Anomalous isothermal compressibility in spin-orbit coupled degenerate Fermi gases

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The spin-orbit coupling (SOC) in degenerate Fermi gases can fundamentally change the fate of s-wave superfluids with strong Zeeman field and give rise to topological superfluids and associated Majorana zero modes. It also dramatically changes the thermodynamic properties of the superfluids. Here we report the anomalous isothermal compressibility \( \kappa_T \) in this superfluids with both SOC and Zeeman field. We formulate this quantity from the Gibbs-Duhem equation and show that the contribution of \( \kappa_T \) comes from the explicit contribution of chemical potential and implicit contribution of order parameter. In the Bardeen-Cooper-Schrieffer (BCS) limit, this compressibility is determined by the density of state near the Fermi surface; while in the Bose Einstein condensate (BEC) regime it is determined by the scattering length. Between these two limits, we find that the anomalous peaks can only be found in the gapless Weyl phase regime. This anomalous behavior can be regarded as a remanent effect of phase separation. The similar physics can also be found in the lattice model away from half filling. These predictions can be measured from the anomalous response of sound velocity and fluctuation of carrier density.

The spin-orbit coupling (SOC) can modify the single-particle band structure [1], thus fundamentally change the behavior of ultracold atoms in the degenerate regime. In bosonic gases, the ground state can carry a finite momentum [2–4], giving rise to either plane wave phase or striped phase, depending on the interactions [5–10]. The transition between these two phases can be described by Dicke model [11–13]. Recently, this platform is used to search the supersolid phases [14–16]. It can also be used to study the universal scaling of defects described by Kibble-Zurek mechanism during quench dynamics [17, 18]. The physics in Fermi gases are totally different due to the exclusive principle. The direct coupling between spin and momentum can make the spin polarization to be momentum dependent, thus when an energy gap is opened by a Zeeman field, pairing is still allowed in the same band with s-wave interaction [19–27]. In case of inversion symmetry breaking, this system can support finite-momentum pairing phases[28–34]. This mechanism was used in experiments for searching of topological phases and Majorana zero modes [35–42]. While the topological phases are widely explored in literatures, their thermodynamic properties are seldom discussed.

In this work, we mainly focus on the effect of SOC and Zeeman field on isothermal compressibility, \( \kappa_T \), which measures fluidity via [43, 44]

\[
\kappa_T = -\frac{1}{\gamma} \left( \frac{\partial V}{\partial P} \right)_{T,N}.
\]

Here the thermodynamic variables \( P, V, T \) and \( N \) correspond to pressure, volume, temperature and total number of particles, respectively. The minus sign in Eq. 1 is used to ensure \( \kappa_T > 0 \) for the stable phases. For an ideal gas, \( \kappa_T = 1/P \); while in solid material, \( \kappa_T = 1/B \), where \( B \) is the corresponding bulk modulus [45]. For ideal gas, this quantity is related to sound velocity via Newton-Laplace formula \( c = \sqrt{\gamma V/N\kappa_T} \), where \( \gamma \) is the isentropic expansion factor [46]. According to this definition, the more fluidity the system is, the larger...
this value will be. For this reason, this value was used in literatures to identify the boundaries between superfluid phases and insulating phases \[ \rho \] as well as the boundary between normal phase and Bose-Einstein condensates (BEC). In BEC, \( \kappa_T \) will divergent since the condensate does not contribute to pressure \[ \rho \text{C} \]. In experiments this quantity has also been explored with both fermions \[ \rho \text{F} \] and bosons \[ \rho \text{B} \].

We investigate the isothermal compressibility in the spin-orbit coupled degenerate Fermi gases. We formulate this quantity based on Gibbs-Duhem equation \[ \rho \text{D} \], and find that due to the implicit dependence of pairing strength on chemical potential and carrier density, this quantity can be divided into two parts: the explicit term related to chemical potential, and the implicit term related to order parameter. In the Bardeen-Cooper-Schrieffer (BCS) limit, this value is determined by the density of state at the Fermi surface, while in the BEC limit it is determined by the scattering length. In the intermediate regime with both spin-orbit coupling and Zeeman field, we find a pronounced enhancement of compressibility in the gapless Weyl superfluid phase regime contributed from the implicit part. This kind of peak can be regarded as the remanent effect of phase separation (PS). The similar features can also be found in an optical lattice away from half filling.

Theory. We work in the grand canonical ensemble and the Gibbs thermodynamic potential \( \rho \text{G} \) and the Gibbs-Duhem equation \[ \rho \text{D} \], \[ \rho \text{F} \] for a two-component system with \( \sigma = \uparrow, \downarrow \). In equilibrium, we have the following Gibbs-Duhem equation \[ \rho \text{D} \],

\[
- S dT + V dP = \sum_{\sigma} N_\sigma d\mu_\sigma, \tag{2}
\]

in which the chemical potential \( \mu_\uparrow = \mu + h_\uparrow \) and \( \mu_\downarrow = \mu - h_\downarrow \), with \( h_\sigma \) being the effective Zeeman field (see below), \( S \) is the entropy of the whole system and \( N = N_\uparrow + N_\downarrow \) is the total number of particle. In the case of fixed temperature, Eq. 2 establishes a direct connection between pressure and carrier density, \( P = P(T, n_\sigma, n_\downarrow) \), with \( n_\sigma = N_\sigma / V \), since pressure is an intensive quantity. Then from the differential chain-rule, we obtain

\[
\frac{1}{\kappa_T} = - V \left( \frac{\partial P}{\partial n_\uparrow} \right)_{T,n_\downarrow} \left( \frac{\partial n_\uparrow}{\partial V} \right)_{T,n_\down\uparrow}, \tag{3}
\]

From the Maxwell relation, \( \frac{\partial P}{\partial N_\sigma} = \frac{\partial \mu_\sigma}{\partial V} \), we have

\[
\frac{1}{\kappa_T} = - \sum_\sigma N_\sigma \left( \frac{\partial \mu_\sigma}{\partial V} \right)_T. \tag{4}
\]

One should notice that the chemical potential is also an intensive quantity, that is, \( \mu_\sigma = \mu(n_\sigma, T) \). Let us define compressibility matrix as \( \kappa_{ij}^{-1} = n_i n_j \frac{\partial \mu_\sigma}{\partial n_\sigma} \), then the isothermal compressibility can be written as,

\[
\frac{1}{\kappa_T} = \sum_{i,j=\uparrow,\downarrow} \frac{1}{\kappa_{ij}}. \tag{5}
\]

This relation can be generalized to arbitrary number of components. In the limiting case when \( n_i \) is independent of \( \mu_j \) for \( i \neq j \), one finds \( \kappa_{ij}^{-1} = 0 \). Otherwise, \( \kappa_{ij}^{-1} \neq 0 \), thus the right hand side is always well-defined. Moreover, in the limiting case when \( \mu_\sigma = \mu \), the above compressibility is reduced to \( \kappa_T = \frac{1}{V} \left( \frac{\partial P}{\partial N} \right)_T \), which was widely used in literatures \[ \rho \text{G} \]. Finally, let us stress that even at zero temperature, this quantity is nonzero.

In following we employ the above theory to understand the fluidity of the spin-orbit coupled superfluids.
are two major results we have obtained as $H_0 = \sum_{k,\sigma} c_{k\sigma}^\dagger c_{k\sigma} + \alpha(k_y \sigma_x - k_z \sigma_y) + h_z \sigma_z \epsilon_{k\sigma} c_{k\sigma}$, where $\xi_k = \epsilon_k - \mu = k^2 - \mu$, $k = (k_x, k_y, k_z)$, $\alpha$ is the SOC coefficient, and $h_z$ is the corresponding Zeeman field between the two components and $\sigma_{x,y,z}$ are Pauli matrices. In the presence of $s$-wave interaction between the two species, one can define a uniform pairing order $\Delta = \frac{1}{g} \sum_k (c_{k\uparrow} c_{-k\downarrow})$, where $g$ is the scattering strength. Let us define the thermodynamic potential $\Omega$ through the partition function $Z = e^{-\beta \Omega} = Tr(e^{-\beta H})$, with $\beta = 1/k_BT$, then

$$\Omega = \sum_k \xi_k - \frac{1}{\beta} \sum_{k,\lambda} \ln \left[ 2 \cosh \left( \frac{\beta E_k}{2} \right) \right] - \frac{V|\Delta|^2}{g}$$

(6)

where $E_k^\lambda = \sqrt{\gamma_k^2 + \xi_k^2 + h_z^2 + |\Delta|^2 + 2\alpha E_0}$ is the excitation spectrum, $E_0 = \sqrt{h_z^2\xi_k^2 + |\Delta|^2 + \gamma_k^2\xi_k^2 \xi_k^2}$, $|\Delta|^2 = \lambda^2(k_x^2 + k_y^2)$ and $\lambda = \pm 1$. The corresponding carrier density and order parameter are determined by $n_a = -\frac{\partial \Omega}{\partial \Delta}$, $k_{\Delta} = 0$. During regularization, in Eq. 6, we have used $\frac{1}{g} = \frac{m}{\pi n_a} - \frac{1}{\beta} \sum_k \frac{1}{k^2 + m}$, with $a$ being the scattering length. For more details, please see Ref. [19].

The important point is that, though $\Delta$ is an important quantity to characterize the interaction between the particles. It is not a thermodynamic variable. Thus to compute $\kappa_T$ in Eq. 5, we may explicitly (e) take derivative of carrier density with respect to chemical potential, or implicitly (i) take derivative of carrier density with respect to order parameter $\Delta$, as following,

$$\left(\frac{\partial n_x}{\partial \mu}\right)_{T,i} = \left(\frac{\partial n_x}{\partial \mu}\right)_{T,i} + \left(\frac{\partial n_x}{\partial \mu}\right)_{T,c}$$

(7)

where $(\frac{\partial n_x}{\partial \mu})_{T,i} = -((\frac{\partial \Omega}{\partial \mu})_{T,D})$ and $(\frac{\partial n_x}{\partial \mu})_{T,c} = \frac{1}{\beta} \frac{2n^2}{D^2 |\Delta|^2}$. In the second term,

$$\left(\frac{\partial n_x}{\partial \mu}\right)_{T,i} = \left(\frac{\partial n_x}{\partial \Delta}\right)_{T,c}$$

(8)

Let’s define $f = \frac{\partial \Omega}{\partial \mu} = 0$, then using df = $\frac{\partial f}{\partial \mu} d\mu + \frac{\partial f}{\partial \Delta} d\Delta = 0$ we find $\left(\frac{\partial n_x}{\partial \mu}\right)_{T,i} = -\frac{(\frac{\partial \Omega}{\partial \mu})_{T,c} \partial \mu}{\partial \Delta}$. Thus

$$\left(\frac{\partial n_x}{\partial \mu}\right)_{T,i} = \left(\frac{\partial \Omega}{\partial \mu}\right)_{T,c}$$

(9)

where their expressions are presented below:

$$\kappa_{T,e} = \frac{1}{2n^2} \sum_{k,\lambda} \left( X_k^\lambda - Y_k^\lambda \right) \left( \frac{\xi_k^2}{E_k} \right)^2 + X_k^\lambda \left( Q_k^\lambda - \lambda \frac{F_k^\lambda}{E_k} \right)^2$$

(10)

and

$$\kappa_{T,i} = \frac{1}{2n^2} \sum_{k,\lambda} \left( X_k^\lambda - Y_k^\lambda \right) \left( \frac{F_k^\lambda}{E_k} \right)^2 - \lambda X_k^\lambda \frac{h_k^4}{E_k}$$

(11)

Here $X_k^\lambda = \tan \theta \left( \frac{\beta E_k^\lambda}{E_k^\lambda} \right) / E_k^\lambda$, $Y_k^\lambda = \beta(1 - \tan \theta \left( \frac{\beta E_k^\lambda}{E_k^\lambda} \right)) / 2$

with $E_k^\lambda$ being the corresponding Zee-ken field, at the isothermal compressibility peaks in Fig. 2. We have setted $k_x = 0$ and $k_y = 0$, which is the case for gapless Weyl points.

![FIG. 4. (Color online) Band structure of $E_k$](image)

(FIG. 4. Color online) Band structure of $E_k$ as the isothermal compressibility peaks in Fig. 2. We have setted $k_x = 0$ and $k_y = 0$, which is the case for gapless Weyl points.

Eq. 10 and 11 are two major results we have obtained in this work. Before presenting our numerical results, let us discuss the implementations of these results in some limiting cases. (i) Without interaction, $\Delta = 0$, the implicit term $\kappa_{T,i} = 0$, and the total carry density $n = \frac{1}{\beta} \sum_k n_{\lambda k}$, thus $\kappa_T = \frac{1}{\beta} \sum_{\lambda} \sum_k \left[ 1 - \tan \theta^2 \left( \frac{\beta E_k^\lambda}{E_k^\lambda} \right) \right]$. Obviously, at zero temperature, $\kappa_T = \frac{1}{2n^2} \rho(\mu) \propto \rho(\mu)$, where $\rho$ denotes for density of state at the Fermi surface. Thus in insulating phase with $\rho(\mu) = 0$, $\kappa_T = 0$. (ii) Without SOC and Zeeman field, we have $E_0 = 0$ and $E_k^\lambda = E_k$, then $\kappa_{T,i} = \frac{1}{2n^2} \sum_{\lambda} \sum_k \left( \frac{\xi_k^\lambda}{E_k^\lambda} \right)^2 \frac{1}{\beta} \sum_{\lambda} \sum_k \left( \frac{\xi_k^\lambda}{E_k^\lambda} \right)^2$. Both the implicit part and explicit part are positive value. This case can also be computed exactly using $\frac{1}{\beta} \sum_k \frac{1}{E_k} = \frac{2}{(\beta^2 + D^2 + 2\beta x)^2 (4\beta^2 \Delta^2 + 4\beta \Delta x)^{-1} + 1}$, where $E(x)$ and $K(x)$, with $x = \frac{1}{2} (1 + \frac{\beta}{\beta^2 + D^2 + 2\beta x})$, are the second kind incomplete and the first kind complete elliptic integrals, respectively. With these expressions, we find that the compressibility $\kappa_{T,e} \gg \kappa_{T,i}$ and $\kappa_{T,i} \sim 0$ in the BCS limit, while in the BEC limit, $\kappa_{T,e} \sim 0$, while $\kappa_{T,i} \propto \sqrt{\mu}$. Notice that in the BEC limit, $\mu \propto \frac{1}{\frac{1}{\beta} \sum_{\lambda} \sum_k \left( \frac{\xi_k^\lambda}{E_k^\lambda} \right)^2}$, we find $\kappa_{T,i} \propto \frac{1}{\beta} \sum_{\lambda} \sum_k \left( \frac{\xi_k^\lambda}{E_k^\lambda} \right)^2$ (see numerical results in Fig. 1). This result also explains the linear behavior of compressibilities in the BEC limit with both SOC and Zeeman field in Fig. 2. (iii) The case with only SOC was investigated in Ref. [60], and our expression can be reduced to the results in Ref. [60] by letting $h_z = 0$. The interesting point is that in the presence of both SOC and Zeeman field, the excitation spectra may become gapless in the Weyl superfluids regime. The expression for $\kappa_{T,i}$ is no longer always larger than zero, giving rise to PS phase. We have utilized this feature.

Numerical results. We determine the value of $\mu$ and $\Delta$ self-consistently at zero temperature [61, 62]. The Fermi momentum $k_F = \sqrt{3n^2}$ and Fermi energy $E_F = \frac{k_F^2}{2m}$ serve as basic scales for momentum and energy, respectively. We first discuss the role of SOC and
Zeeman field individually in Fig. 1. In strong Zeeman field and in the BCS limit, the pairing is completely destroyed when \(|h_z| > |\Delta|\), thus we have a normal gas (NG) phase. In both cases we find that \(\kappa_T\) in the BEC limit is much larger than that in the BCS side. Moreover, since the Zeeman field plays the role of reducing the density of state at the Fermi surface, while SOC plays the opposite role, we find the same trend for the isothermal compressibility. We also find that in the BCS limit, \(\kappa_{T,e} \gg \kappa_{T,i} \sim 0\), while in the BEC side, \(\kappa_{T,i} \gg \kappa_{T,e} \sim 0\), as expected from our theoretical analysis.

The physics is completely changed in the presence of both terms; see Fig. 2. We find a pronouncedly enhancement of isothermal compressibility, by one order of magnitude, in some proper parameter regimes. This enhancement compressibility is more likely to be found in regime with relative larger Zeeman field and weaker SOC. Especially, we find that the peak position depends more strongly on the Zeeman field. In Fig. 2b and d, we find that this peak arises from the implicit part, while the explicit part always shows a smooth behavior. To further pin down the reason for this anomalous peak, we plot the numerator and denominator of \(\kappa_{T,i}\) in Fig. 3. The numerator is always a smooth function of scattering length. However, the denominator exhibits some peculiar behavior with increasing of scattering length from BCS side to the BEC side. The dip in the denominator accounts for the anomalous behavior of compressibility. We find that in the fully gapped regime, the denominator is always very large; it can take a minimal value only in the gapless regimes, which can be realized either with \(\Delta \sim 0\) (BCS limit) or Weyl superfluid phase regime. We illustrate this physics in Fig. 4 by plotting the band structure of the corresponding peaks in Fig. 2, which are always gapless in the Weyl superfluids. With the increasing of scattering length in the BEC side, these Weyl points are destroyed, and the superfluid enter the fully gapped phase, in which the compressibility becomes extremely large due to condensation, and we have \(\kappa_T \propto 1/T^3\).

We plot the compressibility and phase diagram as a function of Zeeman field and SOC in Fig. 5. There is a small regime for PS, which is determined by \(\kappa_T < 0\). In this case the Helmholtz free energy \(F = \Omega + \sum_\sigma \mu_\sigma N_\sigma\) shows two local minimals in space by \(\mu\) and \(\Delta\). The SOC can effectively suppress this PS effect. Near this regime, by tuning of Zeeman field, we can find a dramatic enhancement of isothermal compressibility in Fig. 5a near the boundary between the fully gapped superfluid and the Weyl superfluids with two Weyl points (W2 SF). Th peak position in the anomalous regime depends strongly on the Zeeman field. Thus we may regard this anomalous behavior as the remnant effect of PS, which happens near the boundary between gapped phase and gapless Weyl phase.

Finally we have also examined the same quantity in the lattice model, in which similar anomalous behavior have also been identified. In the optical lattice, the filling factor and particle-hole symmetry about half filling become two important controlling parameters in experiments. We find that near half filling, the implicit compressibility is greatly suppressed, while away from this regime, this kind of anomalous compressibility can always be found. These results will be discussed elsewhere.

To conclude, we present a general theory to study the isothermal compressibility in the superfluids with both SOC and Zeeman field from the Gibbs-Duhem equation. These two terms can modify the band structure and possible pairings, thus dramatically influences its isothermal compressibility. We find that in the BCS limit the compressibility is determined by the density of state at the Fermi surface, while in the BEC limit, it is determined by the scattering length. Between these two regimes, we predicted a pronouncedly enhancement of isothermal compressibility in the gapless Weyl phases. The peak mainly comes from the implicit contribution of isothermal compressibility in the gapless Weyl phases. This kind of behavior can be found in both free space and optical lattice models. The foundation in this work pave the way for exploring other thermodynamic properties in spin-orbit coupled ultracold atoms.

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