Pair Density Wave Instability of Cold Fermionic Atoms in an Optical Lattice

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We show that the band insulating state of cold fermionic atoms in a three-dimensional cubic optical lattice is unstable to forming a pair-density wave (PDW) state in the presence of strong attractive interactions induced by proximity to a Feshbach resonance. The PDW state in this model is a special type of supersolid, which arises from the condensation of predominantly interband Cooper pairs at a nonzero, generically incommensurate, wavevector, and is expected to be accompanied by an induced density modulation. We also discuss the mean field phase diagram of a two-band tight binding model, which exhibits a PDW state, and discuss the relation of the PDW instability in this model to the Halperin-Rice exciton condensation instability in indirect bandgap semiconductors.

Introduction. — The theme of coexisting or competing order parameters is common to several strongly correlated systems, including high temperature cuprate [1] and pnictide [2] superconductors. Most notably, there have been striking experimental indications of stripes or checkerboard patterns of spin and charge modulations, that coexist with superconductivity in several cuprate materials [3, 4, 5, 6, 7]. Motivated by the observation [8] of quasi-two-dimensional superconductivity coexisting with stripe order in the layered superconductor La$_2$CuO$_4$ (LBCO), Berg et al. [9] have proposed, on phenomenological grounds, that a distinct state of matter, named a ‘pair density wave’ (PDW), is realized in this material. In its simplest avatar, the PDW state results from condensing singlet Cooper pairs with nonzero center-of-mass momenta $\pm \mathbf{Q}$ and is accompanied by an induced charge density modulation at momenta $\pm 2\mathbf{Q}$. It is thus similar to the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state of magnetized superfluids [10] except that the PDW does not require broken time-reversal symmetry. In contrast to earlier proposals for a Cooper pair insulator [11, 12] in LBCO, the PDW state is a supersolid, in that it coexists with superfluid and density orders, which break lattice symmetries. However, it is very different from the supersolid state proposed to exist in $^4$He [13, 14], or the supersolids realized in simple lattice boson models [15], since the superfluid order parameter in the PDW state has no uniform Fourier component. The bosonic analog of the PDW may be found in lattice models of bosons in which the kinetic energy is ‘frustrated’ so that the single-particle dispersion has multiple minima, at nonzero momenta, into which bosons can condense [16] without breaking time-reversal symmetry.

In this Letter, we show that there are simple microscopic models of fermions with short-range attractive interactions which support PDW ground states. Our work complements earlier Landau theory descriptions and Josephson junction models of the PDW state [9]. Our first example is a one-channel model of fermionic atoms near a Feshbach resonance [17, 18] confined to a cubic optical lattice. It has been demonstrated recently [19] that this system shows a superfluid to band-insulator transition [20, 21, 22] when the lattice depth is varied at a commensurate density of two atoms per lattice site. Here we show, via a more careful study, that a PDW state is expected to intervene between the uniform superfluid and the band insulator. Our second example is a two-band tight binding model where the chemical potential is chosen to be such that both bands are empty. An appropriate choice of local attractive interactions between the fermions is then shown to lead to a PDW instability of this zero-filling band insulator.

The key physics which leads to the emergence of the PDW state in both these models is the presence of multiple bands and the dominance of interband Cooper pairing. In the cold atom model, we present arguments to show that, in contrast to intraband pairing, the phase space for interband pairing is expanded at nonzero pairing momenta, which stabilizes an incommensurate PDW state. In the two-band tight binding model, the reason for the occurrence of the PDW state is that the lowest energy momentum points in each band differ by a nonzero wavevector $\mathbf{Q}$, which leads to a large Cooper pair susceptibility at this wavevector. For this model, we present the mean field phase diagram and show that the PDW instability is closely related to the Halperin-Rice exciton condensation instability in indirect bandgap semiconductors [23, 24].

Cold Atoms in an Optical Lattice. — We describe fermionic atoms with attractive interactions in a periodic potential [20, 21, 22] using the Hamiltonian ($\hbar = 1$):

$$H = \int d^3r \left[ c_\sigma^\dagger \left( -\frac{\nabla^2}{2m} - \mu + V_r \right) c_\sigma - U c_\uparrow^\dagger c_\downarrow^\dagger c_\downarrow c_\uparrow \right]. \quad (1)$$

Owing to universality in the unitarity regime, this simple theory provides a faithful description of fermionic cold atoms tuned near a broad Feshbach resonance [25]. We will study this model using mean-field theory which is known to be a reasonable approximation near unitarity for the qualitative points we wish to make. Fluctuations...
can be treated systematically using, for example, large-$N$ expansions \cite{21,22,23}, but we will not pursue this here.

We work with a simple cubic lattice potential:

$$V_r = V \left[ \cos \left( \frac{2\pi x}{a_L} \right) + \cos \left( \frac{2\pi y}{a_L} \right) + \cos \left( \frac{2\pi z}{a_L} \right) \right],$$

where $a_L$ is lattice spacing. The quantum numbers of single-particle Bloch eigenstates in this potential are crystal wavevector $k = (k_x, k_y, k_z)$ inside the first Brillouin zone (BZ) $-\pi/a_L \leq k_x, k_y, k_z < \pi/a_L$, and band index $n = (n_x, n_y, n_z)$. We label the Bloch wavefunctions by $\psi_{nk}(r)$ and the corresponding energies by $\epsilon_{nk}$.

Near unitarity, the cutoff-dependent contact interaction parameter $U$ is related to the scattering length $a$:

$$\frac{1}{U} = -\frac{m}{4\pi a} + \sum_n \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\epsilon_{nk}^2} |V_r = 0|.$$  

Band-index cutoff, discussed below, is implicit in (3).

A $T = 0$ superfluid-insulator transition for an even number of fermions per site occurs at a critical value of the lattice amplitude $V_r$, which is a universal function of $a_L/a$ and the fermion density \cite{21,22,23}. Starting from a band-insulating state, the onset of pairing in the mean-field approximation can be extracted from the inverse static pairing susceptibility matrix:

$$\Pi_{Gq;G'q} = \sum_{n_1,n_2} \int \frac{d^3k_1}{(2\pi)^3} \frac{d^3k_2}{(2\pi)^3} f(\xi_{n_1,k_1}) - f(-\xi_{n_2,k_2})$$

$$\times \frac{1}{U} \int \frac{d^3r_{Gq}(r)}{U} \Phi_{Gq}(r) \psi_{n_1,k_1}(r) \psi_{n_2,k_2}(r),$$

where $q$ are first BZ wavevectors, $G$ are reciprocal lattice vectors, $\xi_{nk} = \epsilon_{nk} - \mu$, $f(\xi)$ is Fermi-Dirac distribution function and $G$ are vertex functions:

$$\Gamma_{n_1;k_1;Gq} = \frac{1}{U} \int \frac{d^3r_{Gq}(r)}{U} \Phi_{Gq}(r) \psi_{n_1,k_1}(r) \psi_{n_2,k_2}(r).$$

Since crystal momentum is conserved, $\Pi_{Gq;G'q} = \Pi_{G'q;Gq}$, $\delta(\mathbf{q} - \mathbf{q}')$. We will use the plane wave representation for $\Pi_{Gq;Gq}(q)$, corresponding to the pair wavefunctions $\Phi_{Gq}(r) = e^{i\mathbf{q} \cdot \mathbf{r}}$. All eigenvalues of the matrix $\Pi_{GG'}$ are positive in the band insulating state. When the lowest eigenvalue $\Pi_{Gq}$ becomes negative at some wavevector $\mathbf{q} = \mathbf{Q}$, the insulating state becomes unstable to a superfluid of fermion pairs condensing at momentum $\mathbf{Q}$, which is a PDW state \cite{0} if $\mathbf{Q} \neq 0$.

Normally one would expect the pair condensation to occur at $\mathbf{Q} = 0$. This is certainly true in any single-band model of lattice fermions. However, as we demonstrate below, interband pairing in multi-band models can give rise to pairing instability at a finite $\mathbf{Q}$. Figure 1 shows a contour plot of $\Pi(q)$ for two fermions per lattice site at $T = 0$. Each contour in this plot \cite{1} defines a superfluid-insulator transition for a different scattering length $a$.

Insulators are obtained in the limit of large $V$, so the largest $V$ on the contour for a given $a$ is the critical lattice depth $V_c(a)$ for the onset of pairing. One can see that $V_c(a)$ generally corresponds to a nonzero value of $\mathbf{q} = \mathbf{Q}$. The smooth evolution of $|\mathbf{Q}|$ with the lattice depth in the deep BCS limit indicates that the formed PDW state is incommensurate. As the pairing interactions become stronger moving toward the BEC limit, $|\mathbf{Q}|$ grows and possibly eventually saturates at the BZ edge making the PDW commensurate. Another notable feature is that sometimes a superfluid at not too small $\mathbf{q}$ can be destabilized by both increasing and decreasing $V$ (for example, the dashed contour in Fig. 1). The latter illustrates that interband pairing is responsible for superfluidity at finite $\mathbf{q}$, which can be expected to weaken with decreasing $V$. Note that Mott physics plays no role in this instability, since repulsive interactions between Cooper pairs are captured only by two-boson correlation functions. Also, without knowing such correlations we cannot rule out time-reversal symmetry breaking.

Even though the PDW instability we observe is a weak feature, we found its robust convergence with increasing cutoffs. In the following we provide simple arguments to show why multiband models can favor a PDW instability.

The incommensurate PDW owes its existence to phase-space restrictions for interband pairing. Consider two particular fermion bands along some momentum direction in the first BZ, separated by an indirect ‘gap’ (which may be filled by other bands). For concreteness, let us describe these two bands using a one-dimensional toy model with $a_L = 1$ illustrated in Fig. 1. Since momentum is conserved only modulo reciprocal lattice vectors $G$, we
can rewrite the vertex functions \( \Gamma_{n_1k_1n_2k_2}^{Gq} \) as:

\[
\Gamma_{n_1k_1n_2k_2}^{Gq} = \sum_{G'} A_{n_1n_2}^{Gq}(G') \times 2\pi\delta(k_1 + k_2 - q + G'),
\]

(6)

where the coefficients \( A_{n_1n_2}^{Gq}(G') \) depend on details of the band-structure. In the limit of small lattice depth \( V \) all but one of these coefficients for any fixed \((n_1,n_2,G)\) become small, and must gradually vanish as \( V \to 0 \), when momentum conservation becomes exact. The remaining large coefficient occurs at a value of \( G' \), which depends on \((n_1,n_2,G)\), and approaches unity, as \( V \to 0 \).

For example, pairing into a plane-wave superfluid at \( q \in \text{first BZ} \) is given by \( A_{11}^{11}(G) = \delta_{G,0} \) (intra-band) and \( A_{22}^{11}(G) = A_{21}^{11}(G) = \delta_{G,2\pi\text{sgn}(q)} \) (inter-band) for small \( V \). We simplify the following discussion by focusing only on this pairing channel which reduces the inverse pairing susceptibility matrix \( \Pi_{GG'}(q) \) to a scalar \( \Pi(q) \). The other allowed pairing channels, involving condensate harmonics at larger reciprocal lattice vectors, will be neglected since they have relatively small amplitudes at small \( V \), and only slightly enhance the PDW instability.

Using (3) we find that the main contribution to intra-band pairing for small \( V \) at \( T = 0 \) comes from

\[
\Pi^{(1,1)}(q) \approx -\frac{1}{2\pi} \int dk_1dk_2 \frac{\delta(k_1 + k_2 - q)}{\xi_{1,k_1} + \xi_{1,k_2}},
\]

which is illustrated in Fig. 2(a). Since \( k_1 \) and \( k_2 \) are restricted to the first BZ, the number of states available for intra-band pairing decreases with \( q \). Consequently, the magnitude of \( \Pi^{(1,1)}(q) \) decreases with \( q \) and thus purely intra-band pairing would occur at \( q = 0 \). The dominant interband contribution

\[
\Pi^{(1,2)}(q) \approx -\frac{1}{2\pi} \int dk_1dk_2 \frac{\delta(k_1 + k_2 + 2\pi\text{sgn}(q) - q)}{\xi_{1,k_1} + \xi_{2,k_2}},
\]

illustrated in Fig. 2(b) has the opposite behavior because the number of states available for interband pairing increases with \( q \). Therefore, interband processes alone would prefer pairs to condense at a BZ edge, i.e. at the largest possible value of \( q \).

It is important to note that \( \Pi(q) \sim |q| \) for \( q \to 0 \) due to the boundaries of momentum integrals in all \( \Pi^{(n_1n_2)}(q) \), as can be seen from Fig. 2. Only for \( V = 0 \) and in the tight-binding limit do these linear contributions cancel out, leading to \( \Pi(q) \sim q^2 \). The initially negative slope of \( \Pi(q) \) leads to a local minimum at \( q \neq 0 \). The location of this minimum is determined by the relative strengths of interband and intraband contributions, so that in principle it can be anywhere in the BZ, making the PDW incommensurate. However, for large lattice amplitudes \( V \) a tight-binding limit provides a better description of the system and naturally yields a commensurate PDW as we illustrate below.

A linear \( \Pi(q) \) for \( q \to 0 \) is incompatible with a uniform superfluid instability. Since phase-space restrictions for pairing in the presence of a periodic potential generally result in a linear \( \Pi(q) \), we argue that a PDW supersolid always preempts an ordinary superfluid instability of the band insulator. This is consistent with our numerical findings. Note that fluctuations beyond the mean-field approximation cannot remove the PDW instability unless some accidental cancellations of the linear terms occur.

**Two-band tight binding model.** — Let us next turn to a tight-binding model which is of interest for fermions in deep optical lattices or for strongly correlated solid state materials. We assume a model Hamiltonian

\[
H = -\sum_{\langle i,j \rangle\sigma\eta} t_{ij} c_{i\sigma}^\dagger c_{j\eta} + h.c. + \sum_{\alpha} (\gamma_{\alpha} - \mu) c_{i\alpha}^\dagger c_{i\alpha} - U \sum_{\ell} \lambda_{n_1n_2} c_{i_{n_1}^\dagger} c_{i_{n_2}^\dagger} c_{i_{\ell_1}^\dagger} c_{i_{\ell_2}^\dagger},
\]

(7)

where the fermions \( c \) have a band-index \( n \) in addition to spin \( \sigma \). The noninteracting ground state of this model is either a normal metal or a band insulator, depending on the parameters in the Hamiltonian.

Upon including interactions, we find that the inverse Cooper pair susceptibility of the noninteracting ground state is given by

\[
\Pi(q) = \frac{1}{U} + \frac{1}{N} \sum_{k,n,\ell} \lambda_\ell^2 \frac{f(\xi_{n,k}) - f(-\xi_{\ell,k+q})}{\xi_{n,k} + \xi_{\ell,k+q}},
\]

(8)

where \( \xi_{n,k} = -2t_q (\cos k_x + \cos k_y) + \gamma_n - \mu \), and \( N \) is the number of lattice sites. In contrast to the previous model, the momentum dependence of the susceptibility in this tight binding limit arises only from the band dispersion, while the coupling constants are momentum independent unlike the pairing vertices studied earlier. For simplicity, we focus here on a two-dimensional two-band model and restrict ourselves to the case where \( \lambda_{11} = \lambda_{22} = \cos \theta \) and \( \lambda_{12} = -\lambda_{21} = \sin \theta \), with \( 0 \leq \theta \leq \pi/2 \). With this parametrization, the overall pairing strength is controlled by \( U \), while tuning the angle \( \theta \) takes us from pure intra-band pairing (\( \theta = 0 \)) to pure interband pairing (\( \theta = \pi/2 \)).
We have shown that the PDW state arises in simple and experimentally relevant microscopic lattice fermion models. In the multiband tight binding limit, the PDW state appears to be robust provided one has strong interband interactions. The PDW instability for cold atoms near unitarity in a cubic optical lattice is a comparatively weaker effect at the lattice depths and densities we could explore. Also, the ordering wavevector is incommensurate and small, which could make it difficult to observe this effect in cold atom experiments. However, we expect it to be possible to significantly enhance the PDW modulation by engineering different lattice potentials and using higher atom densities.

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