Sum-rule analysis of radio-frequency spectroscopy of ultracold Fermi gas

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We carried out an analysis based on sum rules and determined the radio-frequency spectroscopy shift observed in Chin *et al.*'s experiment [C. Chin, M. Bartenstein, A. Altmeyer, S. Riedl, S. Jochim, J. Denschlag, and R. Grimm, Science **305**, 1128 (2004)]. It is shown that such a shift can be interpreted as spin correlations peculiar to a BCS-type state. An analytical form for the shift is obtained which enables us to make quantitative comparisons with the experiment throughout the crossover. We also calculated the width of the resonance. An interesting consequence is noticed, which can possibly be tested by future experiments.

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I. INTRODUCTION

With the advent of degenerate Fermi gases [1], considerable effort has been devoted to realize superfluidity in those systems [2–6]. It is well known that in the weakly interacting limit, the transition temperature is very small, as a result of the exponential dependence on the interaction strength, as demonstrated long ago by Gor'kov and Melik-Barkhudarov [7]. However, by using a Feshbach resonance (FR) [8–10], experimentalists can tune the interaction and explore the whole "BEC-BCS crossover" regime, characterized by the dimensionless parameter $\xi=-(k_F a_s)^{-1}$, where k_F is the Fermi wave vector and a_s is the two-body s-wave scattering length. It is generally believed that a high temperature superfluid exists at unitarity, with a transition temperature of the order of the Fermi temperature. It has also become possible to test quantitatively the predictions of the crossover model proposed nearly forty years ago [11–13]. It is quite surprising that, albeit simple, those predictions are in qualitative agreement with most experiments. This suggests that the basic structure of the many-body ground state is not that different from a BCS-type state even in the so-called strongly interacting regime.

In this paper, we discuss the experiment of Chin *et al.* [14], where evidence has been found for the pairing gap in ^{6}Li by the radio-frequency (rf) spectroscopy technique. The Cooper pairing in this case is believed to occur between the lowest two hyperfine Zeeman levels. The data taken at low temperature shows a clear upshift on both the BEC and BCS sides in comparison with the bare atomic transition. On the BEC side, this shift was interpreted as associated with the binding energy of the molecules [15]; on the BCS side, one understood it as the measure of the effective pairing gap [16–19]. Recently, Baym *et al.* [20] attempted a full theory in the whole crossover regime by using the Monte Carlo calculation of Astrakharchik *et al.* [21] to extract relevant quantities which describe the shift. Perali *et al.* [22] have used a diagrammatic approach which includes the final state interaction into their calculation. Here we present a simple calculation based on the "naive" ansatz, and give a consistent theory of the rf shift in the crossover regime. The formula obtained below [Eq. (18)] reduces to known results in the BEC and BCS limits. We note that Eq. (18) can also be applied to the polarized case [23,24]. In addition, we calculate the width of the resonance and find that it is in qualitative agreement with experiment. Let us emphasize that the average shift defined in Eq. (17) is not the same as the peak position of the rf-spectroscopy profile and, moreover, is proportional to Δ^2 within the crossover model, where Δ is the single-particle excitation gap, apart from an explicit magnetic field dependent factor. This fact renders it nontrivial to extract the gap parameter from the experiment.

II. GENERAL SETUP

Let us consider a two-component Fermi gas of ^{6}Li with total number N (including both species with equal mass). The single-particle Hamiltonian can be written as

$$\hat{H}_1 = A\hat{\mathbf{S}}\cdot\hat{\mathbf{I}} - \gamma_e\hbar\hat{S}_z H - \gamma_n\hbar\hat{I}_z H, \tag{1}$$

in which $A=h\times 152$ MHz is the hyperfine coupling of ^{6}Li, γ_e and γ_n are the gyromagnetic ratios of the electron spin and nuclear spin, respectively, $\hat{S}_z$ and $\hat{I}_z$ are, respectively, the z component of the electron spin operator $\hat{\mathbf{S}}$ and nuclear spin operator $\hat{\mathbf{I}}$, and H is the constant external magnetic field, which we shall take to be along the z direction. The single-particle Hamiltonian Eq. (1) can be easily diagonalized and we find that the eigenstates are labeled by the z component of the total electron plus nuclear spin. For ^{6}Li, the internal space (the spin degree of freedom) is six dimensional and we shall label those eigenstates (from lower to higher energies) as $|m\rangle$, $m=1,2,\ldots,6$. To write the explicit spin wave function, we use the following basis, $|\hat{S}_z,\hat{I}_z\rangle$, to denote the spin orientations. In particular, we need in the following calculation the lowest two states

$$|1\rangle = 1/\sqrt{1+\alpha^2}(|-1/2,1\rangle + \alpha|1/2,0\rangle),$$

$$|2\rangle = 1/\sqrt{1+\beta^2}(|-1/2,0\rangle + \beta|1/2,-1\rangle), \tag{2}$$

where α and β are given by the expressions

$$\alpha = -\frac{2\sqrt{2}A}{A-2\gamma_e\hbar H+\sqrt{9A^2-4A\gamma_e\hbar H+4(\gamma_e\hbar H)^2}},$$

$$\beta = \frac{2\sqrt{2}A}{A + 2\gamma_e \hbar H - \sqrt{9A^2 + 4A\gamma_e \hbar H + 4(\gamma_e \hbar H)^2}}. \quad (3)$$

It is to be noticed that due to the small hyperfine interaction as compared with that of the electron Zeeman energy, α and β are normally very small (of the order of $|A/\gamma_e \hbar H|$ and numerically about 1/20 in the realistic experimental conditions). Nevertheless, the small mixing plays a very important role in the radio-frequency transition experiment because the magnetic moments of electron and nuclear spins are very different (see later discussion). Note that in calculating the eigenstates, we have omitted the small nuclear Zeeman energy, which is of the order of a few MHz and can be safely neglected.

The interaction between two atoms (say atoms 1 and 2) can be adequately described by the central part of the interaction potential,

$$\hat{V}_c(\mathbf{r}) = \hat{f}(\mathbf{r}) + \hat{g}(\mathbf{r})\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2, \quad (4)$$

in which $\hat{f}(\mathbf{r})$ and $\hat{g}(\mathbf{r})$ are the direct and exchange interaction, respectively. It is useful to notice that the range r_0 of the potential is of the order of 30 Å, which is much smaller than interparticle spacing, i.e., $r_0 \ll k_F^{-1}$.

It is known that ^{6}Li has a broad Feshbach resonance at around $H_0 = 830$ G with a width of about $\Delta H = 300$ G. The population of the closed channel component can be estimated to scale as δ/δ_c, where $\delta_c = (m/2\hbar^2)\lim_{\delta \to 0}(da_s^{-1}/d\delta)^{-2}$ represents the characteristic energy scale associated with Feshbach resonance, and for this case has a value of about 10^{12} Hz, and $\delta = \Delta\mu(H - H_0)$ is the energy difference between the open and closed channels [10]. Now, around the resonance ($\delta \lesssim \epsilon_F$), this factor is about $10^{-8} - 10^{-7}$, which is tiny compared with α or β. It is thus reasonable to assume that the ground state $|0\rangle$ is composed of only atoms from states $|1\rangle$ and $|2\rangle$. (This assumption should work for the polarized case as well.) In particular, in the case of an equally populated two-component Fermi gas, one can assume the usual naive BCS ansatz at zero temperature,

$$|\mathrm{BCS}\rangle = \prod_{\text{all } \mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} a_{\mathbf{k},1}^\dagger a_{-\mathbf{k},2}^\dagger)|\mathrm{vac}\rangle. \quad (5)$$

Here $|\mathrm{vac}\rangle$ is the vacuum and $a_{\mathbf{k},m}^\dagger$ is the creation operator for a hyperfine Zeeman state $|m\rangle$ with momentum $\mathbf{k}$. $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are the usual variational parameters. For fields far from the resonance, it is likely we need to take into account the closed channel component and, moreover, worry about the adjacent resonances. It is to be emphasized that the general expression [Eq. (18)] obtained in the following does not depend on the specific choice of the ground state wave function, only on the assumption that it contains only the lowest two hyperfine states. In fact, at finite temperature, the same expression [Eq. (18)] holds as well within the same assumption.

If we *assume* that the Cooper pairing is between the lowest two hyperfine Zeeman states, then it is clear that the total spin along the z direction $\hat{m}_F \equiv \Sigma_{i=1}^2(\hat{S}_{iz} + \hat{I}_{iz}) = 0$ for the Cooper pair. In order to drive the atom from $|2\rangle$ to $|3\rangle$, we need to *decrease* the z component of the total spin by 1. This can be accomplished by flipping *either* the electron or the nuclear spin in state $|2\rangle$. However, in view of the facts that $|\gamma_e/\gamma_n| \approx 2000$ and the hyperfine mixing is of order of 1/20, it is easy to convince oneself that the most important contribution to the matrix element of $\hat{H}_{\mathrm{rf}}$ is carried by the electron spin. Thus the original rf coupling is given by

$$\hat{H}_{\mathrm{rf}} = -\gamma_e \hbar \sum_i \hat{S}_{ix} H_{\mathrm{rf}} \quad (6)$$

for the rf field H_{rf} along the x direction. To simplify the calculation, it is desirable to use the "unphysical" coupling, which induces the transition of specific interest in the experiment, namely, state $|2\rangle$ to $|3\rangle$. We thus write [19]

$$\hat{H}'_{\mathrm{rf}} = -\lambda_{23}(H)\sum_i (|3\rangle\langle 2|)_i \equiv -\lambda_{23}(H)\hat{M}, \quad (7)$$

where $\lambda_{23}(H) = \gamma_e \hbar H_{\mathrm{rf}} \langle 3|\hat{S}_x|2\rangle$ is the magnetic field dependent coupling constant and we have defined our truncated "magnetic operator" $\hat{M}$. The subscript i in $(|3\rangle\langle 2|)_i$ signifies that the operator in the bracket refers to the ith atom. In the second quantized form,

$$\hat{M} = \int \psi_3^\dagger(\mathbf{r})\psi_2(\mathbf{r})d\mathbf{r}. \quad (8)$$

It is important to note here the reason for the validity of this assumption: While in the experiment, it is clear that the rf field along the x direction should have induced transitions from $|1\rangle$ to $|4\rangle$, $|1\rangle$ to $|6\rangle$, and $|2\rangle$ to $|5\rangle$, etc. (which shall be referred to as off-resonance transitions in the following), their frequencies are, however, far separated from the $|2\rangle$ to $|3\rangle$ transition. It is thus reasonable to expect that those off-resonance transitions shall not affect the $|2\rangle$ to $|3\rangle$ transition. In particular, we shall assume further that the line shape for the $|2\rangle$ to $|3\rangle$ transition will be determined by the simplified rf coupling as well. A justification of this assumption is given in the Appendix.

The many-body Hamiltonian can be written as

$$\hat{H} = \hat{H}_0 + \sum_{i<j}^{N} [\hat{f}(\mathbf{r}_i - \mathbf{r}_j) + \hat{g}(\mathbf{r}_i - \mathbf{r}_j)\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j], \quad (9)$$

in which $\hat{H}_0 = \Sigma_i^N \hat{H}_i - \mu_1 \hat{N}_1 - \mu_2 \hat{N}_2$ is a sum of single-particle Hamiltonian Eq. (1), with the chemical potential term. Here $\hat{N}_1 + \hat{N}_2 = \hat{N}$, where $\hat{N}$ is the total number operator of the system. In the equally populated case, we can set the chemical potential $\mu_1 = \mu_2 = \mu$, while in the polarized case they are different.

III. rf-SPECTROSCOPY SHIFT AND LINE SHAPE

As discussed before, the rf experiment of Chin *et al.* [14] indicates that once the temperature drops below some value T_C, a secondary peak appears in the rf spectrum together with a visible single atomic peak (apart from some mean field corrections). At the lowest temperature, the atomic peak disappears and only the shifted peak remains, which means that the whole system has entered a new quantum state. Since the ordinary Hartree-Fock term is accounted for in the

experimental calibration of the shift, the shift must come from some new correlations which will also show up in the two-body density matrix. To relate these two quantities, it is easiest to use the sum-rule argument which was first applied in a very similar situation in ^{3}He [25]. Let us thus consider the structure factor associated with the perturbation $H'_{\rm rf}$ at arbitrary temperature T,

$$S_{\hat{M}}(\omega) = \frac{1}{Z}\sum_{m,n} e^{-\beta E_m} |\langle n|\hat{M}|m\rangle|^2 \delta(\hbar\omega - \hbar\omega_{nm}), \tag{10}$$

in which $|m\rangle$ and $|n\rangle$ are *exact* many-body eigenstates of the Hamiltonian Eq. (9) and $\hbar\omega_{nm}=E_n-E_m\equiv\hbar\omega_n-\hbar\omega_m$ is the energy difference between many-body states $|m\rangle$ and $|n\rangle$. Z is the partition function. It is useful to note here that due to the extremely long spin relaxation time in ultracold gases, each spin component will establish its own thermodynamic equilibrium. Thus for a two-component Fermi gas prepared in the lowest two hyperfine states, the Gibbs sum in Eq. (10) should be understood as a constrained sum where the average number of particles $N_1\equiv\langle\hat{N}_1\rangle$ in state $|1\rangle$ and the average number of particles $N_2\equiv\langle\hat{N}_2\rangle$ in state $|2\rangle$ are separately conserved. In other words, μ_1 and μ_2 are independent.

From the definition of $S_{\hat{M}}(\omega)$, one can write down two sum rules as follows [26]:

$$m_0(\hat{M}) \equiv \hbar\int S_{\hat{M}}(\omega)d\omega = \langle 0|\hat{M}^\dagger\hat{M}|0\rangle, \tag{11}$$

$$m_1(\hat{M}) \equiv \hbar^2\int \omega S_{\hat{M}}(\omega)d\omega = \langle 0|\hat{M}^\dagger[\hat{H},\hat{M}]|0\rangle. \tag{12}$$

The evaluation of these two sum rules is straightforward. One obtains, within the assumption that there are only two spin components ($|1\rangle$ and $|2\rangle$) in the ground state (i.e., neglecting the closed channel component) and that higher angular momentum scattering can be neglected, the following results:

$$m_0 = N_2, \tag{13}$$

$$\begin{aligned} m_1 &= N_2(E_3 - E_2) \\ &+ G(H)\int g(\mathbf{r}_1-\mathbf{r}_2)\langle\psi_1^\dagger(\mathbf{r}_1)\psi_2^\dagger(\mathbf{r}_2)\psi_2(\mathbf{r}_2)\psi_1(\mathbf{r}_1)\rangle d\mathbf{r}_1 d\mathbf{r}_2 \\ &+ J(H)\int g(\mathbf{r}_1-\mathbf{r}_2)\langle\psi_1^\dagger(\mathbf{r}_1)\psi_2^\dagger(\mathbf{r}_2)\psi_2(\mathbf{r}_1)\psi_1(\mathbf{r}_2)\rangle d\mathbf{r}_1 d\mathbf{r}_2, \end{aligned} \tag{14}$$

where the functions $G(H)\ll 1$ and $J(H)\ll 1$ are given in terms of α and β,

$$\begin{aligned} G(H) &= \langle 3|\hat{\mathbf{S}}|3\rangle\cdot\langle 1|\hat{\mathbf{S}}|1\rangle + \langle 1|\hat{\mathbf{S}}|1\rangle\cdot\langle 2|\hat{\mathbf{S}}|2\rangle \\ &= \frac{(1-\alpha^2)\beta^2}{2(1+\alpha^2)(1+\beta^2)}, \end{aligned} \tag{15}$$

$$\begin{aligned} J(H) &= \langle 1|\hat{\mathbf{S}}|2\rangle\cdot\langle 2|\hat{\mathbf{S}}|1\rangle - \langle 1|\hat{\mathbf{S}}|3\rangle\cdot\langle 3|\hat{\mathbf{S}}|1\rangle \\ &= \frac{\alpha^2}{2(1+\alpha^2)(1+\beta^2)}. \end{aligned} \tag{16}$$

It is easy to see that the second and third terms in Eq. (14) are associated with direct and exchange scattering, respectively. Note that $G(H)$ and $J(H)$ are of the same order of magnitude ($\sim\alpha^2$).

If we define the shift as that measured from the single-particle hyperfine Zeeman splitting (E_3-E_2), i.e., write $\delta\omega=\omega-\hbar^{-1}(E_3-E_2)\equiv\omega-\omega_{32}$, we can find an explicit expression for the average of the shift $\delta\omega$, which we shall denote as $\overline{\delta\omega}$,

$$\overline{\delta\omega} = \frac{\int S_{\hat{M}}(\omega)(\omega-\omega_{32})d\omega}{\int S_{\hat{M}}(\omega)d\omega}. \tag{17}$$

Using Eqs. (13) and (14), we find

$$\begin{aligned} \overline{\delta\omega} &= \frac{G(H)}{\hbar N_2}\int g(\mathbf{r}_1-\mathbf{r}_2)\langle\psi_1^\dagger(\mathbf{r}_1)\psi_2^\dagger(\mathbf{r}_2)\psi_2(\mathbf{r}_2)\psi_1(\mathbf{r}_1)\rangle d\mathbf{r}_1 d\mathbf{r}_2 \\ &+ \frac{J(H)}{\hbar N_2}\int g(\mathbf{r}_1-\mathbf{r}_2)\langle\psi_1^\dagger(\mathbf{r}_1)\psi_2^\dagger(\mathbf{r}_2)\psi_2(\mathbf{r}_1)\psi_1(\mathbf{r}_2)\rangle d\mathbf{r}_1 d\mathbf{r}_2. \end{aligned} \tag{18}$$

Note that this result is completely general and applies to the polarized case as well [24].

To evaluate Eq. (18) and make a comparison with experiment, we need to evaluate the integral in that expression. Notice that due to the short-range character of the exchange interaction $g(\mathbf{r}_1-\mathbf{r}_2)$, the main contribution to the integral in Eq. (18) comes from the short-range part of the two-body density matrix. It can be shown by writing down the equation of motion for the two-body density matrix that its short-range form ($|\mathbf{r}_1-\mathbf{r}_2|\lesssim r_0$) is the same as that of the two-body Schrödinger wave function, provided that all the many-body energy scales are smaller than the characteristic two-body energy scale, which is certainly the case in an ultracold Fermi gas. Thus, one does not have to worry about the short-range part of the two-body density matrix, which is fixed by the two-body physics. The many-body effect comes into play only through the overall normalization of the two-body density matrix.

To make the above comments more quantitative, let us write the two-body density matrix in the form (using its Hermiticity property)

$$\begin{aligned} \langle\psi_1^\dagger(\mathbf{r}_1)\psi_2^\dagger(\mathbf{r}_2)\psi_2(\mathbf{r}_2)\psi_1(\mathbf{r}_1)\rangle &= \sum_i n_i\chi_i^*(\mathbf{r}_1,\mathbf{r}_2)\chi_i(\mathbf{r}_1,\mathbf{r}_2) \\ &= \sum_i n_i|\chi_i(\mathbf{r}_1,\mathbf{r}_2)|^2, \end{aligned} \tag{19}$$

where the n_i's are the eigenvalues of the two-body density matrix and $\chi_i(\mathbf{r}_1,\mathbf{r}_2)$ are the associated eigenfunctions. Here, the n_i's and the long-range part of the eigenfunctions $\chi_i(\mathbf{r})$ are determined by many-body physics, while the short-range

form of $\chi_i(\mathbf{r})$ is determined by two-body physics in the dilute gas (see a later discussion). This is precisely the reason why one can express the many-body interaction in terms of two-body scattering length. To a first approximation, Eq. (18) reduces to the standard Hartree-Fock energy associated with exchange interactions in the normal state. The Fock energy is very small due to the suppression of higher angular momentum scattering, and the Hartree mean field term is likely to be unaffected by the transition to the superfluid state. Thus in discussing the shift, we can discard those two contributions. In the superfluid case, one of the eigenvalues n_i assumes a macroscopic value and the associated eigenfunction is bound in space; we thus have to take this part into account separately. Let us note that in effect we have defined our shift as the part due exclusively to the pairing effect, where both the zero and finite center of mass momentum pairs contribute. Equivalently, we have calibrated it against the resonant frequency in the absence of the pairing effect, or at high temperature. One has to keep in mind that the Hartree term does depend weakly on temperature and magnetic field and its dependence will be more pronounced in the trapped case. In the following, we shall always understand $\overline{\delta\omega}$ to be the shift measured with respect to that of the mean field peak. Similarly, we can analyze the third term in Eq. (14) in the same way. Here we have instead

$$\langle \psi_1^\dagger(\mathbf{r}_1)\psi_2^\dagger(\mathbf{r}_2)\psi_2(\mathbf{r}_1)\psi_1(\mathbf{r}_2)\rangle = \sum_i n_i \chi_i^*(\mathbf{r}_1,\mathbf{r}_2)\chi_i(\mathbf{r}_2,\mathbf{r}_1). \tag{20}$$

Since Eq. (18) only picks up contributions from the short-range part of the pair wave function $\chi_i(\mathbf{r}_1,\mathbf{r}_2)$, it is reasonable to retain only the s-wave part of $\chi_i(\mathbf{r}_1,\mathbf{r}_2)$ and discard all other higher partial waves, since they vanish in the limit $\mathbf{r}_1 \to \mathbf{r}_2$. With this in mind, we can identify the two integrals in Eq. (18). Since $G(H)$ and $J(H)$ are of the same order, it is clear that the pairing contributions from the direct and exchange terms are of the same order of magnitude.

In the equally populated case, it is well known that if we use the BCS wave function for the ground state, the corresponding macroscopic eigenfunction of the two-body density matrix is that of the Cooper pair wave function, usually denoted as $F(\mathbf{r}_1,\mathbf{r}_2)$. Let us write the gap equation for the BEC-BCS crossover problem in the following form:

$$2E_k F_k + \sum_{k'} V_{k'-k} F_{k'} = 0, \tag{21}$$

in which $F_\mathbf{k} = \Delta_\mathbf{k}/2E_\mathbf{k}$. $E_\mathbf{k} = \sqrt{(\epsilon_\mathbf{k}-\mu)^2 + \Delta_\mathbf{k}^2}$ is the quasiparticle energy, $\epsilon_\mathbf{k} = \hbar^2 k^2/2m$ is the kinetic energy, and $\Delta \equiv \lim_{\epsilon_\mathbf{k}\to\mu} \Delta_\mathbf{k}$ is the gap parameter close to the Fermi surface. It is easy to see now that for $r \lesssim r_0$, or equivalently, $k \gtrsim 1/r_0 \gg k_F$, we have $E_\mathbf{k} \approx \epsilon_\mathbf{k}$, so that Eq. (21) is the same as that for a two-body Schrödinger equation $(2\epsilon_k - E)\phi_k + \Sigma_{k'} V_{k'-k}\phi_{k'} = 0$ in the same limit, since the energy eigenvalue $E \ll \epsilon_\mathbf{k}$. This implies that the short-range pair wave function is essentially nothing but a two-body wave function apart from normalization (cf. above). Now it is essential to notice that the normalization (or more precisely the normalization in the interval $r_0 \ll r \ll a_s, k_F^{-1}$) will, in general, change as we change the magnetic field. Thus our task is now to determine the behavior of the pair wave function $F(\mathbf{r})$ in the interval $r_0 \ll r \ll a_s, k_F^{-1}$.

The spatial form of $F(\mathbf{r})$ $(\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2)$ can be determined as follows. We transform $F(\mathbf{r}) = \Sigma_\mathbf{k} u_\mathbf{k} v_\mathbf{k} \exp[i\mathbf{k}\cdot\mathbf{r}]$ into an integral,

$$F(\mathbf{r}) = \frac{\Delta}{4\pi^2 r}\int_0^\infty \frac{k \sin kr}{E_k} dk. \tag{22}$$

Δ is determined by the gap equation [27–29]

$$\sum_\mathbf{k} \left[\frac{1}{\epsilon_\mathbf{k}} - \frac{1}{E_\mathbf{k}}\right] = \frac{m}{2\pi\hbar^2 a_s}. \tag{23}$$

Let us introduce a cutoff k_c such that $r_0 \ll k_c^{-1} \ll a_s, k_F^{-1}$. Now it is possible to split the integral Eq. (22) into two parts, $k < k_c$ and $k > k_c$. For $k > k_c$ we can approximate E_k by ϵ_k, while for $k < k_c$, we can approximate $\sin kr \approx kr$. Thus the integral in Eq. (22) can then be written as

$$\int_0^\infty \frac{k \sin kr}{E_k} dk = \int_{k_c}^\infty \frac{k \sin kr}{\epsilon_k} dk + r\int_0^{k_c} k^2 \left(\frac{1}{E_k} - \frac{1}{\epsilon_k}\right) dk$$
$$= \frac{m\pi}{\hbar^2}\left(1 - \frac{r}{a_s}\right). \tag{24}$$

In obtaining the last line, we have extended the integrals from 0 to ∞. We thus found that the behavior of $F(\mathbf{r})$ in the region $r_0 \ll r \ll a_s, k_F^{-1}$ to be

$$F(\mathbf{r}) = \frac{m\Delta}{4\pi\hbar^2}\frac{1 - r/a_s}{r}. \tag{25}$$

The factor in the expression of $F(\mathbf{r})$, which is independent of r, is linear in the gap and comes from many-body physics. The r-dependent part is just the two-body wave function in the interval $r_0 \ll r \lesssim a_s$. We have thus successfully decomposed those two contributions. Note that the integral in Eq. (18) then takes the form

$$\overline{\delta\omega} = \frac{1}{\hbar N_2}[G(H) + J(H)]\int g(\mathbf{r})|F(\mathbf{r})|^2 d\mathbf{r}, \tag{26}$$

where, as discussed above, we have neglected the Hartree-Fock term and used the fact that $F(\mathbf{r})$ is an even function. Note that some general conclusions can be drawn from Eq. (26). First of all, once we have taken out the normalization constant in $F(r)$, which depends on the gap parameter, we are left with essentially a two-body wave function normalized in such a way that the radial part approaches 1 for $r_0 \ll r \ll a_s$. The many-body physics, especially that associated with the Feshbach resonance, is entirely encoded in the gap parameter, which one can calculate either from the naive ansatz or by a more elaborate scheme such as quantum Monte Carlo simulation. Second, since nowhere in the argument presented above have we specified the position of the crossover, the expression works throughout the whole crossover regime and gives a consistent interpretation of the rf shift. In the following section, we shall verify indeed that Eq. (26) reduces in the BEC limit to the result of Ref. [15] and in the BCS limit

to that of Ref. [19]. Third, it is easy to see that apart from the magnetic field dependent factor $G(H)+J(H)$, the shift should scale as Δ^2 and, moreover, decrease as one approaches the BCS side (high magnetic field).

However, it is clear both theoretically and experimentally that the rf line shape is not a delta function and one has to understand where the broadening of the peak comes from. In general, we can distinguish two types of contributions to the width of the resonance. The first is associated with the external rf field and goes to zero as the intensity of the rf field tends to zero. The second type is intrinsic to the system and, in general, is fairly complicated. In the following we shall only consider those intrinsic effects as a whole (in a gross way) by calculating the third sum rule. It is clear, by the very construction of the sum rules, that the intrinsic effects are accounted for (with, of course, the proviso that linear response theory is valid).

Now, as we have commented before, it is reasonable to treat the rf coupling as $\int \psi_3^\dagger(\mathbf{r})\psi_2(\mathbf{r})d\mathbf{r}$ even for the consideration of the line shape (see also the Appendix). We can calculate the third sum rule in a straightforward way,

$$m_2(\hat{M}) \equiv \hbar^3 \int \omega^2 S_{\hat{M}}(\omega) d\omega = \langle 0|[\hat{M}^\dagger,\hat{H}][\hat{H},\hat{M}]|0\rangle. \quad (27)$$

The exact form of the line shape is not easy to obtain. However, as a characterization of the rf profile, we can use the Gaussian distribution to represent the line shape with average peak at $\bar{\omega}$ and standard deviation σ^2 (cf. discussions at the end of this section), i.e.,

$$S_{\hat{M}}(\omega) = \text{const}\frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{(\omega-\bar{\omega})^2}{2\sigma^2}\right). \quad (28)$$

From the first sum rule, it is easy to see that const$=\hbar N_2$. From the sum rules m_1, m_2, we find

$$\bar{\omega} = \hbar^{-1}(E_3 - E_2) + \overline{\delta\omega}, \quad (29)$$

$$\bar{\omega}^2 + \sigma^2 = \hbar^{-2}(E_3 - E_2)^2 + 2\hbar^{-1}(E_3 - E_2)\overline{\delta\omega} + \frac{1}{\hbar^2 N_2}\langle 0|[\hat{M}^\dagger,\hat{V}_c][\hat{V}_c,\hat{M}]|0\rangle, \quad (30)$$

where $\overline{\delta\omega}$ is given by expression (18). Thus we find an expression for the width of the resonance,

$$\sigma^2 = \frac{1}{\hbar^2 N_2}\langle 0|[\hat{M}^\dagger,\hat{V}_c][\hat{V}_c,\hat{M}]|0\rangle - (\overline{\delta\omega})^2. \quad (31)$$

Here, $\hat{V}_c(\mathbf{r}) = \hat{f}(\mathbf{r}) + \hat{g}(\mathbf{r})\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2$ is the central part of the interaction between atom 1 and atom 2. Equation (31), in general, involves the three- and four-body density matrices in addition to the two-body density matrix. However, one can discard those higher density matrices if one notices that in a low density system, those will be of higher order in density. More precisely, since the short-range potential which enters into Eq. (31) will have at least three different coordinate variables for the higher order density matrix, the contribution of those will be at least of order $k_F r_0$ as compared with those coming from the two-body density matrix, where as above, r_0 is the typical length scale for the short-range potential.

Thus, let us only retain the two-body density matrix in Eq. (31). We then find

$$\sigma^2 = \frac{1}{\hbar^2 N_2}P(H)\int d\mathbf{r}_1 d\mathbf{r}_2 g^2(\mathbf{r}_1-\mathbf{r}_2) \times[\langle 0|\psi_1^\dagger(\mathbf{r}_1)\psi_2^\dagger(\mathbf{r}_2)\psi_2(\mathbf{r}_2)\psi_1(\mathbf{r}_1)|0\rangle] + \frac{1}{\hbar^2 N_2}Q(H)\int d\mathbf{r}_1 d\mathbf{r}_2 g^2(\mathbf{r}_1-\mathbf{r}_2) \times[\langle 0|\psi_1^\dagger(\mathbf{r}_1)\psi_2^\dagger(\mathbf{r}_2)\psi_2(\mathbf{r}_1)\psi_1(\mathbf{r}_2)|0\rangle] - (\overline{\delta\omega})^2. \quad (32)$$

Here $P(H)$ and $Q(H)$ are given by the following expressions:

$$P(H) = \frac{2\alpha^2 + 2\alpha^2\beta^2 + 2\alpha^2\beta^4 + \beta^4}{4(1+\alpha^2)(1+\beta^2)^2} \sim \frac{1}{2}\alpha^2, \quad (33)$$

$$Q(H) = \frac{\alpha^2\beta^2}{2(1+\alpha^2)(1+\beta^2)^2} \sim \frac{1}{2}\alpha^2\beta^2. \quad (34)$$

Note that $P(H) \ll 1$ and $Q(H)/P(H) \sim \beta^2 \ll 1$. They are both decreasing functions of the magnetic field H. The same discussion given above [below Eq. (19)] applies here as well. Here, the "Fock" energy associated with $g^2(\mathbf{r}_1-\mathbf{r}_2)$ is certainly negligible as explained above. For the Hartree term, we expect it to be the same in the normal and superfluid phase. Moreover, provided the density distribution does not change appreciably when we change the magnetic field (this will be true on the BCS side of the resonance, including the unitary limit, where $\mu \sim \epsilon_F > 0$, where ϵ_F is the Fermi energy of the free gas), the "Hartree" term will stay almost the same. It is important to note here that $\overline{\delta\omega}$ is the total shift given by Eq. (18), which includes the Hartree contribution. Using the naive ansatz, the pairing contribution to the first two terms in Eq. (32) is given by

$$[P(H)+Q(H)]\int d\mathbf{r}|F(\mathbf{r})|^2 g^2(\mathbf{r}), \quad (35)$$

and thus is proportional to Δ^2 by a similar argument as given above for the shift. Note that $\overline{\delta\omega}$ is proportional to Δ^2 apart from the Hartree contribution. Then we find that σ^2 will be proportional to Δ^2 apart from Hartree contributions. Recalling that $P(H)$ and $Q(H)$ are decreasing functions of the magnetic field, we find that at zero temperature the width of the resonance will decrease as one approaches the BCS limit. This is in qualitative agreement with the experiment.

Before concluding the discussions in this section, let us mention that it is not crucial that we make the assumption that the line shape is Gaussian. All we need is a proper definition of the width, which can be clearly defined in the experiment. As in the traditional NMR experiment, we can use the following definition for the width of the resonance:

$$\hbar^2\sigma^2 \equiv \frac{\hbar^3\int(\omega-\bar{\omega})^2 S_M(\omega)d\omega}{\hbar\int S_M(\omega)d\omega} = \frac{m_2}{m_0} - \frac{m_1^2}{m_0^2}. \quad (36)$$

The end result is the same as before.

IV. EXPLICIT RELATIONS TO KNOWN RESULTS ON THE BEC AND BCS LIMITS

In this section, we shall look at two limits of the general expression, Eq. (18), derived above. In particular, we shall show that the shift Eq. (18) reduces to known results in the BEC and BCS limits and thus brings in some coherence in the treatment of rf spectroscopy. Once again we note that in obtaining Eq. (18) the only assumptions made are the validity of the use of linear response theory. Other effects, for example, the interaction of the third state $|3\rangle$ with states $|1\rangle$ and $|2\rangle$ are treated on the same footing as that of $|1\rangle$ and $|2\rangle$ (cf. discussions of Ref. [22]).

To make explicit contact with [15] and [19], we shall use the expression (26), where we have used the naive ansatz Eq. (5). Since the results of [15] and [19] are expressed in terms of the scattering lengths, it is useful to consider the following relation between the potential and the scattering length, which is derived in [10]. Consider two-body radial wave functions $\chi(r)$ in the (12) and (13) channels normalized in such a way that in the range $r_0 \ll r \lesssim a_s$, they have the following form:

$$\chi_{12}(r) = 1 - r/a_{12}, \quad \chi_{13}(r) = 1 - r/a_{13}, \quad (37)$$

in which a_{12} and a_{13} are scattering lengths in Eqs. (12) and (13) channels, respectively, Here instead of comparing two solutions of the radial Schrödinger equation with different potential $V(\mathbf{r})$ in the same channel as in [10], to which we refer for details, we shall compare two solutions corresponding to (12) and (13) channels, respectively. The potential difference $V_{12}(\mathbf{r})$ and $V_{13}(\mathbf{r})$ comes from two places. First, the electronic spin orientation is different for Eqs. (12) and (13) and thus they should have different exchange interactions. The second part of the contribution comes from the difference in magnetic moments in the (12) and (13) channels. This difference is, however, quite small since electron spins are approximately aligned in the z direction in both (12) and (13) channels and in any case much smaller as compared with the hard-core contribution from the exchange interaction $g(\mathbf{r})$ and shall be neglected in the following. We then have the potential difference in (12) and (13) channels as

$$\hat{V}_{12}(\mathbf{r}) - \hat{V}_{13}(\mathbf{r}) = g(\mathbf{r})[(\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2)_{12} - (\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2)_{13}]. \quad (38)$$

Here we have assumed that the magnetic moments of the atom pairs in Eqs. (12) and (13) are approximately the same, as explained above. $(\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2)_{13}$ is the average value of $\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2$ in the (13) channel in the absence of interchannel coupling. We find the following results:

$$a_{12}^{-1} - a_{13}^{-1} = [(\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2)_{13} - (\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2)_{12}]\frac{m}{\hbar^2}\int g(r)\chi_{12}^*(r)\chi_{13}(r)dr. \quad (39)$$

Furthermore, we observe that since the (12) and (13) channels have nearly the same triplet potential, the short-range parts of χ_{12} and χ_{13} are approximately the same. Now since they have been normalized the same way, we can replace χ_{13} with χ_{12} and thus obtain our desired relation,

$$a_{12}^{-1} - a_{13}^{-1} = [(\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2)_{13} - (\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2)_{12}]\frac{m}{\hbar^2}\int g(r)|\chi_{12}(r)|^2 dr$$

$$= [G(H) + J(H)]\frac{m}{\hbar^2}\int g(r)|\chi_{12}(r)|^2 dr. \quad (40)$$

Here we have noted that $(\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2)_{13} - (\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2)_{12} = G(H) + J(H)$.

Now, let us first look at the BEC limit. Here the system consists of tightly bound molecules and one would expect that the shift in the radio frequency should be entirely a two-body effect. Indeed, this is true as one can see from Eq. (26). To write it in a more suggestive way, we shall reexpress them on the BEC side by using quantities from the two-body scattering with scattering length $a_{12} > 0$ and the asymptotic normalized radial wave function $\tilde{\chi}_{12}(r) = \sqrt{2/a_{12}}e^{-r/a_{12}} \approx \sqrt{2/a_{12}}(1 - r/a_{12})$. Using Eqs. (25) and (26), we find

$$\overline{\delta\omega} = \frac{3\pi}{16}[G(H) + J(H)](k_F a_{12})\left(\frac{\Delta}{\epsilon_F}\right)^2\int dr g(r)|\tilde{\chi}_{12}(r)|^2. \quad (41)$$

First, it is straightforward to check that this result reduces to a decoupled two-body problem in the extreme BEC limit, where $\Delta = 4\epsilon_F/\sqrt{3\pi k_F a_s}$. The expression will be $\overline{\delta\omega} = [G(H) + J(H)]\int dr g(r)|\tilde{\chi}_{12}(r)|^2$. Now using the relation (40) derived above and noting the normalizations of $\chi_{12}(r)$ and $\tilde{\chi}_{12}(r)$, we find

$$\overline{\delta\omega} = -\frac{2\hbar^2}{m}\frac{a_{12} - a_{13}}{a_{12}^2 a_{13}}. \quad (42)$$

Note that this expression is positive since $a_{13} < 0$ and $a_{12} > 0$.

To make an explicit correspondence with the results of Ref. [15], we shall take their expression for the Franck-Condon factor and construct the average shift which appears in our calculation. In their notation, the transition frequency measured from the single-atom transition $|2\rangle$ to $|3\rangle$ is denoted by E. It is the same as our $\delta\omega$. One also notes that in Ref. [15], it is important to distinguish bound-bound and bound-free transitions. Let us thus define the mean shift

$$\bar{E} \equiv \overline{\delta\omega} = \int EF_f(E)dE, \quad (43)$$

where F_f is the Franck-Condon factor. By using expression (17) of Ref. [15] in the case when $a_{13} < 0$ and expressions (17) and (18) of Ref. [15] in the case when $a_{13} > 0$ (when a bound state is possible), we find that in both cases, Eq. (43) gives a result identical to Eq. (42).

A question arises regarding the width of the resonance. As has been shown in Ref. [15], the Frank-Condon factor has an asymptotic $1/\omega^{5/2}$ dependence on the perturbed frequency and thus the second moment will be divergent. However, this result is based on the assumption that one can calculate the Frank-Condon factor solely based on the asymptotic wave functions and incorporate the short-range interaction through phase shift [their Eqs. (5)–(8)]. This procedure, while correctly describing the physics on the scale $r \gg r_0$, does not incorporate the short-range details of the potential and the wave functions. Its failure is manifested in the divergence of the second moment of the Frank-Condon factor. In fact, in the range where $r \lesssim r_0$, or equivalently, $\omega \gtrsim \frac{\hbar^2}{2mr_0^2}$, the form of the wave functions [their Eqs. (5) and (6)] and the expansion of the scattering phase shift [their Eq. (7)] is not valid (as indicated in their paper as well). Hence the Franck-Condon factor calculated from those is invalid at high energy $\omega \gtrsim \frac{\hbar^2}{2mr_0^2}$ and thus the divergence is superficial and a correct treatment of the short-range physics will eliminate it. In our calculation, we cannot provide an analytic form of the rf profile; however, by insisting on using the original short-range interactions, we are free of this divergence and, moreover, can draw some general conclusions about the dependence of the width of the resonance.

Second, approaching the resonance from the BEC side, the expression Eq. (41) is well defined. a_s drops out since its occurrence in the normalization of the two-body wave function cancels that in $k_F a_s$ [see Eq. (44) below]. The dependence on interaction is encoded in the parameter Δ, which is a well-defined quantity even in the limit $a_s \to \pm\infty$.

On the BCS side, we can rewrite Eq. (41) in a slightly different form, by using the two-body wave function normalized so that in the asymptotic region $r_0 \ll r \lesssim a_s$, we have $\chi_{12}(r) = 1 - r/a_s$, then we have Eq. (41) as

$$\overline{\delta\omega} = \frac{3\pi}{8}[G(H) + J(H)]k_F\left(\frac{\Delta}{\epsilon_F}\right)^2 \int d\mathbf{r} g(\mathbf{r})|\chi_{12}(r)|^2. \tag{44}$$

Note that the expression in the integral is well defined throughout the resonance and can be taken to be a universal quantity, since we have extracted all the many-body dependence and are left with only two-body dependence, which is complicated but universal for our purpose. The expression Eq. (44) is valid throughout crossover. Using again Eq. (40) derived above, we find, by using $n = k_F^3/3\pi^2$ (total density), that the result reduces to

$$\overline{\delta\omega} = \frac{a_{13} - a_{12}}{a_{13}a_{12}} \frac{m\Delta^2}{2\pi\hbar^2 n}. \tag{45}$$

This is exactly what is obtained in Ref. [16].

V. COMPARISON WITH EXPERIMENTAL RESULTS

In the above section, we have demonstrated explicitly that the general expression Eq. (18) obtained above reduces to the two-body result derived in [15] in the BEC limit, where it is clear that the density distribution in the trap is irrelevant. Molecules form on a length scale much smaller than the typical density variation in the trap, i.e., $a_s \ll R_{\mathrm{TF}}$, where R_{TF} is the Thomas-Fermi length associated with composite bosons with scattering length $a_d = 0.6a_s$ [30]. On the BCS side, it reduces to that derived in [19] using the Hartree-Fock-Bogoliubov approximation for the superfluid phase. Here, however, since the gap parameter depends on the density of the system, one has to take into account density variations in the trap. Note a slight complication here: as discussed before, while in the uniform system, one can argue that the Hartree term is nearly a constant as we lower the temperature, in the trapped case, due to redistribution of atoms in the trap, the Hartree term will change. Moreover, as we change the magnetic field, the Hartree term will change as well. In the following we shall only concentrate on the pairing contributions.

To deal with the nonuniform distribution, we utilize the local density approximation (LDA). Using Eq. (41), we can construct quantities in units of energy on the BCS side. Since apart from the normalization factor Δ in front of the pair wave function $F(\mathbf{r})$, all other quantities are either constants or two-body quantities, we can safely take them as density independent. The resulting dependencies of $\delta\omega_{32}$ then scale as Δ^2/n. In a trap geometry, both Δ and n are position dependent. Our task is to take the average of Δ^2/n over the whole trap; since it is not possible to get a closed form in this case, we shall use numerical integration. As in the experiment, the cloud is cigar shaped, with an aspect ratio about 10 at the lowest temperature; the density distribution is taken for simplicity as the fermionic Thomas-Fermi profile in the trap. We expect such a simplification will not affect the result qualitatively on the BCS side. Now, if we take the shift at magnetic field $H = 822$ G, which is about 6.0 kHz as an input parameter, this gives a value of the shift of 4.4 kHz at a field of 837 G, in agreement with the one observed in the experiment, which is about 3.9 kHz. The value at $H = 875$ G is not so good: The calculation gives a value of about 2 kHz, where the value one gets from experiment is about 0.5 kHz. A possible origin of the discrepancy is that finite temperature effects are more important on the BCS side. Let us recall that at field $H = 875$ G, the scattering length $a_s = -600$ nm and $T_F = 1.2$ μK. We find the parameter $\xi = -(k_F a_s)^{-1} \approx 0.31$. If one estimates the transition temperature from the Gor'kov and Melik-Barkhudarov result [7], one finds that approximately $T_C(H = 875\ \mathrm{G})/T_F \approx 0.2$. The temperature as indicated in the experiment is $T/\epsilon_F < 0.2$ and possibly not very far from that, thus we expect that the finite temperature effect is very important. However, we remark that apart from the magnetic field dependent factor $G(H) + J(H)$, the general behavior of the shift in the resonance regime should follow the $\Delta(T)^2$ scaling law, insofar as the BCS-type state is assumed.

Finally, we note that the shift in the resonance frequency of the rf-induced $|1\rangle$ to $|4\rangle$ transition can be worked out in a similar manner. One finds that the only difference with respect to Eq. (18) is that instead of the function $G(H)$ and $J(H)$, there appears in Eq. (18) another function $G'(H)$ and $J'(H)$, which are given by the following expressions:

$$G'(H) = \frac{(\beta^2 - 1)(1 - \alpha^2\beta^2)}{2(1 + \alpha^2)(1 + \beta^2)^2}, \tag{46}$$

$$J'(H) = \frac{\alpha^2 - 2\beta^2 - \alpha^2\beta^2}{2(1+\alpha^2)(1+\beta^2)^2}. \quad (47)$$

A comparison with $G(H)+J(H)$ shows that $G'(H)+J'(H)$ is larger by a factor $1/\alpha^2$ and negative. The difference comes from the fact that in the (12) channel the electron spins align with each other while in the (24) channel they align in opposite directions. The energy difference is then considerably larger than that resulting from the $|2\rangle$ to $|3\rangle$ transition. As a result, the transition from state $|1\rangle$ to $|4\rangle$ should show a negative shift with a magnitude of the order of several MHz. For example, at a field of 822 G, we would expect a shift of about −1.38 MHz, which is much larger than the Fermi energy. We note here that since the (24) channel is controlled predominantly by the singlet potential, which is much deeper than the triplet potential in the (12) channel, the large shift is due to the bound molecular state in the (24) channel.

VI. CONCLUSION

On the basis of sum rules associated with the magnetization $\hat{M}$, we have derived an expression for the shift in the radio-frequency spectroscopy experiment [14]. We have used the generalized BCS ansatz ("naive ansatz") to rederive the known results in the BEC and BCS limits. Our result is valid throughout the crossover regime and suggests a consistent interpretation of the observed shifts. An interesting consequence of the calculation is that if the rf-field is tuned to a frequency of the order of 2000 MHz, then the predicted shift according to Eqs. (41), (46), and (47) would be of the order of 1.38 MHz near resonance, which is much larger than the Fermi energy.

Note added. Recently, Mueller [31] has argued that the asymmetrical rf profile can be understood as a generic consequence of the nonuniform density distribution in the trap. His discussion in [31] refers to the polarized case (also a brief discussion for the balanced case at the end of the paper) and relies on the assumption that the homogeneous gas will consist of a single delta peak and the broadening comes entirely as a result of the nonuniform density. Our discussion of the width of the resonance is intended for the homogeneous case and thus is different from their discussions. In [32], they have calculated the rf profile for a balanced and uniform Fermi gas at temperature zero, using a restricted set of intermediate states coupled by the rf field. However, the structure factor in their calculation has asymptotic behavior in ω as $\omega^{-3/2}$ and thus has divergent first and higher moments.

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APPENDIX

In this Appendix, we present the justification for using the truncated rf coupling Eq. (8) to calculate the shift and the width of the resonance. We recall that in the actual experiment, the rf field is in the x direction and, in principle, will induce transitions from the lower manifold to the upper manifold of the hyperfine Zeeman levels of ^{6}Li, in addition to the $|2\rangle$ to $|3\rangle$ transition. We can write the original rf coupling $-\gamma_e\hbar\Sigma_i\hat{S}_{ix}H_{rf} \equiv -\gamma_e\hbar\hat{M}_{\text{total}}H_{\text{rf}}$ of the system as a sum of its matrix elements between different hyperfine Zeeman states,

$$-\gamma_e\hbar H_{\text{rf}}\hat{M}_{\text{total}} = -\sum_i \sum_{m,n} \lambda_{mn}(H)(|m\rangle\langle n|)_i, \quad (A1)$$

where $\lambda_{mn} = \gamma_e\hbar H_{\text{rf}}\langle m|\hat{S}_x|n\rangle$ and subscript i in $(|m\rangle\langle n|)_i$ signifies that the operator in the brackets refers to the ith atom, exactly the same as before. We shall single out $\hat{M} = \Sigma_i(|3\rangle\langle 2|)_i$ in (P1) and refer to all other terms as "off-resonance transitions" as before. In the actual experiment, the relevant structure factor, which is probed by the rf field, is $S_{\hat{M}_{\text{total}}}$ and we are only interested in the low frequency part of it. Our aim is to show that to calculate the low frequency part of the structure factor $S_{\hat{M}_{\text{total}}}$, it is enough to use only $\hat{M}$ and calculate the structure factor $S_{\hat{M}}$. We understand in the following that the low frequency part refers to the frequencies around the $|2\rangle$ to $|3\rangle$ transition and high frequency parts are induced by off-resonance transitions, which are separated from low frequency parts by an energy much larger than the many-body energy scale. The proof consists of two parts.

(P1) The truncated operator $\hat{M}$ captures all the low frequency parts of the structure factor $S_{\hat{M}_{\text{total}}}$; in other words, the off-resonance transitions do not contribute to the low frequency part of $S_{\hat{M}_{\text{total}}}$.

(P2) The contribution from high frequency to the sum rules associated with $S_{\hat{M}}$ is small as compared with that from the low frequency part. This condition ensures that we can use the sum rules associated with $S_{\hat{M}}$ to determine the shift and width of the resonance.

Crudely speaking, the first requirement ensures that we do not lose any information about the low frequency part of $S_{\hat{M}_{\text{total}}}$ by using the truncated operator $\hat{M}$. In practice, the closest pair of states that have transition frequency comparable to that of the $|2\rangle$ to $|3\rangle$ transition are $|5\rangle$ and $|6\rangle$. However, since there are no states $|5\rangle$ and $|6\rangle$ in the statistical ensemble we are considering, their contribution is zero and we can neglect this part of the rf coupling. Thus, by using $\hat{M}$ alone, (P1) is satisfied.

The second requirement ensures that when evaluating the sum rules for the truncated operator $\hat{M}$, we do not pick up the contributions from the high frequency part of the spectrum. The demonstration we shall give relies on the following important assumption: Since the many-body energy scale is tiny compared with the atomic energy scale, it is reasonable to assume that the structure factor $S_{\hat{M}_{\text{total}}}$ will consist of distinct peaks centered around the atomic transition frequencies and mildly broadened by the many-body effect. In between those distinct peaks, $S_{\hat{M}_{\text{total}}}$ vanishes.

We can now proceed to show that (P2) is satisfied. For that purpose, we shall check each sum rule one by one. Let

us agree to denote the many-body states in the (mn) channel as $|mn;i\rangle$, where i labels all the many-body states in the channel (mn) and $m,n=1,2,\ldots,6$ labels the hyperfine Zeeman states. It is also convenient to label all the many-body states from different channels by a single index a or b. The many-body ground state we are interested in is denoted by $|0\rangle=|12;i=0\rangle$. The first sum rule is given by

$$m_0 = \langle 0|\hat{M}^\dagger \hat{M}|0\rangle = \sum_a \langle 0|\hat{M}^\dagger|a\rangle\langle a|\hat{M}|0\rangle. \tag{A2}$$

Since operator $\hat{M}$ only couples state $|2\rangle$ to $|3\rangle$, we see that state $|a\rangle$ should be of the form $|13;i\rangle$. This shows that in evaluating the first sum rule, we have only picked up the contribution in the frequency range centered around the $|2\rangle$ to $|3\rangle$ transition and did not mix in contributions from higher frequencies. For the second sum rule

$$m_1 = \langle 0|\hat{M}^\dagger[\hat{H},\hat{M}]|0\rangle, \tag{A3}$$

it is useful to write $\hat{H}=\hat{H}_0+\hat{V}_c$ and recall $[\hat{H}_0,\hat{M}]=(E_3-E_2)\hat{M}$, thus the term associated with $\hat{H}_0$ is the same as m_0 except a multiplication factor E_3-E_2. The term associated with the central part of the interaction $\hat{V}_c$ is given by

$$\langle 0|\hat{M}^\dagger[\hat{V}_c,\hat{M}]|0\rangle = \sum_i \langle 0|\hat{M}^\dagger|13;i\rangle\Big(\sum_a \langle 13;i|\hat{V}_c|a\rangle\langle a|\hat{M}|0\rangle - \sum_b \langle 13;i|\hat{M}|b\rangle\langle b|\hat{V}_c|0\rangle\Big). \tag{A4}$$

We have used the fact that $\hat{M}$ only couples the (12) channel to the (13) channel. The summation over a is restricted to $|13;i\rangle$ because of the factor $\langle a|\hat{M}|0\rangle$. This means that $\hat{V}_c$ only takes the matrix elements between the many-body states in the (13) channel and is entirely determined by many-body effects in the (13) channel, which does not involve any high frequency transitions. A similar analysis for the summation over b shows that $\hat{V}_c$ only takes matrix elements between the many-body states in the (12) channel and does not involve high frequency transitions either.

We now proceed to consider m_2. It is clear that the only term we have to consider is

$$\langle 0|[\hat{M}^\dagger,\hat{V}_c][\hat{V}_c,\hat{M}]|0\rangle, \tag{A5}$$

since terms involving $\hat{H}_0$ reduce to the consideration above for m_0 and m_1. We can decompose this term as well.

$$\langle 0|[\hat{M}^\dagger,\hat{V}_c][\hat{V}_c,\hat{M}]|0\rangle = \sum_b \Big|\sum_a (\langle 0|\hat{M}^\dagger|a\rangle\langle a|\hat{V}_c|b\rangle - \langle 0|\hat{V}_c|a\rangle\langle a|\hat{M}^\dagger|b\rangle)\Big|^2. \tag{A6}$$

Let us first look at the second term in the brackets. Since $\hat{M}$ only couples states from the (12) channel to the (13) channel, it is easy to see that the matrix element for $\hat{V}_c$ will be $\langle 0|\hat{V}_c|12;i\rangle$ and is determined entirely by the many-body effects in the (12) channel. Now let us look at the first term in the brackets. According to the factor $\langle 0|\hat{M}^\dagger|a\rangle$, we see that state $|a\rangle$ should be $|13;i\rangle$. Now the factor $\langle 13;i|\hat{V}_c|b\rangle$ can have transitions between channels and thus gives rise to the large energy difference. However, it can be verified directly by evaluating the matrix element of $\hat{V}_c(\mathbf{r})=\hat{f}(\mathbf{r})+\hat{g}(\mathbf{r})\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2$ that those matrix elements are smaller by a factor of α (or β) as compared with those between the same channel (13). For example, the transition induced by $\hat{V}_c$ from states in the (13) channel to the (35) channel has an atomic matrix element (apart from that associated with many-body wave functions),

$$\langle 35|\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2|13\rangle = \frac{\alpha}{2(1+\alpha^2)}, \tag{A7}$$

while we have

$$\langle 13|\hat{\mathbf{S}}_1\cdot\hat{\mathbf{S}}_2|13\rangle = \frac{1-\alpha^2}{4(1+\alpha^2)}. \tag{A8}$$

Thus, provided that the matrix elements associated with the spatial many-body wave functions do not differ substantially in the case of transition within the (13) channel as compared with the transition from the (13) channel to the (35) channel, we can conclude that the high frequency part constitutes a tiny fraction ($\sim\alpha$) of the m_2 sum rule. We have thus proved (P2).

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