Dynamics of Fluctuations in the BCS-BEC Crossover in Superfluid Fermi Gases

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Abstract. The BCS-BEC crossover phenomenon in a 3D attractive Fermi gas is revisited by using finite temperature Green functions formalism derived from the quantum path integral technique and Mean Field Approximation (MFA). Collective modes for weak and strong coupling particle-particle interaction $g$ are obtained after recovering the dynamical coefficients in the non-linear Time Dependent Ginzburg Landau (TDGL) equation, and numerically simulated under those particular states for the filling energy $\mu \sim 0$ and order parameter $\Delta (x, \tau) \sim \Delta_0$. Explicit formulas for the first order average fluctuations $\langle \eta^2_{\omega} \rangle$ and the scaling law for the thermal energy associated to the non-linear collective modes are also reported.

1. Introduction
The problem of the crossover from BCS theory with cooperative Cooper pairing to the formation and condensation of composite bosons has attracted considerable attention after the discovery of high $T_C$ superconductors. Monte Carlo simulations for the attractive (negative $U$) Hubbard model have shown, for instance, that the crossover region displays highly anomalous correlations in degenerate Fermi system above $T_C$ in the intermediate coupling regime [1]. The crossover phenomenon is also of interest for other problems: excitonic condensates, superconductor-insulator transition and Cooper pair formation in resonant Feshbach channels [2],[3],[4] and more recently, in tunneling properties of bounded Fermi pairs in optical lattices [5] and superfluid Sarma phase critical behavior for unbalanced 2D chemical potentials in ultracold Fermi gases [6],[7]. By using the path integral formalism, we study a 3D continuum model of fermions with attractive interactions at finite temperature, by reconstructing the Time-Dependent Ginzburg Landau (TDGL) equation for the particular case in which the order parameter vanishes at $T = T_C$, and for arbitrary strength coupling $g$ [8]. We show that, in the weak coupling limit, the TDGL coefficients are reduced to the classical ones obtained by Gor’kov (1959) in the framework of the microscopic approximation. This formalism is systematically extended for the broken symmetry case ($T < T_C$), $s$-wave scattering and the Mean-Field Approximation (MFA). In section 4 we derive the complete set of self-consistent equations for collective excitations, and solve them in two particular cases: i) for the weak-coupling interaction limit and ii) and the intermediate/strong attractive interaction potential. We show that our derivation reproduces the value for the sound velocity in the condensate in the first scenario.
2. Time-Dependent Ginzburg Landau Equation (TDGL)

The insertion of the fluctuating (bosonic) fields \( \Delta (\Delta) \) into the effective action functional \( S_{\text{eff}} [\Delta, \Delta] \) has been developed in the framework of the Randeira’s prescription by starting from the Nambu propagator \( (G^{-1}) \) [13]: \( G^{-1} = G_0^{-1} + \Delta \sigma^+ \pm \Delta \sigma^- \). Here \( \sigma^\pm = (\sigma_x \pm \sigma_y)/2 \), and \( \sigma_j \)’s are Pauli’s matrices, \( G_0^{-1} \) represents the non-interacting Green’s propagator given explicitly by:

\[
G_0 = \begin{pmatrix}
  (i\omega_m - \xi_k)^{-1} & 0 \\
  0 & (i\omega_m + \xi_k)^{-1}
\end{pmatrix},
\]

with \( i\omega_m = 2\pi T (m + 1/2) \) as the set of fermionic Matsubara frequencies, and \( \xi_k = k^2/2m - \mu \) defines the non-interacting kinetic energy for particles with momentum \( k \), and chemical potential \( \mu \) at temperature \( T \). The relationship with the effective action \( S_{\text{eff}} [\Delta, \Delta] \) is obtained after applying the well-known Hubbard-Stratonovich transformation over Fermi fields operators \[9],[10]. The remaining (bosonic) fields contribute into \( S_{\text{eff}} [\Delta, \Delta] \) in the form:

\[
S_{\text{eff}} [\Delta, \Delta] = \int d^3x \int_0^\beta d\tau \left[ \left| \frac{\Delta}{g} \right|^2 - \text{Tr} \ln G_0^{-1} - \text{Tr} \ln \left[ 1 + G_0 \left( \Delta \sigma^+ + \Delta \sigma^- \right) \right] \right],
\]

in which the bare interaction between Fermions is primarily encoded through the parameter \( g \). By performing second order expansions in the last term of (2), the effective action can be reduced straightforwardly and the final result resembles the Gaussian structure discussed by Nozières and Schmitt-Rink (NSR) in the frame of the particle-particle scattering t-matrix theory [11]: \( S_{\text{eff}} [\Delta, \Delta] = S_0 + \sum_q | \Delta (q) |^2 \Gamma (q) \). Factor \( \Gamma (q) \) contains the regularization condition for the effective \( s \)-wave interaction on \( g \). Time-Dependent Ginzburg Landau equation (TDGL) becomes now apparent when \( S_{\text{eff}} [\Delta, \Delta] \) includes fourth-order fluctuations in the fields \( | \Delta | \) and under the minimization constraint \( \delta S_{\text{eff}} / \delta \Delta = 0 \). Its final form in the space-time representation takes the form:

\[
\left( a - c \frac{\nabla^2}{2m} + b \right) \Delta (x, t) \left| \Delta (x, t) \right|^2 \frac{\partial}{\partial t} \Delta (x, t) = 0,
\]

where the coefficients in (3) are obtained under specific conditions for a system close to its critical temperature \( T_C \) and slow-time variations in the fields \( \Delta \). Details in the derivation of (3) are given by the author in the reference [12]).

3. Broken Symmetry State at \( T < T_C \)

The previous analysis can be extended for the broken symmetry (superfluid) state at low temperatures. The first stage of our approximation comes from the condition in which the order parameter fluctuations are negligible \( \left( \Delta (x) \approx \Delta_0 \right) \), and \( \delta S_{\text{eff}} / \delta \Delta_0 = 0 \). The relationship between the interaction parameter \( g \) and \( \Delta_0 \) can be obtained by using the standard Gaussian integration technique. The final result can be expressed as: \( 1/g = \sum_k \tanh \left( \beta E_k / 2 \right) / 2E_k \), where \( E_k = \sqrt{\xi_k^2 + \Delta_0^2} \). The regularization condition for the ultraviolet divergence in the gap equation is established by including proper terms associated to the \( s \)-wave scattering length \( a_s \), which directly describes the two-body attraction strength \( g \) in a low density system. The renormalized gap equation then reads:

\[
\frac{m}{4\pi a_s} = \sum_k \left[ \frac{1}{2\epsilon_k} - \frac{\tanh \left( \beta E_k / 2 \right)}{2E_k} \right],
\]

with \( \epsilon_k = k^2/2m \). In order to investigate the nature of the fluctuating fields (denoted by \( \eta (x, \tau) \)) around the saddle point \( \Delta_0 \), we write \( \Delta (x, \tau) = \Delta_0 + \eta (x, \tau) \) while the generic definition for
the Green's propagator in Eq. (1) recasts into: 
\[ G^{-1} = G_0^{-1}(\Delta_0) + \eta \sigma^+ + \tilde{\eta} \sigma^- , \]
where \( G_0(\Delta_0) \) is defined as:
\[ G_0(\Delta_0) = \left( \begin{array}{cc} G_k(\Delta_0) & \mathcal{F}_k(\Delta_0) \\ \mathcal{F}_k^*(\Delta_0) & -G_k^*(\Delta_0) \end{array} \right), \]  
(5)
with \( G_k(\Delta_0) = -(i\omega_m + \xi_k) / (\omega_m^2 + E_k^2) \), and \( \mathcal{F}_k(\Delta_0) = \Delta_0 / (\omega_m^2 + E_k^2) \). The effective action functional must be rewritten in terms of the mean field values \( \Delta_0 \) and their corresponding fluctuating fields \( \eta, \tilde{\eta} \). Hence:
\[ S_{\text{eff}}[\eta, \tilde{\eta}] = \sum_q \left[ \frac{|\eta_q|^2}{g} - \text{Tr} \ln G_0^{-1}(\Delta_0) + \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \text{Tr} (G_0(\Delta_0) \Sigma)^n \right], \]  
(6)
where \( \Sigma \) is a off-diagonal matrix defined as \( \eta_q \sigma^+ + \tilde{\eta}_q \sigma^- \). The index \( q \) in Equation (6) denotes the pair-momentum and the set of Bosonic Matsubara frequencies \( i\nu_n \). It is possible to relate this result with quantities of physical interest such as the generating partition functional and the Helmholtz free energy \( \mathcal{F} \) through \( \mathcal{F} = -kT \ln Z \). Equation (6) can be rewritten in a quadratic form in the fields \( \eta, \tilde{\eta} \) as:
\[ S_{\text{eff}}[\eta, \tilde{\eta}] = S_0 + \sum_q \eta_q^\dagger \left( K_q^{-1} \right) \eta_q, \]  
(7)
with the spinors fields \( \eta^\dagger \equiv [\eta_q, \tilde{\eta}_q] \), and \( K_q \) basically defined in terms of the \( g, a_\sigma \) and \( T \). Calculation of \( \langle \eta_q^2 \rangle \) becomes now evident from Eq. (7). For the case in which the bosonic frequencies \( i\nu_n \) are different from zero, the tensor \( K_q^{-1} \) might be separated into its static component, which has been collected into \( K_q^{-1} \), and its frequency-dependent part denoted as \( K_q^{-1} \), where \( \omega \) is the real frequency that appears after analytic continuation procedure on \( i\nu \), under \( i\nu \rightarrow \omega + i0^+ \). Hence, \( K_q^{-1} = K_q^{-1} + K_q^{-1} \), with \( (K_q^{11})^{-1} = -\sum_k (1 - \Delta_0^2/E_k^2) \tanh (\beta E_k/2) (1 - \omega^2/4E_k^2) \), \( (K_q^{22})^{-1} = -\sum_k \omega \xi_k \tanh (\beta E_k/2) (1 - \omega^2/4E_k^2) \), with \( (K_q^{12})^{-1} = -\sum(q) \). The expression for the partition function \( Z = Z_0 \int D[\eta, \tilde{\eta}] \exp \left[ -\sum_q \eta_q^\dagger K_q^{-1} \eta_q \right] = Z_0 \prod_q \text{det}(K_q) \) might be modified as:
\[ \ln Z = -S_0 + \sum_q \int d\omega \ln [\text{det}(K_q)], \]
where \( \text{det}(K_q^{-1}) = \frac{1}{4} \left[ g^{-1} + \Pi_q^{11} + \Pi_q^{12} + (K_q^{11})^{-1} \right] \times \left[ g^{-1} + \Pi_q^{11} - \Pi_q^{12} + (K_q^{22})^{-1} \right] + \frac{1}{4} \left[ (K_q^{12})^{-1} \right]^2, \]  
(8)
with \( 2K_q^{-1} = g^{-1} + \hat{\Pi}_q \), and \( S_0 = -\sum_q \text{Tr} \ln G_0^{-1}(\Delta_0) \). The expression (8) provides the core result in this section: the complete set of self-consistent equations that describes the Helmholtz free energy associated to Gaussian fluctuations in the field \( \eta \), via the relationship \( \mathcal{F}(\Delta_0, T, \mu) = -\beta^{-1} \ln Z \), for any temperature between \( T \) and \( T_C \), and under the regularization condition in the BSC-BEC crossover scenario (Eq. 4). A similar expression for the full dynamics in the fluctuating field \( \eta(\omega, q) \) is also obtained:
\[ \langle \eta^2 \rangle_{q, \omega} = \text{Tr} \{ K_q^{-1} \} / \text{det}(K_q^{-1}), \]
where \( \text{Tr}\{ \cdots \} \) indicates the Trace operation over the embraced quantity \( \{ \cdots \} \). Explicit expressions for the quantities \( \Pi_q^{11} \) \( \Pi_q^{12} \) are given in Appendix A, while \( \text{Tr} \{ K_q^{-1} \} = g^{-1} + \Pi_q^{11} + (K_q^{11})^{-1} + (K_q^{22})^{-1} \). In the limit of small \( q \)–momenta, \( \Pi_q^{11} \pm \Pi_q^{12} \approx c_{\pm} (\Delta_0, T, \mu) (q^2/2m) \).
4. Collective Modes

Collective modes are calculated in analytical form by applying the condition over the kernel $K_{q,\omega}^{-1}$: $\det\left(K_{q,\omega}^{-1}\right) = 0$. For small values of the momentum and frequencies, we obtain:

$$\left[ A - D\omega^2 + \bar{c}_+ \left( \frac{q^2}{2m} \right) \right] \left[ -R\omega^2 + \bar{c}_- \left( \frac{q^2}{2m} \right) \right] - B^2\omega^2 = 0,$$

with $A, B, \bar{c}_\pm, D$ and $R$ as temperature-dependent functions [12]: $A = \sum_k \Delta_0^2 \bar{X}_k / 2E_k^3$, $R = \sum_k \bar{X}_k / 8E_k^2$, $D = \sum_k (1 - \Delta_0^2 / E_k^2) \bar{X}_k / 8E_k^3$, $B = \sum_k \xi_k \bar{X}_k / 4E_k^3$. The parameters $\bar{c}_\pm$ are given explicitly in the appendix A. Results for numerical simulations are illustrated in figures (1) and (2).

Figure 1: Low-energy topology surface for collective modes mapped through $\omega_q^{\pm}$ at $\mu \approx 0$, and $x = kTC/\varepsilon_F < 1$. $x \to 0$ limit corresponds to BCS regime, while $x \to \infty$ is characteristic to the pure Bose state.

$$\bar{c}_\pm = \sum_k \left[ \left( \frac{\bar{X}_k}{4E_k^2} - \frac{\beta Y_k}{8E_k} \right) Z_k^{\pm} + \frac{\beta^2 \bar{X}_k Y_k}{2} Z_k^{\pm} \right].$$

(10)

Figure (1) illustrates collective excitations of formed pairs in two regimes: for $x \to 0$ which corresponds to the weak interaction coupling, or just the (BCS) state with $\varepsilon_F$ playing the role of an effective cutoff energy [13]; and the strong coupling (labeled as $x \to \infty$), which corresponds to bounded states for a dilute gas of small Cooper pair molecules (Bose gas) with a condensation temperature close to 0.218$\varepsilon_F$. Integrals involving in $A, B, \bar{c}_\pm...$, peak around the Fermi surface at $T \to 0$ (BCS state) for the weak-coupling limit. In these case $A = N_n (\varepsilon_F) / 2$, $B = N_n (\varepsilon_F) / 4\Delta_0 = \bar{c}_-$, $R = N_n (\varepsilon_F) / 8\Delta_0^3$, $D = R/3$, $\bar{c}_+ = 2\pi N_n (\varepsilon_F) / 9\Delta_0$, with $N_n (\varepsilon_F)$ as the normal state density function at zero temperature, which is related with the superfluid density function as $N_n (E_k) dE_k = N_n (\xi_k) d\xi_k$. In the tractable limit at $T \sim T_C$, $\Delta_0 = 0$; $A = 0$, $D = R = 7N (\varepsilon_F) \zeta (3) / 16\pi^2 T_C^2$, $\bar{c}_+ = \bar{c}_- = 4\varepsilon_F D/3$ and

$\langle \eta_n \rangle \sim \langle \varepsilon_n \rangle$ 

Figure 2: Order parameter and average thermal energy activated by the low frequency collective modes as a function of the critical temperature $T_C$. Solid line represents the scaling law for the normalized thermal energy $\langle \varepsilon_n \rangle$. 

$\sim T_C^{4.75}$
\[ B = \left(2\sqrt{2} - 1\right) \zeta(3/2) N \langle \varepsilon_F \rangle / (16\pi T_C \varepsilon_F)^{1/2}. \]

Neglecting terms of the form \( \omega^4, q^4 \) and \( \omega^2 q^2 \), we get a first approach for the collective excitations modes: \( \omega(q) = v_s(T, \Delta_0, \mu) \mid q \mid \), with the sound velocity given by: \( v_s(T, \Delta_0, \mu) = \sqrt{\alpha \mathcal{C} / 2m(B^2 + A R)} \). Under this conditions, the dispersion relationship for \( \omega_q \) at low critical temperature takes the linear form \( \omega_q = \sqrt{\alpha \mathcal{C} / 2m} D q = v_s q \), and \( v_s \), the sound velocity in the condensate, takes the value \( v_s = v_F / \sqrt{3} \), \( ( v_F = \sqrt{2} \varepsilon_F / m \) as the Fermi velocity) which corresponds to the well-known result for the phase mode. Figure (2) illustrates the normalized thermal energy due to the collective excitations

\[ \omega_q^2 = \pm \frac{1}{2} \left[ -B / D \pm \sqrt{(B / D)^2 + 4 (c_- / D)(q^2 / 2m)} \right] \] (in the combination \( \pm; + \)) for a temperature close to the critical temperature \( T_c \). It is defined as \( \langle \varepsilon(T_C) \rangle = \sum_{\mathbf{q}, j} \omega_j^2 n_B(\omega_j, T_C) \), where

\[ n_B^{-1}(\omega_j, T_C) \equiv \left( \exp(\beta_c \omega_j^2) - 1 \right) \]

is the Bose-Einstein statistical factor, \( \beta_c^{-1} = k T_C \). By performing complete integration on the \( q \) space and physically meaningful \( j \)-modes, the thermal energy contribution associated to the collective excitations for the BEC state scales as \( T_C^{4/4} \) in the strong coupling regime, in contrast with the pure linear phase mode contribution in which \( \langle \varepsilon \rangle \sim T_C^4 \). Thermal energy and order parameter at critical temperature behavior have been normalized out of its corresponding values at \( k T_C / \varepsilon_F = 0.3 \), and denoted as \( (\varepsilon_n) \) and \( (\eta_n) \) respectively. Further efforts might be orientated in studying high-order expansions in \( \Sigma \) and their renormalization over coefficients in (9) for different pairing mechanisms [14], as well as specific effects of artificially engineered trapping potentials in ultracold gases arrays of lattices.

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6. Appendix A

The equation (10) is partially decrypted for \( \hat{X}_k = \tanh(\beta E_k/2), \hat{Y}_k = \sech^2(\beta E_k/2) \). Notice that for \( \Delta_0 = 0 \), \( Z_k^+ = Z_k^- \) and \( Z_k^+ = Z_k^- \), results obtained by Randeira et-al. in reference [8]. For \( \Delta_0 \neq 0 \), in simplified notation:

\[ Z^+ = \xi/E (1 - 3\Delta_0^2/E^2) + (\mathbf{k} \cdot \mathbf{n})^2 / m E \left( -1 + 10 (\Delta_0^2/E^2 - \Delta_0^4/E^4) \right); Z'^+ = \Delta_0^4 \xi / 4 E^3 + (\mathbf{k} \cdot \mathbf{n})^2 (1 - 4\Delta_0^2/E^2 + 6\Delta_0^4/E^4) / 4 m E; \]
\[ Z^- = \xi/E - (\mathbf{k} \cdot \mathbf{n})^2 (1 - 3\Delta_0^2/E^2) / m E; Z'^- = (\mathbf{k} \cdot \mathbf{n})^2 (1 - \Delta_0^2/E^2 + 2\Delta_0^4/E^4) / 4 m E; \]
\[ \text{Equation (8) for } \det (K_{q,\omega}) \text{ is completely unveiled with } \]
\[ \Pi_{q}^{11} \pm \Pi_{q}^{12} = \sum_k \frac{E_{k+q} (\xi_0 \mathbf{k} \cdot \mathbf{n} - E_{k+q}^2 + \Delta_0^2)}{2 E_{k+q}} \tanh(\beta E_k/2) - \frac{E_{k+q} (\xi_0 \mathbf{k} \cdot \mathbf{n} - E_{k+q} + \Delta_0^2)}{2 E_{k+q}} \tanh(\beta E_k/2). \]

7. References

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