Flow Equations for the BCS-BEC Crossover

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The functional renormalisation group is used for the BCS-BEC crossover in gases of ultracold fermionic atoms. In a simple truncation, we see how universality and an effective theory with composite bosonic di-atom states emerge. We obtain a unified picture of the whole phase diagram. The flow reflects different effective physics at different scales. In the BEC limit as well as near the critical temperature, it describes an interacting bosonic theory.

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Ultracold gases of fermionic atoms near a Feshbach resonance show a crossover \cite{1} between Bose-Einstein condensation (BEC) of molecules and BCS superfluidity. The controlled microphysics, which can be measured by two-body scattering and the molecular binding energy, and recent experimental breakthroughs \cite{2} can open a new field of quantitatively precise understanding of complex many body physics. On the theory side, this calls for a quantitative and reliable approach to strongly interacting systems. In turn, a precise experimental control of the relevant parameters, namely the scattering length \(a\) acting systems. In this approach, the results of perturbative systems and has already been applied to connected the 'microphysics' to observable 'macrophysics' perturbative methods.

The functional renormalisation group (FRG) directly connects the 'microphysics' to observable 'macrophysics' by a non-perturbative flow equation \cite{3}. It has been used successfully for precision estimates in simple non-perturbative systems and has already been applied to coupled systems of fermions and collective bosonic degrees of freedom in relativistic \cite{4,5} and non-relativistic theories \cite{6,7}. In this approach, the results of perturbative renormalisation near the critical dimension \cite{8} or for a large number of components \(N\) \cite{9} can be recovered by an appropriate level of truncation of an exact functional differential equation. In a certain sense, the FRG can be regarded as a differential form of Schwinger-Dyson or gap equations in a 1PI \cite{10} or 2PI \cite{11} setting, see \cite{12}.

Method and approximation scheme – We study the scale dependence of the average action \(\Gamma_k\) \cite{13}. It includes all quantum and thermal fluctuations with momenta \(q^2 \gtrsim k^2\), or in the presence of a Fermi surface with effective chemical potential \(\sigma > 0\), all \(|q^2 - \sigma| \gtrsim k^2\). For \(k \to 0\), all fluctuations are included and \(\Gamma_{k \to 0}\) generates the 1PI correlation functions. In practice, this is realised by introducing suitable cutoff functions \(R_k(q)\) in the inverse propagators. The dependence of \(\Gamma_k\) on \(k\) obeys an exact flow equation \cite{2},

\[
\partial_k \Gamma_k = \frac{1}{2} \text{STr} \left( \Gamma^{(2)}_k + R_k \right)^{-1} \partial_k R_k. \tag{1}
\]

Here, STTr sums over spatial momenta \(q\) and Matsubara frequencies \(\omega_M\) as well as over internal indices and species of fields, with a minus sign for fermions. The second functional derivative \(\Gamma^{(2)}_k\) represents the full inverse propagator in the presence of the scale \(k\). Both \(\Gamma_k\) and \(\Gamma^{(2)}_k\) are functionals of the fields.

In the present Letter, we demonstrate that already a very simple truncation of \(\Gamma_k\) is sufficient to account for all qualitative features and limits of the crossover problem. We approximately solve Eq. (1) with the ansatz

\[
\Gamma_k = \int_T d^4x \left[ \psi^\dagger (\partial_\tau - \Delta - \sigma) \psi + \varphi^* (\partial_\tau - A_\varphi \Delta) \varphi \right. \\
+ u(\varphi) - h_\varphi \left( \varphi^* \psi_1 \psi_2 - \varphi \psi_1^* \psi_2^* \right). \tag{2}
\]

In addition to the fermionic fields \(\psi\) for the open-channel atoms, we use a collective bosonic di-atom field \(\varphi\). Depending on the region of the phase diagram and the scale \(k\), it can be associated with microscopic molecules, Cooper pairs, effective macroscopic bound states or simply represents an auxiliary field. The bosonic field is renormalised by a wave function renormalisation, \(\varphi = Z^\varphi \tilde{\varphi}\), such that at every scale \(k\) the term linear in the Euclidean time derivative \(\partial_\tau\) has a standard normalisation. (For the fermions, this renormalisation is omitted.) Eq. (1) holds for fixed unrenormalised fields \(\tilde{\varphi}\), i.e., \([\Gamma^{(2)}_k,\varphi]_{\alpha\beta} = \partial^2 \Gamma_k/\partial \tilde{\varphi}_\alpha \partial \tilde{\varphi}_\beta\). We define

\[
Z_\varphi = \left. \frac{\partial \Gamma^{(2)}_k(\omega, q = 0)}{\partial \omega} \right|_{\omega = 0}, \tag{3}
\]

where \(\Gamma^{(2)}_k\) is evaluated for an analytically continued Matsubara frequency \(\omega_M \to i\omega\). The fields and couplings in Eq. (2) are scaled with powers of an appropriate momentum scale \(k\) or energy scale \(k^2/(2M)\) \cite{10}. For nonzero density \(n\), we choose the Fermi momentum \(k_F = (3\pi^2 n)^{1/3}\). Our units are \(\hbar = c = k_B = 1\).

We consider a polynomial effective potential \(u(\varphi)\) written in terms of \(\rho = \varphi^* \varphi\),

\[
u = \begin{cases} 
\frac{m^2}{2} \rho + \frac{1}{2} \lambda \rho^2 & \text{SYM} \\
\frac{1}{2} \lambda \rho (\rho - \rho_0)^2 & \text{SSB} \end{cases} \tag{4}
\]

Here, we distinguish the symmetric regime (SYM), where the minimum of \(u\) is at \(\rho = 0\) and \(m^2 \geq 0\), from the
regime with spontaneous breaking of the U(1) symmetry (SSB), where the potential minimum occurs at $\rho_0(k)$. Superfluidity is signalled by $\rho_0(k \to 0) > 0$, with a gap for single fermionic atoms $\Delta = \hbar \sqrt{\rho_0}$.

The flow starts at some microscopic scale $k_{\text{in}}$ with $\lambda_\varphi = 0$, $m_{\varphi, \text{in}}^2 > 0$ and $A_\varphi = 1/2$. Here $m_{\varphi, \text{in}}^2$ is related to the magnetic field $B$ and relative magnetic moment $\mu$ by $\partial m_{\varphi, \text{in}}^2/\partial B = 2M\mu/k^2$, and reflects the detuning. We will concentrate on the limit of a broad Feshbach resonance, where $m_{\varphi, \text{in}}^2 \to \infty$, $m_{\varphi, \text{in}}^2 \to \infty$. In this limit, the microscopic action is strictly equivalent to a model containing only fermionic atoms with a point-like interaction and scattering length $a$ [10]. Then, the only relevant parameter is the concentration, $c = ak_B$, (or $ak$ for zero density), and the Feshbach resonance is located at $a(B \to B_0) \to \infty$. For broad resonances, the precise initial value of $A_\varphi$ is unimportant.

Finally, we specify the regulator functions $R_k$ for fermions and bosons. We work with optimised cutoffs $[12, 14]$ for space-like momenta $(\xi = q^2 - \theta(\sigma)\sigma)$,

$$ R_k^c = Z_\varphi A_\varphi(2k^2 - q^2)\theta(2k^2 - q^2), $$

$$ R_k^c = (k^2\text{sgn}\xi - \xi)\theta(k^2 - |\xi|). $$

A central object is the flow of the effective potential $u$ with $t = \ln k/k_{\text{in}}$, displayed here for $\sigma \leq 0$,

$$ \partial_t u = \eta_\varphi\rho u' - \frac{k^5}{3\pi^2} \left( \frac{\gamma}{2} \tanh \varphi - 1 \right) + \frac{2\sqrt{2k^5}}{3\pi^2} A_\varphi \left( 1 - \frac{\eta_A + \eta_\varphi}{2} \right) \left( \frac{\alpha + \chi}{\alpha} \right), $$

$$ \partial_t \dot{m}_\varphi^2 = \frac{k^2}{6\pi^2} \frac{k^5}{(k^2 - \sigma)^2}. $$

The condition that $\dot{m}_\varphi^2$ vanishes for $B = B_0$, $\sigma = 0$, $k = 0$ leads to

$$ m_{\varphi, \text{in}}^2 = \dot{m}_{\varphi, \text{in}}^2 = \frac{\hbar^2}{6\pi^2} k_{\text{in}}^2 + \frac{2M\mu}{k^2}(B - B_0) - 2\sigma. $$

In our picture, atom scattering in vacuum is mediated by the formation and decomposition of a collective boson. For the atom phase, one extracts the scattering length for $k \to 0$ [10],

$$ a = \frac{\hbar^2}{8\pi k n_{\varphi}^2} = \frac{\hbar^2}{16\pi M \mu(B - B_0)}. $$

Eq. [11] relates $\dot{m}_{\varphi, \text{in}}^2 = \hbar^2/2$ to the scattering length $a(B)$, thus fixing all parameters of our model. Eq. [11] can also be used for $B < B_0$. Integrating Eq. [9] for $\sigma = \sigma_A < 0$ with the condition $\dot{m}_\varphi^2(k = 0) = 0$ yields the well-known relation between molecular binding energy and scattering length $\epsilon_M = \sigma_A k^2/M = -1/(M\alpha^2)$.

The flow of the renormalised Feshbach coupling $\hbar_\varphi^2$ is determined by the anomalous dimension,

$$ \partial_t \left( \frac{\hbar_\varphi^2}{k} \right) = (-1 + \eta_\varphi) \frac{\hbar_\varphi^2}{k}, \quad \eta_\varphi = \frac{\hbar_\varphi^2}{6\pi^2} \frac{k^5}{(k^2 - \sigma)^3}. $$

For $\sigma = 0$, the rescaled renormalised Feshbach coupling rapidly approaches a fixed-point (scaling solution) given

**FIG. 1:** Chemical potential for $T = 0$ minus half the binding energy $\dot{\epsilon}_M/2 = -\theta(c^{-1})c^{-2}$. We compare our FRG result (solid) to extended mean field theory (dotted) and our previous Schwinger-Dyson result (dot-dashed) [10].

The dimensionless “vacuum chemical potential” $\sigma_A = \epsilon_M M/k^2$ is related to the binding energy $\epsilon_M$ of a molecule, see below. On the BCS side, the bosons experience a gap $m_{\varphi}^2 > 0$ and the low-density limit describes only fermionic atoms. On the BEC side, the situation is reversed: fermion propagation is suppressed by a gap $-\sigma_A$, and the low-density limit describes bound molecules.

In the vacuum limit, we first solve the flow equation for the mass term $m_{\varphi, \text{in}}^2 = Z_\varphi m_{\varphi}^2$ (we choose $Z_{\varphi, \text{in}} = 1$),

$$ m_{\varphi, \text{in}}^2 = m_{\varphi, \text{in}}^2 = \frac{\hbar^2}{6\pi^2} k_{\text{in}}^2 + \frac{2M\mu}{k^2}(B - B_0) - 2\sigma. $$.  

In our formalism, the vacuum correlation functions, that directly yield the cross section [10], are obtained from $\Gamma_{k \to 0}$ in the limit $n \to 0$, $T \to 0$. For fixed $k$ the flow equations then simplify considerably. We find that for $n = T = 0$ the crossover at finite density turns into a second-order phase transition [3, 10] as a function of $m_{\varphi, \text{in}}^2$ or $B$, with

$$ m_{\varphi, \text{in}}^2 > 0, \quad \sigma_A = 0 \quad \text{atom phase (}a^{-1} < 0\text{)} $$

$$ m_{\varphi, \text{in}}^2 = 0, \quad \sigma_A < 0 \quad \text{molecule phase (}a^{-1} > 0\text{)} $$

$$ m_{\varphi, \text{in}}^2 = 0, \quad \sigma_A = 0 \quad \text{resonance (}a^{-1} = 0\text{)} $$
by $\eta_{v} = 1$, $\hbar^{2}/k = 6\pi^{2}$. In the vacuum, we find $A_{v} = 1/2$ and $Z_{v}(\sigma < 0, k \to 0) = 1 + \hbar^{2}/(32\pi\sqrt{-\sigma})$.

Next, we study the equation for the dimensionless four-boson coupling $\lambda_{\varphi} = Z_{\varphi}^{2}/\lambda_{\varphi}$,

$$\partial_{t}\lambda_{\varphi} = -\frac{\hbar^{2}}{4\pi^{2}}\frac{k^{5}}{(k^{2} - \sigma)^{4}} + \frac{2\sqrt{2}A_{v}^{2}}{3\pi^{2}}(2Z_{\varphi}A_{v}k^{2} + m_{\varphi}^{2})^{2}.$$

(13)

There are contributions from fermionic and bosonic vacuum fluctuations, but no contribution from higher $\rho$ derivatives of $u$. For $\sigma = 0$ and large $\hbar^{2}_{\varphi}$, we use the scaling form $Z_{\varphi} = \hbar^{2}_{\varphi}/(6\pi^{2}k)$, $m_{\varphi}^{2} = \hbar^{2}_{\varphi}/(6\pi^{2})$, $A_{\varphi} = 1/2$, $\eta_{\varphi} = 1$, $\eta_{A_{\varphi}} = 0$ and find for the ratio $Q = \lambda_{\varphi}k^{3}/h_{\varphi}^{4}$ the flow equation

$$\partial_{t}Q = 3Q - \frac{1}{4\pi^{2}} + \frac{3\pi^{2}}{\sqrt{2}}Q^{2}.$$

(14)

The infrared stable fixed point $Q_{s} \simeq 0.008$ corresponds to a renormalised coupling

$$\lambda_{\varphi} = \frac{\lambda_{\varphi}}{Z_{\varphi}} = \frac{36\pi^{4}Q_{s}}{k},$$

(15)

to be compared with the effective four-fermion coupling $\lambda_{\varphi,\text{eff}} = -\hbar^{2}/m_{\varphi}^{2} = -6\pi^{2}/k$. The constant ratio between these two quantities is the origin of the universal ratio between the scattering length for molecules and atoms, $a_{M}/a = 2\lambda_{\varphi}/\lambda_{\varphi,\text{eff}}$.

In the molecule phase for $\sigma_{A} < 0$ and $k = 0$, one has $\lambda_{\varphi,\text{eff}} = 8\pi/\sqrt{-\sigma_{A}}$. Omitting the molecule fluctuations, a direct integration of Eq. (13) yields $\lambda_{\varphi} = 8\pi/\sqrt{-\sigma_{A}}$ and therefore $a_{M}/a = 2$, whereas the molecule fluctuations lower this ratio. With the cut-off functions we get $a_{M}/a = 0.92$, while further optimisation of $R_{k}$ leads to $a_{M}/a = 0.71$. Similar diagrammatic approaches give $a_{M}/a = 0.75(4)$, whereas the solution of the 4-body Schrödinger equation yields $a_{M}/a = 0.6$ and with diagrammatic techniques.

Many-body problem – The system is now characterised by two additional scales, the temperature $T$ and the Fermi momentum $k_{F}$. We set $\tilde{k} = k_{F}$ from now on and use tilde instead of hats in order to indicate this specific normalisation. We determine the initial values for the flow in these units by Eqs. (10), (11) in terms of the concentration $c = a_{k_{F}}$ and $h_{\varphi}^{2}$. For large $h_{\varphi}^{2}$ (broad Feshbach resonance), the value of $h_{\varphi}^{2}$ will not be relevant. Finally, we have to adjust $\tilde{\sigma}$ in order to obtain the correct density, which is related to the $\tilde{\sigma}$ dependence of the potential at its minimum. Within our normalisation, this yields the condition $\partial u_{\text{min}}/\partial \tilde{\sigma} = -1/(3\pi^{2})$ for $k = 0$. We follow the flow of $\partial u_{\text{min}}/\partial \tilde{\sigma}$ by taking the $\tilde{\sigma}$ derivative of Eq. (2), starting with an initial value $-\tilde{\sigma}^{1/2}(\tilde{\sigma})/(3\pi^{2})$ at $k_{\text{min}}$. The flow equation integrates out the modes around the Fermi surface for $\tilde{\sigma} > 0$. At least for low $T$, the different contributions on the right-hand side can be identified with the densities in unbound atoms, molecules and the condensate. Our result for $\tilde{\sigma}(c^{-1})$ is shown in Fig. 1. On resonance, we obtain $\tilde{\sigma}(c^{-1} = 0) = 0.55$, while quantum Monte Carlo (QMC) simulations give $\tilde{\sigma}(c^{-1} = 0) = 0.44(1)$, $\tilde{\sigma}(c^{-1} = 0) = 0.42(2)$.

The density and temperature effects modify the flow when $k \approx 1$ or $T \approx T_{1/2}$, i.e., when the wavelength of fluctuations being integrated out is comparable to the interparticle spacing or the de Broglie wavelength. For $T = 0$, in particular, $m_{\varphi}^{2}$ reaches zero for $k_{\text{SSB}} > 0$, and the flow has to be continued in the SSB regime with $\rho_{0}(k < k_{\text{SSB}}) > 0$ until $k \to 0$. We show in Fig. 2 the condensate fraction $\Omega_{C}$ and the gap for single fermionic atoms $\Delta = \hbar\varphi\sqrt{\rho_{0}}$. In the BCS regime, the BCS value $(\Delta(c^{-1})/(\Delta_{BCS}(c^{-1}) = 0.9)$ for the gap parameter is approximately reproduced. On resonance, we find $\Delta(c^{-1} = 0) = 0.6$, to be compared to the QMC value $\Delta(c^{-1} = 0) = 0.54$.

At higher temperature, the effects of fermionic fluc-
tations on the build-up of $\rho_0$ are reduced and the bosonic fluctuations tend to diminish $\rho_0$. At $T_c$ where $\rho_0(k \to 0) \to 0$, we find a second-order phase transition. The critical region is governed by boson fluctuations with universal properties in the $(O(2))$ universality class. From the scaling solution, we find a critical exponent $\eta = \eta_c + \eta_A \approx 0.05$ throughout the crossover. We plot $\Delta(T)/\Delta(0)$ for different values of $c^{-1}$ in Fig. 3. The universal behaviour is visible for $T \to T_c$. On the BCS side, the scale $k_{\text{SB}}$ goes to zero for $c^{-1} \to -\infty$, leading to an exponentially suppressed gap.

The phase diagram in the $(T, c^{-1})$ plane is shown in Fig. 4. In the regime of weak attractive interactions, the BCS critical temperature is reproduced. On the BEC side, we find the shift of the critical temperature $\Delta T_c/T_c^{\text{BEC}} = \kappa(n_M)^{1/3}a_M = (6\pi^2)^{-1/3}\kappa(a_M/a)c^{-1}$ with $\kappa = 1.7$, $a_M = 0.92a$ (short dotted line). Lattice simulations give $\kappa = 1.32(2)$.

In the BEC regime, both at zero temperature and close to $T_c$ the many-body physics reflects the behavior of “fundamental” bosons of mass $2M$ interacting via a scattering length $a_M = 0.9a$. This demonstrates the emergence of an effective bosonic theory, where all memory of the truly fundamental fermionic constituents has been lost, easily understood by the fact that the binding energy of the molecules is the largest scale in this region of the phase diagram. Moving to the unitary and BCS regimes, only a very narrow region around $T_c$ is dominated by bosonic fluctuations, which give rise to the above mentioned critical behavior. Bosonic degrees of freedom are, however, crucial to accommodate the symmetry requirements in the spontaneously broken phase throughout the crossover and form an important building block for our evaluation scheme.

Our present truncation does not yet include the effects of particle-hole fluctuations. They lead to a strong decrease of both the critical temperature and the gap parameter in the regions of the phase diagram where there is a substantial Fermi surface, i.e., in the BCS and unitary regimes. In the BCS regime, the reduction of both $T_c$ and $\Delta(T = 0)$ by a factor $(4e)^{1/3} \approx 2.2$ is well known as Gorkov’s effect. In our formulation, this effect is encoded in the running of an effective four-fermion vertex which is generated by certain mixed boson-fermion diagrams. The relevant diagrams precisely have the topology of the particle-hole diagrams in a purely fermionic setting. This will be discussed in future work.

Conclusion - Our functional renormalization group analysis for ultracold fermionic atoms clearly demonstrates the necessity of the inclusion of bosonic quantum and statistical fluctuations beyond extended mean field theory. Both the BEC regime $(c^{-1} \to \infty)$ and the universal critical behaviour $(T \to T_c)$ are dominated by bosons. The vacuum fluctuations are crucial for the four-boson interaction. The thermal boson fluctuations are needed to establish the expected second-order phase transition. Our method is technically simple and involves only a few running couplings, still enough to resolve the full range of microscopic couplings, i.e., the BCS-BEC crossover, as well as the whole range of temperatures from the ground state to the phase transition. We control all regimes of densities including the physical vacuum $(k_F \to 0)$ where the crossover terminates in a second-order vacuum phase transition. The simplicity of the picture constitutes an ideal starting point for systematic quantitative improvements by extending the truncation. For example, we have not yet included the (many-body) effect of particle-hole fluctuations which will lower $T_c$ in the BCS and crossover regimes. Extended truncations should lead to quantitative precision for the crossover physics.

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