Quantum defect analysis of interacting collisional resonances

Matthew Chilcott, James F. E. Croft, Ryan Thomas, and Niels Kjærgaard

1 Quantum Science Otago, Dodd-Walls Centre, Department of Physics, University of Otago, New Zealand
2 Department of Quantum Science and Technology, Research School of Physics, The Australian National University, Canberra 2601, Australia

(Dated: January 3, 2022)

We use a laser-based collider to study the interplay between a magnetic Feshbach resonance and a shape resonance in cold collisions of ultracold $^{87}$Rb atoms. By exerting control over a parameter space spanned by both collision energy and magnetic field, we can tune the width of a Feshbach resonance over several orders of magnitude. We develop a quantum defect theory specialized for ultracold atomic collisions, and provide a full description and analysis of the experimental observations.

Collision resonances are ubiquitous in atomic and particle physics, where they arise due to coupling between the scattering continuum and a quasi-bound state. Their tell-tale signature is an abrupt suppression or enhancement in scattering as the collision energy is scanned, but they may also emerge when scanning an external field which tunes the energy levels of the system. In ultracold atomic physics, such field-tunable resonances provide an indispensable tool for manipulating the interactions between atoms, which has been exploited in a number of hallmark quantum experiments in atomic systems, including solitons [1], the BEC-BCS crossover [2, 3], and quantum droplets [4].

With the recent push towards experiments with ultracold molecules [5, 6], the interaction between collisional resonances has become a subject of increased interest, due to the high density of states in molecules compared to atoms. Extraordinarily long lifetimes, approaching milliseconds [7–9], have been observed in collisions between nonreactive ultracold molecules in their absolute ground state. These long lifetime have been attributed to the high density of states of molecules [10–12] and suggest the presence of overlapping resonances [13]. Interacting Feshbach resonances are also of importance in collisions of ultracold magnetic lanthanides, such as erbium and dysprosium, and have been used to reveal the chaotic nature of the collision process [14, 15].

Quantum defect theory (QDT) provides a convenient framework for analyzing cold atomic collisions. By separating the scattering problem into energy sensitive and insensitive components, QDT allows for an elegant description of resonance interactions, with the energy dependence encapsulated in a few analytic parameters. Recent demonstrations of the power of QDT include the prediction and interpretation of triplet structures for $d$-wave Feshbach resonances [16] and shape resonances [17].

In this paper, we study the interaction between a shape resonance and a Feshbach resonance in collisions of $^{87}$Rb atoms, with both resonances arising from quasi-bound $d$-wave states of the system. Figure 1 shows an example potential well for the collisional entrance channel (blue line) which describes the interaction as a function of radial separation. When including angular momentum, the effective potential contains a barrier in front of the potential well (orange line), behind which a quasi-bound state can be formed (orange dashed line). For atoms tunnelling through the barrier, such a quasi-bound state gives rise to a scattering resonance. Similarly, Feshbach resonances arise from the coupling to a bound state, but in this case the bound state belongs to a closed channel. A closed channel potential, which is energetically inaccessible for separated particles, is presented in red in Fig. 1. Due to the deep potential well, the closed channel shown becomes accessible at short-range during a collision. If a bound state (red dashed line) is present at the collision energy, incoming atoms can temporarily bind in this state, enhancing their interaction. In the case of a magnetic Feshbach resonance, the different magnetic moments of

* niels.kjaergaard@otago.ac.nz
We show that a simple two-channel QDT model captures the position of the Feshbach resonance in energy. While shape resonances and Feshbach resonances are typically treated in isolation, the tunability of the latter opens the possibility of moving a Feshbach resonance through a shape resonance using an external field. We recently studied the interaction of a pair of such resonances and observed the avoided crossing in the associated $S$ matrix poles [18]. In the current work, we extend our analysis of this resonance pair and give an interpretation in terms of multi-channel quantum defect theory (MQDT). We show that a simple two-channel QDT model captures all the essential physics of the interacting collisional resonances.

I. EXPERIMENTAL METHODS

A. System

We collide atoms of $^87$Rb which are both in the absolute ground hyperfine state $|F, m_F⟩ = |1, 1⟩$. This $|1, 1⟩ ⊕ |1, 1⟩$ entrance channel has a plethora of Feshbach resonances, previously mapped out by loss spectroscopy [19]. In the current study, we utilize a $d$-wave Feshbach resonance corresponding to the closed channel molecular state with the quantum numbers $F_1 = 2, F_2 = 2, ν′ = −5$, and $M = 2$, where $M = m_{F_1} + m_{F_2}$ and $ν′$ is the vibrational quantum number counting from the $F_1 = 2, F_2 = 2$ threshold. For a magnetic field of 930 G, this state becomes located at the $|1, 1⟩ ⊕ |1, 1⟩$-channel threshold where it is predominantly comprised of components from the $|2, 0⟩ ⊕ |2, 2⟩$ and $|2, 1⟩ ⊕ |2, 1⟩$ channels. The $|1, 1⟩ ⊕ |1, 1⟩$ channel also hosts a $d$-wave shape resonance near 300 μK [20, 21].

The Feshbach resonance we employ was predicted by Marte et al. [19] to be located at 930.9 G with a theoretical zero-energy width of $\ll 0.1$ mG; their experiments observed it at $B_0 = 930.02$ G using loss spectroscopy. A subsequent observation has placed this resonance at 930.89 G in photo-association experiments [22]. Our own loss spectroscopy measurements (described in Appendix A) observe the zero-energy resonance at 929.921(3) G.

B. Setup

Our collider is composed of a system of steerable optical dipole traps, formed by pairs of crossed, red-detuned laser beams [23]. A horizontal guide beam defines the axis of the collision, while a vertical beam can be translated by a pair of acousto-optic deflectors, capable of producing multiple time-averaged traps by toggling the frequency drive to the deflectors. We begin each collision experiment by loading a single crossed dipole trap with a cloud of $^87$Rb atoms in the $|2, 2⟩$ state, which we have previously collected in a magneto-optical trap, and then evaporatively-cooled in an Ioffe-Pritchard magnetic trap. The dipole trap then splits into two traps, which are dragged apart by 500 μm along the horizontal beam resulting in two clouds of approximately equal size. The clouds are transferred into the $|1, 1⟩$ state by microwave adiabatic rapid passage [24] with the Zeeman states split by a small bias field. We then lower the power of the horizontal guide beam to allow the atoms to cool further by evaporation, finally attaining temperatures of $\sim 800$ nK with $\sim 3 \times 10^5$ atoms in each cloud. For higher collision energies, we further separate the clouds allowing room for a 2 mm run-up to the collision. We tune the position of the Feshbach resonance by applying a magnetic field with a pair of Helmholtz coils carrying a current controlled at the ppm level [25], before accelerating the clouds towards each other by steering the vertical dipole beams. As the clouds reach the collision energy, all laser beams are turned off and the clouds collide in the absence of trapping.

C. Detection

After the clouds separate post-collision, we apply a pulse of resonant light to acquire an absorption image of the clouds and the halo of scattered atoms. Figure 2a shows examples of such images with the atom distribution projected onto a plane and exhibiting clear $d$-wave character [21, 26]. We integrate the an image (Fig. 2b) in the direction orthogonal to the collision (vertically) and the resulting integral (Fig. 2c) carries a spatial imprint of shapes associated with the interfering $s$ and $d$ partial waves, and the unscattered thermal clouds. By fitting these shapes to the integrated image, we extract the scattered fraction $S$.

The cross-section is related to the scattered fraction by [27]

$$S = \frac{ασ}{1 + ασ}$$

where $σ = σ_s + σ_d$ is the sum of the $s$ and $d$ partial-wave cross-sections, and the parameter $α$ is geometry-dependent and left as a free parameter when fitting the cross-section. For a particular partial wave $ℓ$, the cross-section is

$$σ_ℓ = \frac{4πℏ(2ℓ + 1)}{μE} \sin^2(δℓ),$$

where $δℓ$ is the corresponding partial wave scattering phase shift, $E$ is the collision energy, and $μ$ is the reduced mass. As we are colliding indistinguishable bosons, only even-$ℓ$ partial waves are allowed and Eq. (2) includes an additional factor of 2 compared to the distinguishable particle case. Because the magnetic Feshbach resonance has a $d$-wave character, we take the $s$-wave phase-shift $δ_s$, and consequently $σ_s$ to be constant in magnetic field and only a function of energy. Close to the magnetic resonance, the $d$-wave phase-shift $δ_d$ can be described by the Beutler-Fano model:

$$δ_d(E, B) = δ_{bg}(E) + \tan^{-1}\left(\frac{Γ(E)/2}{B - B_{\text{res}}(E)}\right),$$

where $Γ(E)$ is the width of the scattering cross-section at energy $E$, and $B_{\text{res}}(E)$ is the resonance magnetic field.
FIG. 2. Fractions of scattered atoms from post-collision absorption images. a) Absorption images at a range of magnetic fields over the resonance for a collision energy of \( E/k_B = 300 \mu K \). The collision axis is horizontal. b) Close-up of a collision near 940 G. The scattering here is strongly anisotropic and has the signature of \( d \)-wave scattering [26]. c) The integrated column density (blue), to which our model is fitted in order to extract the parameters of the collision. From the fit the components of unscattered (orange), and the \( s \)-wave (red) and \( d \)-wave (green) scattered atoms are extracted.

For magnetic field \( B \), and collision energy \( E \).

With this resonance model, we extract the \( d \)-wave background phase shift \( \delta_{bg}(E) \), along with the width \( \Gamma(E) \), and position \( B_{res}(E) \) of the Fano lineshape by sweeping the magnetic field at constant energy.

The Beutler–Fano model above is equivalent to the common form of the Fano profile [28],

\[
\sigma \propto \frac{(q + \epsilon)^2}{1 + \epsilon^2},
\]

where \( q \) is the so-called shape parameter and \( \epsilon \) is the scaled, dimensionless parameter in which the resonance occurs. In our case, the required mapping to this form is given by \( q = \cot(\delta_{bg}) \) and \( \epsilon = 2(B - B_{res})/\Gamma \), the inverse of the \( \tan^{-1} \) argument in Eq. (3). Representative Fano

FIG. 3. The Fano profiles observed in the fraction of atoms which scatter during the collision. The behavior is shown at a number of energies, with resulting \( q \) values of both signs. The ability to choose \( q \) by adjusting the collision energy demonstrates the exceptional control possible in ultracold systems.

Profiles measured at four different energies are shown in Fig. 3, illustrating different regimes of the \( q \) parameter. We note that the limiting cases provide a symmetric dip at \( q = 0 \), and a Lorentzian profile at \( |q| \to \infty \), while intermediate values of \( q \) are tied to asymmetric profiles with a ‘polarity’ determined by the sign of \( q \).

II. QUANTUM DEFECT THEORY

The compelling variation in the Fano profiles observed in Fig. 3 results from the interplay between the Feshbach resonance and shape resonance. We employ quantum defect theory (QDT) to characterize and interpret the intriguing resonant scattering behavior.

A. Overarching QDT framework

The QDT approach to cold collisions takes advantage of the separation of energy and length scales common in scattering problems [29–33]. The solid blue line in Fig. 4a,b shows the triplet interaction potential between two \(^{87}\text{Rb} \) atoms as a function of separation. At long-range this potential goes to zero. Atoms at short-range (Fig. 4a) encounter a potential with a depth on the order of a thousand Kelvin, compared to a collision energy of the order of a millikelvin. This separation of energy and length scales allows the important physics of collisions to be captured
by a few analytic parameters [34–38]. Importantly, computing these QDT parameters for a system only requires the long-range form of the interaction potential and the masses of the atoms.

1. Wave functions: signatures at short and long range

To set the scene, we show in Fig. 4b the energy-normalised scattering wave functions in the $|1, 1\rangle \oplus |1, 1\rangle$ channel, generated by full coupled-channel calculations [39] at two different energies ($E/k_B = 300\,\mu K$ and $E/k_B = 500\,\mu K$). These wave functions highlight two salient features shared by all scattering solutions. Firstly, inside the well solutions are oscillatory with a varying local wave number which, crucially, has virtually no dependence on the collision energy $E$; the common waveform differ only in amplitude (see Fig. 4c). This difference in amplitude arises due to the asymptotic energy normalization. Secondly, the long-range asymptotic solutions are sinusoidal with a constant wave number. This wave number will depend strongly, but trivially, on the collision energy $E$ as $k = \sqrt{2\mu E/\hbar^2}$ and for a given energy the sinusoid will display a phase shift $\eta(E)$ with respect to the regular free space solution at that energy (Fig. 4d). The partial (elastic) scattering cross section is determined by this phase shift using Eq. (2), with $\delta_\ell = \eta$. By observing that all scattering solutions share some common ground via the above two highlighted features, the QDT framework will enable us to predict the energy dependence of the phase shift analytically.

2. Coupled channels equations, $K$ matrix and $S$ matrix

The objective of any scattering problem is to obtain the system’s $S$ matrix, as it completely describes the outcome of a scattering experiment. Formally, the $S$ matrix can be constructed from computed wavefunctions, which are solutions to the coupled radial Schrödinger equations.
where the energy $E_i$ for a channel $i$ is measured with respect to its threshold and $V_{ij}$ are the elements of a potential matrix. In our experiments, we consider two atoms entering as $|1,1\rangle \oplus |1,1\rangle$. If we ignore the weak spin-spin dipole interactions, collisions between the atoms 1 and 2 conserve $m_{F_1} + m_{F_2} = 2$ as well as mechanical angular momentum $\ell$ [40]. For the d-wave channel, their coupling is restricted to the channels $|1,1\rangle \oplus |2,1\rangle$, $|1,0\rangle \oplus |2,2\rangle$, $|2,0\rangle \oplus |2,2\rangle$, and $|2,1\rangle \oplus |2,1\rangle$ with $\ell = 2$, which results in an $N = 5$-channel set of equations [41]. Designating the entrance channel $|1,1\rangle \oplus |1,1\rangle$ with $i = 1$, we have $E_1 > 0$ as the asymptotically free incoming $|1,1\rangle$ atoms have a non-zero relative kinetic energy. In our experiment the collision energy is so low that $E_i < 0$ for the remaining four channels; these are all energetically closed and atoms can only leave the collision via the $i = 1$ channel.

Generally, when solving coupled channels problems like Eq. (5), one typically propagates out an $N \times N$ regular solution matrix $F$ [42] where $N = N_o + N_c$ is the sum of the number of open and closed channels. The $N$ columns of $F$ represent $N$ linearly independent solution vectors to Eq. (5) with row $i$ of a solution vector corresponding to the channel $i$. Asymptotically, the solution matrix can be decomposed as [43]

$$F(r) \rightarrow N(r)K,$$

where $K$ is a constant real symmetric matrix, and $J$ and $N$ are diagonal matrices with entries

$$J_{ij}(r) = \begin{cases} rk_{\ell}/2, j_{\ell}(kr), & \text{for open} \\ (kr)^{-\ell/2} I_{\ell+1/2}(kr), & \text{for closed}. \end{cases}$$

$$N_{ij}(r) = \begin{cases} rk_{\ell}/2, n_{\ell}(kr), & \text{for open} \\ (kr)^{-\ell/2} K_{\ell+1/2}(kr), & \text{for closed}. \end{cases}$$

Here, $j_{\ell}$ and $n_{\ell}$ are spherical Bessel functions of the first and second kind, respectively, and $I_{\ell+1/2}$ and $K_{\ell+1/2}$ are modified Bessel functions of the first and third kind, respectively.

The energy dependent $K$ matrix defined by Eq. (6) contains all the scattering behavior of the system. In particular, the $N_o \times N_o$ sub-matrix of $K$ that pertains to only the open channels defines the $S$ matrix [43, 44]:

$$S = [1 + iK_{oo}]^{-1}.$$

We note that $K_{oo}$ is known as the reactance matrix in the literature. In the treatment of identical particles, the wavefunctions must be properly symmetrised [45]. Because we only consider elastic collisions, we simply need to include a factor of 2 in the even-$\ell$ partial-wave cross sections—Eq. (2).

$$\sum_{j=1}^{N} \left\{ \left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\ell(\ell + 1)\hbar^2}{2\mu r^2} \right] \delta_{ij} + V_{ij}(r) \right\} u_j(r) = E_i u_i(r), \quad (5)$$

3. QDT treatment: uncoupled channels at long range

Rather than directly numerically solving Eq. (5) to, in turn, obtain $K$ and $S$, QDT proceeds by assuming that beyond a certain separation, $R_{\text{int}}$, all channels are uncoupled. At long-range, where the interaction potential is $V^{\text{int}}(r)$, the radial wavefunction for the entrance channel is a solution to the (uncoupled) radial Schrödinger equation,

$$\left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\ell(\ell + 1)\hbar^2}{2\mu r^2} + V^{\text{int}}(r) \right] u_1(r) = E_1 u_1(r). \quad (9)$$

For our system, the long-range behavior is well-described by a van der Waals potential, $V^{\text{int}}(r) = -C_6/r^6$, and Eq. (9) takes the specific form

$$\frac{d^2}{dR^2} u_1(R) = \left( \frac{1}{R^6} + \frac{\ell(\ell + 1)}{R^2} - \bar{E}_1 \right) u_1(R), \quad (10)$$

where the radial distance $R$ is measured in units of $\beta = (2\mu C_6/\hbar^2)^{1/4}$ and energy on a scale $E_\beta \equiv \hbar^2/2\mu\beta^2$. We also define the local wave number

$$\bar{k}_1(R) = \sqrt{E_1 - V_{\text{eff}}(R)}. \quad (11)$$

For reference, we note that our particular system has $C_6 = 3.253 \times 10^7 \text{K}^6 \text{A}^6$ for $^{87}\text{Rb}$ [46], which gives $\beta = 87.37 \text{A}$ and $E_\beta = 73.11 \text{mK}$.

B. Long-range considerations ($R \gg 1$)

For $R \gg 1$, $V_{\text{eff}}$ vanishes and the $E_1$-term on the right hand side of Eq. (10) dominates. In this region an energy-normalized solution $u_1(R)$ is sinusoidal, oscillating with the asymptotic wavenumber $\bar{k}_1 \rightarrow \infty \sqrt{E_1}$,

$$u_1(R) \rightarrow \frac{1}{\sqrt{\bar{k}_1}} \sin(\bar{k}_1 R - \ell\pi/2 + \eta_1), \quad (12)$$

where the $\ell\pi/2$-term references the phase shift $\eta_1$ against the regular free particle solution for the given partial wave,

$$u_{\text{free}}(R) = \bar{k}_1 R j_\ell(\bar{k}_1 R) \rightarrow \infty \sin(\bar{k}_1 R - \ell\pi/2). \quad (13)$$

Equivalently, Eq. (12) can be written as

$$u_1(r) \rightarrow c_1 \frac{1}{\sqrt{\bar{k}_1}} \sin \left( \bar{k}_1 R - \ell\pi/2 + \xi_1 \right) + c_2 \frac{1}{\sqrt{\bar{k}_1}} \cos \left( \bar{k}_1 R - \ell\pi/2 + \xi_1 \right), \quad (14)$$

where $c_1$ and $c_2$ are constants.
where the coefficients for the two quadrature components are given by
\[
\begin{bmatrix}
  c_1 \\
  c_2
\end{bmatrix} = \begin{bmatrix}
  \sin \xi_1 & \cos \xi_1 \\
  (1-1)\xi_1 & (-1)\xi_1+1 \sin \xi_1
\end{bmatrix} \begin{bmatrix}
  \sin \eta_1 \\
  \cos \eta_1
\end{bmatrix},
\] (15)
for a particular choice of the arbitrary phase \( \xi_1 \). Guided by Eq. (14), the solution of Eq. (10) can be expressed as
\[
u_1(R) = c_1 f_1(R) + c_2 g_1(R),
\] (16)
where \( f \) and \( g \) are exact solutions to Eq. (10) defined by the boundary conditions
\[
f_1(R) \sim \frac{1}{\sqrt{k_1}} \sin (k_1 R - \ell \pi/2 + \xi_1),
\] (17a)
and
\[
g_1(R) \sim \frac{1}{\sqrt{k_1}} \cos (k_1 R - \ell \pi/2 + \xi_1).
\] (17b)
In Eq. (16) the coefficients \( c_1 \) and \( c_2 \) depend on the choice of the free parameter \( \xi_1 \). In particular, for \( \xi_1 = \eta_1 \), \( c_1 = 1 \) and \( c_2 = 0 \).

C. Short-range considerations \((R \ll 1)\)

For \( R \ll 1 \), the \( E_1 \)-term of Eq. (10) is negligible and the solution \( \nu_1(r) \) becomes reminiscent of the solution \( \nu_1^{(0)}(r) \) of the Bessel equation
\[
\frac{d^2}{dr^2} \nu_1^{(0)}(r) = -\left[ \frac{1}{R^6} - \frac{\ell(\ell+1)}{R^2} \right] \nu_1^{(0)}(R).
\] (18)
\( \nu_1^{(0)}(r) \) can be expressed as a linear combination of
\[
u_+(R) = \frac{\sqrt{\pi}}{2} \sqrt{R} Y_{(2\ell+1)/4} \left( \frac{1}{2R^2} \right),
\] (19a)
and
\[
u_-(R) = \frac{\sqrt{\pi}}{2} \sqrt{R} J_{(2\ell+1)/4} \left( \frac{1}{2R^2} \right),
\] (19b)
where \( J \) and \( Y \) are Bessel functions of the first and second kind, respectively. In Fig. 5 we plot \( \nu_\pm(R) \) for \( \ell = 2 \) and it can be seen how \( \nu_- \) decays as \( R \) increases, while \( \nu_+ \) blows up. This functional behaviour is also captured by the limiting forms \([47]\)
\[
u_+(R) \sim \begin{cases} R^{3/2} \sin \left( \frac{1}{2R^2} - \frac{2\ell+3}{8} \right), & \text{for } R \rightarrow 0 \\ \sqrt{\frac{\pi}{2}} R^{\ell+1}, & \text{for } R \rightarrow \infty,
\end{cases}
\] (20a)
\[
u_-(R) \sim \begin{cases} R^{3/2} \cos \left( \frac{1}{2R^2} - \frac{2\ell+3}{8} \right), & \text{for } R \rightarrow 0 \\ \sqrt{\frac{\pi}{2}} R^{-\ell}, & \text{for } R \rightarrow \infty.
\end{cases}
\] (20b)
Both \( \nu_-(R) \) and \( \nu_+(R) \) are exact solutions to Eq. (18), \( i.e. \), Eq. (10) with \( E_1 = 0 \), valid for all \( R \). For \( E > 0 \), a pair of linearly independent approximate WKB solutions to Eq. (10) around some point \( R_0 \) where the potential \( V_{\text{eff}} \) is deep are given by
\[
w_+(R) = \frac{1}{\sqrt{k_1(R)}} \sin [\theta_{WKB}(R)],
\] (21a)
\[
w_-(R) = \frac{1}{\sqrt{k_1(R)}} \cos [\theta_{WKB}(R)],
\] (21b)
where
\[
\theta_{WKB}(R) = \int_{R_0}^R dR' \tilde{k}_1(R') - \frac{1}{2} R_0^{-2} - \frac{2\ell + 3}{8} + \phi_1.
\] (22)
We note that in the vicinity of \( R_0 \) \( i.e., \) for values of \( R \) where the potential well is deep, \( w_+(R) \) and \( w_-(R) \) are largely insensitive to the channel energy \( E_1 \) and for \( \phi_1 = 0 \), they match the analytic zero-energy solutions \( u_\pm(R) \) at short range \((\text{Fig. 5 shows } w_s \text{ and } w_c \text{ for } E/k_B = 300 \, \mu K)\). The phase \( \phi_1 \) is the key that unlocks QDT’s use of only the long-range potential because it can encapsulate the effects of the complicated multi-channel short-range interaction as a scalar quantity which varies only weakly with energy and hence can be taken to be constant.

Analogous to Eq. (16), the solution \( \nu_1(R) \) to Eq. (10) can be expressed as the linear combination
\[
\nu_1(R) = \hat{c}_1 \tilde{f}_1(R) + \hat{c}_2 \tilde{g}_1(R),
\] (23)
where \( \tilde{f}_1 \) and \( \tilde{g}_1 \) are exact solutions to Eq. (10) defined by the initial values
\[
\{ \tilde{f}_1(R_m) = w_s(R_m), \tilde{f}_1'(R_m) = w_s'(R_m) \} \quad (24a)
\] and
\[
\{ \tilde{g}_1(R_m) = w_c(R_m), \tilde{g}_1'(R_m) = w_c'(R_m) \}, \quad (24b)
\] where \( R_m \) is some point within the potential well (possibly, but not necessarily \( R_0 \)), and the coefficients \( \hat{c}_1 \) and \( \hat{c}_2 \) are determined by the boundary conditions of the physical problem. Individually, \( \tilde{f}_1 \) and \( \tilde{g}_1 \) inherit the energy-insensitivity of \( w_s \) and \( w_c \) inside the potential well.

Figure 5 shows that \( \tilde{f} \) and \( \tilde{g} \) are perfectly tailored to represent the short-range multichannel wave function. Over the range of collision energies of interest they are essentially independent of energy, and the similarity in the wave functions at short range extends analytically to energies below threshold. The functions \( w_s \) and \( f_1 \), which are plotted in Fig. 5 for an energy \( E = 300 \, \mu K \), are both completely equivalent to the zero-energy solution \( u_+ \) at short-range; likewise, \( w_c \) and \( g_1 \) are completely equivalent to the zero-energy solution \( u_- \). We also note that, by construction, for \( \phi_1 = 0 \), \( \tilde{g}_1 \) links up to the purely decaying zero-energy solution to Eq. (18), namely \( u_- \). This choice provides numerically stable reference functions as it corresponds to propagating the maximally linearly independent pair \([48]\).
D. Relating reference functions

The above considerations at short and long ranges provide two pairs of reference functions \( \{ f_1(R), g_1(R) \} \) and \( \{ \hat{f}_1(R), \hat{g}_1(R) \} \). These are all defined for all \( R > R_m \), but while \( f_1 \) and \( g_1 \) refer to boundary conditions at long-range, \( \hat{f}_1 \) and \( \hat{g}_1 \) refer to boundary conditions at short range. Connecting the pairs of reference functions defines the QDT parameters which underpin the QDT framework.

Like \( f_1(R) \), the solution \( \hat{f}_1(R) \) [subject to Eq. (24a)] will be sinusoidal for \( R \to \infty \). The phase of the two reference functions will generally differ, but for a given \( \phi_1 \) the functions can be made to match through the free phase \( \xi_1 \). Next, the amplitudes can be matched by scaling \( \hat{f}_1(R) \) by a factor \( C_1^{-1} \),

\[
    f_1(R) = C_1^{-1} \hat{f}_1(R). \tag{25}
\]

Finally, with both \( \xi_1 \) and \( C_1 \) fixed, \( g(R) \) can be written as a linear combination of \( f_1(R) \) and \( g_1(R) \)

\[
    g_1(R) = C_1 \tan \lambda_1 \hat{f}_1(R) + C_1 \hat{g}_1(R), \tag{26}
\]

as \( \hat{f}_1 \) and \( \hat{g}_1 \) span the solution space. Formally, \( \xi_1, C_1 \) and \( \tan \lambda_1 \) can be found by considering appropriate Wronskians from the short-range form of \( f \) and \( g \), \cite{31, 49}

\[
    C^{-2} = \left( f^2 k + f'^2/\bar{k}_1 \right), \tag{27a}
\]

\[
    \tan \lambda = \frac{k^2 + \gamma u}{k(\gamma - u)}, \tag{27b}
\]

where \( \gamma \) and \( u \) are the log-derivatives, \( \gamma = f'/f \), and \( u = g'/g \). We note that connecting \( \{ f_1(R), g_1(R) \} \) and \( \{ \hat{f}_1(R), \hat{g}_1(R) \} \) as in the above imposes a fixed relationship between \( \phi_1 \) and \( \xi_1 \) at a particular energy, and that the QDT parameters \( C_1 \) and \( \lambda_1 \) describing the transformation

\[
    \begin{pmatrix}
    f_1 \\
    g_1
    \end{pmatrix} =
    \begin{pmatrix}
    C_1^{-1} & 0 \\
    C_1 \tan \lambda_1 & C_1
    \end{pmatrix}
    \begin{pmatrix}
    \hat{f}_1 \\
    \hat{g}_1
    \end{pmatrix}, \tag{28}
\]

will depend on the choice of these interrelated phases.

\( C_1 \) and \( \tan \lambda_1 \) are the QDT parameters for the \( i = 1 \) open entrance channel. To connect this back to our physical system, we will (eventually) pick the pair of \( \phi_1 \) and \( \xi_1 \) such that \( \xi_1 \) reproduces the non-resonant scattering phase-shift \( \delta_{bg} \) [cf. Eq. (3)]. For this choice, \( c_2 = 0 \) in Eq. (16) which renders \( f \) as the scattering wave-function in the non-resonant scenario. As such, \( C_1^{-2} \) is the probability for the two atoms to penetrate to short range in absence of interchannel coupling, while \( \lambda_1 \) is the phase lag between \( g_1 \) and \( \hat{g}_1 \) due to the difference in kinetic energy at long range compared to short range. Together, the parameters \( C_1 \) and \( \tan \lambda_1 \) quantify the breakdown of the WKB approximation [cf. Eq. (21)] near threshold: at energies well above threshold \( C_1 \to 1 \) and \( \tan \lambda_1 \to 0 \) as the WKB treatment becomes evermore valid at all separation ranges.

E. Multichannel QDT

In general, any open channel \( i \) of a system can be subjected to the considerations for \( i = 1 \) above. The rationale behind defining \( \hat{f}_i \) and \( \hat{g}_i \) following the prescription of section II C with a corresponding transformation

\[
    \begin{pmatrix}
    f_i \\
    g_i
    \end{pmatrix} =
    \begin{pmatrix}
    C_1^{-1} & 0 \\
    C_1 \tan \lambda_i & C_1
    \end{pmatrix}
    \begin{pmatrix}
    \hat{f}_i \\
    \hat{g}_i
    \end{pmatrix}, \tag{29}
\]

becomes clear if we write the full complicated many-channel radial scattering wave function in terms of them. Suppose there is some intermolecular distance \( R_{int} \) beyond which the channels are essentially uncoupled, i.e., the same condition for which Eq. (9) emerged. The radial wave function matrix at radii \( R > R_{int} \) can be written

\[
    F(R > R_{int}) \sim \hat{f} + \hat{g} Y. \tag{30}
\]

Here \( \hat{f} \) and \( \hat{g} \) are diagonal matrices containing the \( N = N_c + N_o \) channel reference function and \( Y \) is an \( N \times N \) matrix that plays a similar role to \( K_{so} \), but at short range where all channels are locally open. As noted in section II C, \( \hat{f}_i \) and \( \hat{g}_i \) only depend weakly on the collision energy at short range since here \( |E_i| \ll |V_{eff}(R)| \). \( Y \) can therefore be considered constant with respect to the collision energy. The energy dependence characteristic of the threshold behavior is instead captured by the QDT parameters, through the transformation Eq. (29).

As such, once \( Y \) is known, computing the physical scattering \( S \) matrix at a given energy becomes simply a question of applying the appropriate scattering boundary conditions, as detailed in Ref. \cite{31} and Appendix B2.

In addition to the open entrance channel \( |1, 1 \rangle \oplus |1, 1 \rangle \), the coupled equations in Eq. (5) includes closed channels (four in our case). At short-range, these channels are locally open, so \( \hat{f} \) and \( \hat{g} \) are defined perfectly well following the prescription in section II C. Connecting to the classically forbidden region, where the wavefunction...
exponentially decays, introduces a single QDT parameter \( \nu_i \) in each closed channel such that
\[
\cos \nu_i \hat{f}_i - \sin \nu_i \hat{g}_i \rightarrow \infty \frac{e^{-|k_i|R}}{2\sqrt{|k_i|}},
\]
where \( \hat{f}_i \) and \( \hat{g}_i \) are defined as in section II.C. This identifies the particular linear combination of \( \hat{f}_i \) and \( \hat{g}_i \) which is decaying asymptotically.

Given the QDT parameters in each channel, the asymptotic \( S \) matrix can be obtained from the short range \( Y \) matrix by applying the appropriate scattering boundary conditions [31]. We start from the short-range \( Y \) matrix, which is split into sub blocks representing closed and open channels,
\[
Y = \begin{bmatrix} Y_{oo} & Y_{oc} \\ Y_{co} & Y_{cc} \end{bmatrix}.
\]

The procedure for eliminating the closed channels to connect this short-range coupling matrix to long-range, where the scattering boundary conditions for the \( N_o \) open channels are defined, is described in Appendix B2. Briefly, this relies on incorporating the effect of the closed channels on the open channels using the reduced \( Y \) matrix, \( \tilde{Y} \):
\[
\tilde{Y} = Y_{oo} - Y_{oc} [\tan \nu + Y_{cc}]^{-1} Y_{co},
\]
where \( \tan \nu \) is a diagonal matrix with \( \tan \nu_i \) as diagonal elements. Equation (33) therefore folds in the behavior of Feshbach resonances, which arise due to the closed channels and appear as poles when \( \tan \nu + Y_{cc} \rightarrow 0 \).

The effective reaction matrix, \( \tilde{R} \) is given by [see Eq. (B19)]
\[
\tilde{R} = C^{-1} [\tilde{Y}^{-1} - \tan \lambda]^{-1} C^{-1},
\]
where \( C^{-1} \) and \( \tan \lambda \) are diagonal matrices containing elements \( C_i^{-1} \) and \( \tan \lambda_i \). This introduces the effects of scattering near threshold, such as a shape resonance. Finally, the \( S \) matrix can be recovered as
\[
S = e^{i\xi} [1 + i\tilde{R}] [1 - i\tilde{R}]^{-1} e^{-i\xi},
\]
as detailed in Appendix B2.

\section{Two Channel Model}

The general multichannel QDT framework outlined above in section II.E can be simplified in the case pertaining to a single open channel, and multiple closed channels over which a single isolated resonance resides. In this case an effective two channel QDT model captures the essential physics [38, 41]. In our model, the open channel, \( o \), is the \( d \)-wave entrance channel which contains the shape resonance, and the closed channel, \( c \), contains the quasi-bound state giving rise to the Feshbach resonance.

We choose the short-range reference functions such that the \( Y \) matrix is purely off-diagonal
\[
Y = \begin{pmatrix} 0 & y \\ y & 0 \end{pmatrix},
\]
which we are always free to do in the two channel case [50]. Applying the above MQDT formulae Eq. (33) and Eq. (34) gives
\[
\tilde{R} = \frac{y^2 C^{-2}}{-\tan \nu - y^2 \tan \lambda}.
\]

Writing the \( S \) matrix, in our case just a single complex number, in terms of the scattering phase shift, \( S = e^{2i\delta} \), and using Eq. (35) gives [51]
\[
\delta_d = \xi + \arctan \tilde{R},
\]
which yields the scattering phase shift in terms of the QDT parameters
\[
\delta_d = \xi + \arctan \left( \frac{y^2 C^{-2}}{-\tan \nu - y^2 \tan \lambda} \right).
\]

Using a linear expansion of \( \tan \nu \) which goes to zero in the vicinity of a resonance \( \tan \nu \approx \frac{\partial \nu}{\partial E} (E - E_0) \) and defining \( \frac{1}{2} \tilde{\Gamma} = \left( \frac{\partial \nu}{\partial E} \right)^{-1} y^2 \) gives
\[
\delta_d = \xi + \arctan \left( \frac{\frac{1}{2} \tilde{\Gamma} C^{-2}}{E_0 - E - \frac{1}{2} \tilde{\Gamma} \tan \lambda} \right).
\]

Comparing the above to Eq. (3), we note that \( \xi \) corresponds to our measured background phase shift, \( \delta_{bg} \).

We now consider the resonance position as a function of the external magnetic field. In the closed channel, the bare bound state position in energy is \( E_0 = \delta \mu (B - B_0) \) where \( \delta \mu \) is the difference in magnetic moment between the open and closed channels, and \( B_0 \) is the field at which the (non-interacting) resonance is at threshold [37]. By defining \( \tilde{\Gamma}_B = \tilde{\Gamma} / \delta \mu \),
\[
\delta_d = \delta_{bg} + \arctan \left( \frac{\frac{1}{2} \tilde{\Gamma}_B C^{-2}}{B - (B_0 + E / \delta \mu + \frac{1}{2} \tilde{\Gamma}_B \tan \lambda)} \right).
\]

Within this model, the width and position of the resonance in magnetic field are therefore given by
\[
\Gamma(E) = C^{-2}(E) \tilde{\Gamma}_B, \quad B_{\text{res}}(E) = B_0 + \frac{E}{\delta \mu} + \frac{\tilde{\Gamma}_B}{2} \tan \lambda.
\]

These formulae elegantly demonstrate the advantage of the MQDT approach. The width of the resonance is factorised into one energy-dependent part associated with the long-range threshold effects, \( C^{-2} \), and another energy-independent part, \( \tilde{\Gamma}_B \), associated with the short-range physics. They also demonstrate that threshold effects
modify not only the width of a resonance but also its position [32, 33, 52]. Within Fano’s configuration-interaction approach the shift in the resonance position is due to the off-energy shell interactions [53], which have the effect of mixing in the irregular solution to the bare scattering solution in the open channel. Having chosen the reference function \( f \) to have a phase which matches the physical scattering phase shift \( \delta_{bg} \) in the \( d \)-wave channel (i.e. to be the regular solution), the admixture of the irregular solution \( g \) is completely captured by \( \tan \lambda \) within the QDT formalism, which determines the shift [54].

G. Computations

We now consider the practical computation of the QDT parameters. These can be computed either analytically [55] or numerically [48, 49, 56]. Here we implement the stable numerical approach developed by Ruzic et al. [48]. As discussed by Ruzic et al., reference solutions lose their linear independence when propagating through a centrifugal barrier, so it is optimal to choose reference functions which are purely exponentially growing and decaying in that region. In our case this simply corresponds to choosing \( \phi_1 = 0 \) in Eq. (22), as can be seen in Fig. 5. We then combine this approach with a reference-function rotation to obtain any particular set of reference functions [50, 57, 58]. In our case this corresponds to choosing them such that \( \xi = \delta_{bg} \) as discussed earlier.

The QDT parameters are computed in the same way as detailed in Ref. [31], and here we just give the numerical details specific to this work. Numerical propagation of the reference functions was done using Numerov’s method [59]. The \( f \) reference function was propagated out from \( R_{\text{min}} = 0.1 \) to \( R_{\text{max}} = 25 \) using Eq. (21a) as the short-range boundary condition with \( \phi = 0 \). Matching \( f \) with \( f \) defines \( \xi \) via Eq. (17a). This also defines the reference function \( g \) via Eq. (17b), which serves as a boundary condition to propagate \( g \) back to short range. The QDT parameters can be extracted using Eq. (27). These QDT parameters are then rotated [50, 57, 58] such that \( \xi = \delta_{bg} \) following the procedure in Appendix B 3. We note that because \( \phi \) is defined at short range (where both the collision energy and the centrifugal term are small compared to the depth of the potential) a single energy independent \( \phi \) will reproduce the energy dependent \( \delta_{bg} \) over the entire range of energies we are interested in here.

Figure 6 shows the QDT parameters obtained, both as propagated using \( \phi = 0 \), and following an analytic rotation so that \( \xi \) matches the experimentally observed background scattering phase-shift. The choice of \( \phi = 0 \) produces slowly varying QDT parameters, while those rotated to match the physical scattering phase shift show a peak in \( C^{-2} \) which directly gives the increased probability of tunneling through the \( d \)-wave barrier at the energy of the observed shape resonance.

The QDT parameters are not sensitive to the choice of propagation limits: it is sufficient that at \( R_{\text{min}} \) WKB is valid, and at \( R_{\text{max}} \) the potential has decayed to near-zero. The propagation of the reference functions relies only on knowing the reduced mass \( \mu \), the van der Waals coefficient \( C_6 \), and the angular momentum \( \ell \). This means that the QDT parameters are solely a property of the general long-range potential and account for the threshold effects on the scattering.

III. RESULTS

For a range of energies, we measure of the scattering fraction as a function of magnetic field to obtain scans as those shown in Fig. 3. From these magnetic field scans we extract the resonance parameters shown in Fig. 7, namely the background phase \( \delta_{bg} \), the resonance position \( B_{\text{res}} \), and the resonance width \( \Gamma \), as defined by Eq. (3). These three parameters completely describe the observed resonance features and their variation captures the interplay
A. Experimental Observations

Figure 7a shows the development of the open channel $d$-wave background phase shift with energy. In particular we note its transition through the value $\pi/2$ at the location of the shape resonance. During the course of this, the Fano profile undergoes a $q$-reversal which flips the shape of the Fano profiles shown in Fig. 3. The background phase changes by a total value of less than $3\pi/4$ in this system, while an isolated resonance normally accrues a total phase change of $\pi$ asymptotically—a general feature of resonances in both quantum and classical systems. The discrepancy can be explained by considering that the shape resonance is not a pure, isolated Breit-Wigner resonance: not only are there other resonances in the channel, but the background phase-shift of a channel would normally change near threshold [33, 60].

Figure 7b displays the magnetic field at which the resonance feature is positioned, where we observe a ‘kink’ in the trajectory, shifting by a substantial fraction of the width of the resonance. Above threshold, a Feshbach resonance usually moves linearly in energy as shown by the dashed line, with the slope given by the difference in magnetic moment between the two channels. The deviation from linear is the manifestation of the interaction between states. Indeed, examples of such behaviour has previously been found for a Feshbach resonance interacting with an antibound state [27, 61], and a $p$-wave shape resonance [62].

As shown in Fig. 7c, the Fano profile broadens across the nominal shape resonance energy position by orders of magnitude from the zero-energy width. The Feshbach resonance we inspect is considered narrow [19], and at zero-energy the width is limited by the weak $s$ to $d$-wave coupling, and its observation hence requires a very stable and low noise magnetic field. For experiments conducted above threshold, the shape resonance is, however, readily detected.

B. QDT Analysis

We find the short-range QDT phase $\phi = 0.590\pi$ in the open channel by fitting $\xi$ to the observed background phase in Fig. 7a. The QDT parameters corresponding to this $\phi$ are shown in Fig. 6. By fitting Eq. (43) to $B_{\text{res}}$ (Fig. 7b), we obtain the Feshbach resonance parameters $\bar{\Gamma} = 96 \mu\text{K}$, $\delta\mu = 184 \mu\text{K G}^{-1}$, and $B_0 = 928.7 \text{G}$. The width of the resonance predicted by Eq. (42) is shown as an orange line in Fig. 7c. This is in excellent agreement with the experimental observations and describes the energy dependence of the width entirely through $C^{-2}$. Since $C^{-2}$ quantifies the tunnelling through the centrifugal barrier to short range, we can attribute the broadening of the resonance to the increased amplitude of the wavefunction at short range due to the shape resonance.

The shift in $B_{\text{res}}$ due to the interaction with the open channel is given by the last term of Eq. (43),

$$\delta B = -\frac{\bar{\Gamma}\mu}{2} \tan \lambda. \quad (44)$$

The calculated $\tan \lambda$ for this system, shown in Fig. 6b, explains the non-linear and non-monotone resonance trajectory. We observe that $\tan \lambda$ is non-zero at threshold so the zero-energy position of the Feshbach resonance is already shifted by $\sim 1 \text{G}$ due to the coupling to the open channel, that is, due to the presence of the shape resonance. This is particularly apparent in Fig. 7b which shows the uncoupled resonance position $B_0 + E/\delta\mu$ as a dashed line.
These maxima correspond to positions where the phase winds by $\sim \pi$, which is characteristic of a resonance. Similarly, $B_{\text{res}}$ corresponds to a winding of $\pi$ in field. As is clear from the figure, the positions of the resonances in energy and field do not always line up. In the middle of the kink ($\sim 300 \mu$K), one encounters a magnetic resonance where there is no resonance in energy. As previously discussed, (energy) resonances arise due to the coupling with a quasi-bound state near the collision energy. Here however, one can see that the Fano profile (a dip) arises not from a nearby quasi-bound state, but from the temporary absence of one. This is discussed in our previous work [18], where we have shown that this occurs as the quasi-bound states associated with the two resonances undergo an avoided crossing. The lack of correspondence in energy and field positions is also clear from equations (3) and (41): only $B$ in the denominator changes as a function of magnetic field, giving rise to an isolated Fano profile; in energy, $\Gamma$, $B_{\text{res}}$ and $\delta_{\text{bg}}$ all vary rapidly across the shape resonance, leading to a non-trivial winding of the scattering phase. Raoult and Mies [33] state this another way: one cannot always assign a meaningful energy width to a Feshbach resonance due to the energy shift. Here, we see the energy shift effectively splits the resonance in two. However, we observe that the Fano profile in magnetic field is always singular and well defined: the width of the resonance is clear.

\section*{IV. CONCLUSION}

In this work we have studied the non-trivial interplay between a shape resonance and a Feshbach resonance in ultracold atomic $^{87}$Rb collisions. By manipulating the collision energy and magnetic field we can tune the shape parameter, $q$, of the Fano profile over a range sufficient to observe a full $q$-reversal. In addition to the $q$-reversal we observe strong broadening, and an oscillatory kink in the resonance trajectory as the Feshbach resonance moves over the shape resonance.

To explain this behaviour, we have presented a multichannel quantum defect theory (MQDT) analysis of the experimental data. The MQDT model is able to accurately capture the essential physics of the interactions over the entire range of energy and magnetic field of interest in terms of just 4 constants ($\phi = 0.590\pi$, $\Gamma = 96 \mu$K, $\delta_{\mu} = 184 \mu$K G$^{-1}$, and $B_0 = 928.7$ G) and the three energy dependant QDT parameters ($C^{-2}$, $\tan \lambda$, and $\xi$), which are simply properties of the long range van der Waals potential.

We observe an excellent match between experiment and theoretical predictions, and the MQDT framework demonstrates that the observed resonance behaviour is primarily due to the open-channel, related to the short-range enhancement (determined by $C^{-2}$) and long-range phase rotation (determined by $\tan \lambda$) of the scattering wave-function. In addition to providing additional insight MQDT also proves a vastly simpler tool than complete coupled-channels calculations which require a complex multichannel potential.
Our experimental scheme using an optical collider effectively implements a Feshbach resonance “microscope” which magnifies a narrow zero-energy feature through a shape resonance. While for our particular realization, the Feshbach resonance in question can be resolved at zero energy, in the future the approach may be used to verify predicted ultra-narrow Feshbach resonances that evade experimental observation in conventional loss spectroscopy.

ACKNOWLEDGMENTS

This work was supported by the Marsden Fund of New Zealand (Contract No. UOO1923). J. F. E. Croft acknowledges a Dodd-Walls Fellowship and M. Chilcott a University of Otago Postgraduate Publishing Bursary (Doctoral).

[1] E. A. Donley, N. R. Claussen, S. L. Cornish, J. L. Roberts, E. A. Cornell, and C. E. Wieman, Dynamics of collapsing and exploding Bose–Einstein condensates, Nature 412, 295 (2001).
[2] C. A. Regal, M. Greiner, and D. S. Jin, Observation of resonance condensation of fermionic atom pairs, Phys. Rev. Lett. 92, 040403 (2004).
[3] M. W. Zwierlein, C. A. Stan, C. H. Schunck, S. M. F. Raupach, A. J. Kerman, and W. Ketterle, Condensation of pairs of fermionic atoms near a Feshbach resonance, Phys. Rev. Lett. 92, 120403 (2004).
[4] C. R. Cabrera, L. Tanzi, J. Sanz, B. Naylor, P. Thomas, P. Cheiney, and L. Tarruell, Quantum liquid droplets in a mixture of Bose–Einstein condensates, Science 359, 301 (2018).
[5] K.-K. Ni, S. Ospelkaus, M. H. G. de Miranda, A. Pe’er, B. Neyenhuis, J. J. Zirbel, S. Kotochigova, P. S. Julienne, D. S. Jin, and J. Ye, A high phase-space-density gas of polar molecules, Science 322, 231 (2008).
[6] J. G. Danzl, E. Haller, M. Gustavsson, M. J. Mark, R. Hart, N. Bouloufa, O. Dulieu, H. Ritsch, and H.-C. Nägerl, Quantum gas of deeply bound ground state molecules, Science 321, 1062 (2008).
[7] P. D. Gregory, J. A. Blackmore, S. L. Bronle, and S. L. Cornish, Loss of ultracold $^{87Rb}_{133}Cs$ molecules via optical excitation of long-lived two-body collision complexes, Phys. Rev. Lett. 124, 163402 (2020).
[8] R. Bause, A. Schindewolf, R. Tao, M. Duda, X.-Y. Chen, G. Quémeré, T. Karman, A. Christianen, I. Bloch, and X.-Y. Luo, Collisions of ultracold molecules in bright and dark optical dipole traps, Phys. Rev. Res. 3, 033013 (2021).
[9] P. Gersema, K. K. Voges, M. Meyer zum Alten Borgloh, L. Koch, T. Hartmann, A. Zenesini, S. Ospelkaus, J. Lin, J. He, and D. Wang, Probing photoinduced two-body loss of ultracold nonreactive bosonic $^{23}Na^{87}Rb$ and $^{23}Na^{39}K$ molecules, Phys. Rev. Lett. 127, 163401 (2021).
[10] M. Mayle, G. Quémeré, B. P. Ruzic, and J. L. Bohn, Scattering of ultracold molecules in the highly resonant regime, Phys. Rev. A 87, 012709 (2013).
[11] J. F. E. Croft, J. L. Bohn, and G. Quémeré, Unified model of ultracold molecular collisions, Phys. Rev. A 102, 033306 (2020).
[12] J. F. E. Croft, J. L. Bohn, and G. Quémeré, Anomalous lifetimes of ultracold complexes decaying into a single channel: What’s taking so long in there? (2021), arXiv:2111.09956 [cond-mat.quant-gas].
[13] A. Christianen, G. C. Groenenboom, and T. Karman, Lossy quantum defect theory of ultracold molecular collisions, Phys. Rev. A 104, 043327 (2021).
N. Kjærgaard, Observation of bound state self-interaction in a nano-eV atom collider, Nat. Commun. 9, 4895 (2018).

[28] A. E. Miroshnichenko, S. Flach, and Y. S. Kivshar, Fano resonances in nanoscale structures, Rev. Mod. Phys. 82, 2257 (2010).

[29] M. J. Seaton, Quantum defect theory I. general formulation, Proc. Phys. Soc. 88, 801 (1966).

[30] C. H. Greene, A. R. P. Rau, and U. Fano, General form of the quantum-defect theory, II, Phys. Rev. A 26, 2441 (1982).

[31] F. H. Mies, A multichannel quantum defect analysis of diatomic predissociation and inelastic atomic scattering, The Journal of Chemical Physics 80, 2514 (1984), https://doi.org/10.1063/1.447000.

[32] F. H. Mies and M. Raoult, Analysis of threshold effects in ultracold atomic collisions, Phys. Rev. A 62, 012708 (2000).

[33] M. Raoult and F. H. Mies, Feshbach resonance in atomic binary collisions in the wigner threshold law regime, Phys. Rev. A 70, 012710 (2004).

[34] F. H. Mies and P. S. Julienne, A multichannel quantum defect analysis of two-state couplings in diatomic molecules, J. Chem. Phys. 80, 2526 (1984).

[35] P. S. Julienne and B. Gao, Simple theoretical models for spin-exchange and dipole relaxation rates in atomic hydrogen, Phys. Rev. A 62, 112701 (2000).

[36] C. H. Greene, A. R. P. Rau, and U. Fano, Generalized multichannel quantum defect theory for cold molecular collisions, Phys. Rev. A 87, 012701 (2013).

[37] The coupled-channels calculations, as used in Ref. [18], are generated by propagating the log-derivative of the wavefunction using the technique of Ref. [63], and extracting the wavefunction using the technique of Ref. [64].

[38] E. Tiesinga, C. J. Williams, P. S. Julienne, K. M. Jones, P. D. Lett, and W. D. Phillips, A spectroscopic determination of scattering lengths for sodium atom collisions, J. Res. Natl. Inst. Stand. Technol. 101, 505 (1996).

[39] P. H. Mies, E. Tiesinga, and P. S. Julienne, Manipulation of Feshbach resonances in ultracold atomic collisions using time-dependent magnetic fields, Phys. Rev. A 61, 022721 (2000).

[40] In practice, for reasons of numerical stability, it is more common to propagate the log-derivative of this matrix.

[41] J. M. Hutson, Cold Molecules: Theory, Experiment, Applications (CRC Press, 2009) Chap. Theory of Cold Atomic and Molecular Collisions.

[42] P. G. Burke, R-Matrix Theory of Atomic Collisions (Springer Berlin Heidelberg, 2013).

[43] H. T. C. Stoof, J. M. V. A. Koelman, and B. J. Verhaar, Spin-exchange and dipole relaxation rates in atomic hydrogen: Rigorous and simplified calculations, Phys. Rev. B 38, 4688 (1988).

[44] A. Derevianko, J. F. Babb, and A. Dalgarno, High-precision calculations of Van der Waals coefficients for heteronuclear alkali-metal dimers, Phys. Rev. A 63, 052704 (2001).

[45] M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions (Dover, 1970).

[46] B. P. Ruzic, C. H. Greene, and J. L. Bohn, Quantum defect theory for high-partial-wave cold collisions, Phys. Rev. A 87, 032706 (2013).

[47] J. F. E. Croft, A. O. G. Wallis, J. M. Hutson, and P. S. Julienne, Multichannel quantum defect theory for cold molecular collisions, Phys. Rev. A 84, 042703 (2011).

[48] A. Giusti-Suzor and U. Fano, Alternative parameters of channel interactions. I. Symmetry analysis of the two-channel coupling, J. Phys. B. 17, 215 (1984).

[49] F. H. Mies and M. Raoult, Analysis of threshold effects in ultracold atomic collisions, Phys. Rev. A 62, 012708 (2000).

[50] M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions (Dover, 1970).

[51] Where the trigonometric identity

\[ \arctan z = \frac{1}{2} \log \left( \frac{1 + iz}{1 - iz} \right), \]

is useful.

[52] P. Naidon and L. Pricoupenko, Width and shift of fano-feshbach resonances for van der waals interactions, Phys. Rev. A 100, 042710 (2019).

[53] U. Fano, Effects of configuration interaction on intensities and phase shifts, Phys. Rev. 124, 1866 (1961).

[54] U. Fano, Connection between configuration-mixing and quantum-defect treatments, Phys. Rev. A 17, 93 (1978), qdt.

[55] B. Gao, Solutions of the Schrödinger equation for an attractive 1/r^4 potential, Phys. Rev. A 58, 1728 (1998).

[56] B. Yao and C. H. Greene, Implementation of the quantum-defect theory for arbitrary long-range potentials, Phys. Rev. A 34, 1635 (1986).

[57] R. Osséni, O. Dulieu, and M. Raoult, Optimization of generalized multichannel quantum defect reference functions for Feshbach resonance characterization, J. Phys. B 42, 185202 (2009).

[58] J. F. E. Croft, J. M. Hutson, and P. S. Julienne, Optimized multichannel quantum defect theory for cold molecular collisions, Phys. Rev. A 86, 022711 (2012).

[59] B. V. Nounourov, A Method of Extrapolation of Perturbations, Mon. Not. R. Astron. Soc. 84, 592 (1924).

[60] H. R. Sadeghpour, J. L. Bohn, M. J. Cavagnero, B. D. Esry, I. I. Fabrikant, J. H. Macek, and A. R. P. Rau, Collisions near threshold in atomic and molecular physics, J. Phys. B. 33, R93 (2000).

[61] B. Marcelis, E. van Kempen, B. Verhaar, and S. Kokkelmans, Feshbach resonances with large background scattering length: Interplay with open-channel resonances, Phys. Rev. A 70, 012701 (2004).

[62] D. J. Ahmed-Braun, K. G. Jackson, S. Smale, C. J. Dale, B. A. Olsen, S. J. J. M. F. Kokkelmans, P. S. Julienne, and J. H. Thywissen, Probing open- and closed-channel p-wave resonances, Physical Review Research 3, 033269 (2021).

[63] D. E. Manolopoulos, An improved log derivative method for inelastic scattering, The Journal of Chemical Physics 85, 6425 (1986).

[64] A. E. Thornley and J. M. Hutson, Bound-state wave functions from coupled channel calculations using log-derivative propagators: Application to spectroscopic intensities in ar–HF, J. Chem. Phys. 101, 5578 (1994).

[65] Q. Beaufils, A. Crubellier, T. Zanon, B. Laburthe-Tolra, E. Maréchal, L. Vernac, and O. Gorceix, Feshbach resonance ind-wave collisions, Phys. Rev. A 79, 032706 (2009).

[66] M. Aymar, C. H. Greene, and E. Luc-Koenig, Multichannel Rydberg spectroscopy of complex atoms, Rev. Mod. Phys. 68, 1015 (1996).

[67] B. P. Ruzic, Exploring Exotic Atomic and Molecular Col-
Appendix A: Loss Spectroscopy

We measure the (near) zero-energy position of the Feshbach resonance in magnetic field by observing its effect on a stationary atomic cloud. At the Feshbach resonance, the scattering length between the $^{87}$Rb atoms diverges, resulting in a wildly increased three-body loss rate. We can therefore observe the presence of the Feshbach resonance by counting the number of atoms lost while holding a cloud of atoms in a magnetic field.

To perform the measurement, we perform a procedure initially identical to that laid out in Section I, up to the point where we would split and collide the clouds of atoms. Instead, a single cloud which has been further evaporatively cooled below 400 nK is held in a stationary optical dipole trap and exposed to a magnetic field for 200 ms. An absorption image of the single cloud is then used to estimate the number of atoms remaining in the trap. In such an experiment, the profile of the atom loss can often be well approximated by a Gaussian line shape [19], especially when the width of the Feshbach resonance is greater than the range of collision energies present in a thermal cloud. In our data, we observe an asymmetry that is distinctly non-Gaussian (shown in Fig. 9), requiring us to take into account the thermal distribution of the finite temperature cloud—the Maxwell-Boltzmann distribution is skewed towards high energies with negative energies forbidden and the same skew is imposed upon the shape of the atom loss in magnetic field as the resonance tunes above threshold. Explicitly, we model the coupling rate to the Feshbach state as a Breit-Wigner profile in energy,

$$R(E, B) \propto \frac{\gamma}{\gamma^2 + (E - \epsilon(B))^2},$$  \hspace{1cm} (A1)

for atoms at a given energy $E$, when the Feshbach resonance is at energy $\epsilon(B) = \delta \mu (B - B_0)$. The distribution of kinetic energies (which are strictly positive) are taken to be Maxwellian at a temperature $T$:

$$P(T, E) = kT e^{-E/kT}. \hspace{1cm} (A2)$$

The three-body loss rate $K_3$ is then proportional to the integral of these over energy,

$$K_3(B) \propto \int_0^\infty R(E, B) P(T, E) dE. \hspace{1cm} (A3)$$

If we assume that the loss process does not produce evaporative heating/cooling, and that the loss rate from other processes is negligible, then the loss can be modelled by

$$\dot{N}(B) = -K_3(B) N^2, \hspace{1cm} (A4)$$

where $N$ is the number of atoms remaining. Here we are describing the three-body loss process as second-order in atom number (akin to a two-body loss process) to encapsulate the inverse density and hence $N^{-1}$ atom number dependence of $K_3$ [65]. A fit of this model to experimental data is shown in Fig. 9, and a number of such measurements give us an estimate of the zero-energy Feshbach resonance position $B_0 = 929.921(3)$ G.

Appendix B: QDT Supplementary

1. Scattering wavefunctions

In several places [e.g., Eq. (6) and Eq. (30)], the scattering wavefunction is written in the form

$$F = \mathcal{F} + \mathcal{G}K. \hspace{1cm} (B1)$$

where $\mathcal{F}, \mathcal{G}$ are diagonal matrices. In the case of $\mathcal{F}$ and $\mathcal{G}$ containing the free-particle solutions as in Eq. (6), $K$ is the the open-open part of the scattering reaction matrix. At short range, where all the channels are open, where $\mathcal{F}$ and $\mathcal{G}$ contain the QDT reference function $\hat{f}$ and $\hat{g}$, $K$ is the $Y$ matrix. The general form of a scattering wavefunction is

$$M = \mathcal{F}A + \mathcal{G}B, \hspace{1cm} (B2)$$

where the matrices $A, B$ contain the appropriate coefficients. Then defining [66]

$$F = MA^{-1}, \hspace{1cm} (B3)$$

gives the expression

$$F = \mathcal{F} + \mathcal{G}K, \hspace{1cm} (B4)$$

with

$$K = BA^{-1}. \hspace{1cm} (B5)$$
2. Multichannel scattering in QDT

In this section, we derive the \( S \) matrix from the constant short-range \( Y \) matrix [31, 67].

\[ f, g \]

The true reaction matrix (often called \( \bar{f} \)) wavefunction has the appropriate exponentially decaying form in the closed channels. Defining the transformation

\[ \bar{F} = FT = \left[ f + gY \right] T, \]  

(B7)

where \( \bar{F} \) has dimension \( N \times N_o \). The appropriate asymptotic boundary conditions in block matrix form are

\[ \bar{F}_{oo} \sim \hat{f}_{oo} + g_{oo} Y_{oo}, \]  

(B8a)

\[ \bar{F}_{co} \sim \left[ f_{cc} - \tan \nu_c g_{cc} \right] Y_{co}. \]  

(B8b)

Expanding Eq. (B7),

\[
\begin{bmatrix}
(f_{oo} & 0 \\
0 & f_{cc}
\end{bmatrix}
+ g_{oo} \begin{bmatrix}
0 & 0 \\
0 & g_{cc}
\end{bmatrix}
\begin{bmatrix}
Y_{oo} & Y_{oc} \\
Y_{co} & Y_{cc}
\end{bmatrix}
\begin{bmatrix}
T_{oo} \\
T_{co}
\end{bmatrix}
= \begin{bmatrix}
\bar{F}_{oo} \\
\bar{F}_{co}
\end{bmatrix}.
\]

(B9)

Substituting in Eq. (B8), and finally matching terms yields the \( Y \) matrix. The open-open subblock required for scattering applications is given by

\[ Y_{oo} = Y_{oo} - Y_{oc} \left[ \tan \nu + Y_{cc} \right] Y_{co}. \]  

(B10)

\[ \bar{F}_{oo} \]

is written in terms of the short range reference functions \( \hat{f} \) and \( \hat{g} \) however to make the connection to the physical \( S \) matrix we want the wavefunction to have the form

\[ F \sim f + g\bar{R}, \]  

(B11)

in terms of the energy normalised asymptotic reference functions \( f \) and \( g \). \( \bar{R} \) is an effective reaction matrix. The true reaction matrix (often called \( K \) or \( R \) in the literature) is defined by a form identical to Eq. (B11), with the QDT reference solutions \( f, g \) replaced with the appropriate spherical Bessel solutions in Eq. (6).

The relation between the short- and long-range reference function is

\[ \hat{f}_{oo} = C f_{oo}, \]  

(B12)

\[ \hat{g}_{oo} = C^{-1} g_{oo} - \tan \lambda C f_{oo}. \]  

(B13)

Writing \( \bar{F}_{oo} \) in terms of the long-range reference solutions gives

\[ \bar{F}_{oo} \sim \hat{f}_{oo} + \hat{g}_{oo} Y_{oo}, \]  

(B14)

\[ = C f_{oo} + \left[ C^{-1} g_{oo} - \tan \lambda C f_{oo} \right] Y_{oo} \]  

(B15)

\[ = f_{oo} C \left[ 1 - \tan \lambda Y_{oo} \right] + g_{oo} C^{-1} Y_{oo} \]  

(B16)

\[ \sim f_{oo} + g_{oo} C^{-1} \left[ Y_{oo}^{-1} - \tan \lambda \right]^{-1} Y_{oo} \]  

(B17)

\[ = f_{oo} + g_{oo} \bar{R}, \]  

(B18)

where we note that diagonal matrices commute, and that we have ignored an overall normalisation. Starting from Eq. (B8a), the form of an effective reactance matrix is therefore

\[ \bar{R} = C^{-1} \left( Y_{oo}^{-1} - \tan \lambda \right)^{-1} Y_{oo}^{-1}. \]  

(B19)

The scattering matrix is defined by the asymptotic wavefunction

\[ F \sim h^- - h^+ S, \]  

(B20)

where \( h^\pm \) are the free-particle solutions with incoming and outgoing asymptotic boundary conditions (sometimes called the Riccati-Hankel functions)

\[ h^+ \sim \exp \left[ i \left( kr - \frac{\ell \pi}{2} \right) \right], \]  

(B21)

\[ h^- \sim \exp \left[ -i \left( kr - \frac{\ell \pi}{2} \right) \right]. \]  

(B22)

Writing \( f \) and \( g \) in terms of \( h^\pm \) gives

\[ f \sim \frac{-i}{2} \left[ h^+ e^{i \xi} - h^- e^{-i \xi} \right], \]  

(B23)

\[ g \sim \frac{1}{2} \left[ h^+ e^{i \xi} + h^- e^{-i \xi} \right]. \]  

(B24)

Substituting into Eq. (B11) gives

\[ F \sim \frac{-i}{2} \left[ h^+ e^{i \xi} - h^- e^{-i \xi} \right] + \frac{1}{2} \left( h^+ e^{i \xi} + h^- e^{-i \xi} \right) R \]  

(B25)

\[ \sim h^+ e^{i \xi} \left[ -i + R \right] + h^- e^{-i \xi} \left[ i + R \right] \]  

(B26)

\[ \sim h^+ + h^+ e^{i \xi} \left[ iR + 1 \right] \left[ iR - 1 \right]^{-1} e^{i \xi}. \]  

(B27)

The \( S \) matrix therefore has the form

\[ S = e^{i \xi} \left[ 1 + i R \right] \left[ 1 - i R \right]^{-1} e^{i \xi}. \]  

(B28)
This differs from the usual translation from the reactance matrix to the $S$ matrix, Eq. (8), by the two factors of $e^{i\xi}$. This is because $\tilde{R}$ is defined with respect to the long-range reference functions $f, g$, which differ from the usual sine and cosine free-particle solutions by a phase of $\xi$.

\[ \tilde{\xi} = \arctan \left[ \frac{C^2 \sin \xi (\cos \phi + \tan \lambda \sin \phi) - \cos \xi \sin \phi}{C^2 \cos \xi (\cos \phi + \tan \lambda \sin \phi) + \sin \xi \sin \phi} \right], \quad \text{(B30a)} \]

\[ \tan \tilde{\lambda} = -\frac{2C^4 \tan \lambda \cos 2\phi + [1 + C^4(\tan^2 \lambda - 1)] \sin 2\phi}{2C^4 \cos^2 \phi + 2 \sin \phi \left[ \sin \tilde{\phi} + C^4 \tan \lambda (2 \cos \phi + \tan \lambda \sin \phi) \right]}, \quad \text{(B30b)} \]

\[ \tilde{C} = \left[ \frac{\sin \xi \sin \phi}{C} + C \cos \xi (\cos \phi + \tan \lambda \sin \phi) \right] \times \sqrt{1 + \left[ \frac{\cos \xi \sin \phi - C^2 \sin \xi (\cos \phi + \tan \lambda \sin \phi)}{\sin \xi \sin \phi + C^2 \cos \xi (\cos \phi + \tan \lambda \sin \phi)} \right]^2}, \quad \text{(B30c)} \]

\[ \tilde{\nu} = \nu - \phi. \quad \text{(B30d)} \]

As such, once the QDT parameters have been calculated for $\phi = 0$, it is straightforward to obtain them for any choice of $\phi$. Reference functions for any $\phi$ can therefore be obtained in a numerically stable way.