Quasiparticle excitations in Bose-Fermi mixtures

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I. INTRODUCTION

Recent experimental studies of ultra cold atomic gases cooled to quantum degeneracy and trapped in optical lattice potentials have demonstrated precise control over two-body interactions. The Feshbach resonance, which can be exploited by ramping a magnetic field $\Delta B$ near the resonance $B_0$, can tune the scattering length $a_0$ over a wide range of values, generating both repulsive and attractive interactions (of strength $g_{\alpha\beta}$) between pairs of atoms $\alpha$ and $\beta$. The interaction coupling has the following dependence on key quantities,

$$g_{\alpha\beta} \approx \sqrt{\frac{2\pi a_{bg} \Delta B \delta \sigma_{\alpha\beta}}{m_\psi}}$$

(1.1)

where $\delta \sigma_{\alpha\beta}$ is a field dependent quantity that depends on the mismatch of the magnetic moments and $a_{bg}$ is the background scattering length.

Furthermore, optical lattice systems have provided a remarkably ideal testing ground for new strongly correlated phenomena. In particular, Bose-Fermi mixtures possess a unique physical realization beyond the scope of traditional solid state materials. Several experimental groups have successfully synthesized mixtures of $^6$Li Fermions with both $^7$Li Bosons and $^{23}$Na Bosons, and more recently $^{40}$K Fermions with $^{87}$Rb Bosons. The electrically polar nature of KRb and other heteronuclear diatomic molecules allow for novel quantum states driven by electric dipole-dipole interactions, however for simplicity such effects will not be discussed here. Most recent experiments have reported interspecies Feshbach resonances in mixtures of Rb and Cs atoms.

Earlier theoretical studies have focused on density-density type interspecies interactions. Interesting phenomena utilizing various mean-phase studies has found the precise limits of phase separation. Certain one-dimensional approaches have predicted novel 1D ordered phases where strong coupling theories seem to break down. More recent numerical work by Lewenstein et al. identified several pairing instabilities with a rich phase diagram consisting of various paired phases between the bosons and fermions, with order ranging from CDW to superconductivity. Later studies introduced a 3-particle interaction which explicitly allows for the creation of a boundstate molecular particle, revealing Bose-Einstein condensate depletion and other manifestations of phase separation. In this article we shall focus on the consequences of this type of interaction.

Unlike simple electrons, atoms and molecules have internal degrees of freedom that build composite particles with total spin given by $F = I + S$, where $I$ is the nuclear spin and $S$ is the electron spin. In the case of fermions, the system can exhibit high degeneracy due to hyperfine spin multiplets such as the recently observed $^{173}$Yb Fermi gas, with constituents having spin of $5/2$. Therfore, here we consider such a system, consisting of a degenerate Bose-Fermi mixture containing high spin fermions of degeneracy $N_\psi = 2F + 1$, which can combine with bosonic atoms via resonant scattering. We derive a Fermi-liquid picture of the low-lying excitations of a single molecular level, having an effective quasiparticle weight and broadening width, taking in account non-Gaussian fluctuations at the order $1/N_\psi$. The analysis presented here fundamentally unifies the condensed matter physics with
atomic physics and chemistry, given that the molecular levels which are hybridized through a many-body chemical reaction can be described through the quasi-particle concept. Thus, if the chemical equilibrium conditions can be violated, the components of the mixture will be driven by a steady reaction rate that will deplete one or more atomic or molecular species either by net molecular formation or disassociation.

II. THE MODEL

Here we study a model of a mixture of spin-polarized fermionic atoms and bosonic atoms, both of which can be treated as spinless particles. The canonical annihilation and creation operators are defined for the Bosons - $b, b^\dagger$ and Fermions - $f, f^\dagger$, combined to form fermionic diatomic molecules $\psi, \psi^\dagger$. The most general Hamiltonian can be decomposed into the following parts:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{bb} + \mathcal{H}_{bf}^{2p} + \mathcal{H}_{bf}^{3p}$$  \hspace{1cm} (2.1)

where,

$$\mathcal{H}_0 = \sum_k \epsilon_k^{f} f_k^\dagger f_k + \sum_k \epsilon_k^{b} b_k^\dagger b_k + \sum_k \epsilon_k^{bf} \psi_k^\dagger \psi_k$$  \hspace{1cm} (2.2)

$$\mathcal{H}_{bb} = g_{bb} \sum_{k, k', q} \hat{b}_{k+q}^\dagger \hat{b}_{k'}^\dagger \hat{b}_{k'} \hat{b}_{k+q}$$  \hspace{1cm} (2.3)

$$\mathcal{H}_{bf}^{2p} = g_{bf}^{2p} \sum_{k, k', q} \hat{f}_{k+q}^\dagger \hat{b}_{k}^\dagger \hat{b}_{k} \hat{f}_{k+q}$$  \hspace{1cm} (2.4)

$$\mathcal{H}_{bf}^{3p} = g_{bf}^{3p} \sum_{k, k', q} \psi_{k+q}^\dagger \hat{f}_{k}^\dagger \hat{b}_{k} \hat{b}_{k} \psi_{k+q}$$  \hspace{1cm} (2.5)

The fermionic $s$-wave scattering is usually suppressed due to the Pauli exclusion principle and can be omitted from the outset. Furthermore, we take the regime of net attraction $g_{bf}^{2p} < < g_{bf}^{3p}$ such that $H_{bf}^{2p}$ can be neglected. The kinetic energy part is given by $\mathcal{H}_0$, consisting of dispersion relations that are offset by the respective chemical potentials $\mu$. If the system is truly at chemical equilibrium then the sum of $\mu$’s of the reactants should equal that of the products.

In order to obtain controlled and qualitatively simple analytical results when integrating over momenta, we shall invoke a wide flat-band approximation where the two species of Fermions occupy separate kinetic bands with separate Fermi surfaces, and the effective masses are large enough such that the dispersion relations are slow varying in momentum space near the bottom of the bands: $\epsilon_k^f \approx \epsilon^0_f - \mu_f$, $\epsilon_k^b \approx \epsilon^0_b - \mu_b$. Although the fermionic atoms and molecules occupy decoupled Fermi surfaces the hybridization effects of the molecules with the atoms will manifest through the broadening of the molecular Fermi energy.

The Bosons are sufficiently condensed into a BEC phase such that the total number of Bosons is $N_b^0 \approx L^3 \langle n_b^0 \rangle_{\beta}^{1}$ for a restricted volume $L^3$ with $\epsilon_b^0 = \hbar^2 k_b^2 / 2m_b - \mu_b$. It follows that the two-body and three-particle Bose-Fermi couplings $g_{bf}^{2p}$ and $g_{bf}^{3p}$ can be tuned by a magnetic field via Eq.(1.1), thus driving the formation of molecular bound states or renormalizing the kinetic bands. The vertices associated with the $g_{bf}^{2p}$ type of interaction are shown in Fig I. Term $H_{bb}$ describes Boson-Boson interactions, which affect the condensation fraction $N_b^0 / N_b$ at low temperatures. A sharp transition into the BEC phase occurs when the chemical potential reaches a critical threshold at which $\mu_b^c = E_b^0$, where $E_b^0$ is the lowest energy that the Bosons can occupy. This transition can be understood as the breaking of the $U(1)$ gauge symmetry associated with the change of phase in the many-body wave function. For free Bosons in a box, $\mu_b^c = 0$. However, in a ultra cold atomic systems, the Bosons are usually confined by a superposition of harmonic trapping potentials, resulting in the critical value $\mu_b^c = (\hbar/2)(\omega_1 + \omega_2 + \omega_3)$, where $\omega_i$ is the trapping frequency along the $i$th direction. Hence, in physically realizable ultra cold atomic systems, the condensate fraction $N_b^0 / N_b$ and critical value $\mu_b^c = E_b^0$ strongly depend on the details of the confining potentials in addition to the 2 and 3 body interaction effects. If the condensate fraction is large enough, the Bogoliubov approximation can be employed, resulting in a renormalized Boson mass $m_b$ and dispersion relation which can be redefined in the original Hamiltonian.

III. MEAN FIELD THEORY

A. Derivation of the quasiparticle Hamiltonian

Here we investigate a special case of the system described by the Hamiltonian (2.1) and restrict our analysis to the degenerate molecules at the Fermi surface that hybridize with the same number of flat-band atomic Fermions. We can express the partition function as a functional integral,

$$Z = \int D\psi D\psi^\dagger Df Df^\dagger D\psi D\psi^\dagger \exp \left( - \int_0^\beta L(\tau)d\tau \right)$$  \hspace{1cm} (3.1)
with the Lagrangian given by
\[ \mathcal{L}(\tau) = \]
\[ = \hat{b}_0^\dagger \left( \frac{\partial}{\partial \tau} + \epsilon^b_0 \right) \hat{b}_0 + \sum_{k,m} \hat{f}_{km}^\dagger \left( \frac{\partial}{\partial \tau} + \epsilon^f_k \right) \hat{f}_{km} \]
\[ + \sum_m \hat{\psi}_m^\dagger \left( \frac{\partial}{\partial \tau} + \epsilon^\psi_m \right) \hat{\psi}_m \]
\[ + V \sum_{km} \hat{\psi}_m \hat{f}_{km} \hat{b} + \hat{b}^\dagger \hat{f}_{km} \hat{\psi}_m + \mathcal{H}_{bb} \]  
(3.2)
where the constant \( V \) is proportional to \( g_{bf}^3 \) and the degeneracy index \( m \) is summed to \( N_\psi \). Note that the degeneracy index which is attached to the operator \( \hat{f}_{km} \) reflects stoichiometry, in that the number of fermions that participates in the hybridization is fixed by the molecular level degeneracy. The resulting model described by Eq. (3.2) has a form that at first glance mirrors the slave boson mean-field theory of the infinite U Anderson model, for which the mean-field theory and \( 1/N \) corrections have been thoroughly studied. However the operator constraint which projects out the bosons is replaced by the bosonic repulsion and chemical potential terms. Nevertheless, the two models exhibit distinct phenomena which will be clarified in a later section.

Consider the effect of integrating out either both or one of the \( f \) and \( \psi \) fields. Since the \( H_{bf}^3 \) is linear all fields, we can make use of the Hubbard-Stratonovich transformation. A proper choice of the integration depends on dominant low energy scale of each particle species. Ref.10 for instance, integrates out only the molecular field \( \psi \) as follows,
\[ Z_{eff}^{2p} = Z_0^{\psi} Z_0^{b,f} \int D\hat{b}D\hat{b}^\dagger D\hat{f}D\hat{f}^\dagger e^{-S_{eff}^{2p} - S_{eff}^b - S_{eff}^f} \mathcal{H}_{bb}(\tau) d\tau \]  
(3.3)
where \( Z_0^{\psi} \) is an irrelevant constant and \( Z_0^{b,f} \) is the partition function of the non-interacting \( f,b \) systems. The effective action becomes
\[ S_{eff}^{2p} = \int_0^\beta V^2 \sum_{km} \hat{f}_{km} \left( \frac{\partial}{\partial \tau} + \epsilon^\psi_k \right)^{-1} \hat{f}_{km}^\dagger d\tau \]  
(3.4)
Thus, the resulting attractive 2-body interaction simply offsets the repulsive two-body coupling constant \( g_{bf} \). This binding energy reaches a threshold at which the scattering amplitude vanishes. Beyond this zero energy regime are 3-particle processes shown in Fig. 1 which is the central focus of this article.

On the other hand, if the \( f \) fields are integrated out followed by the \( \psi \) fields, then the partition function becomes
\[ Z_{eff}^b = Z_0^f \int D\hat{b}D\hat{b}^\dagger \exp \left( -S_{eff}^b \right) \]  
(3.5)
with
\[ S_{eff}^b = -NTr \ln \left[ \frac{\partial}{\partial \tau} + \epsilon^\psi_f - V^2 \hat{b}_0 + \hat{f}_{km} \right] \]
\[ + \int_0^\beta d\tau \left( \frac{\partial}{\partial \tau} + \epsilon^b_0 \right) \hat{b}_0 + \mathcal{H}_{bb} \]  
(3.6)
where \( Z_0^f \) is the non-interacting partition function of the fermionic atoms. By approximating this functional integral by the maximum value of its integrand for \( \tau \) independent bosonic fields, we arrive at our version of the mean-field approximation, where the \( \hat{b} \)'s of the low energy ground state will be replaced by their expectation values: \( \hat{b}_0 = \langle \hat{b}_0 \rangle = r \) and \( \hat{b}_0^\dagger = \langle \hat{b}_0^\dagger \rangle = r \), with \( r \) defined as a variational mean-field parameter that minimizes the free energy \( F = -T \ln Z \). Therefore, the following mean field Hamiltonian becomes,
\[ \mathcal{H}_{mf} = \mathcal{H}_{qp} - \mu_b r^2 + g_{bb} r^4 \]  
(3.7)
with the quasiparticle Hamiltonian given by the expression,
\[ \mathcal{H}_{qp} = \sum_k \epsilon^f_k \hat{f}_k^\dagger \hat{f}_k + \sum_m \epsilon^\psi_m \hat{\psi}_m^\dagger \hat{\psi}_m + \sum_{m,\bar{m},\bar{\phi}} \tilde{V} \hat{\psi}_m^\dagger \hat{f}_{m,\bar{\phi}} + \tilde{V}^* \hat{f}_{m,\bar{\phi}}^\dagger \hat{\psi}_m \]  
(3.8)

B. Quasiparticle Thermodynamics

The quasiparticle free energy \( F_{qp} \) can be determined from the partition function,
\[ F_{qp} = -\frac{1}{\beta_0} \ln Z_{qp} \]
\[ = -\frac{N_\psi}{\beta} \int_{-\infty}^\infty \ln \left( 1 + e^{-\beta (\omega - \mu_{qp})} \right) \rho_{qp}(\omega) d\omega \]  
(3.9)
where the quasiparticle density of states is given by
\[ \rho_{qp}(\omega) = \sum_n \delta(\omega - \epsilon_{qp}^n) = \frac{1}{\pi} \text{Im} \left[ \frac{\partial}{\partial \omega} \ln G_{qp}(\omega^{+}) \right] \]  
(3.10)
and the single quasiparticle Green’s function \( G_{qp}(i\omega_n) \) can be determined by solving the coupled equations for a broadened energy level that often appears in the analysis of local magnetic moments in metals,
\[ G_{qp}(i\omega_n)^{-1} = \left( i\omega_n - \epsilon^\psi_f - |\tilde{V}|^2 \sum_k (i\omega_n - \epsilon^f_k) \right)^{-1} \]  
(3.11)
After substituting Eq. (3.10) via Eq. (3.11) into Eq. (3.9)
and integrating by parts we have,

\[ F_{MF} = -\frac{N_\omega}{\pi} \sum_n \ln \left( -i\omega_n + \varepsilon_F^0 + \sum_{\vec{k}} \frac{|\tilde{V}_k|^2}{\omega_n - \varepsilon_F^0} \right) - \mu_b r^2 + g_{bb} r^4 \]

\[ = -\frac{N_\omega}{\pi} \int_{-\infty}^{\infty} \tilde{f}(\omega) \text{Im} [\text{ln} G_{\psi}^{MF}(\omega)] d\omega - \mu_b r^2 + g_{bb} r^4 \]

(3.12)

where the quasiparticle distribution \( \tilde{f}(\omega) \) is given by,

\[ \tilde{f}(\omega) = \frac{1}{e^{\beta(\omega - \mu_{qp})} + 1} \]

(3.13)

and the low temperature behavior follows from a Sommerfeld expansion of each Fermi-Dirac distribution in the equation above,

\[ \int_{-\infty}^{\infty} \tilde{f}(\omega) H(\omega) d\omega \approx \int_{-\infty}^{\mu_{qp}} H(\omega) d\omega + \frac{\mu}{2} T^2 \rho(\omega = \mu_{qp}) + \mathcal{O}(T^4) \]

(3.14)

where \( H(\omega) \) is a function that vanishes at as \( \omega \to 0 \). Next we utilize the wide band limit approximation, where the integration is taken over a width \( 2W \) with a constant density of states \( \rho_0 \), and the summation reduces to

\[ \sum_{\vec{k}} \frac{|\tilde{V}_k|^2}{\omega_n - \varepsilon_F^0} = -i\Delta \text{sgn}(\omega_n), \]

yielding

\[ F_{MF} = -\frac{N_\omega}{\pi} \int_{-W}^{W} \tilde{f}(\omega) \tan^{-1} \left( \frac{r^2 \Delta}{\varepsilon_F^0 - \omega} \right) d\omega - \mu_b r^2 + g_{bb} r^4 \]

(3.15)

and the ground state energy (\( T = 0 \)) evaluates to,

\[ E_{gs} = -\frac{N_\omega \Delta}{\pi} + \frac{N_\omega \varepsilon_F^0}{\pi} \tan^{-1} \left( \frac{\Delta}{\varepsilon_F^0} \right) + \left( \frac{N_\omega \Delta}{2\pi} \right) \ln \left( \frac{\varepsilon_F^0 + \Delta}{\varepsilon_F^0 - \Delta} \right) - \mu_b \Delta \frac{\Delta}{\Delta^2} + g_{bb} \left( \frac{\Delta}{\Delta^2} \right)^2 \]

(3.16)

with \( \Delta = r^2 \Delta \) is determined through a minimization that solves the equation,

\[ \frac{\partial E_{gs}}{\partial \Delta} = \frac{N_\omega}{2\pi} \ln \left( \frac{\varepsilon_F^0 + \Delta}{\varepsilon_F^0 - \Delta} \right) - \mu_b \Delta \frac{\Delta}{\Delta^2} + 2 g_{bb} \frac{\Delta}{\Delta^2} = 0 \]

(3.17)

Next, we invoke the Friedel sum rule, which relates the quasiparticle occupation to the self-energy corrections and broadening factor\( ^{20} \),

\[ n_{\varepsilon_F^0} = \frac{N_\psi}{\pi} \tan^{-1} \left( \Delta / \varepsilon_F^0 \right) \]

(3.18)

Consequently, in order to maintain a finite density of levels as \( N_\psi \to \infty \), then \( \Delta \to 0 \). Taking this limit in Eq. (3.17) leads to the following zero temperature shift of the bosonic chemical potential,

\[ \delta \mu_b(T = 0) = \frac{N_\psi \Delta}{\pi} \ln \left( \frac{k_B T_F^{\psi}}{W} \right) \]

(3.19)

with the thermal energy scale of the molecules defined by \( \varepsilon_F^0 \equiv k_B T_F^{\psi} \) which is valid provided that \( \varepsilon_F^0 \ll W \). Eventually, the BEC will be depleted if this correction shifts the bosonic chemical potential above its lowest available energy. Moreover, the low temperature behavior can be obtained by applying the expansion of Eq. (3.14) in the wide band limit to yield,

\[ \delta \mu_b(T \to \infty) \simeq \frac{\pi N_\psi}{6} \left( \frac{T}{T_F^{\psi}} \right)^2 + \mathcal{O}(T^4) \]

(3.20)

Thus, these corrections determine the large \( N_\psi \), low \( T \) behavior as compared to the characteristic temperature \( T_F^{\psi} \). However, for a proper sense of the behavior near \( T_F^{\psi} \), it is necessary to go beyond the mean field theory.

C. Quasiparticle weight and Fermi liquid theory

In order to formally establish a local Fermi-liquid picture for a broadened molecular level, one must determine the quasiparticle weight and establish a 1 to 1 correspondence between the quasiparticles and original molecular levels. The propagator of the broadened molecular Fermi level is related to the quasiparticle propagator by the relation,

\[ G_\psi(\omega) = |\langle b \rangle|^2 G_{qp}(\omega) \]

\[ = |\langle b \rangle|^2 \left( i\omega_n - \varepsilon_F^0 - |\tilde{V}_k|^2 \left( \sum_{\vec{k}} (i\omega_n - \varepsilon_F^0) \right) \right)^{-1} \]

(3.21)

In the context of the theory of the Fermi liquid, \( |\langle b \rangle|^2 = r^2 \) plays the role of the wave function renormalization factor or quasi-particle weight \( z \). Furthermore, \( z \) can be related to several conservation laws that arise from constraints on the volume of the Fermi surface. Recent studies by Powell et al. have derived such laws given for \( H_{qp} \) by applying Luttinger’s theorem which states that the volume of the respective Fermi surfaces is conserved even in the presence of interactions.\( ^{20} \) These conservation laws take the form,

\[ z = |\langle b \rangle|^2 = N_b - |\langle \psi \rangle|^2 \]

\[ |\langle f \rangle|^2 = N_f - |\langle \psi \rangle|^2 \]

(3.22)

Additionally, by applying the relation above one can then generate conserved charges. Formally, with any conservation law there is an associated quantum number \( Q \) such that quasi particle charges can be defined. However, \( Q \) should vanish if the particle-hole symmetry of the system is strictly upheld. More importantly, the validity of these conservation laws can be tested via the measurement of \( z \) and \( Q \), which should be directly accessible from spectral line broadening measurements and laser absorption that can capture velocity and density distribution profiles to a high degree of precision.\( ^{14} \)
D. Diagrammatic approach

An alternative approach, which will be useful in considering non-Gaussian fluctuations is to derive the preceding results diagrammatically from the standard Green’s function technique involving an expansion in powers of the hybridization $V$. The resulting thermal, one-particle propagator with Lorentzian broadening can be computed from the series in Fig. 2(b). Additionally, another propagator of interest describes the mixed molecule-Fermion propagator with Lorentzian broadening can be computed the hybridization $\tilde{\Sigma}$.

Next we can proceed to determine the change in mean-field free energy of order $N_\psi$. (a) Ring diagram summation and (b) Hartree approximation.

IV. BEYOND MEAN-FIELD THEORY

Previously in the mean field solution, $\hat{b}$ and $\hat{b}^\dagger$ were replaced by their expectation values. Beyond mean field theory we make use of the transformation $\hat{b} = \langle \hat{b} \rangle = \tilde{b} + r$ and $\hat{b}^\dagger = \langle \hat{b}^\dagger \rangle = \tilde{b}^\dagger + r$, where $\tilde{b}$ and $\tilde{b}^\dagger$ are static operators that obey the Bose commutation rules. After making these replacements, the Hamiltonian separates into two parts consisting of the mean-field part given by

\[ G^{MF}_{\psi,f}(i\omega_n) = \frac{(i\omega_n - \varepsilon_{\tilde{f}})^{-1}}{(i\omega_n - \varepsilon_{\tilde{f}}) - \tilde{\Sigma}} \] (3.23)

Next we can proceed to determine the change in mean-field free energy of order $N_\psi$ due to $H_{bf}^{3p}$. The mean-field equations follow from a perturbation series in the usual way involving Feynman diagrams. The first approach follows from the linked cluster expansion where the mean-field free energy is computed from the sum of the ring diagrams as shown in Fig. 3(a). The second approach follows from the Hartree tadpole diagram as shown in Fig. 3(b), which is made to cancel the external field terms, reducing to the desired mean-field equation. In both cases we recover Eq. (3.17).

\[ \mu_{bf} + 2g_0r^3 + \sum_{n,k} \tilde{V}_k G^{MF}_{\psi,f}(i\omega_n) = 0 \] (4.1)

After carrying out the frequency summation and $k$ integration for a wide flat band, we exactly recover Eq. (3.17) and the mean-field result for large $N_\psi$.

A. Hartree approximation

The Hartree approximation can be obtained by analyzing the tadpole diagram of Fig. 3(b), which contains a closed loop of the mixed amplitude $G^{MF}_{\psi,f}(i\omega_n)$, represented by Eq. (3.23) and a static Bose interaction line. Here the mean-field equation can be derived by choosing the external field $r$ such that it cancels the the tadpole diagram. This condition is satisfied by adjusting the terms that are linear in the Bose field to zero as follows:

\[ \mu_{bf} + 2g_0r^3 + \sum_{n,k} \tilde{V}_k G^{MF}_{\psi,f}(i\omega_n) = 0 \] (4.1)

B. Random Phase Approximation

The available expansion parameter in our model is $1/N_\psi$ and in order to justify the Gaussian saddlepoint (mean-field theory) of the previous section it is necessary to examine fluctuations systematically in a $1/N_\psi$ expansion. First we can examine several second order diagrammatic contributions to the Boson propagator,

\[ G_b(i\omega_n) = \left( i\omega_n - \varepsilon_b^b + \Sigma_b \right)^{-1} \] (4.2)

where $\Sigma_b$ is the exact self energy, which can be expanded perturbatively in the usual manner by including various virtual processes generated by Wick’s theorem. Several of these self energy contributions are shown in Fig. 3(b) however only diagram (a) will contribute at order $1/N_\psi$. A proper renormalization of the perturbation series can be accomplished by summing a particular subset of the diagrams to infinite order as shown in Fig. 3(c). This partial diagram summation is known as the Random phase approximation, where in our case the bosonic interaction is effectively renormalized by a pseudo-dielectric response of the Fermion-molecule polarization bubble, which sums to:

\[ \Delta F_{RPA} = \frac{1}{\beta} \sum_n \ln \left( -i\omega_n + \varepsilon_b^b + \Sigma_b^{(2)}(i\omega_n) \right) \] (4.3)
and the irreducible Fermion-molecule bubble of Fig. 5 follows the usual frequency summation rules,

\[ \Sigma_b^{(2)}(i\omega_n) = \frac{N\nu |V|^2}{\beta} \left( \sum_{k,F} \frac{1}{i\omega_n + \varepsilon_{k,F} - \varepsilon^b_F} \right) \left( \sum_{k,F} \frac{|\Sigma_{k,F}|^2}{(i\omega_n + \varepsilon_{k,F} - \varepsilon^b_F)} \right)^{-1} \]

\[ = \frac{N\nu |V|^2}{\beta} \sum_{k,F} \frac{1}{i\omega_n - \varepsilon_k} \left( \frac{1}{i\omega_n - \varepsilon_k} - 1 \right) \frac{1}{(\varepsilon_k - \varepsilon^b_F - \Delta \text{sgn}(\omega_n))} \]  

(4.4)

\[
\delta\mu_b(T = 0) = \frac{N\nu \Delta}{\pi} \ln \left( \frac{\varepsilon_F}{W} \right) + \frac{(N\nu \Delta)^2}{N\nu \pi} \int_{-W}^{0} \frac{de}{\varepsilon_k} \frac{1}{\varepsilon_k - \varepsilon_F} \left( \varepsilon - \frac{\varepsilon^b_F - N\nu \Delta}{\pi} \ln \left( \frac{\varepsilon - \varepsilon^b_F}{W} \right) \right)^{-1}
\]

(4.5)

in which the integral of the RHS of Eq.(4.5) renormalizes the chemical potential. Let us term this integral \( I \) and focus on its bandwidth \( W \) dependence. \( I \) can be conveniently re-expressed as,

\[
I = \frac{\kappa^2 \pi T \psi}{N} \int_{0}^{W/T \psi} dx \frac{x}{1 + x} \left( x + \frac{\varepsilon^b_F}{\varepsilon^F} + \kappa \ln(1 + x) \right)
\]

(4.6)

where \( \kappa \equiv (N\Delta)/(\pi \varepsilon^F) = (N\Delta)/(\pi T \psi) \), for \( k_B = 1 \). This expression can be integrated by parts, retaining the dominant leading order contribution, and dropping higher order logarithmic corrections,

\[
I \sim \frac{\mu^2 \pi}{N\nu} \frac{W - \varepsilon^F}{W/\varepsilon^F + \varepsilon^b_F/\varepsilon^F + \kappa \ln(1 + W/\varepsilon^F)}
\]

(4.7)

This yields the final expression,

\[
\delta\mu_b(T = 0) \propto \frac{N\nu \Delta}{\pi} \ln \left( \frac{\varepsilon_F}{W} \right) + \frac{\mu^2 \pi}{N\nu} \frac{W - \varepsilon^F}{W/\varepsilon^F + \varepsilon^b_F/\varepsilon^F + \kappa \ln(1 + W/\varepsilon^F)}
\]

(4.8)

for the appropriate low temperature dependence one can again apply the Sommerfeld expansion as indicated earlier. Consequently, the convergence of the non-Gaussian fluctuations is verified and such corrections are sufficiently finite that mean field theory is stable at order \( 1/N\psi \), and the quasiparticle description holds in the limit \( N\psi \to \infty \).

V. DISCUSSION: CHEMICAL EQUILIBRIUM AND THE SUPERFLUID-INSULATOR PHASE TRANSITION

The existence of fermions will effect the superfluid-insulator transition of the Boson atoms at large \( g_{bb} \). For \( H_{2p} \) type interactions this effect was explored by Refael and Demler, who found that the superfluid phase was suppressed by fermionic screening fluctuations. On the other hand, Tewari et. al. found a suppression of the Mott insulating lobes arising from a bosonic screening effect. Consequently, the total effect is complex and the phase boundaries can be enhanced in either direction.

For our particular system with finite \( g_{3p} \), the renormalization of \( \mu_b \) has important consequences in different physical phenomena which are experimentally measurable. In the preceding analysis we identified a characteristic crossover temperature \( T_{\psi} \) that directly depends on

FIG. 5: RPA-like corrections to the mean-field free energy
the magnitude of $\varepsilon_F^\psi$. Thus, by adjusting the molecular Fermi level $\varepsilon_F^\psi$, one sets the crossover scale, given that our analysis is valid at temperatures $T \ll T_F$. In accordance with the Kondo-like crossover, we expect $\mu_b$ to develop a local peak indicating that our approximation is breaking down, separating the low and high temperature regimes. This enhancement will affect the $\mu$'s and reaction rates of the other species, given that chemical equilibrium implies that the $\mu$'s of the components obey a rigid sum rule. Since the bosons contain a self interaction term, at very large repulsion the system is expected to undergo a transition into a Mott insulating state, and the mean-field phase diagram contains various insulating lobes separated by fixed values of the ratio $\mu_b$. The Mott insulating states are incompressible implying that $\frac{\partial N}{\partial \mu_b} = 0$ and the phase boundary is governed by a zeros of some function $\phi(\mu_b/U)$. Therefore we predict qualitatively that by adjusting $\varepsilon_F^\psi$ to smaller values, the phase boundaries of the lobes will be shifted downwards via the enhancement of $\mu_b$.

As mentioned earlier we have studied a model of a many-body chemical reaction. Chemical equilibrium requires that $\sum_{i=reactants} \mu_i = \sum_{j=products} \mu_j$. If the binding and disassociation is classical in nature, or $\psi \rightarrow f + b$ then conventional chemical thermodynamics in liquid solution using the law of mass action, relating the relative concentrations $\rho_\psi$ and reaction rate $K$ is appropriate,

$$K = \frac{\rho_b \rho_f}{\rho_\psi} \sim e^\varepsilon_\psi / k_b T$$  \hspace{1cm} (5.1)

which is a thermally activated process that limits $K$ by the activation energy $\varepsilon_\psi$. However, in ultra-cold atomic mixtures with tunable resonant interactions, the sweeping of a magnetic field near the Feshbach resonance will be governed by Fermi's golden rule instead of the law of mass action, controlling the bare coupling $g_{\psi f}$ and subsequently $K$. Hence, this renormalization of the reaction rate is clearly a quantum many body problem beyond the scope of ordinary chemistry.

For an accurate physical interpretation, it is important to make note of certain differences between the Bose-Fermi mixture that we explored here and the slave Boson theory of the infinite $U$ Anderson model. Evidently, the final expression for the bosonic chemical potential corrections given by Eq. (4.8) does not contain any of the problematic infrared divergences of the Kondo problem which are related to the subtle restoration of gauge invariance. There are two primary reasons for this. First it must be made clear that we do not enforce any Lagrange multipliers onto the Hamiltonian $H_0$, as the Bosons and Fermions are real physical particles that do not represent vacancies and occupied states. A Lagrange multiplier that reduces the span of the extended Hilbert space introduces an additional mean field parameter which renormalizes $\varepsilon_F^\psi$. Therefore, taking an additional derivative of the RPA correction of integral $\Delta$ with respect to the renormalized $\varepsilon_F^\psi$ yields an infrared divergent integral. Another difference is that in our unconstrained system, the Bosons or the molecules do not arise from the decomposition of the Hubbard operators, $\hat{X}_{m,0} = \hat{\psi}_m^\dagger \hat{b}$, $\hat{X}_{0,m} = \hat{\psi}_m^\dagger \hat{b}$, $\hat{X}_{0,0} = \hat{b}^\dagger \hat{b}$, $\hat{X}_{m,m} = \hat{\psi}_m^\dagger \hat{\psi}_m$. Such a decomposition for a correlated electron systems retains a local gauge symmetry $\hat{b} \rightarrow e^{i\theta} \hat{b}$, $\hat{b}^\dagger \rightarrow e^{-i\theta} \hat{b}^\dagger$ with a simultaneous change $\psi \rightarrow e^{i\theta} \hat{\psi} \rightarrow e^{i\theta} \hat{\psi}$. This symmetry is absent in our system, therefore there are no local gauge symmetry breaking issues.

One possible deficiency of our unconstrained mean-field theory was that we did not enforce a conservation of the volumes of the two Fermi surfaces. In particular, the conservation laws generated by Powell et al. derives directly from Luttinger’s theorem and a proper mean-field theory that reflects chemical equilibrium should enforce these constraints as Lagrange multipliers onto the Hamiltonian, thus generating a more complicated quasiparticle theory as observed in the Kondo problem, possibly generating an infrared divergence at order $1/N$.

Another important deficiency of our model is from restricting the interactions to the hybridization of one degenerate molecular level with a wide flat atomic band and the excitation spectrum of the Bose-Fermi mixture is qualitatively described by a Lorentzian broadened quasiparticle with width $\Delta$. The final result of Eq. (4.8) describes a bosonic chemical potential with a renormalization controlled by the ratio $\varepsilon_F^\psi / W$, valid in the regime $\varepsilon_F^\psi << W$, which shall ultimately impact the condensation behavior. Although we have specifically chosen an $N_\psi$-fold degenerate at the molecular Fermi surface, the analysis can be generalized to any energy or range of energies that are likely to hybridize with the atoms via $\rho_\psi$.

In conclusion, we have explored a wide variety of phenomena associated with the mean-field description of a tunable many-body chemical reaction that can be described in terms of a local Fermi liquid picture. These features can be probed directly by velocity and density distribution measurements via laser beam absorption. Furthermore, we have demonstrated a unique relationship between the condition for chemical equilibrium and the criteria for incompressibility observed in the Mott insulating phases of the superfluid-insulator transition for the Bosons. Although we only considered a single molecular level it is conjectured that the certain qualitative features of the excitation spectrum of Hamiltonian (2.0) still admit a quasiparticle description, as the restoration of the momentum dependent self-energy corrections do not alter the Lorentzian broadened form of the mean-field Green’s function given by Eq. (5.1) and subsequently the effective bosonic action should be renormalized in a similar fashion. However, it is necessary to restore the explicit momentum dependence in the interactions to study the pairing bubbles of the self-energy that may detect screening/dielectric effects, and the novel possibility of nesting behavior and other Fermi surface instabilities that may
FIG. 6: The contour \( C \) of Eq. (A2) is deformed to the contour \( C' \), allowing for a precise evaluation.

indicate a breakdown of this quasiparticle picture.

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Appendix A: Evaluation of \( \Sigma^{(2)}(\imath \omega_n) \)

Here we carry out the evaluation of the of the second order self-energy term \( \Sigma^{(2)}(\imath \omega_n) \) as discussed in

Ref.\textsuperscript{23,24}. Starting with Eq. (4.3), where \( \omega_\nu = (2\nu + 1)\pi/\beta, \omega_n = 2\pi n/\beta \) for integer values of \( \nu \) and \( n \), the \( \omega_\nu \) integration can be expressed as a contour integral by applying the Matsubara summation procedure. We can approximate the atomic Fermion propagator as,

\[
\sum_k \left( \imath \omega_n + \varepsilon_k^b \right)^{-1} \approx -\imath \pi \rho \text{sgn}(\omega_n) \quad (A1)
\]

which for a constant density of states of width \( 2W \) yields the following contour integral,

\[
\Sigma^{(2)}(\imath \omega_n) = \frac{N_\psi \Delta}{\pi} \ln \left( \frac{\imath \omega_n - \varepsilon_F^\psi + \tilde{\Delta} \text{sgn}(\omega_n)}{\varepsilon_F^\psi - \tilde{\Delta} \text{sgn}(\omega_n)} \right)
\]

\[
+ \frac{N_\psi \Delta}{2\pi} \ln \left( \frac{\varepsilon_F^\psi}{W^2} \right) \quad (A2)
\]

Next to get the RPA free energy correction, the above expression is substituted into Eq. (4.3), and the Matsubara summation over the the Bose frequencies can be performed by extracting the imaginary part and deforming the contour to surround the negative real axis to yield,

\[
\Delta F_{\text{RPA}} = -\frac{1}{\pi} \int_{-W}^{0} \tan^{-1} \left[ \frac{\varepsilon}{\varepsilon - \varepsilon_k^b + (N_\psi \Delta/\pi) \ln \left( \varepsilon_F^\psi - \varepsilon \right)} \right] d\varepsilon \quad (A4)
\]

To the leading order in \( 1/N_\psi \) this is simplified to yield,

\[
\Delta F_{\text{RPA}} = -\frac{1}{\pi} \int_{-W}^{0} d\varepsilon \frac{\tilde{\Delta}}{\pi} \left( \frac{1}{\varepsilon - \varepsilon_F^\psi} + \frac{1}{\varepsilon_F^\psi} \right) \left( \varepsilon - \varepsilon_k^b - \frac{N_\psi \Delta}{\pi} \ln \left| \varepsilon - \varepsilon_F^\psi \right| \right) \quad (A5)
\]
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