left(\frac{1}{2}+2\cos\chi\left(\tau_i^x\tau_j^x-\tau_i^y\tau_j^y\right)\right.$$
$$\left.+2\sin\chi\left(\tau_i^x\tau_j^y+\tau_i^y\tau_j^x\right)-2\tau_i^z\tau_j^z\right). \qquad (16)$$

The appearance of the phase-dependent ground state can be illustrated as follows. For the ferromagnetic spin background the mean-field energy $E_{\rm MF} = \langle\psi_{\rm MF}|H_\chi|\psi_{\rm MF}\rangle$ of the pseudospin subsystem is

$$E_{\rm MF} = \frac{J}{2}\sum_{\langle i,j\rangle}\{1+\cos[\chi-(\varphi_i+\varphi_j)]\sin\theta_i\sin\theta_j$$
$$-\cos\theta_i\cos\theta_j\}, \qquad (17)$$

where we used $\frac{1}{2}+2\mathbf{S}_i\mathbf{S}_j = 1$. Consider now the energy of the antiferromagnetic orbital state. For such a state the mean-field energy per site is

$$E_{\rm MF} = \tfrac{3}{2}J[1-\cos(\chi-2\varphi)\sin^2\theta+\cos^2\theta]. \qquad (18)$$

The minimization of the energy $E_{\rm MF}$ relative to θ and φ gives the twofold-degenerate ground state $E_{\rm g.s.} = 0$ with $\theta = \pi/2$ and $\varphi = \chi/2, \chi/2+\pi$. The resulting direction of the pseudospin $\langle\boldsymbol{\tau}\rangle$ depends on the phase χ. In real space this state describes the situation when the atoms with equal probability are spread over the first and second wells in the notch, but the phase relation between pseudospin states $|1\rangle$ and $|2\rangle$ is tuned by the applied phase χ. The change of χ induces the corresponding variation of the phase φ, which is equivalent to rotation of the pseudospin vector $\langle\boldsymbol{\tau}\rangle$ in the pseudospin space.

IV. CONCLUSION

Optical lattices are quantum simulators of many-particle systems. We have shown that there is a mapping between fermion quantum ordering in the optical superlattices and the spin-orbital physics developed for degenerate d-electron compounds. The effective spin-pseudospin model has been derived. This model is the generalization of the Kugel-Khomskii Hamiltonian for complex hopping amplitudes. We have shown how different ground states of this Hamiltonian correspond to particular nontrivial fermion arrangements on the lattice.

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APPENDIX: PERTURBATIVE EXPANSION IN HOPPING AMPLITUDES

In the subspace of functions $|\Phi^0\rangle$ with occupancy equal to one at each site the hopping term $H_{\rm T}$ creates intermediate states with double occupancy. There are six different intermediate states with double occupancy at a given site i, which differ in the well α and spin σ indices

$$|\psi_1\rangle = \left(\begin{array}{c}\text{——}\\ \uparrow\downarrow\end{array}\right), \quad |\psi_2\rangle = \left(\begin{array}{c}\uparrow\downarrow\\ \text{——}\end{array}\right), \qquad (A1)$$

$$|\psi_3\rangle = \left(\begin{array}{c}\uparrow\\ \uparrow\end{array}\right), \quad |\psi_4\rangle = \left(\begin{array}{c}\downarrow\\ \downarrow\end{array}\right), \qquad (A2)$$

$$|\psi_5\rangle = \left(\begin{array}{c}\downarrow\\ \uparrow\end{array}\right), \quad |\psi_6\rangle = \left(\begin{array}{c}\uparrow\\ \downarrow\end{array}\right). \qquad (A3)$$

Here the lower (upper) level is for the pseudospin state $\alpha = 1$ (2). All of them are eigenstates of the $H_{\rm U}$ with the same energy

U and the first four are also eigenstates of $H_{\rm J}$. Although the term $H_{\rm J}$ mixes the states $|\psi_5\rangle$ and $|\psi_6\rangle$, it mixes them into eigenstate of $H_{\rm U}$.

In second-order perturbation theory for the hopping term $H_{\rm T}$ the effective Hamiltonian has the form [24]

$$H_{\rm TUJ} = -H_{\rm T}\frac{1}{H_{\rm U}+H_{\rm J}}H_{\rm T}. \tag{A4}$$

Assuming that $J_{\rm H} \ll U$, the above expression to first order of $J_{\rm H}/U$ can be simplified as

$$H_{\rm TUJ} = -H_{\rm T}\left[\frac{1}{H_{\rm U}} - \frac{1}{H_{\rm U}}H_{\rm J}\frac{1}{H_{\rm U}}\right]H_{\rm T}. \tag{A5}$$

As we mentioned above, all the intermediate states (A1)–(A3), after mixing them by $H_{\rm J}$, remain eigenstates of $H_{\rm U}$. This enables us to reduce the above expression for $H_{\rm TUJ}$ to the form

$$H_{\rm TUJ} = -\frac{1}{U}\left(H_{\rm T}^2 - \frac{1}{U}H_{\rm T}H_{\rm J}H_{\rm T}\right). \tag{A6}$$

Presentation of Fermi operators through the spin and pseudospin operators, which is originally due to Kugel and Khomskii [19], can be given as

$$c^\dagger_{i\alpha\gamma}c_{i\beta\gamma'} = \left(\tfrac{1}{2}\delta_{\alpha\beta} + \tau_i^a\sigma^a_{\beta\alpha}\right)\left(\tfrac{1}{2}\delta_{\gamma\gamma'} + S_i^b\sigma^b_{\gamma'\gamma}\right). \tag{A7}$$

In the subspace of functions $|\Phi^0\rangle$ the first and the second term of $H_{\rm T}^2$ is reduced to

$$\begin{aligned} H_{\rm T}^2 = \sum_{\langle ij\rangle}\Big\{&{\rm Sp}(t^\dagger t) + {\rm Sp}(t^\dagger\sigma^a t)\tau_i^a + {\rm Sp}(t\sigma^a t^\dagger)\tau_j^a \\ &- \left(\frac{1}{2} + 2\mathbf{S}_i\cdot\mathbf{S}_j\right)\Big[\frac{1}{2}{\rm Sp}(t^\dagger t) + {\rm Sp}(t^\dagger\sigma^a t)\tau_i^a \\ &+ {\rm Sp}(t\sigma^a t^\dagger)\tau_j^a + 2{\rm Sp}(t^\dagger\sigma^a t\sigma^b t)\tau_i^a\tau_j^b\Big]\Big\}, \end{aligned} \tag{A8}$$

$$\begin{aligned} &\frac{1}{U}H_{\rm T}H_{\rm J}H_{\rm T} \\ &= \left(-\frac{J_{\rm H}}{U}\right)\sum_{\langle ij\rangle}\Big\{-\frac{1}{2}{\rm Sp}(t^\dagger\sigma^{a'}t)\tau_i^{a'} \\ &- \frac{1}{2}{\rm Sp}(t\sigma^{a'}t^\dagger)\tau_j^{a'} - {\rm Sp}(t^\dagger\sigma^{a'}\sigma^b t)\tau_i^{a'}\tau_j^b \\ &- {\rm Sp}(t^\dagger\sigma^b t\sigma^{a'})\tau_i^b\tau_j^{a'} + \left(\frac{1}{2} + 2\mathbf{S}_i\cdot\mathbf{S}_j\right) \\ &\times\left[\frac{1}{2}{\rm Sp}(t^\dagger t) + \frac{1}{2}{\rm Sp}(t^\dagger\sigma^{a'}t)\tau_i^{a'} + \frac{1}{2}{\rm Sp}(t\sigma^{a'}t^\dagger)\tau_j^{a'}\right. \\ &\left. - {\rm Sp}(t^\dagger\sigma^z t\sigma^a)\tau_i^z\tau_j^a - {\rm Sp}(t^\dagger\sigma^a t\sigma^z)\tau_i^a\tau_j^z\right]\Big\}. \end{aligned} \tag{A9}$$

The summation over repeated indices $a,b = 1,2,3$ is implied; indices with a prime mean that the summation does not include the third component, i.e., $a',b' = 1,2$. In terms proportional to τ_j^a we used the property of the Hermitian conjugate hopping matrix $t_{ji}^{\alpha\beta} = (t^\dagger)_{ij}^{\alpha\beta}$.

In what follows we omit the constant term ${\rm Sp}(t^\dagger t)$ in $H_{\rm T}^2$. Taking both terms together, we obtain after regrouping the effective Hamiltonian

$$\begin{aligned} H_{\rm TUJ} = \sum_{\langle ij\rangle}\Big[&\frac{1}{4}A_{ij} + A_{ij}\mathbf{S}_i\cdot\mathbf{S}_j + B_{ij}^{ab}\tau_i^a\tau_j^b \\ &- \frac{1}{2}\left(K_{ij}^a\tau_i^a + K_{ji}^a\tau_j^a\right) + 4\mathbf{S}_i\cdot\mathbf{S}_j \\ &\times\left\{D_{ij}^{ab}\tau_i^a\tau_j^b + \frac{1}{2}\left(K_{ij}^a\tau_i^a + K_{ji}^a\tau_j^a\right)\right\}\Big], \end{aligned} \tag{A10}$$

where

$$A_{ij} = \frac{1}{U}{\rm Sp}(t\,t^\dagger)\left(1 - \frac{J_{\rm H}}{U}\right); \tag{A11}$$

$$B_{ij}^{ab} = \frac{1}{U}{\rm Sp}(t^\dagger\sigma^a t\sigma^b)\begin{cases} 1+\frac{2J_{\rm H}}{U}, & a,b = 1,2 \\ 1+\frac{3J_{\rm H}}{2U}, & a = 1,2, b = 3 \\ 1+\frac{J_{\rm H}}{U}, & a = 3, b = 1,2 \\ & a,b = 3; \end{cases} \tag{A12}$$

$$D_{ij}^{ab} = \frac{1}{U}{\rm Sp}(t^\dagger\sigma^a t\sigma^b)\begin{cases} 1, & a,b = 1,2 \\ 1+\frac{J_{\rm H}}{2U}, & a = 1,2, b = 3 \\ 1+\frac{J_{\rm H}}{U}, & a = 3, b = 1,2 \\ & a,b = 3; \end{cases} \tag{A13}$$

$$K_{ij}^a = \frac{1}{U}{\rm Sp}(t^\dagger\sigma^a t)\begin{cases} 1-\frac{J_{\rm H}}{2U}, & a = 1,2 \\ 1, & a = 3. \end{cases} \tag{A14}$$

The vectors K_{ji}^a, which enter in Eq. (A10), are proportional to ${\rm Sp}(t_{ji}^\dagger\sigma^a t_{ji})$. They can be given in terms of t_{ij} using the equality ${\rm Sp}(t_{ji}^\dagger\sigma^a t_{ji}) = {\rm Sp}(t_{ij}\sigma^a t_{ij}^\dagger)$. Note also that for zero Hund's coupling $J_H = 0$, the second-rank tensors are similar $B_{ij}^{ab} = D_{ij}^{ab}$.

The presentation in the form (A10) can be viewed as a generalization of the corresponding Kugel-Khomskii [19] Hamiltonian for complex hopping amplitudes. Below we write the explicit form of all the traces that contribute to the coefficients of the Hamiltonian:

$$\begin{aligned} {\rm Sp}(t^\dagger t) &= |t^{11}|^2 + |t^{22}|^2 + |t^{12}|^2 + |t^{21}|^2, \\ {\rm Sp}(t^\dagger\sigma^z t) &= |t^{11}|^2 - |t^{22}|^2 + |t^{12}|^2 - |t^{21}|^2, \\ {\rm Sp}(t\sigma^z t^\dagger) &= |t^{11}|^2 - |t^{22}|^2 + |t^{21}|^2 - |t^{12}|^2, \\ {\rm Sp}(t^\dagger\sigma^z t\sigma^z) &= |t^{11}|^2 + |t^{22}|^2 - |t^{12}|^2 - |t^{21}|^2, \\ {\rm Sp}(t^\dagger\sigma^x t) &= 2\,{\rm Re}[t^{11}(t^{21})^* + t^{22}(t^{12})^*], \\ {\rm Sp}(t\sigma^x t^\dagger) &= 2\,{\rm Re}[t^{11}(t^{12})^* + t^{22}(t^{21})^*], \\ {\rm Sp}(t^\dagger\sigma^y t) &= 2\,{\rm Im}[-t^{11}(t^{21})^* + t^{22}(t^{12})^*], \\ {\rm Sp}(t\sigma^y t^\dagger) &= 2\,{\rm Im}[t^{11}(t^{12})^* - t^{22}(t^{21})^*], \\ {\rm Sp}(t^\dagger\sigma^x t\sigma^x) &= 2\,{\rm Re}[t^{11}(t^{22})^* + t^{12}(t^{21})^*], \\ {\rm Sp}(t^\dagger\sigma^y t\sigma^y) &= 2\,{\rm Re}[t^{11}(t^{22})^* - t^{12}(t^{21})^*], \\ {\rm Sp}(t^\dagger\sigma^x t\sigma^y) &= 2\,{\rm Im}[t^{11}(t^{22})^* - t^{12}(t^{21})^*], \\ {\rm Sp}(t^\dagger\sigma^y t\sigma^x) &= 2\,{\rm Im}[-t^{11}(t^{22})^* - t^{12}(t^{21})^*], \\ {\rm Sp}(t^\dagger\sigma^x t\sigma^z) &= 2\,{\rm Re}[t^{11}(t^{21})^* - t^{22}(t^{12})^*], \\ {\rm Sp}(t^\dagger\sigma^z t\sigma^x) &= 2\,{\rm Re}[t^{11}(t^{12})^* - t^{22}(t^{21})^*], \\ {\rm Sp}(t^\dagger\sigma^z t\sigma^y) &= 2\,{\rm Im}[t^{11}(t^{12})^* + t^{22}(t^{21})^*], \\ {\rm Sp}(t^\dagger\sigma^y t\sigma^z) &= 2\,{\rm Im}[-t^{11}(t^{21})^* - t^{22}(t^{12})^*]. \end{aligned}$$

For specific choices of $t^{\alpha\beta}$, in particular for those considered in the paper, $K^a_{ji} = K^a_{ij}$ and the general form (A10) is reduced to Eq. (9) of the main text.

For the case of real site-independent hopping amplitudes $t^{11} = t_1$, $t^{22} = t_2$, and $t^{12} = t^{21} = t_{12}$ the Hamiltonian (A10) is reduced to the original Kugel-Khomskii Hamiltonian

$$\begin{aligned} H_{\mathrm{KK}} = \frac{1}{U}\sum_{\langle ij\rangle}\Bigg[& -\left(t_1^2 - t_2^2\right)\left(\tau_i^z + \tau_j^z\right) - \left(1 - \frac{J_H}{2U}\right)2t_{12}(t_1 + t_2)\left(\tau_i^x + \tau_j^x\right) + \frac{J_H}{U}4\left(t_1 t_2 + t_{12}^2\right)\tau_i^x\tau_j^x \\ & + \frac{J_H}{U}4\left(t_1 t_2 - t_{12}^2\right)\tau_i^y\tau_j^y + \frac{J_H}{U}2t_{12}(t_1 - t_2)\left(\tau_i^z\tau_j^x + \tau_i^x\tau_j^z\right) + \left(\frac{1}{2} + 2\mathbf{S}_i\cdot\mathbf{S}_j\right)\Bigg\{\left(1 - \frac{J_H}{U}\right)\frac{1}{2}\left(t_1^2 + t_2^2 + 2t_{12}^2\right) \\ & + \left(t_1^2 - t_2^2\right)\left(\tau_i^z + \tau_j^z\right) + \left(1 - \frac{J_H}{2U}\right)2t_{12}(t_1 + t_2)\left(\tau_i^x + \tau_j^x\right) + 4\left(t_1 t_2 + t_{12}^2\right)\tau_i^x\tau_j^x \\ & + 4\left(t_1 t_2 - t_{12}^2\right)\tau_i^y\tau_j^y + \left(1 + \frac{J_H}{U}\right)2\left(t_1^2 + t_2^2 - 2t_{12}^2\right)\tau_i^z\tau_j^z + \left(1 + \frac{J_H}{2U}\right)4t_{12}(t_1 - t_2)\left(\tau_i^z\tau_j^x + \tau_i^x\tau_j^z\right)\Bigg\}\Bigg]. \end{aligned} \tag{A15}$$

For the diagonal hopping matrix $t_{12} = 0$, $t_1 = t_2 = t$, and the Hamiltonian (A15) is simplified to

$$\begin{aligned} H_{\mathrm{KK}} = {} & \tfrac{1}{4}J_1 + J_1\mathbf{S}_i\cdot\mathbf{S}_j + J_2\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j + 4J_3(\mathbf{S}_i\cdot\mathbf{S}_j)(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j) \\ & - J_3(1 - 4\mathbf{S}_i\cdot\mathbf{S}_j)\frac{J_H}{U}\tau_i^z\tau_j^z, \end{aligned} \tag{A16}$$

where

$$J_1 = \frac{2t^2}{U}\left(1 - \frac{J_H}{U}\right), \tag{A17}$$

$$J_2 = \frac{2t^2}{U}\left(1 + 2\frac{J_H}{U}\right), \tag{A18}$$

$$J_3 = \frac{2t^2}{U}. \tag{A19}$$

The Hamiltonian serves as a starting form for the symmetrical Hamiltonian (11) with independent J_1, J_2, and J_3, if one neglects the anisotropy term ($\propto J_H/U\,\tau_i^z\tau_j^z$) in pseudospin space.

Toy model. To illustrate the meaning of complex phases we have considered herein the case when the hopping process can be described by the toy model

$$t^{11} = 0, \quad t^{22} = 0, \quad t^{12} = t', \quad t^{21} = t'e^{i\chi}. \tag{A20}$$

For such amplitudes the only nonzero traces are

$$\mathrm{Sp}(tt^\dagger) = 2|t'|^2, \quad \mathrm{Sp}(\sigma^z t\sigma^z t^\dagger) = -2|t'|^2, \tag{A21}$$

$$\mathrm{Sp}(\sigma^x t\sigma^x t^\dagger) = -\mathrm{Sp}(\sigma^y t\sigma^y t^\dagger) = 2|t'|^2\cos\chi, \tag{A22}$$

$$\mathrm{Sp}(\sigma^x t\sigma^y t^\dagger) = \mathrm{Sp}(\sigma^y t\sigma^x t^\dagger) = 2|t'|^2\sin\chi. \tag{A23}$$

The Hamiltonian H_{TUJ} can be rewritten as

$$H_\chi = J\sum_{\langle ij\rangle}\left(\frac{1}{2} + 2\mathbf{S}_i\cdot\mathbf{S}_j\right)\left(\frac{1}{2} + 2B^{ab}\tau_i^a\tau_j^b\right), \tag{A24}$$

where the effective exchange is $J = 2|t'|^2/U$ and $B^{12} = B^{21} = \sin\chi$, $B^{11} = -B^{22} = \cos\chi$, and $B^{33} = -1$. Equation (A24) can be rewritten in the form (16).

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