

Observation of the p -wave shape resonance in atom-molecule collisions


Baruch Margulis¹,^{*} Prerna Paliwal,^{1,*} Wojciech Skomorowski,² Mariusz Pawlak³,
Piotr S. Żuchowski⁴, and Edvardas Narevicius^{1,†}

¹*Department of Chemical and Biological Physics, Weizmann Institute of Science, 7610001 Rehovot, Israel*

²*Centre of New Technologies, University of Warsaw, Banacha 2c, 02-097 Warsaw, Poland*

³*Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Gagarina 7, 87-100 Toruń, Poland*

⁴*Institute of Physics, Faculty of Physics, Astronomy and Informatics,
Nicolaus Copernicus University, Grudziądzka 5, 87-100, Toruń, Poland*

 (Received 19 January 2022; revised 5 April 2022; accepted 28 September 2022; published 18 October 2022)

We observe a p -wave resonance in the collisions between metastable neon and rovibrationally ground state HD molecules at a collision energy of $k_B \times 22$ mK. This is the first observation of the lowest quasibound angular momentum state in molecular collisions. This measurement was enabled by the reduction of the lowest collision energy achieved without laser cooling, using the phase-space correlation in cold molecular beams. We demonstrate that contrary to higher l -state resonances, the p -wave resonance allows sensitive probing of the leading term of the van der Waals intermolecular interaction. Furthermore, the same sensitivity to the long range part of the interaction potential allows an accurate estimation of p -wave resonance lifetime using only fundamental constants and the dispersion coefficient.

DOI: [10.1103/PhysRevResearch.4.043042](https://doi.org/10.1103/PhysRevResearch.4.043042)

I. INTRODUCTION

Many processes in nature at low collision energies are slow and occur mainly via quantum resonance states. For example, collision products can be either blocked by a potential barrier as in $F+H_2$ reaction [1,2] or be suppressed by quantum symmetry as in the case of atom-ion spin exchange [3], molecular fine structure changing collisions [4] and Penning ionization (PI) reactions [5]. PI is an ionization by impact process between two neutral particles [6]. Shape type resonances in particular are identified by a well-defined angular momentum quantum number and are formed by tunneling through a centrifugal barrier which arises due to the addition of the centrifugal term $\frac{\hbar^2 l(l+1)}{2\mu R^2}$ to the intermolecular potential. Partial wave resonances in molecular scattering experiments were first observed in elastic scattering [7] and later in reactive and inelastic collisions using merged beams technique [8] as well as in low intersection angle collisions [4]. These resonances are excellent probes of intermolecular potentials [9], enable the direct probe of interaction anisotropy [10], and serve as a benchmark for modern quantum chemistry theories [11]. Observation of partial wave resonances requires collision energies of $k_B \times 1$ K and below. The low collision energies limit the number of accessible angular momentum states, enabling

observation of a well-resolved resonance state, eventually reaching the point where the resonance collision complex possesses a single quanta of angular momentum. This allows a full control not only over the internal molecular degrees of freedom but also the intermolecular ones, constraining all the quantum numbers involved in the collision. Although previously observed in cold atomic collisions [12,13], to date, molecular collisions experiments using small angle scattering were only able to probe the onset of a p -wave resonance [14]. A Feshbach type resonances appearing in the p -wave channel have been observed in several systems [15,16].

Here we present the first measurement of the lowest possible angular momentum quasibound state, the p -wave resonance state, in molecular scattering. We demonstrate that such low angular momentum states are particularly important in sensing the leading terms in the van der Waals part of the long-range intermolecular interaction. The same sensitivity allows us to accurately estimate the p -wave resonance lifetime without any knowledge of short-range physics using a semiclassical approach together with a truncated potential. This approach is complementary to the estimation of the low energy scattering length [17]. This is a useful result, since in many experiments the measured resonance linewidth does not necessarily correspond to lifetime, it may be limited by the energy resolution. Using our method we can now estimate the natural p -wave resonance lifetime from fundamental constants and the dispersion parameter alone.

We detect the fully resolved p -wave resonance in PI collisions between metastable neon atoms and neutral hydrogen deuteride molecules at a collision energy of $k_B \times (22.2 \pm 5.4)$ mK. We observe this resonance state using the merged beam technique, taking advantage of the phase space correlation within two overlapping particle bunches with nearly identical mean velocities.

^{*}Present address: Department of Chemistry, University of Basel, 4056 Basel, Switzerland.

[†]edvardas.narevicius@weizmann.ac.il

Published by the American Physical Society under the terms of the [Creative Commons Attribution 4.0 International](https://creativecommons.org/licenses/by/4.0/) license. Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.

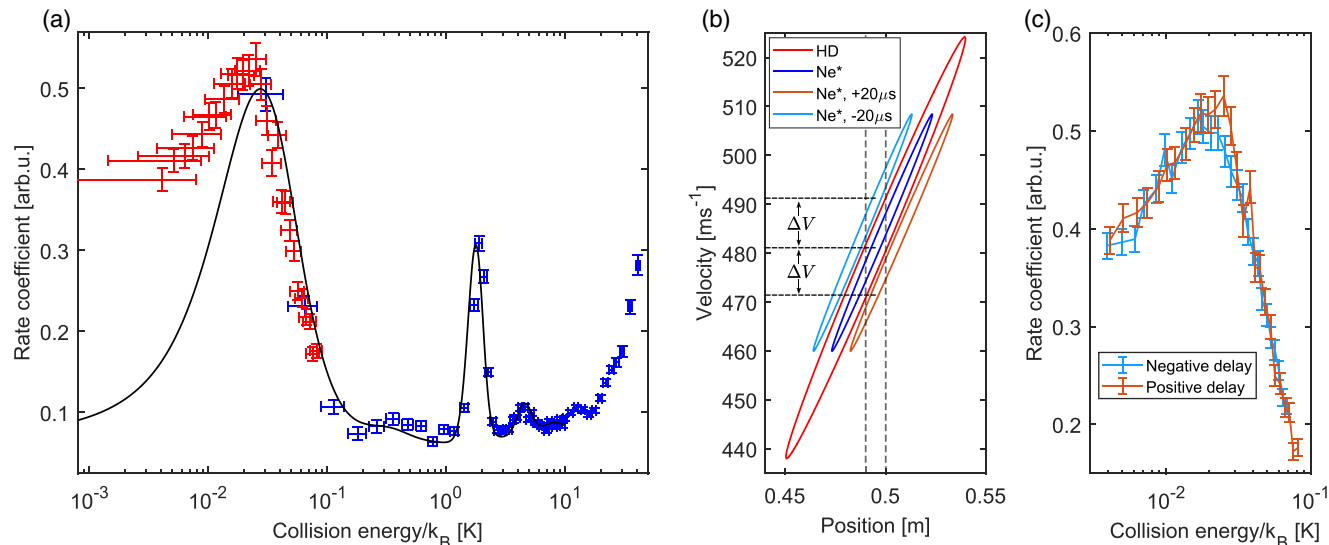


FIG. 1. (a) The data points with error bars represent measured rate coefficients for the Ne^* -HD PI reaction and their uncertainties. The black curve depicts the calculated rate coefficients using the interaction potential, obtained at the CCSD(T)/d-aug-cc-pV5Z+midbond level of theory with additional 2.9% scaling of the electron correlation energy. Vertical error bars represent statistical errors. Horizontal error bars represent the uncertainty in collision energy as derived from the uncertainty in individual beam velocity. (b) Phase space distributions snapshot of the Ne^* and HD beams assuming the experimental velocity distributions at the low-energy regime in the interaction region of our detector. For the red curve, the delay between the beams is set for a maximal overlap at the center of the VMI detector. Blue and orange contours represent a shift of $\pm 20 \mu\text{s}$ in delay between the valves, respectively. Vertical dotted lines represent the edges of the detection region. (c) Comparison of the measured shape of the low-energy resonance for negative and positive beam delay scans.

II. EXPERIMENTAL SETUP

The experimental setup is described in detail elsewhere [18]. In short, two pulsed supersonic beams of pure Ne and a 50/50 mixture of HD and Ne are generated by two Even-Lavie valves [19]. The Ne beam is excited to the 3P_2 metastable state (Ne^*) by a dielectric barrier discharge which is located directly after the valve nozzle [20]. The Ne^* beam is merged with the HD beam using a curved 20-cm magnetic guide leading to a zero relative angle between the beams. Product ions are extracted and detected using a velocity map imaging (VMI) spectrometer, which operates in ion count mode. HD molecules are generated in their ground rovibrational state by supersonic expansion. The Ne^* beam velocity and standard deviation, σ , are characterized by measuring the time-of-flight (TOF) information using an on-axis multichannel plate. The HD beam is characterized using a TOF mass spectrometer (TOF-MS) which contains an electron impact ionization element. The collision energy is determined by the mean relative velocity between the beams. The rate coefficient is calculated according to the ratio between counts of ions and the intensity of the reactant beams at the intersection point. Every measurement of product ions is followed by a measurement of background ions, which is deducted from the overall count.

III. RESULTS

We present the measured rate coefficient as a function of collision energy together with the results of the theoretical calculations in Fig. 1. The experimental data consists of two sets of measurements. For the first set, the collision energy

is tuned by manipulating the mean value of the velocity of the HD beam while simultaneously setting the TOF delay between the valves such that the beams merge at the center of the detection region. The first set is represented by blue data points and includes collision energies between $k_B \times 30$ mK and $k_B \times 40$ K. For this set, the Ne^* beam velocity is kept constant at 470 m/s ($\sigma = 11.2$ m/s) while the HD beam velocity is tuned between 485 m/s ($\sigma = 35$ m/s) and 982 m/s ($\sigma = 49$ m/s) by changing the HD valve temperature between 64 and 210 K. Each data point represents events accumulated over 5000 repetitions. Our merged beam setup allows us to scan collision energy in a low energy range with high resolution using the phase space correlation, which develops during the beam propagation from the source to the detection region [21]. Since beam generation time is much shorter as compared to the time of flight, velocity distribution in the detection volume becomes squeezed, with the standard deviation of 2 m/s for the Ne^* beam. In order to scan the relative velocity between two such beams, we can either change the center velocity of one beam relative to the other as is done in most experiments or change the time delay between two near-matched velocity beams as shown in Fig. 1(b). The second data set acquired using phase space correlation is represented by red data points for collision energies between $k_B \times 4$ mK and $k_B \times 75$ mK. For this set, both the Ne^* and HD beams' velocities are kept constant at 484 m/s ($\sigma = 11$ m/s) and 475 m/s ($\sigma = 33$ m/s), respectively. The collision energy is tuned by changing the time delay between the valves opening time in the range of 0 to 45 μs . Each point represents data acquired in 10 000 repetitions. By shifting the valve opening time of one beam relative to the other, once in the positive direction and once in the negative direction, we are able to probe the

low energy regime in two separate measurements [Fig. 1(c)]. This allows us to obtain an accurate value for the HD beams' generation time therefore, reducing the uncertainty in the TOF of the HD beam from around 20 μ s, which is the valve opening time, to 0.5 μ s. For the Ne* beam, the generation time is accurately defined by the ignition instance of the dielectric discharge which is 45 μ s.

IV. THEORY

Theoretical rate coefficients are estimated using an *ab initio* complex-valued potential energy surface. The real part of the potential is calculated using the supermolecular approach and the coupled-cluster method with single, double, and approximate noniterative triple excitations [CCSD(T)] in a very large, diffused basis set (d-aug-cc-pV5Z+midbond, i.e., doubly augmented correlation consistent polarized valence quintuple zeta with midbond functions). The potential is smoothly merged between $R = 15$ and $R = 20 a_0$ with an analytical function representing the long-range interaction. The van der Waals coefficients C_6 and C_8 were found by fitting to the *ab initio* potential energy curve computed up to $R = 50 a_0$. The imaginary part of the potential is obtained using the Fano-Feshbach approach combined with equation-of-motion coupled-cluster single and double wave function [23], and with a bound-domain projection operator adapted to the PI problem. To construct final (continuum) electronic states of the system in the Feshbach theory, the orbital describing the outgoing electron is approximated with a Coulomb wave centered at the midpoint of the HD molecule. The primary source of uncertainty in the real part of the interaction potential is the electron correlation energy which depends on the truncation of the basis set and the coupled-cluster excitation accuracy level. The electron correlation energy is adjusted to match the experimental findings by scaling it by 1.029. The rotational wave function of the HD molecule in the ground rotational state is spherically symmetric, and the anisotropy resulting from the spatial distribution of the excited metastable neon atom is negligible, similar to the interactions with He and Ar atoms [24]. Hence, only the isotropic part of the intermolecular potential, expanded in renormalized spherical harmonics, is considered in the calculation. To this end, the *ab initio* calculations are carried out using the linear and T-shaped geometries of the complex. The scattering wave function is propagated from 7 to 500 a_0 , where a_0 is the Bohr radius, applying the log-derivative method [25]. The reaction rate coefficient is convoluted according to the experimental resolution which is expressed by the spread in relative velocity per collision energy. The latter is estimated using 1D particle trajectory simulations, taking into account the experimental spread in individual beam velocities and the size of the VMI extraction area. The theoretical result is shown as a black curve in Fig. 1(a).

We observe three scattering resonances at $k_B \times (22.2 \pm 5.4)$ mK, $k_B \times (1.92 \pm 0.13)$ K, and $k_B \times (4.51 \pm 0.20)$ K. Figure 2 presents the calculated partial wave contribution to each resonance state and the numerically calculated resonance state wave functions. We identify the resonance at $k_B \times 22$ mK as arising from the *p*-wave partial wave state.

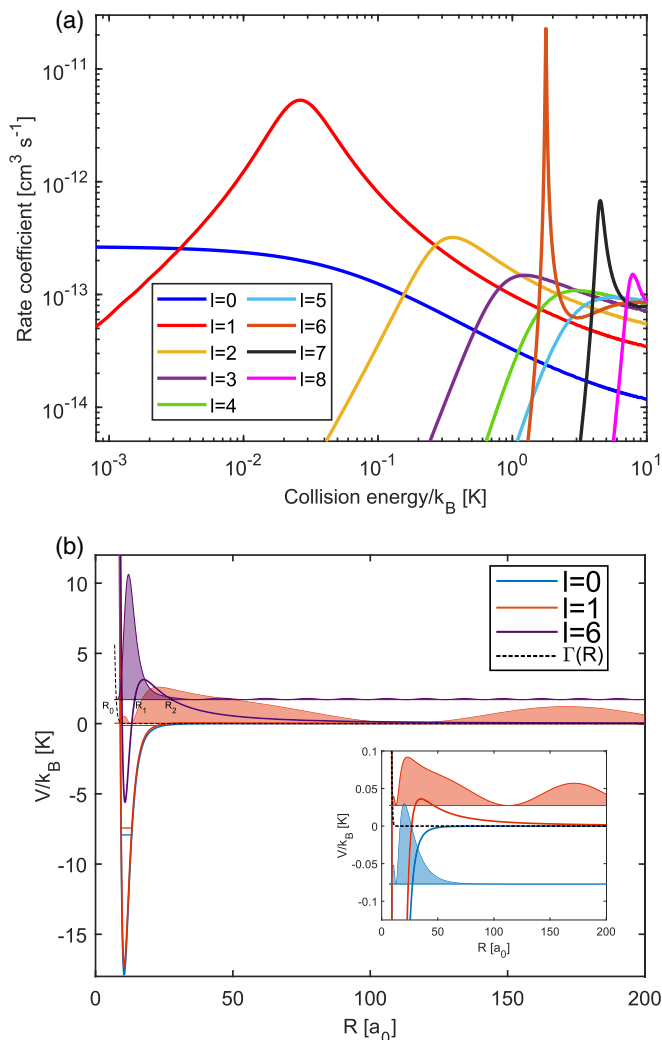


FIG. 2. (a) Partial wave selected PI rate coefficient as a function of collision energy. (b) Effective potentials for the $l = 0, 1$ and 6 states of collision. $\Gamma(R)$ is the ionization probability which is related to the imaginary part of the intermolecular potential $\text{Im}(V(R)) = -\Gamma(R)/2$. Resonance wave functions for the partial waves $l = 1$ and $l = 6$ are shown by shaded orange and purple areas, respectively. Bound state energies for $l = 0$ and $l = 1$ are depicted by orange and blue horizontal lines. The inset shows a zoomed-in view where the *p*-wave barrier can be seen. The wave function of the excited bound state for $l = 0$ is presented as a shaded blue curve. Wave functions and energies are calculated using discrete variable representation [22].

The higher energy resonances at $k_B \times 1.9$ K and $k_B \times 4.5$ K arise from the $l = 6$ and $l = 7$ states accordingly.

V. SENSITIVITY TO THE LONG RANGE PART OF THE INTERACTION

Surprisingly, the *p*-wave and $l = 6$ resonances have nearly identical widths although the $l = 6$ resonance is stronger confined by the centrifugal barrier. The shape type resonance width, Γ , which is inversely proportional to the lifetime $\tau = \hbar/\Gamma$, can be estimated using semiclassical Gamow approximation, which introduces two parameters. One is the

TABLE I. Resonance positions and widths calculated by the CAP method ($E_{\text{res}} = E_{\text{exact}} - i\frac{\Gamma_{\text{exact}}}{2}$), semiclassical widths obtained using exact resonance energies (Γ_{sc}), tunneling probabilities (P_{sc}), and widths for the truncated potential ($\Gamma_{\text{sc}}^{\text{trunc}}$). All energy values are in units of Kelvin.

l	E_{exact}	Γ_{exact}	P_{sc}	Γ_{sc}	$\Gamma_{\text{sc}}^{\text{trunc}}$
1	0.023	0.030	0.50	0.045	0.046
6	1.781	0.033	0.023	0.036	0.047
7	4.47	0.59	0.59	0.64	0.83

tunneling probability through a centrifugal barrier whereas the second parameter defines the time scale given by the nuclear motion frequency [26,27]:

$$\Gamma = \frac{\hbar^2}{2\mu} \left[\int_{R_0}^{R_1} \frac{1}{k(R)} dR \right]^{-1} \exp \left[-2 \int_{R_1}^{R_2} |k(R)| dR \right], \quad (1)$$

where R_0 , R_1 , and R_2 are the classical turning points as indicated for the $l = 6$ resonance state in Fig. 2(b). $k(R) = \sqrt{2\mu(E - V(R))}/\hbar$ is the semiclassical wave vector.

For resonance states where tunneling probability is $\ll 1$, this leads to a characteristic exponential decay or a Lorentzian line shape in the energy spectrum. A very unusual situation arises for resonances that are located near the top of the centrifugal barrier where tunneling probability approaches unity. In such a case the decay time is mainly defined by the time it takes particles to reach the centrifugal barrier. For p -wave resonances, the top of the centrifugal barrier is located near the threshold. This leads to both high tunneling probability and slow nuclear dynamics since particles spend most of the time exploring the long range part of the interaction potential. As a result, the linewidth of such shape resonances can be orders of magnitude narrower as compared to orbiting resonances that have been detected earlier [18].

A comparison of the numerically exact width as calculated using complex absorbing potential [28,29] and semiclassical approximation is given in Table I. The semiclassical approximation reliably estimates the width within an order of magnitude. The p -wave and $l = 6$ resonance lifetimes are nearly identical despite the order of magnitude difference in tunneling probabilities. Since the tunneling probability for the p -wave resonance approaches unity, the lifetime becomes limited by the time scale of the nuclear motion behind the barrier, given by the first term in (1). For the p -wave resonance, the slow nuclear dynamics timescale results in a resonance width which is larger as compared to the resonance energy position leading to a distinct non-Lorentzian form of the resonance peak indicating a non-exponential decay. For the $l = 7$ resonance state, which has a similar magnitude of tunneling probability, the real part of the resonance energy is by two orders of magnitude higher leading to a 20 fold shorter lifetime.

The p -wave centrifugal barrier is located at intermolecular distance that is described by the long-range dispersion interaction alone. Since the p -wave resonances are located close to the threshold we show that the lifetime can be calculated using the semiclassical approximation with a truncated potential which includes only the long range part and the centrifugal

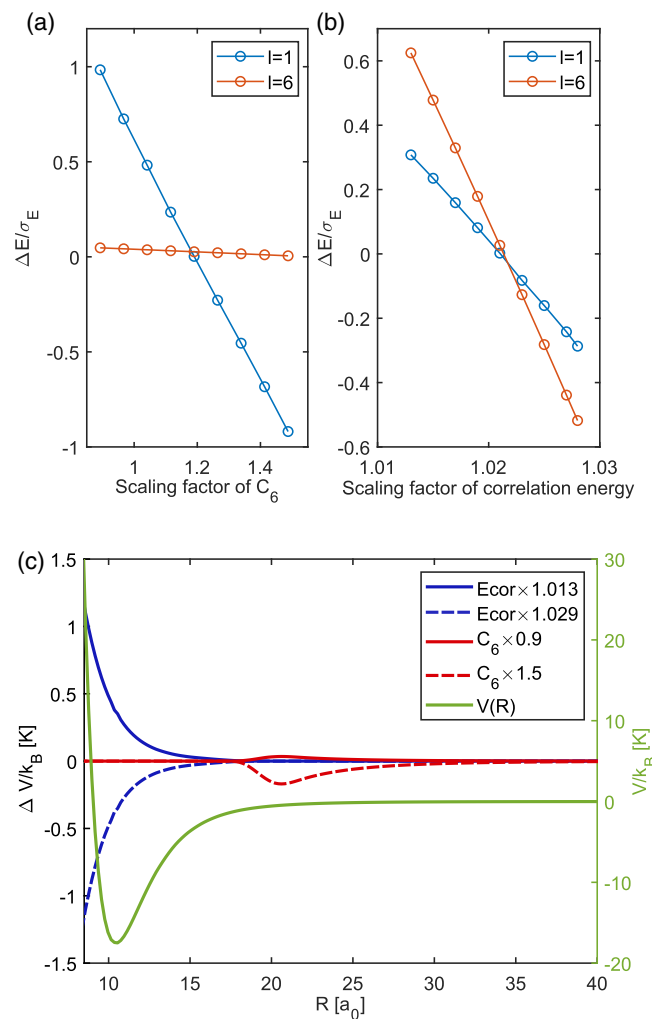


FIG. 3. Shift in position of $l = 1$ and $l = 6$ resonances as a function of the scaling of the C_6 coefficient (a) and the electron correlation energy (b). The shift is expressed in the units of the width of the measured resonance (σ_E). For C_6 scaling, the potential is smoothly modified between $R = 17$ and $R = 22 a_0$. Calculations are performed around scaling values which provide the lowest error for both resonance positions simultaneously. (c) Addition to the intermolecular potential due to scaling of the electron correlation energy (blue curves) and scaling of C_6 (red curves). The interaction potential is presented by a green curve.

term: $V_{\text{lr}}(R) = -\frac{C_6}{R^6} - \frac{C_8}{R^8} + \frac{\hbar^2 l(l+1)}{2\mu R^2}$. We choose the truncation position at a potential minimum, although our result is not sensitive to the exact truncation point. For the p -wave resonance, the semiclassical lifetime evaluated using only the long-range part of the interaction agrees well with the full calculation, resulting in a relative error of less than 1%. This demonstrates that the lifetime of p -wave resonance is nearly universal quantity that can be estimated using the reduced mass and the leading terms in the long-range interaction potential.

Whereas the p -wave resonance lifetime is sensitive only to the long-range part of the interaction, the energy position depends both on the short- and the long-range parts of the interaction. However, since the two lowest energy resonance states occupy different areas in the phase space we

expect different sensitivity to the interaction potential details. An accurate description of shape resonance position requires potential energy surface exceeding the accuracy achievable with the “gold standard” of current quantum chemistry methods [11]. As a result, calculated potential surfaces are usually uniformly scaled within the estimated error limits [30,31] or modified only at the short range by scaling the electron correlation energy [10]. By independently scaling the electron correlation energy and the leading van der Waals coefficient (C_6), we separately modify the short- and long-range parts of the interaction potential, respectively, as shown in Fig. 3. The latter allows us to demonstrate that different angular momentum shape resonances probe different parts of the interaction potential.

For every modification of the interaction potential, we calculate the position of the $l = 6$ and $l = 1$ resonances and express the shift in resonance position in units of the measured resonance width (σ_E) which is limited by the experimental resolution. The results are shown in Figs. 3(a) and 3(b). Scaling of the correlation energy in the range from 1.013 to 1.029 resulted in a shift of $1.1\sigma_E$ for the $l = 6$ state and $0.6\sigma_E$ for the $l = 1$ state [Fig. 3(b)]. On the other hand, scaling of the C_6 coefficient by 0.9 to 1.5 has altered the position of the p -wave resonance by $1.9\sigma_E$, whereas the $l = 6$ resonance was shifted only by $0.04\sigma_E$ [Fig. 3(a)]. While the position of the $l = 6$ resonance is by a factor of 2 more sensitive to the short-range interaction, the position of the p -wave resonance is by a factor of 50 more sensitive to the strength of the long-range

interaction. The simultaneous probing of the shape resonance phenomenon in the few kelvin and millikelvin energy regimes effectively probes the intermolecular potential at all regions of the interaction.

VI. OUTLOOK

The experimental ability to constrain a collision process to a single, low-value total angular momentum state may further improve the imaging resolution in molecular collision experiments. In PI electron-ion coincidence experiments, information about the final state distribution resulting from the postionization ion-neutral dynamics is blurred by the increasing number of accessible angular momentum states. Improved resolution may enable for example, the detection of different Feshbach resonances which are located close to the dissociation threshold [32].

ACKNOWLEDGMENTS

We thank Christiane Koch and Yuval Shagam for helpful discussions. B.M., P.P. and E.N. acknowledge funding from the Israel Science Foundation. P.S.Z. is grateful to Narodowe Centrum Nauki (2019/34/E/ST4/00407) for funding the project Sonata Bis 9. The work of W.S. was supported by the Polish National Agency for Academic Exchange within Polish Returns Programme.

-
- [1] J. B. Kim, M. L. Weichman, T. F. Sjolander, D. M. Neumark, J. Klos, M. H. Alexander, and D. E. Manolopoulos, Spectroscopic observation of resonances in the $F + H_2$ reaction, *Science* **349**, 510 (2015).
- [2] M. Tizniti, S. D. Le Picard, F. Lique, C. Berteloite, A. Canosa, M. H. Alexander, and I. R. Sims, The rate of the $F+H_2$ reaction at very low temperatures, *Nat. Chem.* **6**, 141 (2014).
- [3] T. Sikorsky, M. Morita, Z. Meir, A. A. Buchachenko, R. Ben-Shlomi, N. Akerman, E. Narevicius, T. V. Tscherbul, and R. Ozeri, Phase Locking between Different Partial Waves in Atom-Ion Spin-Exchange Collisions, *Phys. Rev. Lett.* **121**, 173402 (2018).
- [4] S. Chefdeville, Y. Kalugina, S. Y. T. van de Meerakker, C. Naulin, F. Lique, and M. Costes, Observation of partial wave resonances in low-energy O_2-H_2 inelastic collisions, *Science* **341**, 1094 (2013).
- [5] E. Lavert-Ofir, Y. Shagam, A. B. Henson, S. Gersten, J. Klos, P. S. Żuchowski, J. Narevicius, and E. Narevicius, Observation of the isotope effect in sub-kelvin reactions, *Nat. Chem.* **6**, 332 (2014).
- [6] P. E. Siska, Molecular-beam studies of Penning ionization, *Rev. Mod. Phys.* **65**, 337 (1993).
- [7] J. P. Toennies, W. Welz, and G. Wolf, Molecular beam scattering studies of orbiting resonances and the determination of van der Waals potentials for $H-Ne$, Ar , Kr , and Xe and for H_2-Ar , Kr , and Xe , *J. Chem. Phys.* **71**, 614 (1979).
- [8] A. B. Henson, S. Gersten, Y. Shagam, J. Narevicius, and E. Narevicius, Observation of resonances in Penning ionization reactions at sub-kelvin temperatures in merged beams, *Science* **338**, 234 (2012).
- [9] S. N. Vogels, T. Karman, J. Klos, M. Besemer, J. Onvlee, A. van der Avoird, G. C. Groenenboom, and S. Y. T. van de Meerakker, Scattering resonances in bimolecular collisions between NO radicals and H_2 challenge the theoretical gold standard, *Nat. Chem.* **10**, 435 (2018).
- [10] A. Klein, Y. Shagam, W. Skomorowski, P. S. Żuchowski, M. Pawlak, L. M. C. Janssen, N. Moiseyev, S. Y. T. van de Meerakker, A. van der Avoird, C. P. Koch, and E. Narevicius, Directly probing anisotropy in atom-molecule collisions through quantum scattering resonances, *Nat. Phys.* **13**, 35 (2017).
- [11] A. G. Császár, I. Simkó, T. Szidarovszky, G. C. Groenenboom, T. Karman, and A. van der Avoird, Rotational-vibrational resonance states, *Phys. Chem. Chem. Phys.* **22**, 15081 (2020).
- [12] R. Thomas, K. O. Roberts, E. Tiesinga, A. C. J. Wade, P. B. Blakie, A. B. Deb, and N. Kjærgaard, Multiple scattering dynamics of fermions at an isolated p -wave resonance, *Nat. Commun.* **7**, 12069 (2016).
- [13] M. Chilcott, R. Thomas, and N. Kjærgaard, Experimental observation of the avoided crossing of two S -matrix resonance poles in an ultracold atom collider, *Phys. Rev. Res.* **3**, 033209 (2021).
- [14] T. de Jongh, M. Besemer, Q. Shuai, T. Karman, A. van der Avoird, G. C. Groenenboom, and S. Y. T. van de Meerakker, Imaging the onset of the resonance regime in low-energy NO-He collisions, *Science* **368**, 626 (2020).

- [15] H. Son, J. J. Park, Y.-K. Lu, A. O. Jamison, T. Karman, and W. Ketterle, Control of reactive collisions by quantum interference, *Science* **375**, 1006 (2022).
- [16] A. Green, H. Li, J. H. See Toh, X. Tang, K. C. McCormick, M. Li, E. Tiesinga, S. Kotochigova, and S. Gupta, Feshbach Resonances in p -Wave Three-Body Recombination within Fermi-Fermi Mixtures of Open-Shell ${}^6\text{Li}$ And Closed-Shell ${}^{173}\text{Yb}$ Atoms, *Phys. Rev. X* **10**, 031037 (2020).
- [17] G. F. Gribakin and V. V. Flambaum, Calculation of the scattering length in atomic collisions using the semiclassical approximation, *Phys. Rev. A* **48**, 546 (1993).
- [18] P. Paliwal, N. Deb, D. M. Reich, A. van der Avoird, C. P. Koch, and E. Narevicius, Determining the nature of quantum resonances by probing elastic and reactive scattering in cold collisions, *Nat. Chem.* **13**, 94 (2021).
- [19] U. Even, J. Jortner, D. Noy, N. Lavie, and C. Cossart-Magos, Cooling of large molecules below 1 K and He clusters formation, *J. Chem. Phys.* **112**, 8068 (2000).
- [20] K. Luria, N. Lavie, and U. Even, Dielectric barrier discharge source for supersonic beams, *Rev. Sci. Instrum.* **80**, 104102 (2009).
- [21] Y. Shagam and E. Narevicius, Sub-kelvin collision temperatures in merged neutral beams by correlation in phase-space, *J. Phys. Chem. C* **117**, 22454 (2013).
- [22] D. T. Colbert and W. H. Miller, A novel discrete variable representation for quantum mechanical reactive scattering via the S -matrix Kohn method, *J. Chem. Phys.* **96**, 1982 (1992).
- [23] W. Skomorowski and A. I. Krylov, Feshbach–Fano approach for calculation of Auger decay rates using equation-of-motion coupled-cluster wave functions. I. Theory and implementation, *J. Chem. Phys.* **154**, 084124 (2021).
- [24] M. Hapka, G. Chałasiński, J. Klos, and P. S. Żuchowski, First-principle interaction potentials for metastable $\text{He}({}^3\text{S})$ and $\text{Ne}({}^3\text{P})$ with closed-shell molecules: Application to Penning-ionizing systems, *J. Chem. Phys.* **139**, 014307 (2013).
- [25] B. R. Johnson, The multichannel log-derivative method for scattering calculations, *J. Comput. Phys.* **13**, 445 (1973).
- [26] G. Gamow, Zur quantentheorie des atomkernes, *Z. Phys.* **51**, 204 (1928).
- [27] S. A. Gurvitz and G. Kalbermann, Decay Width and the Shift of a Quasistationary State, *Phys. Rev. Lett.* **59**, 262 (1987).
- [28] U. V. Riss and H.-D. Meyer, Calculation of resonance energies and widths using the complex absorbing potential method, *J. Phys. B* **26**, 4503 (1993).
- [29] R. Santra and L. S. Cederbaum, Non-Hermitian electronic theory and applications to clusters, *Phys. Rep.* **368**, 1 (2002).
- [30] A. O. G. Wallis, E. J. J. Longdon, P. S. Żuchowski, and J. M. Hutson, The prospects of sympathetic cooling of NH molecules with Li atoms, *Eur. Phys. J. D* **65**, 151 (2011).
- [31] S. Chefdeville, T. Stoecklin, A. Bergeat, K. M. Hickson, C. Naulin, and M. Costes, Appearance of Low Energy Resonances in $\text{CO-}para\text{-H}_2$ Inelastic Collisions, *Phys. Rev. Lett.* **109**, 023201 (2012).
- [32] B. Margulis, J. Narevicius, and E. Narevicius, Direct observation of a Feshbach resonance by coincidence detection of ions and electrons in Penning ionization collisions, *Nat. Commun.* **11**, 3553 (2020).