Spin-charge-density wave in a rounded-square Fermi surface for ultracold atoms

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Abstract – We derive and discuss an experimentally realistic model describing ultracold atoms in an optical lattice including a commensurate, but staggered, spin-flip term. The resulting band structure is quite exotic; fermions in the third band have an unusual rounded picture-frame Fermi surface (essentially two concentric squircles), leading to imperfect nesting. We develop a generalized theory describing the spin and charge degrees of freedom simultaneously at the random-field-approximation level, and show that the system can develop a coupled spin-charge-density wave order. Our generic approach can be used to study spin and charge instabilities in many materials, such as high-$T_c$ superconductors, organic compounds, graphene, and iron pnictides.

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Introduction. – Ultracold atoms in optical lattices have recently emerged as a class of condensed-matter systems, where the properties of the many-body Hamiltonian are under exquisite experimental control. Interfering laser beams in one, two or three dimensions (D) create standing waves: nearly perfect optical lattices for atoms with lattice spacing and topology set by the laser geometry and wavelength [1]. Optical lattices not only allow for the implementation of different lattice models without defects, but also open a wide range of possibilities to manipulate the parameters of the model describing ultracold bosons, fermions, or mixtures thereof. For example, the hopping parameters, local chemical potential, and often even the interaction strength can be tuned at will.

Most optical-lattice experiments use atoms in a single spin state [2]; however, some experiments study mixtures of atoms in two or more atomic “spin” states, each of which can experience different lattice potentials [3–5]. We derive a lattice model, equally applicable to bosons and fermions, with a staggered spin-flip term, which can be described as a fictitious staggered Zeeman field [6]. In condensed-matter systems, the Zeeman field can break local time-reversal invariance as required for topological insulators [7,8].

For particles with two spin states, our lattice model has four low-energy bands, and the third is shaped as a squarish, deformed, Mexican hat for a wide range of system parameters. By filling the system with fermions, we obtain a peculiar Fermi surface, consisting of the boundaries of a squarish ring, essentially two concentric squircles [9]. The particular shape of the Fermi surface suggests that nesting effects should be expected. To account for interactions, we develop a description of the coupled charge and spin degrees of freedom at the random-phase-approximation (RPA) level. Imperfect nesting along the diagonal connecting corners of the Fermi surface gives rise to a coupled spin-charge-density wave (SCDW) instability at a critical interaction strength $U_c$. We calculate the imaginary part of the trace of the RPA susceptibility to study the collective excitations of the system. At the interaction strength $U_c$, a soft mode arises at the optimal nesting wave vector $Q$. The SCDW instability is in general incommensurate with the lattice, and is tunable by external parameters. In contrast with the usual behavior in 1D, our results show that in 2D a combined treatment of spin and charge degrees of freedom is essential to capture the possible instabilities of the system.

Our new theoretical approach is applicable to many materials including high-$T_c$ superconductors, iron-pnictides, organic charge-transfer solids, and graphene.
While some, limited, theories previously studied coexisting SCWDs in quasi-2D organic compounds (a few coupled chains were considered [10]) and in the striped phase of high-Tc superconductors (weakly coupled 1D systems [11]), the lack of a 2D analytical formalism prevented a complete treatment. Our full 2D theory is applicable in both cases. Simply enlarging our matrices allows direct access to complex multi-band materials such as the iron pnictides. Likewise, different lattice topologies such as honeycomb or graphene can be studied by changing a few matrix elements.

The system under study (figs. 1(a), (b)) is a sample of ultracold atoms illuminated by two optical and rf magnetic fields. The latter, linearly polarized in the $\hat{x}$ direction, is free from magnetic anisotropy and the Zeeman effect of the optical light. Our model includes a static magnetic field $B_0$ along $\hat{x}$ and a rf magnetic field $B_\text{rf}$ with angular frequency $\delta \omega$ along $\hat{z}$; rf coupling between atoms in spin-dependent lattices has been studied both experimentally [5] and theoretically [12], where the resulting non-trivial real-space lattices suggested potential application to many-body systems and quantum computation. In our case, the spin dependence results from the interplay of the laser and rf-magnetic fields.

As was observed in refs. [6,13,14], conventional spin-independent (scalar, $U_s$) optical-lattice potentials acquire additional spin-dependent terms near atomic resonance: the rank-1 (vector, $U_v$) and rank-2 tensor light shifts [14]. For the alkali atoms, adiabatic elimination of the angular momentum $J = 1/2$ (D1) and $J = 3/2$ (D2) excited states yields an effective Hamiltonian $H_0 = U_v (\mathbf{e} \cdot \mathbf{e} + i \mathbf{e} \times \mathbf{e})/\hbar$ for the $J = 1/2$ ground-state atoms. (The rank-2 term is very small for the parameters studied here.) $\mathbf{e}$ is the unit polarization vector of the optical electric field and $U_v = -2U_{\text{fs}} \delta \omega / \hbar$ is the fine-structure splitting; $\hbar \omega_{1/2} - \hbar \omega_{3/2}$ are the D1 and D2 transition energies; and $\Omega = (2 \omega_{1/2} + \omega_{3/2})/3$ is a suitable average. $U_v$ and $U_s$ can be independently specified with informed choices of laser frequency $\omega$ and intensity. Here the lasers detuning $\omega_0 - \omega \gg \delta \omega$ minimizes spontaneous emission and implies $|U_s| \gg |U_v|$ and $U_s < 0$. We express momentum and energy in dimensions of $\hbar \sigma$ and $E_s$, the single-photon recoil momentum and energy, respectively.

The atomic Hamiltonian for the laser and magnetic fields in figs. 1(a), (b) is $H_0 = U_s (\cos^2 k_+ x + \cos^2 k_+ y) + U_{B_\text{RF}} J \cdot \mathbf{B}_\text{RF}$ with a Zeeman field $B_\text{RF} = B_0 \hat{x} + B_\text{RF} \cos(\delta \omega t + \phi) \hat{z} + \zeta (U_{\text{fs}}/2g_B) \cos(\delta \omega t) \cos(k_+ x) \cos(k_+ y)$ where $B_\text{RF} \gg B_0, U_{\text{fs}}/2g_B$. Here, $\mu_B$ is the Bohr magneton and $g$ is the Landé $g$-factor. $B_\text{RF}$ includes a contribution from the vector light shift: a fictitious Zeeman field. We select $\hat{x}$ as the quantizing axes, transform into the frame rotating at $\dot{\omega}$, and make the rotating wave approximation to find

$$B_\text{RF} \cdot \hat{z} \text{ reaches its extremum on the sites of the optical lattice, giving a bias plus staggered fictitious Zeeman fields [6]. While } B_\text{RF} \text{ formally appears in the Hamiltonian as a magnetic field, it results not from a real magnetic field, but instead the vector light shift and the transformation into the rotating frame. This proposal requires the simple retro-reflection of the existing “Raman” lasers discussed in ref. [15], which were used to create an artificial magnetic field (there, } B_\text{RF} \text{ was used only for state preparation.) On Raman resonance, } g_B B_0 = \hbar \delta \omega, \text{ and when } |U_s| \gg |U_v|, |g_B B_\text{RF}| \text{ the conventional tight-binding model [16], valid when } U_s \geq 5E_s, \text{ is slightly modified by the fictitious magnetic field evaluated on the lattice sites, yielding}

$$H_0 = -t \sum_{(i,j),s} c_{i,j}^\dagger c_{j,i} + \Omega_{RF} / 2 \sum_j \left( e^{i\phi} c_{j,\downarrow}^\dagger c_{j,\uparrow} + \text{h.c.} \right) + \Omega_{RF} / 2 \sum_j \left[ e^{i\sigma(x_j + y_j)} c_{j,\uparrow}^\dagger c_{j,\downarrow} + \text{h.c.} \right].$$

$c_{i,j}$ is an annihilation operator (bosonic or fermionic) on site $j$ with spin $s$; the hopping matrix element $t$ can be computed from the band structure of a sinusoidal lattice (for a $U_s = 5E_s$ scalar lattice $t \approx 0.07E_s$); $\Omega_{RF} = g_B B_\text{RF}$; and $\Omega_{RF} = U_s/2$. Since we focus on very small $\Omega_{RF} \tau$, the detuning from atomic resonance can be quite large. For
While the single-particle spectrum is valid for fermions and bosons, we define spinor field operators $\psi_j \equiv (\psi_{j,\uparrow}, \psi_{j,\downarrow})^T$ and three-component vectors $S_j = (S^0_j, S^\pi_j, S^2_j)^T = \sigma \vec{c} \psi_j / 2$, where $\sigma$ is the Pauli matrices. Owing to the fictitious staggered Zeeman field, we introduce sublattices $A_+$ and $A_-$, where $A_{\pm} = \{ (j_x, j_y) \mid (-1)^{j_x+j_y} = \pm 1 \}$ and we define $a_{j,\pm} \equiv \psi_j$ for $j \in A_{\pm}$. In addition, we introduce vectors $B_{\pm} = \{ \Omega_{\epsilon} \sin(\phi) \pm \Omega_R, -\Omega_{\epsilon} \sin(\phi), 0 \}^T$ describing Zeeman fields on the $A_{\pm}$ sublattices. In this notation, the bare Hamiltonian is

$$H_0 = -i \sum_{(k,j)} \left( a_{k,j,\uparrow}^\dagger a_{j,k,\downarrow} + h.c. \right) + \sum_{j \in A_+} S_j^+ B_+ + \sum_{j \in A_-} S_j^+ B_- .$$

In terms of momentum field operators $\psi_k \equiv (\psi_{k,\uparrow}, \psi_{k,\downarrow}, a_{k,\uparrow}, a^\dagger_{k,\downarrow}, a_{k,-}, a^\dagger_{k,\downarrow})$, the Hamiltonian becomes

$$H_0 = \sum_k \psi_k^\dagger H_0 \psi_k \text{ where }$$

$$H_0 = \begin{bmatrix} \tilde{\Delta} \cdot B_+ / 2 - t \gamma_k \mathbf{I} \\ -t \gamma_k \mathbf{I} & \tilde{\Delta} \cdot B_- / 2 \end{bmatrix} .$$

Here, $\gamma_k = 4 \cos(k/2) \cos(k/2)$, with $k = \pi \pm \epsilon (k_x \pm k_y) / k_r$, $k_r = (k_+ - k_-)$ and $\mathbf{I}$ is the $2 \times 2$ identity matrix. The summation goes over the entire Brillouin zone $-\pi < k_x, k_+ \leq \pi$, i.e., $\gamma_k > 0$. The four eigenvalues of $H_0$ are

$$\epsilon_k^2 = (\gamma_k)^2 + \left( \frac{\Omega_{\epsilon}}{\gamma} \right)^2 + \left( \frac{\Omega_R}{2} \right)^2 \pm \Omega_{\epsilon} \sqrt{ (\gamma_k)^2 + \left( \frac{\Omega_R}{2} \cos(\phi) \right)^2 } ;$$

together these eigenvalues constitute four bands (fig. 1(c)). The most interesting one is the third band, which can be shaped as a squarish, deformed Mexican hat.

**Spin-charge-density wave.** While the single-particle spectrum is valid for fermions and bosons, we now focus on spin-1/2 fermions with a Hamiltonian,

$$H = H_0 + H_{\text{int}}; \quad H_{\text{int}} = U \sum_j \left( c_{j,\uparrow} c_{j,\uparrow}^\dagger + c_{j,\downarrow} c_{j,\downarrow}^\dagger \right) .$$

The interaction strength $U$ is proportional to the s-wave scattering length, and the Fermi energy is chosen to be in the third band. The resulting squarish Fermi surface is depicted by the white contours in fig. 1(c) and is shaped like two concentric squircles. Nesting and local fermion-fermion interactions lead to spin- and charge-ordered phases in this system. We anticipate a second-order phase transition when the coefficient of the second-order term in the Landau free energy vanishes. Formally, we use the Hubbard-Stratonovich transformation [17] to treat the interactions within a saddle point approximation (analogous to the time-dependent Hartree-Fock approximation).

Conventional approaches to study SDW instabilities in the 2D Hubbard model neglect the contribution of charge density fluctuations [17,18], which are important here. In the following, we develop a generalized solution of 2D tight-binding models with local interactions and obtain a theory of SCDW instabilities.

In the coherent states formalism, the grand-canonical partition function is $Z = \int \mathcal{D}[\phi] e^{-\mathcal{S}[\phi]/\hbar}$, where $S = \int_0^{h_{k_b}} d\tau \left[ \sum_j \partial^2 \psi_j / (\partial \phi \partial \phi) \right]$ is the Euclidean action and $\beta = 1 / k_B T$. We express the interaction term in a $SO(3,1)$ invariant form $c_{j,\uparrow} c_{j,\downarrow} c_{j,\downarrow} / (1/2) S^2_j \psi_j$ with $n_j = c_{j,\uparrow} c_{j,\downarrow}$. The $SO(3)$ invariance is required by rotational symmetry; the fact that the spin and charge terms have different signs reflects the Pauli principle, which requires a vanishing self-energy for a polarized state. The Hubbard-Stratonovich transformation renders the action quadratic in the fermion operators by introducing auxiliary bosonic fields, $\rho_\pm$ and $M_\pm$, which couple to charge and spin densities, respectively. For repulsive interactions the charge density term leads to a divergent integral. We resolve this problem by integrating along a contour parallel to the imaginary axis for $\rho_\pm$. Next, we introduce a source field $J$ that couples to the charge and spin densities at each sublattice, and an eight-component vector $M_{k,n} = (\rho_{k,+}, M_k, +, n, \rho_{k,-}, M_{k,-} - , n, M_{k,-} - , n)^T$ expressed in terms of momentum $\mathbf{k}$ and Matsubara frequency $\omega_n = \pi (2n + 1) / h \beta$. After integrating out the fermionic fields, we obtain a path-integral over the auxiliary bosonic field $M_{k,n}$, which we evaluate in the saddle-point approximation. Hence, we determine $Z[J]$, and by performing a Legendre transformation [17], we find the free energy

$$\beta F(\langle M \rangle, J) = \frac{1}{2 h \beta^2} \left( \Delta (M,j) \right)^j \cdot \langle \langle \langle \rho \rangle \rangle \rangle \cdot \Delta (M,j)$$

where $\Delta (M,j) \equiv \langle M,j \rangle - \langle M \rangle_0$ and the generalized RPA susceptibility $\langle \langle \rho \rangle \rangle = \chi_0^R - \epsilon \eta$ is an $8 \times 8$ matrix [19]. The matrix $\eta = \text{Diag}(-1, 1, 1, 1, -1, 1, 1, 1)$ is a metric signature corresponding to the $SO(3,1) \times SO(3,1)$ group and $\chi_0$ is the bare susceptibility for the renormalized Hamiltonian theory. For homogeneous phases, the susceptibility and the Hamiltonian become diagonal in momentum and frequency space. The $k$-dependent susceptibility at zero source $\chi_0$ then reads

$$\chi_k = \chi_k^{\rho \rho'} = \chi_k^{\nu \nu'} = \frac{1}{N} \sum_{\alpha, \beta} \rho_{\alpha, \beta} \rho_{\beta, \alpha}$$

and

$$T_{p,k,p,k} \equiv - \frac{1}{N} \text{Tr} \left[ \rho_{\alpha, \beta} \rho_{\beta, \alpha} \right]$$

Here $\Omega_n$ is the bosonic Matsubara frequency; $N$ is the number of sites in a sublattice; $n_F(z)$ is

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the Fermi distribution function; energy is measured with respect to the chemical potential \( \mu \). The instability condition for repulsive interactions requires \( U > U_c \), where \( U_c \) is determined by \( \text{det}(\chi^{-1} - U_I) = 0 \). Since we avoid the van Hove singularity, the susceptibility is finite and the critical value \( U_c \) is nonzero. It is related to the largest eigenvalue \( \lambda_Q \) of the matrix \( \chi_{k}(0) \) by \( U_c^{-1} = \max_{k} \lambda_{k} \). Thus, the instability condition becomes \( \lambda_Q U > 1 \), analogous to the Stoner criterium. Figure 2(a) shows \( \lambda_Q \) for the Fermi surface in fig. 1. \( \phi = \pi/4 \), \( \Omega_B = 2t \), \( \Omega_t = 4t \), \( \mu = t \), and \( k_B T = 10^{-3}t \). We calculated \( \chi_{k}(0) \) numerically on each point of a mesh with 240 \( \times \) 240 points. The peak with \( \lambda_Q = 0.172(6) \), corresponding to the critical value of interactions \( U_c/t = 5.78(6) \), is located at \( Q = (\pi/4, \pi/4) \), where we expect an imperfect nesting between inner and outer lines of the Fermi surface (fig. 1(c)), with \( \epsilon_{Q}^{(3)} \approx \epsilon_{Q}^{(3)} \). For these system parameters, the eigenvector \( V_Q \) corresponding to this eigenvalue is a mixture of both SDW and CDW, hence a SCDW. The details of the mixture are not universal.

The period of the SCDW \( 2\pi/|Q| \) is in general incommensurate with the lattice period and is freely tunable by changing the vectors \( \mathbf{B}_k \), and the chemical potential \( \mu \). Nesting can also occur for other momenta, which give the smaller peaks in the pattern shown in fig. 2(a).

Had we neglected the coupling with charge and considered only the spin susceptibility, we would find at the same value of \( Q \) a much lower value for the critical interaction strength: \( U_c/t = 4.26(6) \) compared with \( U_c/t = 5.78(6) \) in the full calculation. In addition, when considering only charge excitations, no CDW instability occurs for repulsive interactions \( U > 0 \). Thus, the coupling of charge and spin excitations, as developed here, is essential to the realization of a phenomenon which otherwise would only occur for attractive interactions \( U < 0 \).

**Experimental detection.** – Equation (3) allows us to study the collective excitation spectra by analytically continuing \( i\Omega_n \to \omega + i\Omega \) and looking at the imaginary part of the trace of the RPA susceptibility \( \text{Tr}[\text{Im} \chi^{(RPA)}_{k}(\omega)] \). For \( \kappa = 0.02 \) we find a linear dispersion spectrum in fig. 2(b) in the long-wavelength region (the Landau zero sound), which could have been anticipated, since we are considering a compressible zero-temperature Fermi liquid. At the interaction value \( U_c/t = 5.78(6) \) a soft linearly dispersing mode starting from \( k = Q \) appears, signaling the onset of instability (fig. 2(d)). The dynamic structure factor \( S(k, \omega) \) directly reflects the collective excitation spectrum; in condensed-matter systems \( S(k, \omega) \) is measured by neutron scattering, and with cold atoms it can be probed with energy- and momentum-sensitive Bragg spectroscopy [20,21]. In ref. [21] a moving lattice is formed by a pair of “Bragg” lasers with wavelength \( \lambda_B \) intersecting at angle \( \theta_B \) and differing in frequency by \( \omega_B/2\pi \). The population of atoms diffracted from this moving lattice is proportional to \( S(k_B, \omega_B) \), where \( |k_B| = (4\pi/\lambda_B) \sin(\theta_B/2) \) is the momentum transferred by the two lasers. \( S(k, \omega) \) is qualitatively similar to the imaginary part of the trace of the susceptibility (fig. 2(b)–(d)), and will indicate the onset of SCDW order by the appearance of zero-energy spectra weight at \( k = Q \). Indeed, recent experiments detecting Bragg scattering of light from atoms in an arrayed in an optical lattice demonstrated the power of this technique [22].

In \( ^{40} \text{K} \), the collective excitation spectrum can be experimentally studied with an atomic analog of angle-resolved

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**Fig. 2:** (Colour on-line) (a) Largest eigenvalue of the static susceptibility \( \chi_{k}(0) \) as a function of \( k_+ \) and \( k_- \). The peaks indicate the \( Q \) vectors for SCDW instabilities, and the largest peak marks the location of the most prominent nesting vector. (b)–(d) Imaginary part of the trace of the susceptibility \( \text{Tr}[\text{Im} \chi_{k}(\omega)] \) in logarithmic scale in the \( k_+\omega \) plane, with \( k_+ = 0 \), i.e., \( k_+ = -k_- \). (b) Without interactions a linearly dispersing sound mode is observed for small \( k_+ \). (c) For \( U/t = 5.20(6) \), spectral weight builds up for a second linear-dispersing mode, which starts from \( \omega = 0 \) at \( \pi k_+/k_r = \pi/4 \). (d) For \( U/t = 5.78(6) \), the sharp increase of the intensity at \( \omega = 0 \) with \( \pi k_+/k_r = \pi/4 \) signals the onset of SCDW instability. 
photoemission spectroscopy [23]. In this technique —already applied to the BEC-BCS crossover in $^{40}$K—an rf pulse detuned by $\delta \omega_{rf}$ from rf resonance transfers a small fraction of atoms into a non-interacting final state. The momentum distribution $n(k)$ of these atoms is the single-particle spectral function $A(k, \omega)$: the transition probability from the ground to all excited states with energy $\hbar \omega = \hbar k^2/2m - \hbar \omega_{rf}$ when an atom with momentum $\hbar \mathbf{k}$ is removed from the many-body system. Like $S(k, \omega)$, it is expected to reflect SCDW with a tunable energy probability from the ground to all excited states with single-particle spectral function $\mathcal{A}(k, \omega)$.

Conclusions. — We showed how to construct a system with a unique Fermi surface consisting of concentric squircles. The system has peculiar collective excitations, which we analyze in the RPA including both charge- and spin-density excitations. Our studies predict an instability combining both CDW and SDW with a tunable incommensurate wave vector, determined by the nesting properties of the Fermi surface, for sufficiently strong interactions. Moreover, we find that the usual approach —neglecting the coupling with density fluctuations— significantly underestimates the critical value of the interaction strength.

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