Renormalized atomic interaction and quadrupole excitations of cold Fermi gas near Feshbach resonance

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(Dated: January 13, 2022)

We present a model space particle-hole Green’s function calculation for the quadrupole excitations of cold Fermi gas near Feshbach resonance using a simple model where atoms are confined in a harmonic oscillator potential. Both the Tamm-Dancoff and random phase approximations are employed. By summing up exactly the ladder diagrams between a pair of interacting atoms to all orders, we obtain a renormalized atomic interaction which has well defined and identical limits as the scattering length tends to $\pm \infty$. The experimentally observed abrupt rise in the excitation spectrum and its associated large decay width are satisfactorily reproduced by our calculation.

PACS numbers: pacs

Introduction: The Feshbach resonance was originally used in nuclear physics \cite{1}, to describe a resonance in neutron scattering due to the formation of a quasi-bound state between the scatterer and the incident particle. During the past several years, this resonance was experimentally realized in ultracold alkali gases \cite{2,3}. It has many interesting features and has opened a new era to the study of ultracold gases. It serves as an experimental control mechanism to tune the scattering length over a wide range, essentially from positive to negative infinity. Through such process, the inter-atomic effective interaction could also be experimentally controlled. As a result, ultracold alkali gases have provided us a unique many-body system with tunable interactions, and they have been the focus of many theoretical studies (See, e.g. \cite{4,5}). As the magnetic field is tuned across the Feshbach resonance, ultracold Fermi gases have been observed to undergo the well known BCS-BEC crossover \cite{6,7,8}.

Collective oscillations of trapped cold Fermi gas have been recently measured \cite{9,10}, with important and very interesting findings for the collisional-, collisionless- and particularly the transitional-regime in between. In the collisional regime, the oscillation frequency is lower than the trap frequency and it varies continuously across the collisional regime, the oscillation frequency is lower than particularly the transitional-regime in between. In the collisionless regime, the frequency is essentially constant, close to the trap frequency. In the transitional regime, however, an abrupt rise of frequency together with a strong damping rate were observed. To explain these findings has been a challenging task. In the collisional regime, pioneering hydrodynamical studies \cite{11,12} have been carried out.

In this Letter, we would like to carry out a microscopic study for the quadrupole excitations of trapped cold Fermi gas, aiming primarily at the transitional and collisionless regimes. We shall use a particle-hole Green’s function framework which has been commonly used in nuclear physics \cite{13,14,15}. When applying this method to nuclear systems, nucleons are placed in an oscillator well and particle-hole excitations are treated to all orders using either the Tamm-Dancoff or random-phase approximations, commonly referred to as TDA and RPA respectively. We shall use a similar approach for the above gas system, with its atoms trapped in a harmonic oscillator potential.

In the following section, we shall first briefly describe the model space particle-hole Green’s function method \cite{14} which we shall employ. A specific feature of the atomic interaction for cold Fermi gases is that it is divergent at Feshbach resonance. \cite{4,16,17,18,19} This interaction is not suitable for being used directly in microscopic calculations; it needs to be renormalized (or tamed) beforehand. We shall discuss that the well known Brueckner reaction matrix method, which has been widely and successfully used in nuclear matter \cite{23,24,25} and finite nuclei \cite{26}, is very useful in this regard. We shall use this method to derive a renormalized atomic interaction which is smooth and well behaved at the Feshbach resonance. Our results together with some calculational details will be reported and discussed in the last section. A summary will also be presented.

Model space particle-hole Green’s function method: In this section we briefly describe the model space particle-hole (ph) Green’s function method \cite{14} for calculating the quadrupole excitations of cold Fermi gas. We consider atoms as spin $1/2$ fermions confined in a spherical harmonic oscillator potential of oscillator spacing $\hbar \omega_{osc}$ and oscillator length $a_{osc} = \sqrt{\hbar/m\omega_{osc}}$. In our present calculation, we assume the atoms remain normal throughout. As pointed out in \cite{12}, in trapped fermi gas experiments, the superfluid component always resides in the interior of the trap and had little contribution to the quadrupole excitation. We shall use $\hbar \omega_{osc}$ and $a_{osc}$ respectively as the units for energy and length.

We treat the trapped gas as a closed shell system of $N_F$ closed shells. For example, the $N_F = 6$ system has 112 atoms and in its unperturbed ground state the lowest 6 oscillator shells are completely filled. The excitation energies, denoted by $E_n$, of the system are calculated by solving the ph RPA equation \cite{14,15}

$$AX_n + BY_n = E_n X_n,$$

$$-B^* X_n - A^* Y_n = E_n Y_n. \quad (1)$$

Here $A$ represents the sum of the unperturbed ph energy
gap and the TDA vertex function, namely
\[ A(\phi h, \phi' h') = (\epsilon_p + S(p) - \epsilon_h - S(h))\delta_{\phi h, \phi' h'} + \Sigma(\phi h, \phi' h'), \tag{2} \]
where \( S \) denotes the one-body vertex function and \( \Sigma \) the two-body \( \phi h \) vertex function. They are composed of irreducible diagrams as illustrated in Fig. 1. Here each dashed-line represents the vertex of the effective atomic interaction \( V \). Note that the diagrams are time ordered with retarded single particle propagators \[14]. \( B \) denotes the ground-state correlation vertex, whose diagrammatic structure is also illustrated in Fig. 1. All the diagrams contained in the vertex function must be irreducible in the sense that any intermediate state of such diagrams must be orthogonal to the \( \phi h \) model space \[14].

![Fig. 1: Diagrams for one- and two-body vertex functions. The dotted line vertex represents a \( \phi \)-\( h \) vertex of the effective atomic interaction.](image)

The transition amplitudes \( X \) and \( Y \) of Eq.(1) are \( X_n(\phi h) = \langle \Psi_n | a^\dagger_{\phi h} | \Psi_0 \rangle \) and \( Y_n(\phi h) = \langle \Psi_n | a^\dagger_{\phi h} | \Psi_0 \rangle \), where \( \Psi_n \) and \( \Psi_0 \) represent the \( n \)th excited- and ground-state wave functions respectively. When the ground state correlation vertex \( B \) is suppressed, Eq.(1) becomes the TDA equation. We consider that the atomic gas is trapped by a harmonic oscillator potential. Thus \( \epsilon \) of Eq.(2) is the harmonic oscillator single particle energy.

In carrying out the RPA/TDA calculations, a restricted model space near the Fermi surface is employed. We use a hole space consisted of three major shells immediately below the Fermi surface, namely shells \( N_F \) to \((N_F - 2)\), and for particles one major shell immediately above. The external lines \( \phi, h, \phi' \) and \( h' \) of the vertex function diagrams of Fig. 1 are all confined in this space. That we use a restricted model space requires a model-space renormalization, so that the effects from the orbitals outside the model space are taken care of. The inclusion of the higher order diagrams in the vertex functions is for this renormalization purpose. As an example, let us consider the third order diagrams of Fig. 1. They all have a common “ladder” structure, with repeated interactions between a pair particle lines. The intermediate states of them include all the particle states outside the model space, so that our \( \phi h \) calculation within a small model space have renormalization contributions from the space outside. As discussed later, this type of “ladder” diagrams can be summed up to all orders, giving rise to the reaction matrix interaction.

**Separable reaction matrix interaction:** In carrying out our microscopic particle-hole calculations, we must first have an atomic interaction on which our many-body calculation is based. This interaction \[4, 16, 17, 18, 19\] has a specific form and is commonly given as
\[ V = \frac{4\pi}{m} a_s \delta(r), \tag{3} \]
where \( m \) denotes the atomic mass, and \( a_s \) is the s-wave scattering length which can be tuned across the Feshbach resonance, essentially from \(-\infty \) to \(+\infty \). The above is an effective interaction for one hyperfine channel, in the sense that we consider atoms as of only one hyperfine state with the other hyperfine states having been integrated out by renormalization. In our calculation we assume atoms interacting with s-wave interactions only.

The above interaction is clearly divergent at the Feshbach resonance (the unitary limit) where \( a_{s} \rightarrow \pm \infty \), and there is difficulty in using it in microscopic calculations. As described in section 2, to carry out the TDA/RPA calculations, we need first calculate the vertex functions \( S \), \( \Sigma \) and \( B \). As illustrated in Fig. 1, these vertex functions are composed of irreducible diagrams. Near the Feshbach resonance, the above atomic interaction is divergent and consequently every diagram in the figure is divergent; calculation cannot go on unless we use a different approach. This type of difficulty has been well known in nuclear matter theory and has been overcome by the Brueckner reaction matrix theory \[23, 24, 25\]. There each vertex of the bare nucleon-nucleon interaction \( V_{NN} \) is nearly divergent because of its very strong repulsive core. However, the Brueckner reaction matrix \( G \) given by the all order summation of the \( V_{NN} \) interactions between a pair of nucleons is finite and well behaved.

We apply a similar reaction matrix approach to our present atomic gas calculation. Let us consider the diagrams for the one-body vertex function \( S \) of Fig. 1. Clearly they have the structure of a geometric series and can be summed up to all orders. Let us define a reaction matrix \( R \) as
\[ R = V + V Q e \langle \omega - H_0 + i0^+ \rangle Q e V + V Q e V Q e V + \ldots = V + V Q e R, \tag{4} \]
where \( e \) stands for \( \langle \omega - H_0 + i0^+ \rangle \) and \( Q \) the Pauli exclusion operator. (Recall that we use time-ordered diagrams with retarded single particle propagators.) \( H_0 \) is the unperturbed Hamiltonian for the pair of interacting atoms, and \( \omega \) is the starting energy which we shall discuss later. The role of \( Q \) is to ensure that the intermediate states of \( R \) must be outside of the chosen model space. In terms of \( R \), the sum of all the ladder-type diagrams as shown by \( S(p) \) of Fig.1 is now \( \langle \phi h | R | \phi h \rangle \). Similarly the sum for \( \Sigma \) is \( \langle \phi h' | R | \phi h' \rangle \) and for \( B \) is \( \langle \phi p' | R | hh' \rangle \). We shall include only diagrams first order in \( R \) for the vertex function as listed in Fig.2.
In calculating $R$, we shall use an angle average approximation \[24\] for the Pauli operator, namely $Q$ is approximated by $Q_{av}(q, k_F)$ where $q$ is the relative momentum and $k_F$ is an average Fermi momentum which can be estimated by using for example a local density approximation. In addition, we shall use plane-wave intermediate states and an average starting energy $\omega$. Accurate methods for calculating the nuclear reaction matrix have been developed \[26\], and we plan to use them in a future work. With these approximations, the above $R$ matrix becomes

$$R(k, k', \omega) = V(k, k') + \frac{2}{\pi} \int_0^\infty V(k, q) \frac{Q_{av}(q, k_F)}{\omega - q^2 + i0^+} R(q, k', \omega) q^2 dq,$$  \hspace{1cm} (5)

where $k, k', q$ are the relative momenta.

Let us now consider the above $R$ matrix for the scattering length dependent potential of Eq.(3). Schematically, $R$ is given by $R = V/(1 - VQ/e)$ and may have well defined limits as $V \to \pm \infty$. But how to obtain them accurately is a difficult task in general, and it may not be feasible to obtain them reliably using numerical methods. We feel that $R$ has to be solved analytically in order to obtain the above limits reliably. In this regard, we resort to the separable potential approach which has been widely used in nuclear physics \[20, 21, 22\]; the reaction matrix with this approach can be analytically solved. We shall use a separable potential which corresponds to a short range non-local Yukawa potential of the form $a_s e^{-r \mu} e^{-r' \mu}/(\mu^2 r r')$, $\mu^{-1}$ being the range of the interaction and $r$ and $r'$ the inter-atomic radial distance. We shall use large $\mu$ to simulate short range potential. In momentum space this potential becomes

$$V(k, k') = a_s \alpha f(k) f(k'); \quad f(q) = \frac{1}{\mu^2 + q^2}, \quad \alpha = 8\pi \frac{k^2 \mu^3}{m a_{osc}}.$$  \hspace{1cm} (6)

With this separable potential, the reaction matrix, which is complex, is also separable and is obtained analytically as

$$R(k, k', \omega) = [\eta_{rc}(\mu, \omega) + i\eta_{im}(\mu, \omega)] f(k) f(k'),$$  \hspace{1cm} (7)

with

$$\eta_{rc}(\mu, \omega) = \frac{\lambda(\mu, \omega)}{D(\mu, \omega)},$$
$$\eta_{im}(\mu, \omega) = \frac{-\lambda(\mu, \omega)^2 \sqrt{\omega}}{D(\mu, \omega) (\mu^2 + \omega^2)},$$
$$D(\mu, \omega) = 1 + \frac{\omega \lambda(\mu, \omega)^2}{(\mu^2 + \omega^2)},$$
$$\lambda(\mu, \omega) = \frac{a_s \alpha}{1 - a_s \alpha I(\mu, \omega)}.$$  \hspace{1cm} (8)

Note that $\eta_{im} = 0$ if $\omega < 0$. In the above, $I$ is the integral

$$I(\mu, \omega) = \frac{2}{\pi} P \int_0^\infty \frac{Q_{av}(k, k_F)}{(\omega - k^2)(\mu^2 + k^2)^2} k^2 dk,$$  \hspace{1cm} (9)

where $P$ denotes principal value integration. In a recent study of fermionic atoms in optical lattices \[27\], a Gaussian separable interaction is employed and its strength has similar dependence on $a_s$ as the above $\lambda$.

It is readily seen that $R$ has well defined limits as $a_s \to \pm \infty$. Only the factor $\lambda$ of Eq.(8) is dependent on $a_s$, and at the above limits it becomes

$$\lambda_{\pm \infty}(\mu, \omega) = \frac{-1}{I(\mu, \omega)}.$$  \hspace{1cm} (10)

Thus our $R$-matrix has a common well defined limit at the Feshbach resonance, being the same whether $a_s \to +\infty$ or $a_s \to -\infty$.

For dilute systems, $k_F$ should be small. We have calculated the above $R$ matrix for several values of $k_F$, and found that the results for $R$ calculated with $k_F$ ranging from 0 to 1 are quite close to each other. For the case of $k_F = 0$ and $\omega > 0$, the integral of Eq.(9) becomes

$$I(\mu, \omega) = \frac{\omega - \mu^2}{2\mu(\omega + \mu^2)^2},$$  \hspace{1cm} (11)

which is only weakly energy dependent if $\omega$ is much smaller than $\mu^2$. Thus our $R$-matrix interaction is nearly energy independent for cold (small $\omega$) dilute (small $k_F$) system with a short-range (large $\mu$) interaction.

Results and discussion: We now describe some details about our calculations for the energy and decay width of the quadrupole excitation. They are obtained from the solutions of the RPA/TDA equation (1), using the vertex functions given by the diagrams of Fig. 2. These diagrams are calculated from the $R$-matrix interaction, using the methods detailed in \[26\]. Since $R$ is complex, Eq.(1) is now a complex equation and its eigenvalues $E_n$ are generally complex. We write $E_n$ as $(ReE_n - i\Gamma_n)$, with the decay width given by $\Gamma_n$. In Fig.3 we present results for the lowest $2^+$ state of an $N_F = 8$ (240 atoms) model system, using parameters $k_F = 0.3$, $\omega = 1$ and $\mu = 20$. (We have also calculated $N_F = 6$ and 7 systems, with results both being highly similar to those of $N_F = 8$.) These parameters should be suitable for
cold dilute systems interacting with a short range interaction. The above choice has the advantage of making $R$-matrix weakly energy dependent as we have $\mu^2 >> \omega$. As shown, our calculated energy at Feshbach resonance (FR) is about 1.7 $\hbar\omega_{osc}$ with nearly zero width, both being smooth functions there.

The shapes of our calculated spectrum and decay width are worth noting. Starting from the left end of Fig. 3, Re$E$ exhibits a gradual drop followed by an abrupt rise and finally remains nearly constant. At both ends, Re$E$ approaches to 2. Most importantly, the decay width $\Gamma$ is peaked concurrently with the abrupt rise, both happening right at $a_\lambda$. These specific features of our results agree remarkably well with experiments [9, 10].

The above abrupt rising feature is mainly due to the $R$-matrix interaction. The factor $\lambda$ of Eq.(8) has a pole when $a_\omega = -a_\lambda = -1/(\alpha I)$. It is readily seen that at $a_\lambda$ the imaginary part of the $R$ matrix is peaked with a Lorentzian form, while its real part vanishes. In addition, $R$ is positive to the left of $(-a_{osc}/a_\lambda)$, and negative on the other side. These properties of $R$ determine the general shapes of our results. For small $k_F$ and $\omega$, $a_\omega$ is close to $a_{osc}/4\pi$. In fact for $k_F=0$ and $\omega = 0$, $a_\omega$ is exactly equal to $a_{osc}/4\pi$, independent of $\mu$. As shown in the figure, the abrupt rising takes place very close to $4\pi$. We note that RPA and TDA give nearly identical results far from $a_\lambda$. Near $a_\lambda$, Re$E$ for RPA tends to negative indicating the system being unstable.

Last but not least, $\Gamma$ is discontinuous at $a_\lambda$ as shown. We have found that the wave functions $X$ and $Y$ of Eq. (1) are also discontinuous at $a_\lambda$. We plan to further study the nature of this “transition” in a future work.

In summary, we have carried out a particle-hole shell model calculation for the quadrupole excitations of trapped cold Fermi gas. An essential step is the use of a reaction matrix renormalized interaction. Using a separable potential approach, this interaction has been derived analytically and it is a smooth function at Feshbach resonance although the atomic interaction before renormalization is divergent there. Our results demonstrate that, in between the collisional and collisionless regimes, trapped cold Fermi gas undergoes a transition with abrupt variations in both energy (frequency) and decay width (damping rate), in good qualitative agreement with experiments.

Acknowledgement: We sincerely thank G.E. Brown, E. Shuryak and Tom Bergman for many helpful discussions. Partial support from the US Department of Energy under contract DE-FG02-88ER40388 is gratefully acknowledged.

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