Effective theory for ultracold strongly interacting fermionic atoms in two dimensions

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We propose a minimal theoretical model for the description of a two-dimensional (2D) strongly interacting Fermi gas confined transversely in a tight harmonic potential, and present accurate predictions for its equation of state and breathing mode frequency. We show that the minimal model Hamiltonian needs at least two independent interaction parameters, the 2D scattering length and effective range of interactions, in order to quantitatively explain recent experimental measurements at nonzero filling factor \( \frac{N}{N_{2D}} \), where \( N \) is the total number of atoms and \( N_{2D} \) is the threshold number to reach the 2D limit. We therefore resolve in a satisfactory way the puzzling experimental observations of reduced equations of state and reduced quantum anomaly in breathing mode frequency, due to small yet non-negligible \( \frac{N}{N_{2D}} \). We argue that a conclusive demonstration of the much-anticipated quantum anomaly is possible at a filling factor of a few percent. Our establishment of the minimal model for 2D ultracold atoms could be crucial to understanding the fermionic Berezinskii-Kosterlitz-Thouless transition in the strongly correlated regime.

Two-dimensional (2D) quantum many-body systems are of great interest, due to the interplay of reduced dimensionality and strong correlation, which leads to enhanced quantum and thermal fluctuations \( \text{[1]} \) and a number of ensuing quantum phenomena such as Berezinskii–Kosterlitz–Thouless (BKT) physics \( \text{[2, 3]} \). In this respect, the recently realized 2D Fermi gas of ultracold \(^6\text{Li} \) and \(^{40}\text{K} \) atoms under a tight axial confinement provides a unique platform \( \text{[4, 5]} \), with unprecedented controllability particularly on interatomic interactions. To date, many interesting properties of ultracold 2D Fermi gases have been thoroughly experimentally explored \( \text{[6]} \), including the equation of state (EoS) at both zero temperature \( \text{[7, 8]} \) and finite temperature \( \text{[9, 10]} \), radio-frequency spectroscopy \( \text{[11]–[13]} \), pair momentum distribution \( \text{[13]} \), first-order correlation function and BKT transition \( \text{[14]} \), and quantum anomaly in breathing mode frequency \( \text{[15]–[17]} \). These results may shed light on understanding other important strongly correlated 2D systems, such as high-\( T_c \) layered cuprate materials \( \text{[18]} \), \(^3\text{He} \) submonolayers \( \text{[19]} \), exciton-polariton condensates \( \text{[20]} \) and neutron stars \( \text{[21]} \).

The present theoretical model of ultracold 2D Fermi gases is simple \( \text{[4, 5]} \). Under a tight harmonic confinement with trapping frequency \( \omega_z \) along the axial \( z \)-axis and a weak confinement \( \omega_\perp \) in the transverse direction, the kinematic 2D regime is reached when the number of atoms \( N \) is smaller than a threshold \( N_{2D} \approx (\omega_z/\omega_\perp)^2 \), so all the atoms are forced into the ground state of the motion along \( z \). The interatomic interactions are then described by a single \( s \)-wave scattering length \( a_{2D} \), which is related to a 3D scattering length \( a_{3D} \) via the quasi-2D scattering amplitude \( \text{[22]} \). Various experimental data have been compared and benchmarked with different theoretical predictions of the simple 2D model \( \text{[22–32]} \). For EoS, i.e., the chemical potential and pressure at essentially zero temperature, good agreements were found \( \text{[4, 5]} \). But, at the quantitative level the experimental data in the strong interacting regime somehow lie systematically below the accurate predictions from auxiliary-field quantum Monte Carlo (AFQMC) simulations \( \text{[6, 8]} \). The discrepancy is not so serious and might be viewed as an indicator of small deviation from the 2D kinematics \( \text{[3]} \), in spite of the fact that the 2D condition \( N \ll N_{2D} \) is well satisfied. However, a serious problem does arise when two experimental groups measured the breathing mode frequency in the deep 2D regime most recently \( \text{[16, 17]} \). The observed frequency turned out to be much smaller than the well-established theoretical prediction in the strongly interacting regime \( \text{[23, 26]} \). This discrepancy is at the qualitative level, suggesting that the simple 2D model with a single parameter \( a_{2D} \) may not be sufficient for the description of ultracold 2D Fermi gases \( \text{[33]} \).

The purpose of this Letter is to provide a minimal theory of ultracold 2D Fermi gases, with the inclusion of a properly defined effective range of interactions (see Fig. 1). The proposed model Hamiltonian is then solved at zero temperature by taking into account strong pair fluctuations at Gaussian level and beyond (Fig. 2), with the help of a correlation energy from AFQMC in the zero-range limit \( \text{[30]} \). This enables us to predict accurate EoS (Fig. 3 and Fig. 4), as well as reliable breathing mode frequency (Fig. 5). The puzzling quantitative and qualitative discrepancies, observed in the previous comparisons between experiment and theory \( \text{[3, 6, 8, 16, 17]} \), are therefore naturally resolved in a satisfactory way. Our results emphasize the important role played by the effective range of interactions in 2D strongly interacting Fermi systems, which may also be found in cuprate superconductors \( \text{[18]} \) and neutron stars \( \text{[21]} \).

**Effective range of interactions.** We start by considering the collision of two fermions with mass \( M \) and unlike spin in a highly anisotropic harmonic trapping potential,
In general, one thus obtains a momentum-dependent length to parameterize the quasi-2D collision using a 2D scattering amplitude \( A \approx 0 \), where \( R = 2 \ln(\sigma a_2) \). The 2D scattering amplitude \( \sigma \) is evaluated at a characteristic collision momentum \( q \), which in the zero-energy limit takes the form \( q \equiv \sqrt{2/M\mu} \). In the simplest treatment, one may parameterize the quasi-2D collision using a 2D scattering length \( a_{2D} \), by setting the 2D scattering amplitude \( f_{2D}(k; a_{2D}) = -2\pi/\ln[k a_{2D}(k)/1] = f_{2D}(k; a_{2D}, a_z) \). In general, one thus obtains a momentum-dependent \( a_{2D}(k) \), which in the zero-energy limit takes the form \( a_{2D}(k \to 0) = a_z \equiv a_z/\sqrt{\pi} \exp[-(2\pi/2 a_z/a_{2D})] \). The advantage of this simple treatment is that the description universally depends on a single parameter \( a_{2D} \), to be evaluated at a characteristic collision momentum \( k_0 \), i.e., \( k_0 = \sqrt{2M\mu}/\hbar \), where \( \mu \) is the chemical potential that does not include the two-body binding energy \( B \).

A more adequate parametrization of the 2D collision is to include an effective range of interactions \( R_e \) in the 2D scattering amplitude \( f_{2D}(k; a_{2D}, R_e) \).

\[
f_{2D}(k; a_z, R_e) = \frac{4\pi}{-2\ln(k a_z) - R e k^2 + i\pi},
\]

where \( a_z \equiv \sqrt{\hbar/(M\omega_z)} \) is the harmonic oscillator length along the \( z \)-axis and the function \( \varpi(x) \) has the expansion \( \varpi(x \to 0) \sim -\ln(2\pi x/B) + (2\ln 2)x + i\pi \) with \( B \approx 0.905 \). In the simplest treatment, one may consider the effective range \( R_e \), which is well defined at \( R_e \to 0 \) \( \sigma \) or \( R_e \) for two colliding atoms at distance within \( a_z \) of each other. The effective range obtained in this way is reported in Fig. 1. It decreases monotonically from \( R_{e=0} \equiv -2\ln(2 a_z^2) \) with increasing \( a_z/a_{2D} \) (main figure) or binding energy \( B \) (inset). We note that \( R_{e=0} \) can be easily derived from the second expansion term in \( \varpi(x \to 0) \) and its magnitude, i.e., \( R_{e=0} \sim a_z^2 \), is a clear indication of the quasi-2D nature of atom collisions \( B \). As the wavelength of two colliding atoms at distance within \( a_z \) is set by the full 3D contact interaction potential, these collisions can never be purely 2D. They can only be approximately treated as 2D, out of the range \( a_z \).

When should we care about the effective range \( R_e \)? The answer depends on the characteristic collision momentum \( k_0 \) or the dimensionless effective range \( k_0^2 R_e \). By taking the chemical potential of a non-interacting trapped Fermi gas, i.e., \( \mu \equiv N\hbar\omega_1/2 \), we find \( k_0^2 R_e \equiv -(2\ln 2)\sqrt{N/N_{2D}} \), which could be very significant, even though the 2D condition \( N \ll N_{2D} \) is well satisfied.

**Many-body theory.** To account for the effective range \( R_e \), it is convenient to adopt a two-channel model Hamiltonian (the area \( S = 1 \)).

\[
H = \sum_{k \sigma = \uparrow, \downarrow} \xi_k c_{k \sigma}^\dagger c_{k \sigma} + \sum_q (2\xi q/2 + \nu) b_q^\dagger b_q + \sum_{k q} \left( b_q c_{q/2 + k \downarrow}^\dagger c_{q/2 - k \downarrow}^\dagger + \text{h.c.} \right),
\]
where $\xi_p = \hbar^2 p^2 / (2M) - \mu$, and $\epsilon_{k\sigma}$ and $b_q$ are the annihilation operators of atoms and molecules in the open- and closed-channel, respectively. The channel coupling $g$ is related to $R_s$, via $R_s = 4\pi^2\hbar^4 / (M^2 g^2)$, and the detuning $\nu$ of molecules is tuned to reproduce the binding energy $\epsilon_B$, i.e., $\nu = - \epsilon_B + g^2 \sum_k \hbar^2 k^2 / (M + \epsilon_B)$. It is useful to emphasize that, a finite effective range leads to non-negligible closed-channel population $\langle b_q^\dagger b_q \rangle \neq 0$. These are simply virtual excitations above the ground-state along the $z$-axis, necessarily created from quasi-2D collisions.

We solve the model Hamiltonian at different orders of approximation at zero temperature. Formally, the ground-state energy $E$ may be decoupled as,

$$E \left[ \ln (k_F a_s), k_F^2 R_s \right] = E_{MF} + \Delta E_{GPF} + \Delta E_c,$$

where $k_F = (2\pi n)^{1/2}$ is Fermi wavevector and $\epsilon_F = \hbar^2 k_F^2 / (2M)$ is Fermi energy for a system with number density $n$. The mean-field (MF) theory provides the leading term $E_{MF}$, while the major correction arising from strong pair fluctuations at Gaussian level can be obtained by using the Gaussian pair fluctuation (GPF) theory \cite{38, 33, 32, 11}, i.e., $\Delta E_{GPF} = E_{GPF} - E_{MF}$. The effect of pair fluctuations beyond Gaussian level may be characterized by a correlation energy $\Delta E_c$, which is anticipated to be much smaller than $\Delta E_{GPF}$. To see this, in Fig. 2(a) we plot the ground-state energy in the zero-range limit ($R_s = 0$), predicted by mean-field theory, GPF theory \cite{29} and AFQMC simulation \cite{31}. Indeed, the correlation energy given by the difference between the GPF and AFQMC energies is notably smaller than $\Delta E_{GPF}$. In particular, $\Delta E_c$ becomes vanishingly small in the tight-binding limit of $\ln (k_F a_s) \rightarrow -\infty$ \cite{29}. It is then useful to define a beta function $\beta = \Delta E_c / \Delta E_{GPF} \ll 1$, which varies as functions of the two dimensionless interaction parameters $\ln (k_F a_s)$ and $k_F^2 R_s$. For small $k_F^2 R_s$, however, it seems plausible to assume that $\beta$ relies on a single parameter $\epsilon_B / \epsilon_F$, whose dependence can be readily extracted in the zero-range limit using the accurate AFQMC data, as shown in the inset of Fig. 2(a).

We thus establish a viable procedure to calculate the ground-state energy at nonzero effective range. For a given set $(k_F a_s, k_F^2 R_s)$, we first calculate the binding energy $\epsilon_B / \epsilon_F$ and determine the value of $\beta$. Both mean-field and GPF theories are then applied to obtain $E_{MF}$ and $\Delta E_{GPF}$, and consequently $\Delta E_c = \beta \Delta E_{GPF}$. In Fig. 2(b), we present $E = E_{GPF} + \Delta E_c$ in black line for a fixed ratio $R_s / a_s^2 \simeq -0.2511$, at which we may benchmark our prediction against available diffusion Monte Carlo (DMC) data (i.e., the single green dot) \cite{38, 42}. We find that the correction $\Delta E_{GPF}$ becomes smaller at nonzero effective range. Towards the non-interacting limit ($a_s \rightarrow \infty$) and hence large $k^2_F R_s$, $\Delta E_{GPF}$ vanishes quickly. This is understandable, since pair fluctuations become weaker with decreasing channel coupling $g$ and even mean-field theory may provide accurate prediction at sufficiently large $k^2_F R_s$ \cite{38}. The correlation energy also significantly reduces at finite effective range and we find $|\Delta E_c| < 0.02 N \epsilon_F$ at all interaction strengths. The agreement between our theory with DMC is excellent. The difference is less than 0.01 $N \epsilon_F$ and is comparable to the systematic error of standard QMC simulation \cite{29}.

**Equation of state.** Once the ground-state energy $E$ of a uniform 2D Fermi gas is determined, we calculate directly the chemical potential $\mu$ and pressure $P$ using standard thermodynamic relations. Experimentally, these homogeneous EoS can be extracted from a low-temperature trapped Fermi gas, by using the local density approximation \cite{43}, which assigns a local chemical potential $\mu(r) = \mu_{\text{peak}} - V(r)$ to each position $r$ in the potential $V(r) = M \omega_r^2 r^2 / 2$. Both the peak chemical potential $\mu_{\text{peak}}$ and the in situ density distribution $n(r)$ can be experimentally measured \cite{6, 6, 4}, from which one deduces the homogeneous density EoS $n(\mu)$. By further using the force balance condition \cite{4}, $\nabla P(r) = -n(r) \nabla V(r)$, the homogeneous pressure EoS $P(n)$ can also be determined.

In Fig. 3, we show the experimental data for the peak chemical potential $\mu_{\text{peak}}$, measured at different magnetic fields (i.e., $a_{s3D}$) and hence at different $\ln (k_F a_s)$ \cite{38, 43}. Our predictions for the peak chemical potential, calculated under the same experimental condition, are plotted by the black solid line. We find a good agreement between theory and experiment. Due to the large effective range of interactions in the experiment (i.e., $k^2_F R_s \lesssim -1.2$ at $N \simeq N_{2D}$ \cite{4}), the zero-range predic-

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**FIG. 3.** Chemical potential with the two-body bound state contribution subtracted, as a function of $\ln(k_F a_s)$ at the number of atoms $N = N_{2D}$. The predictions of AFQMC (i.e., for zero effective range) \cite{31} and our theory with a realistic effective range as in the experiment \cite{3} are shown by orange dashed line and black solid line, respectively, and are compared with the experimental data for $\mu_{\text{peak}}$ (blue circles) measured at $N \simeq N_{2D}$ \cite{4, 44}. The inset shows the chemical potential as a function of $\ln(k_F a_s)$, where $a_{s2D}$ is the effective scattering length adopted in the experiment \cite{3].
gas. Using the peak density of an ideal trapped Fermi

tatively understand the experimental measurement. We

determine effective range should be used, in order to quanti-

ify the experimental data lie systematically below the zero-range

towards the weakly interacting limit, the finite-temperature

effect may become sizable and up-shift the pressure data [6].

The inset shows the peak density (in units of $n_F^{\text{HO}}$) as a function of $\ln(k_F a_F)$, where $n_F^{\text{HO}}$ and $k_F^{\text{HO}} = (2\pi n_F^{\text{HO}})^{1/2}$ are the peak density and wave-vector of an ideal Fermi gas in traps.

The inset shows the peak density (in units of $n_F^{\text{HO}}$) as a function of $\ln(k_F a_F)$, where $n_F^{\text{HO}}$ and $k_F^{\text{HO}} = (2\pi n_F^{\text{HO}})^{1/2}$ are the peak density and wave-vector of an ideal Fermi gas in traps.

Breathing mode and quantum anomaly. We now turn
to consider the breathing mode frequency, which was newly measured in two experiments at $N \approx 0.2N_{2D}$ [16, 17], as shown in Fig. 5 by green circles and blue squares. Theoretically, the zero-temperature breathing

mode frequency can be conveniently calculated by using the sum-rule approach [45, 46],

$$\hbar^2 \omega_2^2 = -2 \left\langle r^2 \right\rangle \left[ \frac{d \left\langle r^2 \right\rangle}{d \left( \omega_\perp^2 \right)} \right]^{-1},$$

where $\left\langle r^2 \right\rangle = N^{-1} \int d^2 r [r^2 n(r)]$ is the squared radius of

the Fermi cloud at a given trapping frequency $\omega_\perp$. In the classical treatment, a 2D Fermi gas is scale-invariant [47] and acquires a polytropic density EoS, $\mu(n) \propto n^2$. As a result, the mode frequency is pinned to $2\omega_\perp$, regardless of temperature and interactions [47]. The deviation of the breathing mode frequency away from $2\omega_\perp$ can be viewed as a quantum anomaly [25, 26], arising from strong quantum pair fluctuations in 2D [48].

As readily seen from Fig. 5, the observed quantum anomaly in the two experiments is far below the prediction from AFQMC for zero-range interactions with a single 2D scattering length [49]. It can only be understood when we use the proposed minimal model for 2D ultracold fermions and take into account the realistic finite effective range at $N \approx 0.2N_{2D}$. The quantitative differences between our theory and experiment at $0 < \ln(k_F a_F) < 1$ could be caused by the finite temperature in the two ex-

periments, which is in the range $[0.10 - 0.22]T_F$.

It turns out that the breathing mode frequency or quantum anomaly depends sensitively on the effective range. The zero-range result of AFQMC can hardly be asymptotically approached, even we decrease the number of atoms down to just a few percent of $N_{2D}$ (see the red dot-dashed line at $N = 0.02N_{2D}$). In this case, however,
the deviation from the classical limit of $2\omega_\perp$ is very significant and its experimental observation will constitute as a convincing proof of long-sought 2D quantum anomaly in cold atoms \[48\].

Conclusions. We have established a minimal model to describe ultracold interacting fermions confined in two dimensions and have solved it accurately. We have shown that the confinement-induced effective range of interactions has to be included, in order to understand the recent measurements on quantum anomaly in a qualitative manner and on equation of state at quantitative level. Our results pave the way to investigate the crucial role played by effective range in other two-dimensional quantum many-body systems and provide an excellent starting point to address the fermionic Berezinskii-Kosterlitz-Thouless transition with cold-atoms \[14, 50\].

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[44] We have used the peak chemical potential data $\mu = \mu_{peak} + \varepsilon_B / 2$ listed in Table III of Supplemental Material of Ref. [8]. To have a robust procedure of measurement, in the experiment the chemical potential with the two-body binding energy subtracted ($\mu$) was assumed to be proportional to the local Fermi energy, $\mu = \varepsilon_F / c^2$. A ratio $1 / c$ was then obtained by fitting the linear relation at different densities and was supposed to provide the same information as $\mu_{peak}$ at the trap center. The ratio $1 / c$ is slightly smaller than $\mu_{0} / \varepsilon_F$, and is plotted in Fig. 1 of Ref. [8].

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