

Lellouch-Lüscher Relation for Ultracold Few-Atom Systems under Confinement

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We derive an analog of the Lellouch-Lüscher (LL) relation for few-body bosonic systems, linking few-body scattering loss rates to the energies and widths of the corresponding harmonically trapped few-body states. Three-body numerical simulations show that the LL relation applies across a broad range of interaction strengths and energies and allows the determination of scattering rates within a single partial wave. Our Letter establishes a robust theoretical framework for understanding the role of the finite-volume effect in few-body observables in optical lattice and tweezer experiments, enabling precise determination of multibody scattering rates.

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Over the past few decades, trapped ultracold atoms and molecules have become a versatile platform for exploring and exploiting quantum phenomena, driving advances in atomic, molecular and optical physics, condensed matter, chemistry, and quantum information science and technology [1–9]. This success stems from the unparalleled level of control provided by ultracold atomic systems over internal states, interatomic interactions, and trapping dynamics [10–14]. More recent advances in optical lattices and optical tweezers have further expanded the versatility of ultracold atoms by introducing deterministic control of the atom number (up to a few) in a single trap site [15–18]. These techniques enable novel approaches to quantum simulation [19] and allow deeper insight into the fundamental processes governing chemical reactions [20–23]. Furthermore, they pave the way for using trapped few-atom systems for quantum information applications, the exploration of multibody interactions [24], and the study of many-body states created atom by atom [25].

In many ways, atoms and molecules trapped in optical lattices or tweezers form an ideal system for studying various fundamental aspects of few-body interactions. While in ultracold gas experiments few-body interactions

are typically characterized by scattering rates, in trapped systems the key observables are the on-site interatomic interaction and the lifetime of individual trapped states [24–32]. Optical tweezers, in particular, have enabled the creation of fully isolated two- and three-atom systems, allowing measurements of such physical observables at the single-event level [33–35]. While offering unprecedented control over few-body systems, such experiments also encounter two central challenges: how to relate measurements in confined setups to free-space scattering parameters and how confinement itself influences collision dynamics and system stability. Similar challenges arise in high-energy physics, particularly in lattice quantum chromodynamics, where calculations are performed in a finite volume. A breakthrough in that context was the development of the well-known Lellouch-Lüscher (LL) relations [36–45], which provide a rigorous way to extract scattering observables—such as decay rates and cross sections—from the discrete energy levels of finite-volume simulations. A closely related treatment was established in hadronic atoms and is commonly referred to as the Deser-Trueman formula [46–50]. The development of a similar approach for trapped few-atom systems has the potential to provide a more accurate and controllable procedure to determine few-atom scattering rates than in ultracold bulk gases. Isolated few-body systems allow for a clearer and more systematic way to distinguish scattering rates from processes involving varying numbers of atoms [35], a task that proves to be more challenging in bulk gases [51–54]. Moreover, the ability of preparing trapped few-body states in well-defined quantum states [21,24,55–59] can enable the direct measurement of individual partial-wave scattering rates, providing a much more sensitive probe for

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resonance and interference effects often obscured by thermal effects in gases [60,61].

In this Letter, we derive the analog of the LL relation for ultracold few-body systems under harmonic confinement and provide numerical evidence for its validity. In particular, we consider a system of three identical bosons in an isotropic harmonic trap and focus on extracting the free-space energy-dependent three-body loss (recombination) rate coefficient, $L_3(E)$, characterizing the process where three free atoms collide at energy E to form a diatomic molecule. Our key finding is an LL relation that connects $L_3(E_q)$ at the energy $E_q > 0$ ($q = 0, 1, 2, \dots$) of the q th gaslike trapped three-body state in the lowest partial wave [62–64] to its width, Γ_q :

$$L_3(E_q) = C \frac{\hbar^4}{m^3} \frac{\Gamma_q}{\omega_{\text{ho}}[E_q^2 - (\hbar\omega_{\text{ho}})^2]}, \quad (1)$$

where m is the atomic mass, ω_{ho} the angular trap frequency and $C = 72\sqrt{3}\pi^3$, a universal constant. Conversely, if $L_3(E)$ is known, the LL relation predicts the lifetime, $\hbar/\Gamma_q$, of the trapped three-body states [65]. We numerically verify our LL relation through simulations of ^{85}Rb and ^{87}Rb atoms using the hyperspherical adiabatic representation [66–68]. We show that the LL relation remains valid for states in which $|a| \ll r_{\text{ho}}(q) \simeq (E_q/m\omega_{\text{ho}}^2)^{1/2}$, where $r_{\text{ho}}(q)$ is the characteristic size of the q th trap state and a is the two-body scattering length characterizing the strength of the interatomic interaction [10]. We generalize the LL relation to a system of N identical bosons opening up a path for the determination of multibody scattering rates [24,69]. These results provide a direct theoretical framework for interpreting few-body observables in optical lattice and tweezer experiments, where finite-volume effects play a central role.

In adiabatic hyperspherical representation [66,67], three-body observables are determined from the solution of the hyperradial Schrödinger equation [66,67]

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dR^2} + W_\nu(R) - E \right] F_\nu(R) + \sum_{\nu' \neq \nu} W_{\nu\nu'}(R) F_{\nu'}(R) = 0, \quad (2)$$

with the adiabatic potentials W_ν and the nonadiabatic couplings $W_{\nu\nu'}$ obtained by solving the adiabatic hyperangular equations at fixed values of the hyperradius R (see Supplemental Material [70] for more details). Here, ν is the set of quantum numbers necessary to characterize each channel, F_ν is the three-body hyperradial wave function and $\mu = m/\sqrt{3}$ the three-body reduced mass. In Fig. 1(a) we show the adiabatic potentials W_ν for three-body loss in free space and in a harmonic trap. Here, $W_{\nu=\lambda}$ are continuum channels that describe the collision between

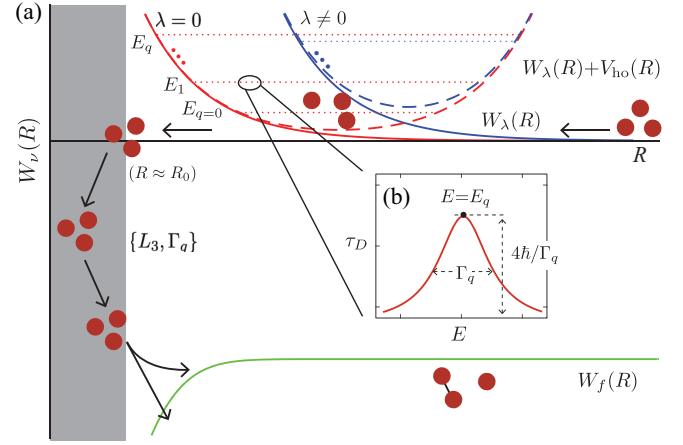


FIG. 1. (a) Schematic illustration of three-body losses in free space and in a harmonic trap. In free space, three atoms in continuum channels $W_\lambda(R)$ (solid) undergo inelastic transitions near $R \lesssim R_0$ (shaded) to atom-dimer channels $W_f(R)$, characterized by the recombination rate constant L_3 . In a trap, discrete states E_q (dotted) form in $W_\lambda(R) + V_{\text{ho}}(R)$ channels (dashed) and decay into atom-dimer channels with rate $\Gamma_q/\hbar$ [70]. (b) Trapped-state energies E_q and widths Γ_q manifest as Lorentzian resonances in the time delay $\tau_D(E)$ (see text).

three free atoms or, in a trap, support discrete three-body states. They are labelled by the hyperangular momentum $\lambda \geq 0 \in \mathbb{Z}$, which sets the hyperradial centrifugal barrier at large R [70]. (For bosonic systems the lowest value of λ is $\lambda_{\text{min}} = 0$ while for fermionic systems $\lambda_{\text{min}} \neq 0$ [76].) In Fig. 1(a), $W_{\nu=f}$ denote an atom–dimer channels, which serve as the primary decay pathways leading to atomic losses.

The central physical quantities in the LL relation (1) can be extracted from the solutions of Eq. (2) in both free space and trapped systems. In free space, the rate constant for three-body recombination at collision energy E is defined as

$$L_3(E) = \sum_J \sum_{\lambda, f} 96\pi^2 \hbar \frac{(2J+1)}{\mu k^4} |S_{f\lambda}^J|^2 = \sum_J L_3^J(E), \quad (3)$$

with $k = (2\mu E/\hbar^2)^{1/2}$, f running over all final W_f (atom-dimer) channels, λ running over the initial W_λ (three-body continuum) channels, and the corresponding S matrix obtained from the solution of Eq. (2) [67]. In the above equation, L_3^J is the partial-wave contribution to L_3 for the total orbital angular momentum, J . For ultracold bosonic gases, the total rate $L_3(E)$ is dominated by the $J = 0$ partial rate, with all other J contributions vanishing as $E \rightarrow 0$ [77,78], only becoming important for energies beyond $E_c = \hbar^2/ma^2$ [60]. In the present Letter, we study $L_3^{J=0}$ recombination and its connection to the lifetime of the $J = 0$ trapped three-body states.

By introducing the harmonic trap $V_{\text{ho}}(R) = \mu\omega_{\text{ho}}^2 R^2/2$ into Eq. (2), each W_λ channel will support a series of trapped states with energy E_q and width Γ_q , arising from the decay into W_f channels [illustrated in Fig. 1(a); see further details in Ref. [70]].

Here, we focus on trapped states associated with the $\lambda = \lambda_{\text{min}} = 0$ channel, as this is the dominant channel for $L_3^{J=0}(E)$ [67]. As we will see below, our numerical calculations show that the widths Γ_q for trapped states associated with $\lambda \neq 0$ are extremely narrow, indicating the weak decay from such channels. (Note that we omit J and λ in our following notation unless stated otherwise.) Here, the energies and widths of the trap states are determined via the time delay $\tau_D(E)$,

$$\tau_D(E) \equiv 2\hbar \frac{d}{dE} \delta_S(E), \quad (4)$$

with the eigenphase-shift sum, δ_S , obtained from the corresponding S -matrix elements [79] extracted from the solutions of Eq. (2) with the trap $V_{\text{ho}}(R)$. As usual, near the energy of a trapped state, the time delay exhibits a Lorentzian line shape [see Fig. 1(b)], reaching its maximum at $E = E_q$, with a width determined by $\Gamma_q = 4\hbar/\tau_D(E_q)$. See Ref. [70] for details on our numerical procedure to determine E_q and Γ_q .

After having introduced the theoretical framework for calculating $L_3(E)$, E_q , and Γ_q , we now present a simple analytical approach to derive the relationship between free-space and in-trap observables, i.e., the LL relation (1). We assume weak interactions ($|a|/a_{\text{ho}} \ll 1$, where $a_{\text{ho}} = \hbar^{1/2}/(m\omega_{\text{ho}})^{1/2}$ is the oscillator length), but also weak trapping ($r_{\text{vdW}}/a_{\text{ho}} \ll 1$, with r_{vdW} being the van der Waals (vdW) length [10,70]). Our key observation is that the mechanism controlling both Γ_q and L_3 is identical; i.e., the inelastic transitions occur primarily at short distances $R \leq R_0 \sim r_{\text{vdW}}$, as illustrated in Fig. 1(a). Accordingly, we define the following relation [79–81]:

$$\frac{\Gamma_q}{\hbar} = \frac{L_3(E_q)}{3} \mathcal{D}_q, \quad (5)$$

where the factor 3 accounts for the loss of three atoms per event, and $\mathcal{D}_q$ is the reactive three-body probability density defined as the probability density to find particles in the q th state within the reaction region ($R \leq R_0$), with hyperspherical volume $\mathcal{V}_0 = \pi^3 R_0^6/6$. In Ref. [70] we show that $\mathcal{D}_q$ is closely related to the three-body correlation function [35]. In hyperspherical representation, $\mathcal{D}_q$ is given by

$$\mathcal{D}_q = \frac{1}{\mathcal{V}_0} \int_0^{R_0} F_q(R)^2 dR, \quad (6)$$

where F_q is the (noninteracting) hyperradial wave function for the q th trapped three-body state [82] associated with the

W_λ channel. For $\lambda = 0$, F_q is given by

$$F_q(R) = \frac{R^{5/2}}{N_q^{1/2} a_{\text{ho}}^3} L_q^{(2)} \left(\frac{R^2}{\sqrt{3} a_{\text{ho}}^2} \right) \exp \left(-\frac{R^2}{2\sqrt{3} a_{\text{ho}}^2} \right), \quad (7)$$

with energy $E_q = (2q+3)\hbar\omega_{\text{ho}}$. Here, $L_q^{(a)}$ is the generalized Laguerre polynomial and $N_q = 3\sqrt{3}(q+1)(q+2)/2$ is a normalization constant. To leading order, the reactive probability density can be expressed as [70]

$$\mathcal{D}_q = \frac{m^3 \omega_{\text{ho}} (E_q^2 - \hbar^2 \omega_{\text{ho}}^2)}{24\pi^3 \sqrt{3} \hbar^5}, \quad (8)$$

independent of the specific choice of R_0 . Substituting Eq. (8) into (5), we finally obtain the LL relation (1),

$$\Gamma_q = \frac{1}{C} \frac{m^3}{\hbar^4} L_3(E_q) [E_q^2 - (\hbar\omega_{\text{ho}})^2] \omega_{\text{ho}}, \quad (9)$$

with $C = 72\sqrt{3}\pi^3$. The above derivation of the bosonic $J = 0$ ($\lambda_{\text{min}} = 0$) LL relation [Eqs. (1) and (9)] can be readily extended to other bosonic and fermionic systems with arbitrary J (λ_{min}) [76].

We note that beyond the weakly interacting regime ($|a|/a_{\text{ho}} \ll 1$), interactions induce measurable shifts in both the energy and the spatial extent of the trapped states. Since $\mathcal{D}_q$ [Eq. (8)] quantifies the probability density within the reaction region, it becomes sensitive to interaction-induced changes of the state size. The use of the numerically obtained energy E_q in $\mathcal{D}_q$ [Eq. (8)] and the LL relations [Eqs. (1) and (9)], rather than the noninteracting form $E_q = (2q+3)\hbar\omega_{\text{ho}}$, incorporates leading-order interaction-induced modifications to the reaction volume [71,72] while preserving the model structure. Furthermore, as q increases, the size of the trapped state grows as $r_{\text{ho}}(q) \simeq (2q+3)^{1/2} a_{\text{ho}}$, reducing interaction effects and improving the accuracy of the LL relation. [Accordingly, the condition $|a|/r_{\text{ho}}(q) \ll 1$ provides a more appropriate criterion for its validity than $|a|/a_{\text{ho}} \ll 1$.] These aspects were verified numerically and discussed in more depth in Ref. [70].

We now test the validity of the LL relation through three-body numerical simulations of ^{85}Rb and ^{87}Rb atoms. Our numerical model employs reduced interatomic interaction potentials derived from Born-Oppenheimer potentials while incorporating the full atomic hyperfine spin structure [68,83] (see also Ref. [70]). This interaction model encompasses more than 100 atom-dimer channels, with three-body potentials that span an energy range several thousands times the characteristic vdW energy scale, $E_{\text{vdW}} = \hbar^2/mr_{\text{vdW}}^2$, below the three-body breakup threshold ($E \leq 0$) [70].

The two isotopes of Rb atoms we use have vastly different physical properties: at zero-magnetic-field, the effective interaction between ^{85}Rb atoms is strong and attractive, characterized by the large and negative value of

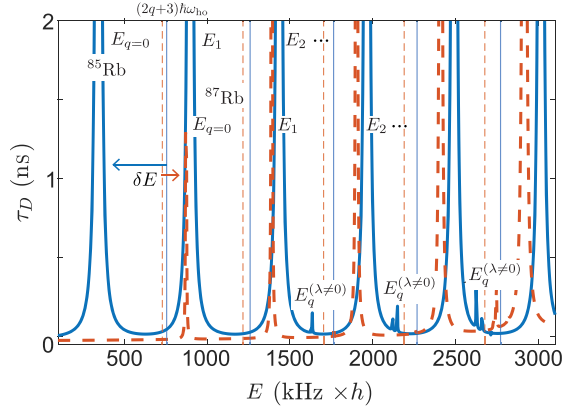


FIG. 2. A typical time delay plot for ^{85}Rb at $\omega_{\text{ho}} = 2\pi \times 252$ kHz or, equivalently, $|a|/a_{\text{ho}} = 1.11$ (solid line) and for ^{87}Rb at $\omega_{\text{ho}} = 2\pi \times 243$ kHz, or $|a|/a_{\text{ho}} = 0.24$ (dashed line). Both frequencies correspond to $a_{\text{ho}} = 5r_{\text{vdW}}$. The vertical lines indicate the energy levels of three non-interacting atoms, $(2q+3)\hbar\omega_{\text{ho}}$. Arrows indicate the shift $\delta E \propto a/a_{\text{ho}}$ from the ground state energy $3\hbar\omega_{\text{ho}}$ due to interactions. E_q denotes the energies for states of the $\lambda = 0$ channel and $E_q^{(\lambda \neq 0)}$ otherwise.

$a = -5.56 r_{\text{vdW}}$ while for ^{87}Rb the effective interaction is weak and repulsive with $a = 1.21 r_{\text{vdW}}$ [70]. In the trap, interactions induces energy shifts ($\delta E \propto a/a_{\text{ho}}$) from the noninteracting energy levels, $(2q+3)\hbar\omega_{\text{ho}}$ [62,70]. This effect can be observed in Fig. 2 for the time delay for three ^{85}Rb (solid line) and ^{87}Rb (dashed line) atoms under strong confinement ($a_{\text{ho}} = 5 r_{\text{vdW}}$). Figure 2 shows $\lambda = 0$ trapped states for both atomic species manifested by the resonance feature (sudden increase) of the time delay near $E = E_q$, shifted by δE from the non-interacting energies (vertical lines). Note that the narrow and unresolved features in

Fig. 2 are associated with trapped three-body states belonging to $\lambda \neq 0$ channels, highlighting their relative insignificance compared to the $\lambda = 0$ states [67]. More notably, while the resonances for ^{85}Rb are generally broad, with Γ_q largely insensitive to E_q , those for ^{87}Rb display a clear transition from narrow to broad as E_q increases. In the following, we show that the LL relation provides a clear interpretation of these two distinct physical behaviors, attributed to the energy dependence of $L_3(E)$.

In Fig. 3, we validate our LL relation (9) by comparing the calculated Γ_q values (symbols) with LL predictions (solid lines), using our results for $L_3(E)$. Figure 3 presents the results for trapping frequencies ranging from 60 kHz to 250 kHz, showing excellent agreement with the LL relation (9) in the regime $|a|/a_{\text{ho}} \ll 1$, with deviations emerging as $|a|/a_{\text{ho}}$ increases. For ^{87}Rb , since interactions are weak, all the values for $|a|/a_{\text{ho}}$ in Fig. 3(a) fall well within the $|a|/a_{\text{ho}} \ll 1$ regime, the agreement with the LL relation (9) holds for all values of E_q , including those with energy comparable to $E_{\text{vdW}} \approx 6000 \text{ kHz} \times h$, therefore, beyond the ultracold regime $E_q \ll E_{\text{vdW}}$. For ^{85}Rb [Fig. 3(b)], however, due to its strong interactions, even at the lowest trap frequency, the ratio $|a|/a_{\text{ho}}$ (≈ 0.56) is not deep in the $|a|/a_{\text{ho}} \ll 1$ regime, leading to a deviation from the LL relation for the lowest few E_q . For higher excited states, deviations become relatively small as E_q increases, confirming that the LL relation remains valid for $|a|/r_{\text{ho}}(q) \ll 1$, as noted previously.

Also evident in Figs. 3(a) and 3(b) is the contrasting behavior of Γ_q for ^{87}Rb and ^{85}Rb : for ^{87}Rb , Γ_q is strongly dependent on E_q , while for ^{85}Rb , it is relatively independent of E_q . According to the LL relation (9), this contrasting

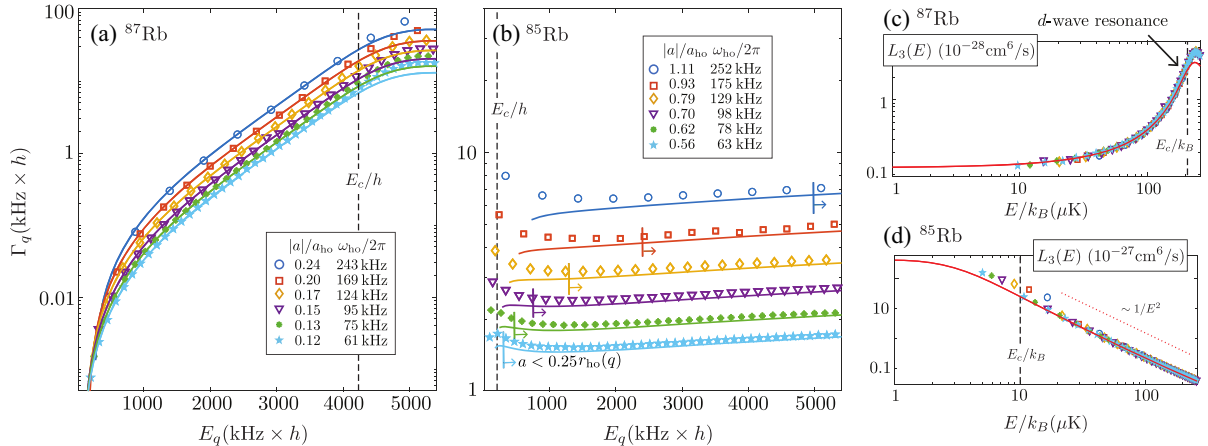


FIG. 3. Numerical values for the width Γ_q of the three-body states (symbols) as a function of their energy E_q for (a) ^{87}Rb , and (b) for ^{85}Rb . Solid lines correspond to the results for Γ_q from the LL relation (9), obtained from our free-space numerical simulations of $L_3(E)$. The colored arrows in (b) mark the regime $a < 0.25r_{\text{ho}}(q)$, and all data points in (a) fall within this regime. For both Rb isotopes the frequencies correspond to $a_{\text{ho}}/r_{\text{vdW}} = 5, 6, 7, 8, 9$, and 10 . Symbols in (c) and (d) correspond to $L_3(E_q)$ from the LL relation (1) obtained from the numerical calculations for E_q and Γ_q shown in (a) and (b). The vertical dashed lines indicate the value of $E_c = \hbar^2/(ma^2)$.

behavior can be understood as arising from the distinct energy dependence of $L_3(E)$ for the two isotopes. For ^{85}Rb atoms, the primary factor influencing $L_3(E)$ results from its strong interactions ($a = -5.56 \text{ } r_{\text{vdW}}$). In such cases, the expected threshold behavior, $L_3(E) = \text{const}$, deteriorates for $E \gtrsim E_c = \hbar^2/(ma^2)$, with $L_3(E)$ reaching its unitary behavior, $L_3(E) = C_\eta/E^2$, where $C_\eta = 72\sqrt{3}\pi^2\hbar^5/m^3(1 - e^{-4\eta})$ and η being the three-body inelasticity parameter characterizing, for instance, the Efimov states lifetime and other universal properties of Efimov physics [60,76]. [For ^{85}Rb , $E_c \approx 200 \text{ kHz} \times h$ (or $10 \text{ } \mu\text{K}/k_B$) and displayed in Fig. 3 as a vertical dashed line.] Figure 3(d) shows this change in behavior in our numerical calculations for $L_3(E)$ (solid line) along with the results for $L_3(E_q)$ obtained from the LL relation (1) (symbols), using our calculated values of E_q and Γ_q shown Fig. 3(b). As can be seen in Fig. 3(d), for ^{85}Rb , most of the states are in the $E_q > E_c$ regime where $L_3 = C_\eta/E_q^2$, in which case the LL relation (9) predicts $\Gamma_q = \Gamma_u[1 - (\hbar\omega_{\text{ho}})^2/E_q^2] \simeq \Gamma_u[1 - 1/(2q + 3)^2]$, thus consistent with Γ_q being weakly dependent on E_q for states beyond $E_q = E_c$ [see Fig. 3(b)]. The unitary width, $\Gamma_u = \hbar\omega_{\text{ho}}(1 - e^{-4\eta})/\pi$, provides a direct mean of extracting η from trap systems. In contrast, for ^{87}Rb atoms, the interaction is weak ($a = 1.21 \text{ } r_{\text{vdW}}$) and $L_3(E)$ is expected to be constant within a broader energy range [$E_c \approx 4000 \text{ kHz} \times h$ (or $200 \text{ } \mu\text{K}/k_B$) for ^{87}Rb]. However, for ^{87}Rb , $L_3(E)$ is enhanced within this region due to the presence of a d -wave diatomic shape resonance [84], as shown by our numerical calculations for L_3 (solid line) in Fig. 3(c). Therefore, according to the LL relation (9), the primary mechanism responsible for the enhancement of Γ_q for ^{87}Rb trapped states in Fig. 3(a) traces back to the presence of the d -wave diatomic resonance. We note that the deviations shown in Fig. 3(c) near the position of the d -wave resonance are likely due to the couplings from other $\lambda \neq 0$ three-body channels, not included in our derivation of the LL relation.

We note that typical experiments with trapped few-atom systems require loading atoms from an ultracold gas into a single trapped state. Without a dedicated cooling scheme (see, for instance, Refs. [21,24,55–59]), atoms will instead be loaded into the trap at some finite temperature, typically $k_B T \gg \hbar\omega_{\text{ho}}$. In such cases, if the system is in thermal equilibrium, the LL relation can be extended by averaging Eq. (9) under a thermal distribution of quantum trapped states (see End Matter).

The LL relation (9) can be generalized to N -atom systems ($N \geq 2$), in which case we obtained

$$\Gamma_{N,q} = \frac{1}{C_N} \frac{m^{\frac{3N-3}{2}}}{\hbar^{3N-5}} L_N(E_{N,q}) \times E_{N,q}^{\frac{3N-9}{2}} [E_{N,q}^2 - 4\alpha_N(\hbar\omega_{\text{ho}})^2] \omega_{\text{ho}}, \quad (10)$$

with $C_N = \pi^{(3N-3)/2} N^{\frac{5}{2}} 2^{(3N-5)/2} \Gamma[(3N-3)/2]$ and $\alpha_N = (N-1)(3N-7)(3N-5)/64$ (see details and further numerical tests at $N = 2$ in Ref. [70]). Here, $\Gamma_{N,q}$ and $E_{N,q}$ are the width and energy of the trapped N -body state, respectively, and L_N the free-space N -body loss coefficient [69,85] for the $J = 0$ and $\lambda = 0$ partial wave. For $N > 3$, the width of an N -body trap state is typically determined by different decay pathways that may involve all or only some of the atoms. In Ref. [24], for instance, it was found experimentally that for Sr atoms in a $q = 0$ state the decay rate for $N = 3, 4$, and 5 is approximately proportional to the number of triads, indicating that three-body processes remain the dominant decay pathway. In reality, the direct experimental observable is the total decay rate, including all higher-order processes, defined as

$$\frac{\Gamma_{N,q}^{\text{tot}}}{\hbar} = \sum_{K=3}^N \binom{N}{K} \frac{\Gamma_{K,q}}{\hbar} = \binom{N}{3} \frac{\Gamma_{3,q}}{\hbar} + \binom{N}{4} \frac{\Gamma_{4,q}}{\hbar} + \cdots + \frac{\Gamma_{N,q}}{\hbar}, \quad (11)$$

with fundamental few-body decay rates $\Gamma_{K,q}/\hbar$ given in Eq. (10). In an experiment such as Ref. [24], where trapped states containing $N = 3, 4, 5, \dots$ atoms are prepared and their decay rates $\Gamma_{N,q}^{\text{tot}}/\hbar$ measured, the corresponding fundamental rates can be extracted by inverting Eq. (11),

$$\frac{\Gamma_{N,q}}{\hbar} = \sum_{K=3}^N (-1)^{N-K} \binom{N}{K} \frac{\Gamma_{K,q}^{\text{tot}}}{\hbar}, \quad (12)$$

allowing for the determination of N -body scattering rates L_N via the LL relation (10), in a much more controlled way than in ultracold gas experiments [51–54,85].

In summary, we have derived the Lellouch-Lüscher (LL) relation connecting the energy and width of few-body states in a harmonic trap to the corresponding loss constants in free space, and demonstrated its validity through three-body numerical calculations. A unique feature of the LL relation is that, when atoms are prepared in trapped states of a single partial wave—typically $J = 0$ for bosons—it enables the measurement of individual partial-wave contributions to loss rates. This makes trapped few-body systems a more sensitive probe of scattering resonances and interference phenomena, including those associated with Efimov physics [76,86], which are often obscured in bulk-gas measurements due to thermal averaging over multiple partial waves [60]. We further show that the generalized N -body LL relation provides a systematic path to precise determinations of multibody scattering rates [24,69]. Taken together, the results from the LL relation framework help to establish trapped few-body systems as a powerful platform for advancing our understanding of complex quantum phenomena.

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Data availability—The data that support the findings of this article are openly available [87].

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End Matter

LL relation in thermal equilibrium—In experiments, loading a few atoms from the bulk into an isolated trap generally leads to $k_B T \gg \hbar \omega_{\text{ho}}$, producing a thermal ensemble instead of a single trap state. The corresponding lifetime $\hbar/\Gamma_{\text{th}}$ of the thermal state can be estimated by assuming a Boltzmann distribution of energies E_q as

$$\Gamma_{\text{th}}(T) \equiv \frac{\sum_q e^{-E_q/k_B T} \Gamma_q}{\sum_q e^{-E_q/k_B T}}. \quad (\text{A1})$$

Provided that the initial state (prior to loading) has a low enough temperature ($k_B T_{\text{in}} \ll E_c$) the populated trap states will predominantly be that of the $J = 0$ (and $\lambda = 0$) partial wave. This allows us to use the LL relations [Eq. (9) or (10)] to derive simple results in two limiting cases, namely, the threshold ($|k_{\text{th}} a| \ll 1$) and unitary

($|k_{\text{th}} a| \gg 1$) regimes, with $\hbar k_{\text{th}} = (m k_B T)^{1/2}$. In fact, while in the threshold regime most of the states that contribute to Eq. (A1) are those with $\hbar \omega_{\text{ho}} \ll E_q \sim k_B T \ll E_c$, where $L_3(E_q) \approx L_3(0)$, the states contributing to Eq. (A1) in the unitary regime will be those with $\hbar \omega_{\text{ho}} \ll E_c \ll E_q \sim k_B T$, where $L_3(E_q) = C_\eta/E_q^2$. Assuming $E_q \simeq (2q+3)\hbar \omega_{\text{ho}}$ and using the LL relation (9), the thermal loss rate in Eq. (A1) can be expressed as

$$\Gamma_{\text{th}} = \begin{cases} 2 \frac{1}{C} \frac{m^3}{\hbar^4} L_3(0) (k_B T)^2 \omega_{\text{ho}}, & \text{for } |k_{\text{th}} a| \ll 1, \\ (1 - e^{-4\eta}) \hbar \omega_{\text{ho}} / \pi = \Gamma_u, & \text{for } |k_{\text{th}} a| \gg 1, \end{cases} \quad (\text{A2})$$

for which a brief derivation and numerical test will be presented below. We note that for $|k_{\text{th}} a| \ll 1$ the thermal

decay rate is quadratic in $(k_B T)$ and is a factor 2 larger than the rate obtained by the LL relation (9), for $E_q = k_B T$ and $L_3(E_q) \simeq L_3(0)$. For $|k_{th}a| \gg 1$, however, the thermal decay rate is independent of the temperature. This unexpected result is a direct consequence of the LL relation (9). Similar results can be obtained for N atoms in thermal equilibrium using the total decay rate in Eq. (11) and the corresponding LL relations (10).

To derive Eq. (A2), we define the individual contribution of the q th trapped state to Γ_{th} as

$$\gamma_q = \frac{e^{-E_q/k_B T} \Gamma_q}{\sum_q e^{-E_q/k_B T}}, \quad (A3)$$

such that $\Gamma_{th} = \sum_q \gamma_q$. Due to the Boltzmann factor $e^{-E_q/k_B T}$, temperature acts as a natural cutoff: a state will contribute significantly to Γ_{th} only if its energy E_q is of the order of $\sim k_B T$ or smaller. Consequently, in the threshold regime where $k_B T \ll E_c = \hbar^2/m a^2$, the major contributing states have energies $\hbar\omega_{ho} \ll E_q \ll E_c$. This is demonstrated in Fig. 4(a) by using the following toy model for $L_3(E)$:

$$L_3(E) = \frac{L_3(0)}{1 + \alpha(E/E_c)^2}, \quad (A4)$$

where $\alpha = L_3(0)E_c^2/C_\eta$. [This toy model is designed to capture the two limiting behaviors of $L_3(E)$: $L_3(E) \rightarrow L_3(0)$ as $E \rightarrow 0$ (threshold limit) and $L_3(E) \rightarrow C_\eta/E^2$ as $E \rightarrow \infty$ (unitary limit), thus providing a suitable framework for the analysis in this section].

As the majority contribution to Γ_{th} comes from the states with $\hbar\omega_{ho} \ll E_q \ll E_c$, we are allowed to replace the energy dependence $L_3(E)$ with $L_3(0)$ and $[E_q^2 - \hbar^2\omega_{ho}^2]$ with E_q^2 in Eq. (A1). By further assuming $E_q \simeq (2q + 3)\hbar\omega_{ho}$, we get

$$\Gamma_{th} = \frac{1}{C} \frac{m^3}{\hbar^2} L_3(0) \omega_{ho}^3 g\left(\frac{\hbar\omega_{ho}}{k_B T}\right), \quad (A5)$$

with

$$\begin{aligned} g(x) &= 5 + 4 \coth(x) + 2 \operatorname{csch}^2(x) \\ &= \frac{2}{x^2} + \frac{4}{x} + \frac{13}{3} + O(x), \end{aligned} \quad (A6)$$

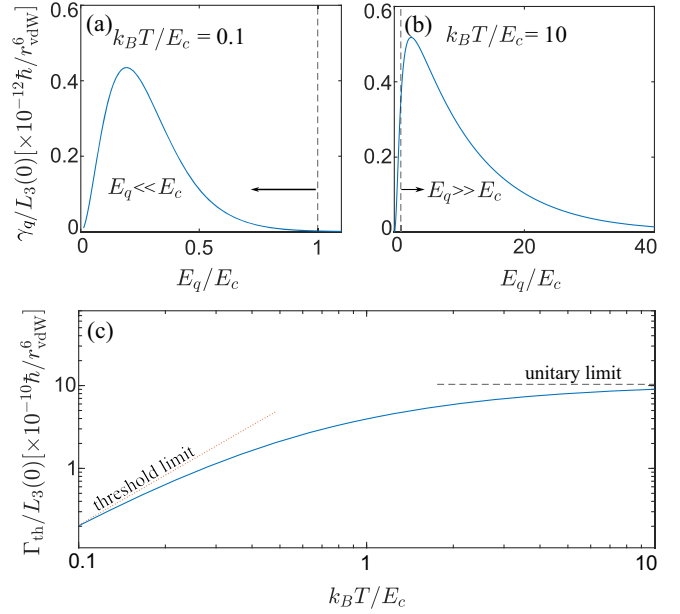


FIG. 4. The distribution of the individual contribution, γ_q , of the trap state to Γ_{th} in the threshold regime of $k_B T/E_c = 0.1$ (a) and in the unitary regime of $k_B T/E_c = 10$ (b). The vertical dashed lines indicate that $E_q = E_c$. (c) shows the temperature-dependence behavior of the Γ_{th} calculated from Eqs. (A1) and (A2) at threshold limit (dotted line) and unitary limit (dashed line). The displayed result is obtained by using Eq. (A4) for $L_3(E)$ with $\alpha = 1$, $E_c = 0.1 E_{vdW}$ and $\hbar\omega_{ho} = 0.001 E_{vdW}$ and Eq. (9) for Γ_q , for instance.

where the leading order gives Eq. (A2) at $|k_{th}a| \ll 1$. The validity of our Eq. (A2) is demonstrated in Fig. 4(c), where it is compared to the numerical result using the expression (A4) for $L_3(E)$.

At the unitary limit where $k_B T \gg E_c$, the states that contribute to Γ_{th} still have an E_q of the order of $\sim k_B T$ or smaller. However, in this regime, a majority of these states can satisfy $E_q \gg E_c \gg \hbar\omega_{ho}$ [see Fig. 4(b)], such that $L_3(E_q) = C_\eta/E_q^2$. To further simplify the derivation, we assume $C_\eta = L_3(E_q)E_q^2$ for all states. Plugging this expression into Eq. (A1) and by considering $[E_q^2 - \hbar^2\omega_{ho}^2] \rightarrow E_q^2$, we get the simple relation in Eq. (A2), i.e., $\Gamma_{th} = \Gamma_u$. The validity of Eq. (A2) in this limit is also confirmed in Fig. 4(c) by comparing it to the numerical result from the toy model.