Spin-Dependent Hubbard Model and a Quantum Phase Transition in Cold Atoms

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We describe an experimental protocol for introducing spin-dependent lattice structure in a cold atomic fermi gas using lasers. It can be used to realize Hubbard models whose hopping parameters depend on spin and whose interaction strength can be controlled with an external magnetic field. We suggest that exotic superfluidities will arise in this framework. An especially interesting possibility is a class of states that support coexisting superfluid and normal components, even at zero temperature. The quantity of normal component varies with external parameters. We discuss some aspects of the quantum phase transition that arises at the point where it vanishes.

I. INTRODUCTION

Cold atom systems can be used to explore important problems of condensed matter physics in new ways. For example, recent rapid development of the ultracold atomic gas in optical lattices [1, 2] supported the observation of the superfluid-Mott insulator transition in cold atomic bosons confined in an optical lattice [3, 4, 5, 6]. In a wider context, methods of “engineering” various lattice model systems with bosonic and fermionic atoms have been proposed [7, 8, 9, 10, 11, 12, 13, 14, 15, 16], opening prospects for exploring exotic new phases. In recent years achieving superfluidity in cold atomic fermions has become a major goal, involving several experimental programs [17, 18, 19, 20, 21, 22, 23, 24, 25]. Here we consider techniques that permit one to introduce both sorts of complexity in one system, with controlled band structures and interactions that depend on spin. They involve counterpropagating laser beams, that together generate a standing light wave which leads to different AC Stark shifts for the spin up and spin down components of alkali atoms (such as K) in their ground state [2, 8]. We then discuss an interesting new phase transition between this state and conventional Bardeen-Cooper-Schrieffer (BCS) superfluidity.

II. SPIN-DEPENDENT OPTICAL LATTICES FOR COLD FERMIONIC ATOMS

In this section we describe how to realize, using cold atoms in an optical lattice, a rather general band Hubbard-type model, with separate, tunable effective masses and filling factors for the two spins [8, 12].

A. The setup of an optical lattice model

Atoms in an off-resonant laser field exhibit a second order AC Stark shift of their ground state levels. This shift is proportional to the light intensity. The intensity may vary in space, for example, by forming a standing light wave from counterpropagating laser beams. For the center-of-mass motion of the atoms, spatially varying AC Stark shifts play the role of a conservative potential. In particular, a standing light wave leads to a periodic intensity pattern which results in a periodic potential, i.e. an optical lattice. By superimposing lattice beams from different directions and different intensity an effectively 1D, 2D or 3D lattice can be built.

Consider a cloud of cold fermionic atoms in 3D optical lattice [15]. We assume that only two of the internal ground states participate in the dynamics, which we call spin up and down, |↑⟩ and |↓⟩. The corresponding effective Hamiltonian is

\[
H = \sum_\sigma \int d^3x \left[ \frac{-\hbar^2}{2m} \nabla^2 + V_\sigma(x) \right] \psi_\sigma(x) - \delta \int d^3x \psi_\uparrow(x) \psi_\downarrow(x) \\
+ \frac{\Omega_0}{2} \int d^3x \left[ \psi_\downarrow(x) \psi_\downarrow(x) + \psi_\uparrow(x) \psi_\uparrow(x) \right] + h.c. \\
+ \frac{4\pi a_s \hbar^2}{m} \int d^3x \psi_\uparrow(x) \psi_\downarrow(x) \psi_\downarrow(x) \psi_\uparrow(x)
\] (1)

with \(\psi_{\sigma=\uparrow,\downarrow}(x)\) fermionic field operators obeying the usual anticommutation relations. The various terms contributing to the Hamiltonian are illustrated in Fig. 1.

The first line in (1) contains the the kinetic energy and the optical lattice potential \(V_\sigma(x)\) generated by the laser beams, obtained in second order perturbation theory for coupling of the ground state levels to the excited atomic states. In the simplest case of three orthogonal laser beams this potential has the form

\[
V_\sigma(x) = \sum_{\ell=1}^3 V_{\sigma\ell}^{(0)} \sin^2 kx_\ell.
\] (2)
FIG. 1: Spin-dependent lattice: two counterpropagating laser beams generate a standing light wave which leads to different AC Stark shifts for the spin up and spin down components of the ground state atoms ($\sigma = \uparrow, \downarrow$). As a result the tunneling matrix elements $t_\sigma$ for the two spin components are different. The spin up and down components are coupled by a Raman laser with Rabi frequency $\Omega_0$ and detuning $\delta$.

Here $k = 2\pi/\lambda$ is the wave vector of the light, $V^{(0)}_\sigma(x)$ is proportional to the lattice beam intensity in the direction $\ell$ and the dynamic atomic polarizability at the laser frequency of the level (spin state) $\sigma$.

Note that in Eq. (1) we have ignored cross AC Stark terms coupling two different spin components. These are negligible for the situation indicated in Fig. 2 where the AC Stark shifts are much smaller than the (bare) energy of the atomic levels, which can be achieved, e.g., by applying a magnetic field to split the magnetic sublevels of the atoms. Furthermore, we have assumed in (2) that the AC Stark shifts of lattice beams in different directions can be added. Depending on the laser configuration there may be interference terms. However, for lattice beams in different directions with (slightly) shifted optical frequencies (obtained by modulating the lattice beams), these interference terms will average to zero. We have also ignored contributions from spontaneous emission. These can, for sufficiently large detunings of the lattice beams from the excited states, be made arbitrarily small. Indeed, for large detuning $\Delta \gg \Gamma$ from excited states with width $\Gamma$, the spontaneous emission rate scales as $\Gamma/\Delta^2$ while the lattice potential scales as $1/\Delta$, so spontaneous emission becomes, on the relevant dynamical timescale, negligible.

A key element in (1) is the assumption that the lattice potential $V_\sigma(x)$ is spin dependent, as illustrated graphically in Fig. 1. Immediately below we will discuss in detail specific atomic and laser configurations that allow us, by varying laser parameters, to engineer this spin dependence.

The second line in Eq. (1) describes the coupling of the two spin states via a Raman transition with effective two-photon Rabi frequency $\Omega_0$, and Raman detuning $\delta$. The Hamiltonian has been written in the frame, where the optical frequencies have been transformed away, so that only the detuning $\delta$ appears in (1).

Finally, the last term in (1) is the usual atom-atom interaction described by a pseudo potential with scattering length $a_s$. In atomic experiments the sign and magnitude of the scattering length can be manipulated, for example, with an external magnetic field via Feshbach resonances $^{21, 22, 23}$. The derivation of (1) assumes explicitly that the scattering length is much smaller than the lattice spacing (given by $\lambda/2$). In more general circumstances, the interaction will extend beyond nearest neighbors.

For single atoms the energy eigenstates in the optical lattice are conveniently described by a band structure and Bloch wave functions. An appropriate superposition of the Bloch wave functions forms a set of Wannier states which are localized at the various lattices sites. For typical experimental parameters the frequencies associated with dynamics of cold atoms in the lattice are much smaller than the excitation energies in the optical potential (excitation to higher Bloch bands). Expanding the field operators in the set of Wannier functions of the lowest Bloch band, $\psi_\sigma(x) = \sum_n w_\sigma(x-x_n)\tilde{\psi}_{n\sigma}$, we obtain the Hubbard (single band) Hamiltonian $^6$

$$H = -\sum_{\sigma(i,j)} t_\sigma \left(c_{\sigma i}^\dagger c_{\sigma j} + \text{h.c.}\right) + \hbar \sum_i \left(c_{\uparrow i}^\dagger c_{\uparrow i} - c_{\downarrow i}^\dagger c_{\downarrow i}\right)$$

$$+ \frac{\Omega_0}{2} \sum_i \left(c_{\uparrow i}^\dagger c_{\downarrow i} + \text{h.c.}\right) - U \sum_i c_{\uparrow i}^\dagger c_{\uparrow i} c_{\downarrow i} c_{\downarrow i}.$$

In the Hamiltonian (4), $h = -\delta/2$ plays the role of “magnetic field”, $t_\sigma$ is a spin dependent hopping term which follows from the spin dependent optical potential, and $U$ is an onsite interaction. The dependence of the hopping amplitude $t_\sigma$ and onsite interaction $U$ on the optical lattice parameters is given by $t_\sigma = E_R(2/\sqrt{\pi})(V_{\sigma}/E_R)^{3/4}\exp(-2(V_{\sigma}/E_R)\lambda/2)$ and $U = E_R ka_s e^{i}\pi(V_{\sigma}/E_R)^{3/4}$ with $E_R = \hbar^2 k^2/2m$ the recoil frequency of the atoms, and $k = 2\pi/\lambda$ the wave vector of the light. Thus the ratio of tunneling to onsite interaction can be controlled via the depth of the optical lattice.

B. Tuning spin-dependent tunneling

For alkali atoms, i.e. the atoms used in present cold fermi gas experiments, the difficulty in obtaining a spin dependent lattice arises from the s-wave character of the ground state. It implies that the AC Stark shift induced by far off-resonant driving fields is the same for all (hyperfine) ground state levels. Fortunately, however, heavy alkali atoms such as $^{40}K$, have a large fine structure splitting of the first excited state. This permits us to obtain a spin dependent optical potential by tuning the lattice lasers between the fine structure levels, still remaining far off resonance to suppress spontaneous emission. As illustrated in Fig. 2, the ground states $^2S_{1/2} M = \pm 1/2$ states couple to excited states
keeping only the dominant contributions from the lowest lying excited states. Here the detuning from the $^2P_{3/2}$ state is denoted $\Delta$, $\Delta_{fs}$ is the fine structure splitting, and the dipole matrix elements for the transitions from the ground state are $\mu_{3/2,1/2}$. We see that for detunings between the fine structure states $0 < \Delta < \Delta_{fs}$ the AC Stark shift $\Delta E_{2 S_{1/2}M_{-1/2}}$ switches from positive to negative values, while $\Delta E_{2 S_{1/2}M_{+1/2}}$ is always negative, giving rise to a strongly spin dependent lattice potential. We can vary the strength of the Stark shift by varying laser power.

Thus, the laser configuration consisting of unbalanced right and left circularly polarized polarization components gives rise to a spin dependent lattice, where the resulting AC Stark shifts are a sum of the shifts in the first and second line of Eq. (3), weighted according to their fraction of $\sigma^+$ and $\sigma^-$ component. For linearly polarized light the AC Stark shifts of the two states are equal.

\[
\begin{align*}
\Delta E_{2 S_{1/2}M_{+1/2}} &= \frac{\mu_{3/2,1/2}^2 \sigma^+}{\hbar \Delta} \\
\Delta E_{2 S_{1/2}M_{-1/2}} &= \frac{\mu_{3/2,1/2}^2 \sigma^-}{\hbar \Delta} + \frac{\mu_{3/2,1/2}^2 \sigma^+}{\hbar \Delta}.
\end{align*}
\]

This shows how to create a 1D spin dependent lattice in counterpropagating laser beams of unbalanced $\sigma^\pm$ polarization. The set-up is readily generalized to higher dimensions. For example, a 3D lattice is obtained by first applying a magnetic field to provide a Zeeman splitting of the hyperfine ground states (to suppress the cross AC Stark terms), and then applying three standing wave $\sigma^+$ polarized beams which are tilted by 45° relative to the magnetic field. Figs. 3 and 4 summarize the corresponding results for the $M_F = 9/2$ and $7/2$ hyperfine structure ground states (compare the level scheme in Fig. 2b). For these states the squares of the relevant Clebsch-Gordan coefficients (as defined above) are given by $|a|^2 = 1/9$ and $|b|^2 = 8/9$. Fig. 3 plots the AC Stark shift of the $M_F = 9/2$ (solid line) and $M_F = 7/2$ (dashed line) as a function of the laser detuning $\Delta$. The detuning interval covers the region of the $^3P_{1/2}$ and $^3P_{3/2}$ excited fine structure states, which are separated by $\Delta_{fs}$. We see that for a detuning $\Delta \approx 0.248 \Delta_{fs}$ the AC Starkshift of the $M_F = 7/2$ state has a zero while the shift of the $M_F = 7/2$ varies comparatively slowly. For detunings in the range $0.248 < \Delta/\Delta_{fs} < 1$ the AC Stark shift of both states $M_F = 9/2, 7/2$ is negative, i.e. the minima of the optical wells $V_{\sigma}(x)$ coincide but the wells have different depths giving rise to a spin-dependent tunneling. The AC Starkshifts in this region between the two fine

FIG. 3: AC Starkshift (in arbitrary units) of the $^{40}$K hyperfine $M_F = 9/2$ (solid line) and $M_F = 7/2$ (dashed line) states (compare Fig. 2b) as a function of the detuning $\Delta$. The value of $\Delta = 0$ corresponds to the $^3P_{1/2}$ excited fine structure state, while $\Delta = \Delta_{fs}$ is the $^3P_{3/2}$ resonance. We note the strong spin dependence (i.e. dependence on the internal state) for detuning between the two fine structure states.
structure states are plotted in Fig. 4, where again the $M_F = 9/2$ level is represented by the solid line, and the $M_F = 7/2$ level of $^{40}$K is given by the dashed line. In Fig. 4, we give the ratio of the corresponding hopping matrix elements as a function of $\Delta$ in the same interval. Here we have chosen a light intensity so that we keep the depth of the optical potential $V_{\uparrow\downarrow}(\ell=1,2,3)$ at a fixed given value $V_0$ for the whole range of detunings, while $V_{\downarrow\downarrow}(\ell=1,2,3)$ varies. Thus the ratio of $t_{\uparrow\downarrow}/t_{\downarrow\downarrow}$ varies. From Fig. 4 we see that the ratio of the tunneling elements can be varied by more than an order of magnitude when we approach the interference minimum at $\Delta \approx 0.248 \Delta_{fs}$.

Besides the alkali atoms discussed above, experimental progress might soon allow the realization of quantum degenerate fermion gases with alkaline earth atoms, e.g., with Sr atoms. Alkaline earth atoms have besides their singlet ground states longlived electronic excited triplet states. Applying an off-resonant laser field, these states will in general have quite different AC Stark shifts. Identifying the ground and metastable excited state with the spin-up and spin-down states, we thus can also have a natural realization of a Hubbard model with a spin-dependent interaction.

C. Remarks on spin superposition by Rabi coupling

The model we have been able (conceptually) to engineer contains a Rabi coupling that is not present in the conventional Hubbard model (8). A few remarks about this issue are in order.

$\Omega_0 = 0$ corresponds to the case that the particle number in each spin species is conserved separately. For $\Omega_0 \neq 0$ only total particle number conserved, while the relative particle number can vary. This point will be important for our discussion of exotic phases.

To treat the effect of the Rabi term theoretically, we should first diagonalize the quadratic part of the Hamiltonian. This is best done in momentum space. In principle, we can always find a unitary transformation of the original fermion fields,

$$\tilde{c}_\sigma(k) = \mathcal{U}_{\sigma\sigma'}(k) c_{\sigma'}(k),$$  \hspace{1cm} (5)

that transforms the Hamiltonian into

$$\hat{H} = \sum_{k\sigma} \tilde{c}^\dagger_{\sigma} k^z_{\sigma\sigma} \tilde{c}_{\sigma} k$$  \hspace{1cm} (6)

with $V_{\sigma_1...\sigma_4;k_1...k_4} = U \delta^4(k_1 + k_2 - k_3 - k_4) \mathcal{U}_{\sigma_1\dagger}(k_1) \mathcal{U}_{\sigma_2\dagger}(k_2) \mathcal{U}_{\sigma_3\dagger}(k_3) \mathcal{U}_{\sigma_4\dagger}(k_4)$ in $d$-spacial dimensions. The explicit form of the unitary transformation matrix $\mathcal{U}(k)$ for each mode $k$ can be found easily after some elementary algebra, but is not essential to our discussion here.

The important point is that the new, effective energy bands $\tilde{\epsilon}_k$ remain spin dependent. The free parameters $\hbar$, $\Omega_0$, and $t'$s allow great freedom of tuning the new band mass ratio and the Fermi surface difference of the effective up and down fermions. Instead of working with the Hamiltonian of the original fermions, we could just as well start with the Hamiltonian of the effective fermions. The new interaction term will contain not only terms $s$-wave spin-singlet terms, but also other higher angular and spin terms. As far as our main interest, $s$-wave spin-singlet pairing, is concerned, the theoretical treatment does not differ substantially from the model.
III. BP TO BCS TRANSITION

Recently there has been considerable discussion of the possible existence of homogeneous zero-temperature phases wherein a superfluid condensation coexists with one or more Fermi surfaces, where the gap vanishes. We have in mind that these are full-fledged codimension 1 Fermi surfaces (e.g., two-dimensional surfaces, which bound three-dimensional regions, in a three-dimensional system) where the gap vanishes. The roots of this idea go back to early work of Sarma; the issue has arisen again, under several different names, in several new contexts, including high-density QCD and (as emphasized here) cold atom systems. There are delicate issues of stability involved, which have been mishandled in much of the literature. We believe that a careful and correct discussion is supplied in Ref. [39]. We shall not repeat the analysis given there, but we rely on the conclusion: there are a number of physically interesting circumstances in which two-component interacting Fermi systems, of the general type discussed in the preceding section, can support a continuous “breached pairing” (BP) to BCS quantum phase transition (i.e., a “superfluid → normal → superfluid” transition at zero temperature).

Stability of the BP phase, which has coexisting, homogeneous superfluid and normal components at zero-temperature, appears to require momentum-dependent interactions, same-species repulsion, or some other complication not present in the simplest Hubbard Hamiltonian with two states defining a quasi-spin degree of freedom. For the sake of simplicity and concreteness, however, we shall work with this Hamiltonian. The qualitative, universal features of the phase transition ought not to depend on this idealization. Then,

\[
H = -\sum_{\sigma(i,j)} t_{ij} \left( c_{\sigma i}^\dagger c_{\sigma j} + h.c. \right) + h \sum_i \left( c_{\uparrow i}^\dagger c_{\uparrow i} - c_{\downarrow i}^\dagger c_{\downarrow i} \right) -U \sum_i c_{\uparrow i}^\dagger c_{\downarrow i}^\dagger c_{\downarrow i} c_{\uparrow i} \ .
\]

where as usual, \( c_{\sigma i} \) and \( c_{\sigma i}^\dagger \) are fermion annihilation and creation operators at site \( i \), with \( \sigma = \uparrow, \downarrow \) indicating two internal quantum states.

The Hamiltonian \( \mathbf{37} \) appears to be a simplified version of \( \mathbf{35} \), by assuming that the Rabi coupling term is transformed away through \( \mathbf{36} \). An important difference is that the spin up and down internal states are coherent now. The two quasi-spin states could well be two hyperfine spin levels for the case of cold atoms, as we discussed in detail above.

A. Nature of quantum phase transition between BCS and BP states

The general nature of the transition can be gleaned from Fig. 5. The BP to BCS transition is continuous, at least in mean field theory. To characterize its critical dynamics, we must use parameters that characterize its singular behavior — in particular, the appearance or disappearance of low-energy degrees of freedom. The magnitude of the superconducting order parameter is evidently not a suitable order parameter, since it evolves smoothly (at the level of mean field theory) and is non-vanishing at both sides of the transition. Furthermore, there is no evident change in symmetry at the transition. We propose that a good order parameter for the BP to BCS transition is the quasi-spin polarization (see Section \[ \mathbf{III.D} \]).

B. Quasiparticle excitations

We shall assume a uniform pairing, with order parameter, \( \Delta = U \langle c_{\uparrow i}^\dagger c_{\downarrow i} \rangle = \text{const} \). To find the spectrum of low energy quasiparticle excitations, we diagonalize the mean field Hamiltonian

\[
H_m = \sum_k \Psi_k^\dagger \left( \begin{array}{cc} 2t \Theta_k + h - \mu & \Delta \\ \Delta^* & -(2t \Theta_k - h) + \mu \end{array} \right) \Psi_k \ ,
\]

where

\[
\Psi_k \equiv \left( \begin{array}{c} c_{\uparrow -k}^\dagger \\ c_{\downarrow k}^\dagger \end{array} \right)
\]

FIG. 5: Quantum phase transition seen from change of quasiparticle spectra. The critical value \( h = h_c \) is determined by requiring that \( E_2 \) branch be of just one solution at zero energy. For \( h > h_c \), one should imagine a three dimensional momentum space in which two surfaces, defined by \( \Theta_k = \Theta^\uparrow \) and \( \Theta_k = \Theta^\downarrow \), are gapless for the \( E_2 \) branch. a) BCS superfluid; b) Quantum critical state; c) “superfluid+normal” BP state. For convenience, \( t_{\uparrow} \geq t_{\downarrow} \) is always assumed throughout the paper.
and

$$\Theta_k = - \sum_{l=1..d} \cos(k_la).$$

(Here $d = 3$ for three dimensional space.) There are two physical branches of (Bogoliubov) quasiparticle excitations that have distinct property in a BP state. They are

$$E_{1,2}(k) = (h + t_\pm \Theta_k) \pm \sqrt{(t_\pm \Theta_k - \mu)^2 + |\Delta|^2} \tag{9}$$

where we have adopted the short-hand notation $t_\pm \equiv t_\uparrow \mp t_\downarrow$. We will assume $t_\uparrow \geq t_\downarrow$ and $h > h_x \equiv -(t_-/t_+).$

By definition, $h_x$ is the value of the magnetic field for which the spin up and down bands have the same Fermi surface.

Fig. 4 shows how the two branches of excitations evolve with $h$. A quantum phase transition takes place at the critical value of $h = h_c$ with

$$h_c = -\frac{\mu_- + 2|\Delta|\sqrt{t_+}}{t_+}. \tag{10}$$

An important feature of the BP state is that the $E_2$ branch of excitations crosses the zero energy axis at two two-dimensional surfaces in three-dimensional momentum space, defined to be $\Theta_k = \Theta^-$ and $\Theta_k = \Theta^+$. Their values are

$$\Theta^\pm = \frac{(\mu_+ + ht_-) \pm \sqrt{(ht_+ + \mu_-)^2 - 4|\Delta|^2 t_+ t_-}}{4t_+ t_-}. \tag{11}$$

At the critical point $h = h_c$, the two gapless “Fermi” surfaces merge into a single one,

$$\Theta^- = \Theta^+ = \Theta_c \equiv \frac{\mu_+ + h_c t_-}{4t_+ t_-}. \tag{12}$$

Excitation spectra similar to Fig. 4(c) are also found in ferromagnetic metals. It was argued in \[44\] that superconductivity could coexist with ferromagnetism.

C. As a Lifshitz topological transition

Lifshitz (topological) transitions \[42\] can take place in metals and alloys at the motion of von Hove singularities of the electron density of states across Fermi surfaces (for review, see, e.g., Blanter et al. \[45\]). The transition from BCS to BP actually falls into this universality class.

To illustrate the topological nature of the transition, we start with the many-body wavefunctions for the BP and BCS states,

$$|\Psi_{BCS}\rangle = \prod_k (u_k + v_k c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger)|0\rangle, \tag{13}$$

$$|\Psi_{BP}\rangle = \prod_{k: \Theta_k < \Theta^-} (u_k + v_k c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger) \prod_{k: \Theta_k \in [\Theta^-, \Theta^+]} c_{k\downarrow}^\dagger \times \prod_{k: \Theta_k > \Theta^+} (u_k + v_k c_{k\uparrow}^\dagger c_{k\downarrow}^\dagger)|0\rangle. \tag{14}$$

Here, $u_k$ and $v_k$ are complex numbers satisfying $|u_k|^2 + |v_k|^2 = 1$; their amplitudes are determined by diagonalizing the mean field Hamiltonian \[46\].

$$\left\{ \frac{|u_k|^2}{|v_k|^2} \right\} = \frac{1}{2} \left( 1 \pm \frac{t_+ \Theta_k - \mu}{\sqrt{(t_+ \Theta_k - \mu)^2 + |\Delta|^2}} \right). \tag{15}$$

There is a manifold of degenerate states featuring an overall relative phase between the $u_k$ and $v_k$ factors, corresponding to the broken U(1)$_\text{charge}$. (Note that by our convention of $h > h_x$, there are more particles in the spin $\downarrow$ species than the $\uparrow$ species.

The occupation numbers of both spin up and down fermions are readily determined. For the BCS state,

$$n_{k\uparrow} = n_{k\downarrow} = |v_k|^2, \quad (\text{for all } k). \tag{16}$$

while for the BP state:

if $\Theta_k \in [\Theta^-, \Theta^+]$: $n_{k\uparrow} = 0$, $n_{k\downarrow} = 1$;

otherwise: $n_{k\uparrow} = n_{k\downarrow} = |v_k|^2. \tag{17}$

In the BCS state the occupation numbers are equal, while for the BP state they differ. Since the BCS state is maintained for a finite range of parameters, its continuous evolution to the BP state is non-analytic. This signals a (zero-temperature, quantum) phase transition.

The phase transition associated with a change in topology of the Fermi sea. This kind of transition is generally known as Lifshitz transition. As shown in Fig. 5, the quantum phase transition connects states of a simply connected Fermi sea and of isolated two regions.

FIG. 6: An illustration of changing topology of the spin up Fermi sea. Shown are cross-sections at $k_x = \pi/2a$ in a 3D first Brillouin zone for (a) BCS and (b) BP; momenta units for $k_x, k_y$ are $\pi/a$ where $a$ is the cubic lattice constant. As usual, the occupied states spread out over the entire Brillouin zone due to pairing interaction. The shading in the graph indicates that the region has a non-vanishing occupation number. The dotted lines indicate the original free Fermi surfaces of spin ups (inner curve) and spin downs (outer curve). The solid lines in (b) are energy surfaces defined by $\Theta_k = \Theta^-$ and $\Theta_k = \Theta^+$. For small $\Delta \to 0$, they merge with the free Fermi surfaces (dotted lines), respectively. The phase transition occurs at the point in which a simply connected Fermi sea is isolated into two regions.
A transition between superfluid phases of different topology in momentum space is also known to occur, for instance, $^3$He-B phase. There, the superfluid velocity with respect to a container drives a quantum phase transition from a fully gapped state to a state of (gapless) fermi surface [44, 45].

D. The order parameter

We now come to discuss the order parameter that characterizes the quantum phase transition. It is spin polarization, $M \equiv \langle S_z(\mathbf{x}) \rangle = n_\uparrow - n_\downarrow$. However, unlike a usual Landau-Ginzburg type theory, no obvious spontaneously broken symmetry is involved at the transition. The spin polarization density is given by

$$M = -\int_{\Theta^-}^{\Theta^+} d\Theta N(\Theta),$$

where

$$N(\Theta) \equiv \sum_k \delta(\Theta - \Theta_k)$$

plays the role of (dimensionless) density of states. Near the critical point $h = h_c$, both $\Theta^-$ and $\Theta^+$ approach $\Theta_c$. So the spin polarization may be approximated to the lowest order in $h - h_c$ by

$$M \simeq N(\Theta_c)(\Theta^- - \Theta^+) = -N(\Theta_c)\sqrt{(\mu t_- + h t_+)^2 - 4\Delta^2 t_+ t_-} = -N(\Theta_c)\frac{t_+}{2t_+ t_-}\sqrt{(h - h_c)(h + h_c - 2h_x)}.$$  

(19)

The spin polarization may be thought being derived from the grand thermodynamical potential $\Omega$ by viewing it as a functional of $h$:

$$M = \frac{\delta \Omega[h]}{\delta h}.$$  

This formula can be inverted. Define $h_M$ as the magnetic field for which the above equation has a prescribed value $M$. Then the quantum effective potential $\Gamma[M]$ is defined (as a functional of $M$, not $h$) by the Legendre transformation

$$\Gamma[M] = -h_M + \Omega[h],$$

with

$$h = h_M$$

fixed. The form of $\Gamma[M]$ is determined by requiring that the equation of state,

$$\frac{\partial \Gamma[M]}{\partial M} = -h_M,$$

(20)

produce what is equivalent to Eq. (19) upon inverting the latter. This leads to

$$\Gamma[M] = \frac{t_-}{t_+} \mu M + \frac{\Delta \sqrt{t_+ t_-}}{t_+} \left[ |M| \sqrt{1 + \left( \frac{M}{M_\Delta} \right)^2} + M \Delta \text{arcsinh} \left( \frac{|M|}{M_\Delta} \right) \right]$$

(21)

where $M_\Delta$ is a constant, $M_\Delta \equiv \Delta N(\Theta_c)/\sqrt{t_+ t_-}$. In deriving Eq. (21), we have treated $\Delta$ as a magnetic field-independent parameter to effectively represent the coupling strength. The effective potential is not analytic in $M$; the appearance of $|M|$ is a consequence of selecting the physically stable solution of it. The physical origin is due to the presence of two gapless “Fermi” surfaces. For small $M$ (and also $M < 0$ in our particular case of $t_+ > t_-$ and $h > h_x$), we could expand $\Gamma[M]$ in powers of $M$. Then, in the presence of external magnetic field $h$, the final effective potential reads

$$V(M) \equiv hM + \Gamma[M]$$

$$= (h - h_c)M + \frac{\Delta \sqrt{t_+ t_-}}{3t_+ M_\Delta^2} |M|^3 + \cdots$$

(22)

For $h > h_c$, $V(M)$ always has a minimum at a nonzero $M$. From either Eq. (19) or (22), one can immediately verify the following power-law (scaling) relation for the spin polarization at mean field level (for $h$ near $h_c$)

$$M = \begin{cases} -\frac{N(\Theta_c)(t_+ \Delta)^{2/3}}{(t_+ t_-)^{1/3}} (h - h_c)^{1/2}, & \text{if } h > h_c, \\ 0, & \text{otherwise}. \end{cases}$$

(23)

The results are sketched in Fig. 7. The behavior of spin polarization near the point $h = h_c$ suggests that the quantum phase transition is of second order.

![Fig. 7: Quantum phase transition shown by spin polarization M. For the BCS (BP) state, $M = 0$ ($M \neq 0$).](image-url)
### E. Scaling theory of $z = 2$ gapless fermions

At the critical point, the $E_2(k)$ branch of quasiparticle excitations is gapless at a single ‘Fermi surface’ defined by $\Theta(k) = \Theta_c$. What makes the critical point special is that the spectrum disperses quadratically near the surface:

$$-E_2(k) = \frac{l^2}{2m_s^2}, \quad k \equiv K + l$$

(24)

where $K$ is a vector on the critical Fermi surface and $l$ a vector of (small) fluctuating momentum orthogonal to the Fermi surface. $m_s^2$ is effective band mass that is implicitly determined from Eq. (14). The dispersion relation implies that the dynamical exponent is $z = 2$ (at least at tree-graph level) in contrast with $z = 1$ in a nominal (metallic) Fermi liquid [46].

The critical properties of the $E_2(k)$ fermions appear to define a new universality class. To begin understanding it, let us consider the relevant operators. Consider a theory of gapless fermions described by an effective free action plus possible quartic interactions,

$$I_\psi = \int dt d^{d-1}K d\mathbf{l} \psi^\dagger(k) \left( i\partial_t - \frac{l^2}{2m_s^2} \right) \psi(k) + g \int dt \prod_{j=1,4} [d^{d-1}K_j d\mathbf{l}_j] \psi^\dagger(k_1) \psi^\dagger(k_2) \psi(k_3) \psi(k_4) \delta^d(k_1 + k_2 - k_3 - k_4)$$

$$+ \psi\psi^\dagger\psi + \psi^\dagger\psi\psi\psi \ldots$$

(25)

where $\psi$ is the gapless fermion field.

One can perform a simple renormalization group analysis to find out how the interactions should scale. When we scale down the fluctuating momentum $l$ by a factor $s < 1$, $l \rightarrow sl$, the quasiparticle energy scales down with a dynamical exponent $z = 2$ as

$$\omega \rightarrow s^2 \omega$$

for a quadratic dispersion relationship. So, in general, the momentum and time in the above action should scale as follows:

$$dt \rightarrow s^{-2} dt, \quad d^{d-1}K \rightarrow s^0 d^{d-1}K, \quad d\mathbf{l} \rightarrow s^1 d\mathbf{l}, \quad \partial_t \rightarrow s^2 \partial_t, \quad 1 \rightarrow sl, \quad \text{with} \quad s \rightarrow 0.$$

Note that the momentum $K$, being attached onto the critical Fermi surface, does not scale. Accordingly, the fermion field scales as

$$\psi \rightarrow s^{1/2} \psi.$$

The scaling dimension of potential interaction operators can now be derived by straightforward power counting. We find that a generic four-fermion scattering operator is marginal. That is,

$$g \rightarrow \left\{ \begin{array}{ll}
    & s^0 g, \quad \text{(generic scatterings)} \\
    \frac{s^0}{s^2} g, \quad \text{(BCS or forward scatterings)}
\end{array} \right.$$

This result contrasts dramatically with what is found in the standard renormalization group theory of a conventional Fermi liquid (see, for instance, the review by Shankar [46]). In that context, only special momentum configurations are marginal.

We next turn to the scaling property of the order parameter correlation function. We now attempt to derive the critical theory of quantum fluctuations of the order parameter field $M$. While the static part of it is already derived in Eq. (22), its dynamical part can be obtained by calculating the spin-spin correlation, which is just the fermion polarization bubble diagram, i.e., $\langle S_z(k, i\omega)S_z(-k, -i\omega) \rangle = \Pi(k, i\omega)$ (in imaginary time formalism), where $S_z(k, i\omega)$ is defined as the Fourier transform of

$$S_{zi} = \frac{1}{2} \left( c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow} \right)$$

at site $i$ and time $t$. The quadratic part of the action for $M$ is given by $\Pi(k, i\omega)$. Near the critical point, we find the quantum effective action of $M$ takes the form,

$$S[M] = \int d^d x d^t \left[ \frac{c_t}{2} (\partial_t M)^2 + \frac{c_s}{2} (\nabla M)^2 + \frac{r}{2} M^2 + \frac{g}{3!} M^3 + \cdots \right]$$

(26)

where

$$r = \frac{2(t^*_\uparrow t^*_\downarrow)^{3/2}}{N(\Theta_c)(t^*_+ \Delta)^{3/2}} \left( h - h_c \right)^{1/2}, \quad g = \frac{2(t^*_\uparrow t^*_\downarrow)^{3/2}}{N^2(\Theta_c)t^*_+ \Delta},$$

(27)

and

$$c_t = \frac{\partial \Pi(k, i\omega)}{\partial (\omega^2)}, \quad c_s = \frac{\partial \Pi(k, i\omega)}{\partial (k^2)}.$$
with \( k, \omega \to 0 \) (long wavelength limit). In deriving the effective action, we have shifted the position of the minima of \( V(M) \) to eliminate the linear term of Eq. 22.

One recognizes that the effective theory of spin polarization field \( M \) bears superficial resemblance to Fisher’s \cite{17} \( \phi^4 \) famous field theory of the Yang-Lee edge singularity in a ferromagnetic Ising model. However, the two theories differ fundamentally in that the cubic interaction term here, \( |M|^3 \), is both non-analytic and real (as opposed to analytic and purely imaginary).

Further investigation of the new critical theory, including interactions between the low-energy fermion modes and the order parameter, is reserved for future work.

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