RF sum rule and "dimer projection" contact measure

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I. BASIC ARGUMENT: EXISTENCE OF THE DIMER FEATURE IN CONTACT SPECTROSCOPY

Consider the RF spectrum of an interacting spin-half Fermi gas, with $E_F \equiv E_{F,1}$, for a balanced $N_1 = N_2 = N/2$ gas, where states $|1\rangle$ and $|2\rangle$ interact with scattering length a_{12}. Spectroscopy flips atoms from $|2\rangle$ to $|3\rangle$, in which channel atoms interact with scattering length a_{13}. If $a_{13} > 0$, there is a dimer bound state in the 13 channel, with binding energy $E_d \approx \hbar^2/ma_{13}^2$; however even when $a_{13} < 0$, we will define a positive $x_d \equiv (\hbar^2/ma_{13}^2)/E_F$.

The contact C governs two well-known properties of the spectrum. Let's define a dimensionless frequency $x = \hbar\omega/E_F$, a dimensionless contact $\widetilde{C} = C/Nk_F$ (for which $k_F = k_{F,1}$), and spectrum normalized such that $\int dx\, \gamma = 1$. Then:

- The positive-frequency side of the spectrum as an asymptotic limit

$$\gamma \to A_+ \widetilde{C} \frac{x^{-3/2}}{1 + x/x_d} \tag{1}$$

  where $A_+ = \pi^{-2}2^{-1/2}$ (see App. B). This spectrum is typically probed in the $1 \ll x \ll x_d$ limit to measure $\widetilde{C}$.

- The sum over all frequencies gives the "clock shift":

$$\bar{x} = \int dx\, x\gamma(x) = -\frac{1}{\pi}\frac{1}{k_F a_{13}}\widetilde{C} = -\mathrm{sgn}(a_{13})\frac{\widetilde{C}}{\pi\sqrt{2}}\sqrt{x_d} \tag{2}$$

  where we have used the shallow-dimer approximation $x_d = (\hbar^2/ma^2)/E_F = 2/(a^2k_F^2)$ so that $\sqrt{x_d/2} = 1/(k_F a)$. Note that the symmetric part of the spectrum ($\gamma_s = \gamma(x)/2 + \gamma(-x)/2$) does not contribute to $\bar{x}$.

Case I. First, let's consider the case of $a_{13} < 0$. From Eq. (2), $\bar{x} > 0$. Let's assume that the only (antisymmetric) spectral feature is the contact tail, given by Eq. (1). Indeed, one can show that these are consistent by integrating from $x = x_i > 0$ to $x = \infty$:

$$\begin{aligned} \bar{x}|_+ &= A_+\widetilde{C}\int_{x_i}^{\infty} dx\, x\frac{x^{-3/2}}{1 + x/x_d} = 2A_+\widetilde{C}\sqrt{x_d}\,\mathrm{atan}\,\sqrt{x_d/x_i} \\ &\approx \pi\sqrt{x_d}\widetilde{A}_+ C = \frac{\widetilde{C}}{\pi\sqrt{2}}\sqrt{x_d} \qquad \text{for} \quad x_d \gg x_i \end{aligned} \tag{3}$$

where the atan $\sqrt{x_d/x_i} \approx \frac{\pi}{2}$ approximation is motivated by the typical $x_d/x_i \sim 10^2$, for ^{40}K near the usual Feshbach resonance. We see that this $x_i \to 0$ result matches Eq. (2).

Case II. Now consider a positive a_{13}, but with equal magnitude to the one considered above. Also, we will keep the same a_{12}, temperature, etc, so that the contact is the same as in case I. The first moment of the positive-frequency tail is still as calculated in Eq. (3). However from the sum rule, the clock shift is now negative, so that the $\bar{x}|_+ = -\bar{x}$. In order to arrive at the correct total clock shift, there must be a *negative-frequency part of the spectrum with first moment* $+2\bar{x}$*:* $\int_{-\infty}^{0} dx\, x\gamma(x) = 2\bar{x}$.

For a weakly interacting final state, the two-particle spectrum suggests that a single delta function exists, at $\omega = -E_d/\hbar$, i.e., $x = -x_d$. Since the dimer enters into the f-sum-rule, and since the positive-frequency part of the f-sum rule is proportional to the contact, we postulate that the weight of the dimer resonance must also be proportional to the contact. So we write

$$\gamma_d = A_d\widetilde{C}\delta(x + x_d) \tag{4}$$

such that weight $W_d = A_d\widetilde{C}$ and first moment $M_{1,d} = -x_d A_d\widetilde{C}$. Its contribution to the clock shift is $-A_d\widetilde{C}x_d$; and by the above argument, this must be $= 2\bar{x}$. Thus

$$A_d = \frac{2\bar{x}}{-\widetilde{C}x_d} = \frac{-2\,\mathrm{sgn}(a_{13})\frac{\widetilde{C}}{\pi\sqrt{2}}\sqrt{x_d}}{-\widetilde{C}x_d} = \frac{\sqrt{2}}{\pi\sqrt{x_d}} \tag{5}$$

This is the central result of this section: that for $a_{13} > 0$, the clock shift requires a dimer feature, whose form is

$$\gamma_d(x) = \frac{\sqrt{2}}{\pi\sqrt{x_d}}\widetilde{C}\delta(x + x_d)\,. \tag{6}$$

where, as a reminder, γ is the rf spectrum normalized as $\int \gamma dx = 1$, and $x = \hbar\omega/E_F$.

II. SPECTRAL WEIGHTS

A. How much of the spectrum is in the dimer feature and in the contact tail?

We can separate the symmetric and antisymmetric parts of the spectrum,

$$\gamma = \gamma_s + \gamma_a \qquad \text{with} \qquad \gamma_{s,a} = \gamma(x)/2 \pm \gamma(-x)/2 \tag{7}$$

The dimensionless spectral weight of each of these is $W_s = \int dx\gamma_s(x)$ and $W_a = \int dx\gamma_a(x)$, such that $W_s + W_a = 1$.

Assuming a lower cutoff x_i, we can estimate the spectral weight W_+ as

$$W_+/A_+\widetilde{C} = \int_{x_i}^{\infty} dx\, \frac{x^{-3/2}}{1 + x/x_d} = \frac{2}{\sqrt{x_i}} - \frac{2\,\mathrm{atan}\sqrt{x_d/x_i}}{\sqrt{x_d}} \approx \frac{2}{\sqrt{x_i}} - \frac{\pi}{\sqrt{x_d}} \approx \frac{2}{\sqrt{x_i}} \quad \text{for } x_d \gg x_i \tag{8}$$

So, while the first moment (calculated in the previous section) is insensitive to x_i in the small-x_i limit, the spectral weight is not. It's interesting to note that for this tail alone , $\bar{x}/W_+$ is roughly the geometric mean of x_i and x_d, and independent of $\widetilde{C}$. [1] However $\bar{x}/W_+$ of the tail alone does not depend on the contact: it is the *amplitude*of the tail that is tied to the contact. The spectral weight in the positive-frequency contact tail is then

$$W_+ \approx 2A_+\widetilde{C}/\sqrt{x_i} \approx \frac{\sqrt{2}}{\pi^2\sqrt{x_i}}\widetilde{C} \tag{10}$$

which is roughly $0.13\widetilde{C}/\sqrt{x_i}$, so perhaps at the 10% level for $\widetilde{C} \sim 1$. Normalization requires that $1 = W_s + W_a$, such that $W_+ < 1$, of course; we see that for large values of $\widetilde{C}$ our treatment will have some issues. In reality, the $x^{-3/2}$ scaling does not continue to low frequency, and for higher values of $\widetilde{C}$ the anti-symmetric part of the spectra must be modeled more carefully.

For the negative-frequency $\gamma_d = A_d\widetilde{C}\delta(x + x_d)$, the spectral weight is $W_d = A_d\widetilde{C}$. For $x_d \sim 200$, approximately $W_d = A_d\widetilde{C} \approx 0.03\widetilde{C}$, or 3% (for $\widetilde{C} \sim 1$) of the spectral weight is in the dimer feature. [2]

B. Utility of dimer feature for fast contact spectroscopy

The spectral weight of the dimer feature occurs at a specific RF frequency: $x = -x_d$. At an equivalent detuning in the positive-frequency tail, where $x \approx +x_d$, the spectral density is $\gamma_a/\widetilde{C} = \pi^{-2}2^{-3/2}x_d^{-3/2} \sim 10^{-5}$. Assuming one integrates over a width Δx to to Fourier broadening, the ratio of transferred fraction would be

$$\left.\frac{\int_{\Delta x} dx\,\gamma_d}{\int_{\Delta x} dx\,\gamma_+}\right|_{x\approx x_d} = \frac{2^{1/2}\pi^{-1}x_d^{-1/2}\widetilde{C}}{2^{-3/2}\pi^{-2}x_d^{-3/2}\widetilde{C}\Delta x} = 4\pi x_d/\Delta x \tag{12}$$

Where we have assumed that $\Delta x \ll x_d$, so that the dimer feature simply gets is weight. For a 1-μs pulse and $E_F/\hbar \sim 10^5\mathrm{s}^{-1}$, then $\Delta x \sim 10$. This would suggest a ratio of nearly 10^3 in response. However, one would typically

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[1] This can be seen from

$$\frac{\bar{x}|_+}{W_+} = \frac{2x_d/\sqrt{x_i} - x_d W_+/A_+\widetilde{C}}{W_+/A_+\widetilde{C}} \approx -x_d + \frac{2x_d x_i^{-1/2}}{2x_i^{-1/2} - \pi x_d^{-1/2}} \approx -x_d + \frac{x_d}{1 - (\pi/2)x_i^{1/2}x_d^{-1/2}} \approx \frac{\pi}{2}\sqrt{x_i x_d}\,. \tag{9}$$

[2] This weight is also lost from the central feature:

$$W_s = 1 - W_+ - W_d \approx 1 - \left(\frac{\sqrt{2}}{\pi^2\sqrt{x_i}} + \frac{\sqrt{2}}{\pi\sqrt{x_d}}\right)\widetilde{C} \tag{11}$$

Interestingly, this model suggests that measuring the weight in the symmetric part of the rf spectrum would in principle also be an indication of contact. However, as noted above, the effective value of x_i must change with $\widetilde{C}$, at least for large values, such that this technique would require calibration.

not use the high-frequency tail at $x \approx x_d$, since the response is small there, and uneccessarily detuned. Instead, choosing only $x \gg \Delta x$ for spectroscopy using the $x^{-3/2}$ tail,

$$\frac{\int_{\Delta x} dx'\, \gamma_d}{\int_{\Delta x} dx'\, \gamma_+(x+x')} = \frac{A_d}{A_+ x^{-3/2}(1+x/x_d)^{-1}\Delta x} = 2\pi \frac{(x+x_d)x^{3/2}}{x_d^{3/2}\,\Delta x} \tag{13}$$

Since $x \gg \Delta x$ is required to avoid the single-particle feature,[3] let's choose $x = 10\Delta x$; then,

$$\frac{\int_{\Delta x} dx'\, \gamma_d}{\int_{\Delta x} dx'\, \gamma_+(x+x')} = 2\pi \frac{(10\Delta x + x_d)(10\Delta x)^{3/2}}{x_d^{3/2}\,\Delta x} \approx 2\pi 10^{3/2} \frac{x_d(\Delta x)^{1/2}}{x_d^{3/2}} \sim 200 \left(\frac{\Delta x}{x_d}\right)^{1/2} \tag{14}$$

Now we see that the advantage of using the dimer peak is $\gtrsim 1$ when $\Delta x \gtrsim 10^{-5} x_d$, or $\Delta\omega \gtrsim 10^{-5}\omega_d$. In terms of pulse length, $T \sim 1/\Delta\omega \lesssim 10^5/\omega_d$. For $\omega_d/2\pi$ 4 MHz, this is $T \lesssim 4$ ms. This sounds wrong... As a check, for our typical 40 μs pulse, $1/T\omega_d \sim 10^{-3}$, so the above expression would then predict a signal ratio of $200/\sqrt{T\omega_d} \sim 6$. Do we get 6 times the signal, for a 40 μs pulse, when using the dimer?

III. T-MATRIX CALCULATION

With a contact interaction of strength $\bar{g}$, the T-matrix is found by summing diagrams, to be

$$T(z) = \frac{\bar{g}}{1 - \frac{\bar{g}}{V}\sum_k \frac{1}{z - k^2/m}} \tag{15}$$

where $z = p^2/m + 0^+$ is the energy, p and k are collision momenta, $m = 2\mu$ is the bare mass, $\bar{g}$ is the bare (unrenormalized) coupling constant, and V is the volume. Completing the sum into an integral with a momentum cutoff Λ,

$$\begin{aligned}
T(z)^{-1} &= \frac{1}{\bar{g}} - \frac{1}{V}\sum_k^{\Lambda} \frac{1}{z - k^2/m} \\
&= \frac{1}{\bar{g}} - \frac{4\pi m}{(2\pi)^3}\int_0^{\Lambda} dk\, \frac{k^2/m - z + z}{z - k^2/m} \qquad \text{using} \quad \frac{1}{V}\sum \to \int \frac{d^3k}{(2\pi)^3} \\
&= \frac{1}{\bar{g}} - \frac{m}{2\pi^2}\int_0^{\Lambda} dk \left(-1 + \frac{z}{z - k^2/m}\right) \\
&= \left(\frac{1}{\bar{g}} + \frac{m\Lambda}{2\pi^2}\right) - \frac{m}{2\pi^2}\int_0^{\Lambda} dk\, \frac{z}{z - k^2/m} \\
&\equiv \frac{1}{g} + I(z,\Lambda) \qquad \text{where} \quad g^{-1} = \bar{g}^{-1} + m\Lambda/2\pi^2
\end{aligned} \tag{16}$$

where we have defined a *renormalized coupling constant* g and an energy-dependent term $I(z,\Lambda)$. The low-energy coupling strength relates the measured s-wave scattering length a as $g = 4\pi a/m$. (We show below that Λ gives the effective range correction to the scattering phase, and can be written in terms of r_e, with which one can find the bare coupling strength $\bar{g}$ in terms of measured a and r_e.)

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[3] For our standard 40 μs pulse, we choose 50 kHz detuning, such that $T\omega \sim 12$; i.e., if the broadening is $1/T$, then we have chosen $12/T$. So, using $x \sim 10\Delta x$ is reasonable.

The energy-dependent part of the T-matrix is

$$\begin{aligned} I(z,\Lambda) &= -\frac{m}{2\pi^2}\int_0^\Lambda dk\,\frac{z}{z-k^2/m} \\ &= \frac{zm^2}{2\pi^2}\int_0^\Lambda dk\,\frac{1}{k^2-mz} \\ &= \frac{zm^2}{4\pi^2\sqrt{mz}}\int_0^\Lambda dk\,\left(\frac{1}{k-\sqrt{mz}}-\frac{1}{k+\sqrt{mz}}\right) \qquad \text{using} \quad \frac{1}{k-\sqrt{j}}-\frac{1}{k+\sqrt{j}}=\frac{2\sqrt{j}}{k^2-j^2} \\ &= \frac{z^{1/2}m^{3/2}}{4\pi^2}\left[\ln\frac{k-\sqrt{mz}}{k+\sqrt{mz}}\right]_0^\Lambda \\ &= \frac{z^{1/2}m^{3/2}}{4\pi^2}\left(\ln\frac{\Lambda-\sqrt{mz}}{\Lambda+\sqrt{mz}}-\ln(-1)\right) \qquad \text{in which } -\ln(-1)=+i\pi \quad \text{(a choice of branch cut)} \\ &= \frac{mp}{4\pi}\left(\frac{1}{\pi}\ln\frac{1-p/\Lambda}{1+p/\Lambda}+i\right) \qquad \text{using } mz=p^2 \end{aligned} \tag{17}$$

So far, we have a T-matrix that is

$$T^{-1}(p,\Lambda)=\frac{m}{4\pi}\left(\frac{1}{a}+ip+\frac{p}{\pi}\ln\frac{1-p/\Lambda}{1+p/\Lambda}\right) \tag{18}$$

To identify the effective-range term, we make a low-energy expansion of the logarithm. Substituting $mz=p^2$, and taking the limit $p\ll\Lambda$, we have

$$\ln\frac{\Lambda-\sqrt{mz}}{\Lambda+\sqrt{mz}}=\ln(1-p/\Lambda)-\ln(1+p/\Lambda)\approx 2p/\Lambda \tag{19}$$

such that

$$T^{-1}=\frac{m}{4\pi}\left(\frac{1}{a}-\frac{2p^2}{\pi\Lambda}+ip\right) \qquad \text{which we compare to} \quad T^{-1}=\frac{m}{4\pi}\left(-p\cot\delta+ip\right) \tag{20}$$

where δ is the scattering phase, and at low energy $\cot\delta\approx -a^{-1}+\frac{1}{2}r_e p^2+\ldots$ is the usual way of writing out the effective-range approximation. We thus identify that the only choice of Λ that gives the correct low-energy behaviour is

$$\Lambda=\frac{4}{\pi}r_e^{-1} \tag{21}$$

and thus we can make this replacement in the T matrix, fixing the cutoff using the measured (or calculated) effective range.

In sum, we have

$$\boxed{T^{-1}(p,a,r_e)=\frac{m}{4\pi}\left(\frac{1}{a}+ip+\frac{p}{\pi}\ln\frac{1-\frac{\pi}{4}pr_e}{1+\frac{\pi}{4}pr_e}\right)} \tag{22}$$

Here, we keep the full energy-dependent term, instead of using Eq. 19, because k/Λ is of order unity for the bound state found in §III.A.

A. Pole

Next, let's find the pole in the T-matrix. Here, we will take $p\to i\kappa$, with $\kappa>0$. Using the identity

$$\tan^{-1}(x)=\frac{i}{2}\ln\frac{1-ix}{1+ix}$$

we have

$$T^{-1}(i\kappa)=\frac{m}{4\pi}\left(\frac{1}{a}-\kappa+\frac{2\kappa}{\pi}\tan^{-1}(\frac{\pi}{4}\kappa r_e)\right) \tag{23}$$

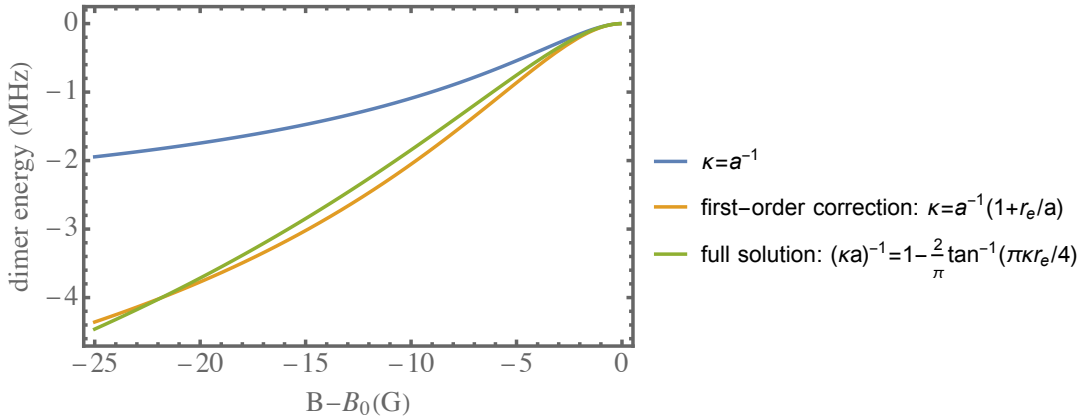

FIG. 1 Bound-state energy versus field for ^{40}K near an s-wave Feshbach resonance. Here, using a fixed $r_e = 107\,a_0$. At the ab resonance, 22.1 G below the ac resonance, the predicted binding energy is -4.04 MHz. (Plot currently uses parameters ($a_{\rm bg}$, Δ, and s) of the ab resonance, assuming that apart from B_0, the ac resonance is otherwise identical.)

The pole equation $T^{-1} = 0$ then gives

$$0 = \frac{1}{a} - \kappa\left(1 - \frac{2}{\pi}\tan^{-1}(\frac{\pi}{4}\kappa r_e)\right) \tag{24}$$

As a check, we can recover the low-energy root. A linear expansion of the arctangent in Eq. (26) gives $(a\kappa)^{-1} \approx 1 - \frac{1}{2}r_e\kappa$, whose quadratic solution give two roots for $a > 0$: $\kappa = (2r_e)^{-1}(1 \pm \sqrt{1 - 4r_e/a})$. The negative root gives the low-energy solution,

$$\kappa \approx \frac{1}{a}\left(1 + \frac{r_e}{a}\right) + \mathcal{O}(r_e^2/a^3) \tag{25}$$

...recovering the $1/a^2$ binding energy in the small-r_e limit.

For larger κ, the nonlinear equation must be solved:

$$\boxed{\frac{1}{a\kappa} = 1 - \frac{2}{\pi}\tan^{-1}\left(\frac{\pi}{4}\kappa r_e\right)} \tag{26}$$

One can show[4] that this is equivalent to

$$\frac{1}{a\kappa} = \frac{2}{\pi}\tan^{-1}\left(\frac{4}{\pi\kappa r_e}\right)$$

...although this simpler-looking form cannot be expanded easily, since the argument of the arctangent is large.

Using the parameterization of $r_e(B)$ described in App. A for ^{40}K, Fig. 1 shows the bound-state energy versus field. The corrected bound state is roughly a factor of 2 below the $1/a^2$ root. Or alternatively, $\kappa a_{13} \approx 1.48$.

IV. EFFECTIVE-RANGE CORRECTION TO THE SUM RULE

The clock shift Ω_c for a balanced gas $N_1 = N_2 = N/2$ is (Punk and Zwerger, 2007; Baym *et al.*, 2007; Zhang and Leggett, 2009; Braaten *et al.*, 2010)

$$\frac{\Omega_c}{E_F} = \frac{4}{mk_F}\frac{\bar{g}_{13}}{\bar{g}_{12}}\left(\frac{1}{\bar{g}_{12}} - \frac{1}{\bar{g}_{13}}\right)\widetilde{C} \tag{27}$$

[4] using $\tan(\frac{\pi}{2} - \theta) = \cot\theta$, so that if $\tan^{-1} x = \theta$, then $\frac{\pi}{2} - \tan^{-1} x = \tan^{-1}(1/x)$.

where $\widetilde{C}$ is the contact written in dimensionless form as $\widetilde{C} = C/Nk_F$, $g^{-1} = \bar{g}^{-1} + m\Lambda/2\pi^2$ for both initial (12) and final (13) channels, and we use $\hbar = 1$ for this section. The numerical prefactor is discussed in App. C

Using $\Lambda = \frac{4}{\pi} r_e^{-1}$ and $g^{-1} = m/4\pi a$ we have

$$\bar{g}_{12}^{-1} = \frac{m}{4\pi}\left(a_{12}^{-1} - \frac{8}{\pi^2} r_{e,12}^{-1}\right) \qquad \text{and} \qquad \bar{g}_{13}^{-1} = \frac{m}{4\pi}\left(a_{13}^{-1} - \frac{8}{\pi^2} r_{e,13}^{-1}\right) \tag{28}$$

such that

$$\frac{mk_F}{4}\frac{\tilde{\Omega}_c}{\tilde{C}} = \frac{m}{4\pi}\frac{a_{13}^{-1} - \frac{8}{\pi^2} r_{e,13}^{-1}}{a_{12}^{-1} - \frac{8}{\pi^2} r_{e,12}^{-1}}\left(a_{12}^{-1} - \frac{8}{\pi^2} r_{e,12}^{-1} - a_{13}^{-1} + \frac{8}{\pi^2} r_{e,13}^{-1}\right) \tag{29}$$

At unitarity, we have

$$\pi k_F \left.\frac{\tilde{\Omega}_c}{\tilde{C}}\right|_{a_{12}\to\infty} = \frac{a_{13}^{-1} - \frac{8}{\pi^2} r_{e,13}^{-1}}{-\frac{8}{\pi^2} r_{e,12}^{-1}}\left(-\frac{8}{\pi^2} r_{e,12}^{-1} - a_{13}^{-1} + \frac{8}{\pi^2} r_{e,13}^{-1}\right) \tag{30}$$

In a simple limit, the final-state scattering length is also large ($a_{13} \gg r_{e,13}$), and the initial- and final-state scattering lengths are the same ($r_{e,13} = r_{e,12}$), such that

$$\pi k_F \left.\frac{\tilde{\Omega}_c}{\tilde{C}}\right|_{a_{12}\to\infty} \approx -a_{13}^{-1} \qquad \text{(Uncorrected sum rule 1: } r_{e,13} = r_{e,12} \text{ and } a_{13} \gg r_{e,13}\text{)} \tag{31}$$

For ^{40}K spectroscopy at ab unitarity (202.1 G), $r_{e,13}/a_{13} \sim 0.5$, so the uncorrected sum rule is not a good approximation. However, a reasonable approximation is that the initial- and final-state r_e are the same: we estimate only a 20% difference. Then, one finds:

$$\pi k_F \left.\frac{\tilde{\Omega}_c}{\tilde{C}}\right|_{a_{12}\to\infty} = \frac{a_{13}^{-1} - \frac{8}{\pi^2} r_e^{-1}}{-\frac{8}{\pi^2} r_e^{-1}}\left(-a_{13}^{-1}\right) = -a_{13}^{-1}\underbrace{\left(1 - \frac{\pi^2}{8} r_e a_{13}^{-1}\right)}_{\approx 0.37} \qquad \text{(for } r_{e,13} = r_{e,12}\text{)} \tag{32}$$

where the quantitative value uses the geometric mean of $r_{e,12} \approx 124\, a_0$ and $r_{e,13} \approx 104\, a_0$. By comparison, the correction factor from the full expression, Eq. (30), gives 0.36. In sum, the effective-range corrections to the clock shift reduce it by a factor of ≈ 3 below the uncorrected value.

An alternate "naive" rule refers to the dimer binding energy. In the zero-range limit, $\sqrt{E_b} = m^{-1/2}\kappa$. Dropping the factors of mass, we then expect that

$$\pi k_F \left.\frac{\tilde{\Omega}_c}{\tilde{C}}\right|_{\text{dimer}} \approx -\kappa \qquad \text{(“dimer” version of the naive sum rule, at Unitarity)} \tag{33}$$

How wrong is this? Let's say we use the correct κ (as found by Eq. (26)). Comparing to Eq. (32), the corrective factor now needs an additional factor of κa_{13}:

$$\begin{aligned} \pi k_F \left.\frac{\tilde{\Omega}_c}{\tilde{C}}\right|_{a_{12}\to\infty} &= -\kappa\underbrace{(\kappa a_{13})^{-1}\left(1 - \frac{\pi^2}{8} r_e a_{13}^{-1}\right)}_{\approx 0.25} \\ &\approx -\kappa\underbrace{(1 + r_e a_{13}^{-1})^{-1}\left(1 - \frac{\pi^2}{8} r_e a_{13}^{-1}\right)}_{\approx 0.24} \end{aligned} \tag{34}$$

where in the second line we have used Eq. (25) to give an approximate expression for κa_{13} (more accurate than it deserves to be: see Fig. 1).

Conclusions:
(I) The clock shift at unitarity is $\tilde{\Omega}_c \approx -0.08(\kappa/k_F)\tilde{C}$. Since $\kappa/k_F \sim 12$ and $\tilde{C} \sim 1$ for our typical conditions, then we expect $\tilde{\Omega}_c \approx -1$.
(II) I think Eq. (34) implies that the back-of-the-envelope argument of §I and §II, based on Eq. (33), over-estimates the weight of the dimer feature by a factor of four.

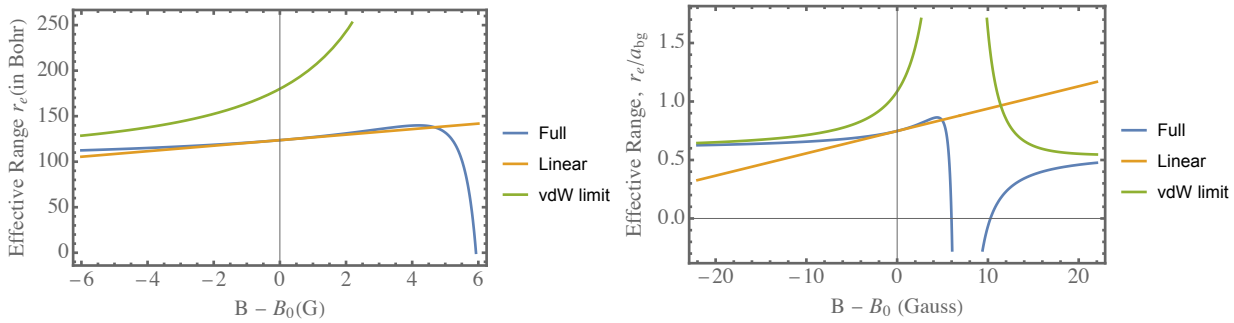

FIG. 2 Effective range versus B-field detuning from resonance. **Left:** r_e for the ab channel, within on Δ_a of resonance. We see little variation, that follows the linear approximation near resonance, but deviates strongly near the zero-crossing of a, at $B - B_0 \sim +7\,\mathrm{G}$. **Right:** At a larger scale, we see that as $a \to a_{\rm bg}$, the two-channel expression for r_e approaches a background value, given by Eq. (A7).

Appendix A: B-field-dependence of the s-wave effective range

As a preliminary, we note that without a Feshbach resonance, the energy and length scales of the open channel are set by the long-range van der Waals interaction $-C_6/r^6$ between neutral ground-state atoms. We can then define a characteristic van der Waals length (along the lines of $C_6 = \hbar^2\beta_6^4/m$), however there are (at least) three distinct conventions:

$$\beta_6 = \left(\frac{2m_r C_6}{\hbar^2}\right)^{1/4} \qquad \text{or} \qquad R_{\rm vdW} = \frac{\beta_6}{2} \qquad \text{or} \qquad \bar{a} = \frac{2\pi}{\Gamma(1/4)^2}\beta_6\,. \tag{A1}$$

For ^{40}K, $R_{\rm vdW} = 65.02\,a_0 \approx 65a_0 = 3.4\,\mathrm{nm}$ (Falke *et al.*, 2008), where $a_0 = 0.053\,\mathrm{nm}$ is the Bohr length. Thus $\beta_6 \approx 130\,a_0$, and $\bar{a} = 4\pi/\Gamma(1/4)^2 \approx 62a_0$ is nearly equal to $R_{\rm vdW}$.

In contrast, the scattering length is widely variable. Near an isolated Feshbach resonance,

$$a(B) = a_{\rm bg}(1 - \Delta_a/\delta B) \qquad \text{where} \qquad \text{and} \quad \delta B = B - B_0\,. \tag{A2}$$

For the most commonly used Feshbach resonance in the ab channel, $B_0 = 202\,\mathrm{G}$, $\Delta_a = 6.9\,\mathrm{G}$, and $a_{\rm bg} \approx 167a_0$. Note that (for ^{40}K), both $a_{\rm bg}$ and r_e are on the order of $R_{\rm vdW}$.

The theory of contact parameters typically assume that r_e and a are independent parameters. However, in the laboratory we cannot vary them independently: scattering is tuned by the Feshbach mechanism, which affects both r_e and a. This means that, near a Feshbach resonance, the change in $r_e(B)$ is linked to the change in $a(B)$. In other words, there is a *special path in the* $\{a^{-1}, r_e\}$ *parameter space that is traversed with variable magnetic field.* A parameterization of $r_e[a(B)]$ is given by (Gao, 2011; Werner and Castin, 2012; Chapurin *et al.*, 2019) as

$$r_e(B) = -2\frac{\bar{a}}{s_{\rm res}}\left(1 - \frac{a_{\rm bg}}{a(B)}\right)^2 + r_e^{\rm vdW}(a(B)) \tag{A3}$$

where the prefactor of the first term is also written as $R^* = \bar{a}/s_{\rm res}$ (Is there a physical interpretation of R^*?) [5]

The second term is given by the open-channel van der Waals potential:

$$r_e^{\rm vdW}(a(B)) = r_{\rm e0}^{\rm vdW}\left(1 - 2\bar{a}a^{-1} + 2\bar{a}^2a^{-2}\right) \tag{A5}$$

which may require that $|a| \gg \bar{a}$, and where

$$r_{\rm e0}^{\rm vdW} = \frac{\Gamma_{1/4}^4\bar{a}}{6\pi^2} \approx 2.8R_{\rm vdW} = 180a_0 = 9.6\,\mathrm{nm} \approx 1.1a_{\rm bg} \tag{A6}$$

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[5] For an isolated resonance, we can write these parameters in terms of the differential magnetic moment of the (bare) dimer branch:

$$s_{\rm res} = \frac{a_{\rm bg}\,\Delta_a}{\bar{a}}\frac{\delta\mu}{\bar{E}} \approx 2.2 \qquad \text{or} \qquad R^* = \frac{\bar{a}}{s_{\rm res}} = \frac{\bar{E}}{a_{\rm bg}\,\Delta_a\,\delta\mu} \approx 28\,a_0 \approx 1.5\,\mathrm{nm} \tag{A4}$$

where the value is given for ^{40}K, from (Chin *et al.*, 2010; Baur *et al.*, 2012), and $\bar{E} \equiv \hbar^2/m\bar{a}^2$. However, it has been shown that for ^{40}, three channels may need to be taken into account, so $\delta\mu$ defined implicitly above should not be taken as quantitative.

Here, values are given for ^{40}K. `It seems like Chapurin (S7) differs by a factor of 2 in the last term.` Since $a \to 0$ at $\delta B = \Delta_a$, we see that the expression (A5) for $r_e(B)$ diverges at the same place. (However, I think the expression is derived only for large scattering lengths?)

`To do with this appendix: 1) extend plots to -22G; (2) Get correct numbers for the ac channel.`

Figure 2 compares Eqs. (A3) and (A5) alone. We see that far from the Feshbach resonance, the closed-channel contribution vanishes. This is evident by inspection of Eq. (A3), for $a \to a_{\rm bg}$. Instead, we are left only with

$$r_e(a \to a_{\rm bg}) = r_{e0}^{\rm vdW} \underbrace{\left(1 - 2\bar{a}a_{\rm bg}^{-1} + 2\bar{a}^2 a_{\rm bg}^{-2}\right)}_{\approx 0.53} \tag{A7}$$

such that the background $r_e \approx 97\, a_0$.

A linearized expression gives, for $|\delta B| \ll |\Delta_a|$,

$$\begin{aligned} r_e(B) &\approx \left[r_{e0}^{\rm vdW} - \frac{2}{s_{\rm res}}\bar{a}\right]\left\{1 + \left[\left(2 - \frac{r_{e0}^{\rm vdW} s_{\rm res}}{a_{\rm bg}}\right)^{-1} + \left(\frac{2\bar{a}}{a_{\rm bg}} - \frac{4\bar{a}}{r_{e0}^{\rm vdW} s_{\rm res}}\right)^{-1}\right]^{-1}\frac{\delta B}{\Delta_a}\right\} \\ &\equiv r_{e0}\left\{1 + \frac{\delta B}{\Delta_r}\right\} \end{aligned} \tag{A8}$$

In the case of ^{40}K, since $s \sim 2$, this *reduces* the on-resonant effective range by $\bar{a}$, or roughly a third:

$$r_{e0} = r_{e0}^{\rm vdW} - \frac{2}{s_{\rm res}}\bar{a} \quad \approx 124 a_0 = 6.6\,{\rm nm} \sim 0.7 r_{e0}^{\rm vdW} \tag{A9}$$

Also the linear variation is smaller, by a factor of ~ 6, than for the inverse scattering length:

$$\Delta_r/\Delta_a = \left(2 - \frac{r_{e0}^{\rm vdW} s_{\rm res}}{a_{\rm bg}}\right)^{-1} + \left(\frac{2\bar{a}}{a_{\rm bg}} - \frac{4\bar{a}}{r_{e0}^{\rm vdW} s_{\rm res}}\right)^{-1} \quad \approx 41\,{\rm G} \sim 6\Delta_a \tag{A10}$$

Since the linear expressions are only valid within $\pm\Delta_a$ of resonance, we see that the r_e changes less than $\pm 10\%$ within the validity of the linear approximation. Also note from Eqs. (A9) and (A10), that in the limit of a broad resonance, $s_{\rm res} \gg 1$, we recover Eq. (**??**).

In summary, near the 202 G Feshbach resonance for the ab channel, the on-resonant effective range is $124\, a_0 \sim 1.9 R_{\rm vdW}$, and the final-state effective range is $104\, a_0 \sim 1.6 R_{\rm vdW}$ from Eq. (A3). The latter is not far from the asymptotic open-channel value of r_e: $97\, a_0 \sim 1.5 R_{\rm vdW}$.

Appendix B: High-frequency s-wave contact tail

The rf spectrum of spin-state σ is $I_\sigma(\omega)$, which obeys the sum rule $\int I_\sigma\, d\omega = N_\sigma$. When transferring to a continuum, we measure I_σ as $\Gamma = \frac{\pi}{2}\Omega^2 I_\sigma$. Note that for N_σ two-level systems, the FGR sum rule gives $\int \Gamma\, d\omega = \frac{\pi}{2}\Omega^2 N_\sigma$. (Note that the matrix element here is $\hbar\Omega/2$; there is sometimes confusion about whether Ω is the bare or rotating-wave Rabi frequency. `Note that (Braaten et al., 2010) gives` $\int \Gamma = \pi\Omega^2 N_\sigma$`!`) With dimensionless transfer rate $\tilde{\Gamma} = \frac{1}{2}(E_F/\hbar N_\sigma) I_\sigma$, and dimensionless frequency $x = \hbar\omega/E_F$, the sum rule is $\int \tilde{\Gamma}\, dx = \frac{1}{2}$.

The contact tail is then

$$\tilde{\Gamma} \to \frac{1}{2^{3/2}\pi^2}\underbrace{\frac{C}{Nk_F}}_{\equiv \widetilde{C}} x^{-3/2} \qquad \text{or} \qquad \frac{\tilde{\Gamma}}{\int \tilde{\Gamma} dx} \to \frac{1}{2^{1/2}\pi^2}\underbrace{\frac{C}{Nk_F}}_{\equiv \widetilde{C}} x^{-3/2} \tag{B1}$$

where we have now assumed that $N_\sigma = N/2$, where N is the total number of atoms. In §I, we normalized $\gamma(x)$ as $\int \gamma\, dx = 1$. In that case,

$$\frac{\gamma(x)}{\int \gamma dx} = \gamma(x) \to \frac{1}{2^{1/2}\pi^2}\widetilde{C}\, x^{-3/2} \tag{B2}$$

In relation to the "lab standard", $\gamma = I_\sigma/N_\sigma$, such that $\int \gamma\, dx = 1$.

To check, the explicit relation in (Braaten *et al.*, 2010) is (without $\hbar$'s)

$$\begin{aligned}
\Gamma &\to \frac{\Omega^2}{4\pi\sqrt{m}} C\omega^{-3/2} \\
\frac{\Gamma}{\int \Gamma d\omega = \pi\Omega^2 N_2} &\to \frac{1}{4\pi^2\sqrt{m}} \frac{C}{N_2} \omega^{-3/2} \\
\frac{\Gamma}{\int \Gamma dx = \pi\Omega^2 N_2/E_F} &\to \frac{E_F}{E_F^{3/2}} \frac{1}{4\pi^2\sqrt{m}} \frac{C}{N/2} x^{-3/2} \\
&= \frac{1}{(k_F^2/2)^{1/2}} \frac{1}{2\pi^2} \frac{C}{N} x^{-3/2} \\
&= \frac{1}{2^{1/2}\pi^2} \frac{C}{N k_F} x^{-3/2} = \frac{1}{2^{1/2}\pi^2} \widetilde{C}\, x^{-3/2} \qquad \text{(Good.)}
\end{aligned} \tag{B3}$$

A correction for final-state interactions is given by (Braaten *et al.*, 2010):

$$\gamma \to \frac{1}{2^{1/2}\pi^2} \widetilde{C}\, x^{-3/2} \times \frac{(a_{12}^{-1} - a_{13}^{-1})^2}{a_{13}^{-2} + m\omega} \tag{B4}$$

In the unitary limit, $a_{12}^{-1} \to 0$, such that

$$\gamma \to \frac{1}{2^{1/2}\pi^2} \widetilde{C}\, x^{-3/2} \times \left(1 + \frac{m\omega}{a_{13}^{-2}}\right)^{-1} = \frac{1}{2^{1/2}\pi^2} \widetilde{C}\, \frac{x^{-3/2}}{1 + x/x_d} \qquad \text{(Unitarity)} \tag{B5}$$

where we have defined $x_d = (m a_{13}^2)^{-1}/E_F$, the dimer energy in the final state channel, in the shallow-dimer limit that $a_{13} \gg r_{e,13}$.

1. Contact tail formula with effective-range correction?

`Is there an expression for the` $\omega^{-3/2}$ `tail that includes the effective-range corrections?`

Appendix C: Forms of the clock-shift sum rule

This Appendix gets the factors of 2 and π correct in the clock shift, for use in Eqs. (2) and (27).
(Haussmann *et al.*, 2009) gives

$$\hbar\bar{\omega} = \frac{4\epsilon_F^2}{n_2} \left(\frac{1}{g} - \frac{1}{g_f}\right) \frac{\mathcal{C}}{k_F^4} \tag{C1}$$

We then replace $\mathcal{C}/n_2$ by C/N_2 (assuming a uniform gas with volume V, such that $N_2 = n_2 V$ and $C = \mathcal{C}V$), divide through by $\epsilon_F = E_F$, expand the remaining $E_F = k_F^2/2m$, to find

$$\frac{\Omega_c}{E_F} = \frac{2}{m k_F} \frac{\bar{g}_{13}}{\bar{g}_{12}} \left(\frac{1}{\bar{g}_{12}} - \frac{1}{\bar{g}_{13}}\right) \frac{C}{k_F N_2} = \frac{4}{m k_F} \frac{\bar{g}_{13}}{\bar{g}_{12}} \left(\frac{1}{\bar{g}_{12}} - \frac{1}{\bar{g}_{13}}\right) \frac{C}{k_F N} \tag{C2}$$

(Braaten *et al.*, 2010) uses the extensive contact C in the sum rule.

$$\int d\omega\, \omega\, \Gamma = \frac{\Omega^2}{4m} (a_{12}^{-1} - a_{13}^{-1}) C \tag{C3}$$

As discussed in §B, they use a different normalization for Γ than our standard, perhaps due to differing definition of Ω. So let's instead calculate

$$\begin{aligned}
\Omega_c \equiv \frac{\int d\omega\, \omega\, \Gamma}{\int d\omega\, \Gamma} &= \frac{1}{4\pi m} (a_{12}^{-1} - a_{13}^{-1}) \frac{C}{N_2} \\
&= \frac{1}{4\pi m} \frac{4\pi}{m} (g_{12}^{-1} - g_{13}^{-1}) \frac{C}{N/2} \\
&= \frac{2}{m^2} (g_{12}^{-1} - g_{13}^{-1}) \frac{C}{N}
\end{aligned} \tag{C4}$$

using $g^{-1} = (m/4\pi)a^{-1}$. In dimensionless form,

$$\tilde{\Omega}_c = \frac{\Omega_c}{E_F} = \frac{4}{mk_F}(g_{12}^{-1} - g_{13}^{-1})\frac{C}{Nk_F} \tag{C5}$$

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