

Delta-kick collimation of heteronuclear Feshbach molecules

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We present a theoretical study of delta-kick collimation (DKC) applied to heteronuclear Feshbach molecules, focusing on both condensed and thermal ensembles across various interaction and temperature regimes. We demonstrate that DKC enables significant reductions in molecular cloud expansion energies and beam divergence, achieving expansion energies in the picokelvin range, comparable to state-of-the-art results obtained experimentally with atoms. Furthermore, we show that vibrational and translational motions remain strongly decoupled throughout the process, and that the vibrational energy remains well below the molecular binding energy, thereby ensuring molecular stability during the delta kick. This work paves the way for advanced experimental sequences involving degenerate ground-state molecules, light-pulse molecular interferometry, and applications of dual-species precision measurements, such as testing the universality of free fall.

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I. INTRODUCTION AND MOTIVATION

Magnetic Feshbach resonances play an important role in the study of ultracold gases, providing a versatile tool for a wide range of applications [1]. By applying a bias magnetic field, these resonances enable precise tuning of the interparticle interactions, universally characterized by the atomic scattering length a , spanning regimes from strongly attractive or repulsive to noninteracting. Moreover, Feshbach resonances allow the adiabatic formation and dissociation of extremely weakly bound diatomic molecules. These Feshbach molecules [2,3] are instrumental in the study of various physical phenomena, such as the BEC-BCS crossover [4–12], the creation of ultracold polar molecules [13–23], and the study of universal few-body phenomena [24,25]. They also enable the controlled creation of entangled states [26–36], and serve as a platform for testing variations of fundamental constants [37–40]. However, in most cases, the kinetic temperature at which the Feshbach molecule is created is a critical factor that can limit its applicability. Reducing the free-expansion rate (i.e., energy) of atomic ensembles and Bose-Einstein condensates (BECs) [41,42] is a crucial step allowing for the precise control of the system’s dynamics and minimization of systematic errors [43,44]. Various collimation techniques have been developed to address this issue [45–50]. The most successful results to date relied on the delta-kick collimation (DKC) technique in rubidium systems [51–53]. Recently, the control of interactions using a

Feshbach resonance coupled with a matter-wave lensing protocol has allowed the collimation of ^{39}K BECs to sub-nK energies [54] in the presence of gravity, with the prospect of reaching double-digit pK energies by incorporating a DKC stage [46]. It is natural to seek to extend the advantages of operating at ultralow energies to dual-species systems. However, extending these techniques to the simultaneous collimation of dual-species gases presents significant challenges, primarily due to mismatches in trap frequencies and different in-trap dynamics of the two species [55]. Similarly, despite the remarkable progress in collimating ultracold atomic ensembles using DKC, its extension to molecular systems, particularly heteronuclear Feshbach diatomic molecules, remains largely unexplored. The additional complexities arising from coupled molecular degrees of freedom, such as vibrational and translational motions, as well as the potential for species-specific dynamics, present significant challenges to the straightforward application of existing techniques. Addressing these challenges is critical for advancing the control of ultracold molecular ensembles and unlocking their potential for precision measurements and quantum technologies.

In this work, we aim to bridge this gap by revisiting the DKC technique to extend its application range for Feshbach molecular ensembles in both thermal and condensed regimes. Specifically, we investigate the performance of DKC across various temperature and interaction regimes, providing insights into its feasibility and scalability for molecular systems. A successful experimental implementation of such a collimation would open a range of potential applications especially since the recent report of the first BEC of dipolar molecules [56]. Notably, improved collimation could enable longer interrogation times in experiments using ultracold molecular ensembles [57] or collimated molecular beams [58,59], paving the way for the observation of universal molecular

dynamics and for molecular interferometry [60] over extended durations. Molecular DKC could also provide an improved foundation for the preparation of more complex molecular states, including Efimov triplets [61,62] and larger multiplets [63,64]. Last but not least, it could allow the collimation of dual-species gases, eliminating the need for multiple lensing techniques [65], and thereby facilitate differential atom interferometry experiments aimed at testing the universality of free fall (UFF), a fundamental principle of Einstein's general theory of relativity [66–69].

In addition, this work explores the interplay between vibrational and translational degrees of freedom during the DKC process. In particular, we analyze the energy transferred to the molecular vibrational coordinate, as excessive excitation could jeopardize the stability of the Feshbach molecules. A detailed understanding of this energy exchange is essential for validating the theoretical model used to describe the cloud dynamics and for ensuring the integrity of the molecule throughout the collimation sequence.

The remainder of this paper is organized as follows. In Sec. II, we present our theoretical framework, key assumptions, and the trapping potential used to model the DKC process. Section III evaluates the performance of molecular DKC across condensed, hydrodynamic, and thermal regimes, highlighting key scaling behaviors and interaction effects. Finally, in Sec. IV, we summarize our findings, discuss their implications for experimental realizations, and outline future research directions.

II. THEORETICAL MODEL

A. Molecular system

While the results presented here are applicable to a wide range of diatomic molecules, this study specifically examines bosonic Feshbach molecules formed from ^{41}K and ^{87}Rb atoms. These atoms are particularly well suited for many of the previously mentioned dual-species gas studies due to their broad heteronuclear Feshbach resonances and the existence of weakly bound ^{41}K ^{87}Rb states at magnetic bias fields below 100 Gauss.

Before molecular association, both atomic species are assumed to be independently cooled and trapped. Although microgravity can enhance the efficiency of this association [70,71], successful ground-based formation of heteronuclear Feshbach molecules has been demonstrated for multiple species, including NaCs, NaK, NaRb, and KRb [56,72–76].

We assume that the Feshbach molecules are sufficiently large to neglect couplings between $\ell = 0$ and higher partial waves due to magnetic and induced dipole-dipole interactions. Furthermore, the molecules are assumed to be initially sufficiently cold that the effects of higher partial waves in molecule-molecule interactions are also neglected. In this regime, the resulting molecular ensemble interacts exclusively via s -wave ($\ell = 0$) interactions.

While one-photon rotational transitions are suppressed when the trapping light is far detuned from all excited levels, two-photon transitions tend to be more probable. In a dipolar trap generated by a laser beam with well-defined polarization, rotational excitations will not be driven, as each

two-photon stimulated emission releases the same amount of angular momentum that it gained during the initial absorption. In addition, even if polarizations are mixed through some mechanism, rotational excitations remain constrained by parity laws. Finally, during the DKC process, the optical potential is applied very briefly to the molecular ensemble so Fourier broadening defines the minimum spectral width of the applied potential. If this width becomes broad enough for the two-photon detuning to match a rotational excitation, parasitic rotational excitations might happen. However, rotational transitions are typically in the microwave regime, meaning that the two-photon detuning would be far too large for such effects to occur efficiently. What remains is the coupled dynamics of the vibrational and translational motions, which is addressed in Sec. II C.

In contrast to bosonic Feshbach molecules formed with fermionic atoms [15], ^{41}K ^{87}Rb molecules suffer from inelastic loss processes due to both atom-molecule and molecule-molecule collisions [25]. To avoid atom-molecule collisions, it is essential to purify the molecular sample by removing all residual atoms, as losses from such collisions are significantly faster than those from molecule-molecule collisions due to the lower molecular densities, as demonstrated for bosonic NaRb molecules in Ref. [77]. Purification of the sample can be achieved through several methods, including resonant pulses (particularly if the molecular BEC has to be prepared in a lower vibrational state), Stern-Gerlach-type separation (taking advantage of the distinct magnetic moments of K, Rb, and KRb), or other techniques tailored to the system. During a time-of-flight (TOF) sequence applied to the molecular ensemble, relaxation into lower vibrational states may still occur due to molecule-molecule collisions. This relaxation imposes a time scale on the TOF duration, which depends on the molecular density but also the specific molecular species. Note, however, that long TOF durations and ultracold low-density gases can be achieved in microgravity environments [70,71].

B. Trapping potential

We consider an optical dipole trap created by a nonuniform intensity distribution denoted as $\mathcal{I}$. Within the trapping region, we assume that the spatial variation of this intensity is harmonic and isotropic. Experimentally, such a harmonic intensity distribution can be achieved over distances on the order of a millimeter using time-averaged (painted) potentials [49,50,54]. The potential experienced by the molecules is represented by $V_{\text{Mol}}(\mathbf{R}, \mathbf{r})$, where $\mathbf{R} = (m_{\text{K}} \mathbf{r}_{\text{K}} + m_{\text{Rb}} \mathbf{r}_{\text{Rb}})/(m_{\text{K}} + m_{\text{Rb}})$ denotes its center-of-mass position, and $\mathbf{r} = \mathbf{r}_{\text{Rb}} - \mathbf{r}_{\text{K}}$ represents the internuclear coordinate. $\mathbf{r}_{\text{K}}$ and $\mathbf{r}_{\text{Rb}}$ are the atomic coordinates, and m_{K} and m_{Rb} are the atomic masses of K and Rb, respectively. Assuming an atomic approach, which is accurate at large internuclear distances [78], we write

$$V_{\text{Mol}}(\mathbf{R}, \mathbf{r}) = V_{\text{int}}(r) + \alpha_{\text{K}} \mathcal{I}(\mathbf{r}_{\text{K}}) + \alpha_{\text{Rb}} \mathcal{I}(\mathbf{r}_{\text{Rb}}), \quad (1)$$

where $V_{\text{int}}(r)$ is the interaction energy between the two atoms, and α_{K} and α_{Rb} are the dynamic polarizabilities of K and Rb, respectively. If the variation of $\mathcal{I}$ over the spatial extent of the molecule is negligible, then $\mathcal{I}(\mathbf{r}_{\text{Rb}}) \simeq \mathcal{I}(\mathbf{R}) \simeq \mathcal{I}(\mathbf{r}_{\text{K}})$, which

allows us to approximate the molecular potential as

$$V_{\text{Mol}}(\mathbf{R}, \mathbf{r}) \simeq V_{\text{int}}(r) + [\alpha_K + \alpha_{\text{Rb}}] \mathcal{I}(\mathbf{R}). \quad (2)$$

This approximation naturally gives rise to the emergence of the molecular polarizability, written as

$$\alpha_{\text{Mol}} = \alpha_K + \alpha_{\text{Rb}}. \quad (3)$$

It should also be noted that in this approximation, the molecular potential becomes separable in the $(\mathbf{R}, \mathbf{r})$ coordinate system. In the harmonic and isotropic case considered here we can write

$$V_{\text{Mol}}(\mathbf{R}, \mathbf{r}) \simeq V_{\text{int}}(r) + \frac{1}{2} M \omega_{\text{Mol}}^2 R^2, \quad (4)$$

where $M = m_K + m_{\text{Rb}}$ is the total molecular mass. This approximation assumes that the intensity remains constant over a distance on the order of the molecular size. This condition imposes a constraint on the characteristic size a_{Mol} associated with the harmonic trap, given by

$$a_{\text{Mol}} = \sqrt{\frac{\hbar}{M \omega_{\text{Mol}}}} \gg a \quad (5)$$

where a , the scattering length between the two atoms, is taken as an upper bound for the typical size of the Feshbach molecule [79]. Nevertheless, it is useful to note that even if such a criteria is satisfied, it would ensure that molecules in the center of the trap would not be significantly impacted by the DKC. Therefore, regarding molecules near the edge, a more thorough investigation is required. Such a study is carried on in Sec. II C.

We now set aside the approximation introduced in Eq. (2) and revert to the exact expression for the molecular potential given in Eq. (1). For the harmonic case considered here, the potential takes the form

$$V_{\text{Mol}}(\mathbf{R}, \mathbf{r}) = V_{\text{int}}(r) + \frac{1}{2} [m_K \omega_K^2 \mathbf{r}_K^2 + m_{\text{Rb}} \omega_{\text{Rb}}^2 \mathbf{r}_{\text{Rb}}^2], \quad (6)$$

where the second term (the trapping potential) can be conveniently rewritten as

$$V_{\text{Mol}}^{(t)}(\mathbf{R}, \mathbf{r}) = V_{\text{CM}}(R) + V_{\text{rel}}(r) + V_{\text{coup}}(\mathbf{R}, \mathbf{r}) \quad (7)$$

where the different terms are defined as follows:

$$V_{\text{CM}}(R) = \frac{1}{2} M \omega_{\text{Mol}}^2 R^2, \quad (8a)$$

$$V_{\text{rel}}(r) = \frac{1}{2} \mu \omega_r^2 r^2, \quad (8b)$$

$$V_{\text{coup}}(\mathbf{R}, \mathbf{r}) = -\mu \omega_c^2 \mathbf{R} \cdot \mathbf{r}. \quad (8c)$$

The reduced mass is given by $\mu = m_K m_{\text{Rb}} / M$ and the harmonic frequencies ω_{Mol} , ω_r , and ω_c are defined by

$$M \omega_{\text{Mol}}^2 = m_K \omega_K^2 + m_{\text{Rb}} \omega_{\text{Rb}}^2, \quad (9a)$$

$$M \omega_r^2 = m_{\text{Rb}} \omega_K^2 + m_K \omega_{\text{Rb}}^2, \quad (9b)$$

$$\omega_c^2 = \omega_K^2 - \omega_{\text{Rb}}^2. \quad (9c)$$

From the preceding expressions (6) and (7), it can be seen that the total molecular potential becomes separable, with $V_{\text{Mol}}(\mathbf{R}, \mathbf{r}) \simeq V_{\text{CM}}(R) + [V_{\text{int}}(r) + V_{\text{rel}}(r)]$, when the coupling $V_{\text{coup}}(\mathbf{R}, \mathbf{r})$ between center-of-mass and relative motions is negligible. Under this condition, the two degrees of freedom can be treated independently. To determine whether this condition is satisfied, we now express the frequencies ω_r and

ω_c in terms of the center-of-mass frequency ω_{Mol} , which is used as the input parameter for the simulations. Moreover, it is worth noting that the DKC procedure is preceded by an initial free expansion, which makes the molecular cloud much bigger than its initial size. It is due to the kinetic expansion or interactions in the thermal and BEC regimes, respectively. Consequently, the effects from the coupling from Eq. (8c) are much more important than in static trapping experiments where molecules remain near their initial positions. This reinforces the need of a study of the energy exchanges during the DKC procedure.

With the present harmonic and isotropic potential, we obtain from Eqs. (1) and (6) $\alpha_K \nabla^2 \mathcal{I} = 3m_K \omega_K^2$ and $\alpha_{\text{Rb}} \nabla^2 \mathcal{I} = 3m_{\text{Rb}} \omega_{\text{Rb}}^2$. In the limit where the condition (5) is satisfied, we also derive from Eqs. (2) and (4) that $\alpha_{\text{Mol}} \nabla^2 \mathcal{I} = 3M \omega_{\text{Mol}}^2$. Consequently, we can write

$$\frac{m_K}{\alpha_K} \omega_K^2 = \frac{m_{\text{Rb}}}{\alpha_{\text{Rb}}} \omega_{\text{Rb}}^2 = \frac{M}{\alpha_K + \alpha_{\text{Rb}}} \omega_{\text{Mol}}^2. \quad (10)$$

Defining the ratio between the two dynamic polarizabilities of the atoms as $p = \alpha_{\text{Rb}} / \alpha_K$, we can finally express the harmonic trapping frequencies ω_r and ω_c as

$$\omega_r = \left[\frac{m_{\text{Rb}}^2 + p m_K^2}{(p+1) m_K m_{\text{Rb}}} \right]^{1/2} \omega_{\text{Mol}}, \quad (11a)$$

$$\omega_c = \left[\frac{m_{\text{Rb}} - p m_K}{(p+1) \mu} \right]^{1/2} \omega_{\text{Mol}}. \quad (11b)$$

Since the ratio p of the dynamic polarizabilities is fixed at a given wavelength, it follows that selecting one of the frequencies ω_{Mol} , ω_r or ω_c automatically determines all the others.

C. Coupled dynamics of molecular motions

In the following, two key hypotheses will be made: the separability of the vibrational motion from the overall translational motion and the stability of the Feshbach molecule. To support these hypotheses, it is first necessary to establish a model for estimating both the extent of coupling between these two degrees of freedom and the energy transferred to the vibrational degree of freedom during a typical DKC process. To this end, and to maintain the simplicity of our approach, we adopt a classical model to describe the coupled nuclear motions.

It is important to note that the interaction potential between the atoms, $V_{\text{int}}(r)$, induces fast oscillatory motion compared to the slower oscillatory dynamics of the trapping potential. For instance, in a Feshbach molecule with a binding energy $E_b = \hbar^2 / (2\mu a^2)$ for a scattering length $a = 1000$ a.u., the rapid classical period T_r of oscillation in the potential well $V_{\text{int}}(r)$ can be estimated as

$$T_r = 2\sqrt{2\mu} \int_{r_{\text{min}}}^{r_{\text{max}}} \frac{dr}{\sqrt{-E_b - V_{\text{int}}(r)}}, \quad (12)$$

which is typically on the order of a fraction of a microsecond [80]. In contrast, the trapping frequencies, typically around a hundred Hz, correspond to slow oscillatory periods that are approximately 10^4 times larger. To address the long-time trapping dynamics, we thus employ the adiabatic approximation, replacing the interaction potential $V_{\text{int}}(r)$ in

the system Hamiltonian with its mean value over a fast oscillatory period, $\langle V_{\text{int}} \rangle$. Assuming zero angular momentum, the system Hamiltonian becomes

$$H(r, p_r, R, p_R) = \frac{p_r^2}{2\mu} + V_{\text{rel}}(r) + \langle V_{\text{int}} \rangle + \frac{p_R^2}{2M} + V_{\text{CM}}(R) + V_{\text{coup}}(\mathbf{R}, \mathbf{r}). \quad (13)$$

The coupling potential $V_{\text{coup}}(\mathbf{R}, \mathbf{r})$, as defined in Eq. (8c), is proportional to $\mathbf{R} \cdot \mathbf{r} = rR \cos(\theta)$, where θ is the angle between the two coordinates. The coupling is therefore maximum when $\mathbf{R}$ and $\mathbf{r}$ are collinear, i.e., when $\theta = n\pi$. In the following, we will consider the worst-case scenario of maximum coupling, given by

$$V_{\text{coup}}(R, r) = -\mu \omega_c^2 R r. \quad (14)$$

Using this expression, the classical Hamiltonian equations of motion for both coordinates can be written as follows:

$$\ddot{R} + \omega_{\text{Mol}}^2 R = (\mu/M) \omega_c^2 r, \quad (15a)$$

$$\ddot{r} + \omega_r^2 r = \omega_c^2 R, \quad (15b)$$

and the eigenfrequencies associated with the coupled system are given by

$$2\omega_{\pm}^2 = \omega_{\text{Mol}}^2 + \omega_r^2 \pm \sqrt{(\omega_{\text{Mol}}^2 - \omega_r^2)^2 + 4(\mu/M)\omega_c^4}. \quad (16)$$

The normal modes corresponding to these eigenfrequencies $\omega_{\pm}$ can be expressed as

$$z_+ = R - r \cdot \gamma / (1 + \gamma), \quad (17)$$

$$z_- = R + r \cdot 1 / (1 + \gamma), \quad (18)$$

where γ denotes the mass ratio $\gamma = m_{\text{Rb}}/m_{\text{K}}$. It is worth noting that this change of coordinates is independent of the frequencies ω_{Mol} , ω_r , and ω_c . To follow the coupled dynamics during the DKC process, we implement linear on/off ramps for the harmonic trap, described by

$$\omega_{\text{Mol}}^2(t) = \begin{cases} \omega_0^2 \cdot t/t_r, & \text{for } 0 \leq t < t_r, \\ \omega_0^2, & \text{for } t_r \leq t \leq t_{\text{DKC}} - t_r, \\ \omega_0^2 \cdot (t_{\text{DKC}} - t)/t_r, & \text{for } t_{\text{DKC}} - t_r < t \leq t_{\text{DKC}}, \end{cases}$$

where t_r is the duration of the on/off ramps, and t_{DKC} is the total duration of the DKC. Here, ω_0 represents the maximum trapping frequency achieved during the DKC. From Eqs. (11a) and (11b), it follows that the frequencies ω_r and ω_c become themselves time dependent. In the new system of coordinates, Eqs. (15a) and (15b) become

$$\ddot{z}_+ + \omega_+^2(t) z_+ = 0, \quad (19a)$$

$$\ddot{z}_- + \omega_-^2(t) z_- = 0 \quad (19b)$$

and are fully uncoupled. From Eqs. (11a), (11b), and (16), it follows that $\omega_{\pm}^2(t) = \alpha_{\pm} \omega_{\text{Mol}}^2(t)$, where $\alpha_+ = (1 + \gamma)/(1 + p)$ and $\alpha_- = p\alpha_+/\gamma$. Consequently, the squared frequencies $\omega_{\pm}^2(t)$ remain constant for $t_r \leq t \leq t_{\text{DKC}} - t_r$ and vary linearly with time during the on/off ramps. The solutions $z_+(t)$ and $z_-(t)$ of Eqs. (19a) and (19b) are thus analytical and can be written as linear combinations of the Airy functions of the first

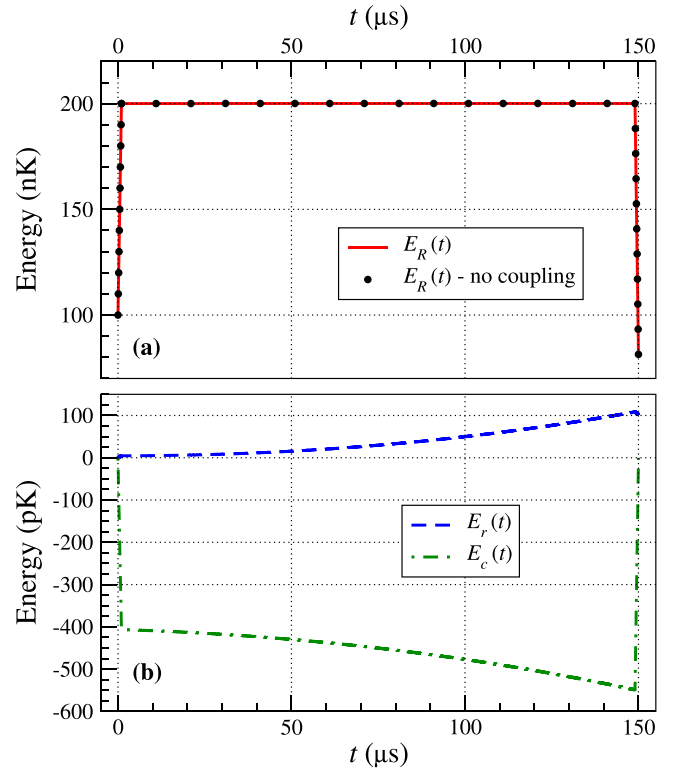


FIG. 1. Time evolution of the energies $E_R(t)$ [red solid line and black dots in panel (a)], $E_r(t)$ [blue dashed line in panel (b)], and $E_c(t)$ [green dash-dotted line in panel (b)] during a typical DKC process. The solid red line represents results obtained, including the coupling between the center-of-mass and vibrational motions, while the black dots correspond to calculations where this coupling is neglected. Note that the vertical scale of panel (b) highlights sub-nK variations, emphasizing that even weak couplings can be rigorously quantified in absolute energy terms, which is essential when addressing near-threshold bound states such as Feshbach molecules.

and second kinds during the switch-on ramp

$$z_{\pm}(t) = a_{\pm} \text{Ai}[-\eta_{\pm}t] + b_{\pm} \text{Bi}[-\eta_{\pm}t], \quad (20)$$

as trigonometric functions for $t_r \leq t \leq t_{\text{DKC}} - t_r$

$$z_{\pm}(t) = c_{\pm} \cos[\alpha_{\pm}^{1/2} \omega_0 t] + s_{\pm} \sin[\alpha_{\pm}^{1/2} \omega_0 t], \quad (21)$$

and again as Airy functions during the switch-off ramp

$$z_{\pm}(t) = a'_{\pm} \text{Ai}[\eta_{\pm}(t - t_{\text{DKC}})] + b'_{\pm} \text{Bi}[\eta_{\pm}(t - t_{\text{DKC}})]. \quad (22)$$

Here, the frequencies $\eta_{\pm}$ are given by $\eta_{\pm} = (\alpha_{\pm} \omega_0^2/t_r)^{1/3}$. The coefficients $a_{\pm}$, $b_{\pm}$, $c_{\pm}$, $s_{\pm}$, $a'_{\pm}$, and $b'_{\pm}$ are determined by the boundary conditions at times $t = 0$, $t = t_r$, and $t = t_{\text{DKC}} - t_r$. By inverting Eqs. (17) and (18), we finally obtain the exact solutions $R(t)$ and $r(t)$ for the coupled dynamics described by Eqs. (15a) and (15b).

Figure 1 shows the temporal evolution of the energies associated with the center-of-mass motion

$$E_R(t) = \frac{1}{2} M [\omega_{\text{Mol}}^2(t) R^2(t) + \dot{R}^2(t)], \quad (23)$$

the molecular vibration

$$E_r(t) = \frac{1}{2} \mu [\omega_r^2(t) r^2(t) + \dot{r}^2(t)], \quad (24)$$

and the coupling term

$$E_c(t) = -\mu \omega_c^2(t) R(t) r(t) \quad (25)$$

for a typical DKC process. These results are based on the assumption that the optical dipole trap operates at a wavelength of $\lambda = 2000$ nm which, as discussed below, is actually a worst-case scenario. At this wavelength, the ratio p of the dynamic polarizabilities of Rb and K is approximately $p = \alpha_{\text{Rb}}/\alpha_{\text{K}} \simeq 1.10$ [81,82]. The total duration of the DKC is $t_{\text{DKC}} = 150$ μs , including the switch-on and switch-off ramps, each of them lasting 1 μs . The maximum trapping frequency is set to $\omega_0 = 2\pi \times 100$ Hz. The initial conditions are chosen as follows. For the R coordinate, corresponding to the center-of-mass motion, the total initial energy is set to 200 nK, a value chosen to be within the typical order of magnitude for Bose-Einstein condensate energies. This energy is equally partitioned between its kinetic and potential components, each contributing 100 nK. Specifically, this corresponds to $R(0) = 4.06$ μm and $\dot{R}(0) = 2.55$ $\mu\text{m/ms}$. For the vibrational coordinate r , we consider a very weakly bound molecule formed via Feshbach resonance. Such molecules are likely to be at very large internuclear distances, near or beyond the outer turning point of the molecular potential. The initial condition for this coordinate is set to $r(0) = 1000$ a.u., with an initial velocity of $\dot{r}(0) = 0$.

In part (a) of Fig. 1, the solid red line shows the time evolution of the center-of-mass energy $E_R(t)$ [Eq. (23)] in a calculation that includes the coupling with the vibrational motion. At the initial time $t = 0$, this energy is 100 nK, as the harmonic potential is off at this point. By the end of the switch-on ramp, after 1 μs , the total energy reaches the expected value of 200 nK. Subsequently, this energy remains nearly constant throughout the collimation process, before decreasing during the switch-off ramp to a final value of approximately 81 nK. This residual energy, though small, must be carefully assessed to rule out nonadiabatic excitations. The black dots on the same graph represent the results of a similar calculation in which the coupling with the vibrational degree of freedom has been neglected. The results of this second simulation are superimposed on those obtained when the coupling is included. At $t = t_{\text{DKC}} = 150$ μs , the relative difference between the two final energies is only 0.045%. We can conclude that, with respect to the center-of-mass dynamics, the coupling with the vibrational degree of freedom can be safely neglected. It is therefore justified to disregard this coupling when describing the DKC process of the molecular cloud.

In part (b) of Fig. 1, the blue dashed line represents the evolution of the vibrational energy $E_r(t)$ [Eq. (24)], while the green dash-dotted line shows the evolution of the coupling energy $E_c(t)$ [Eq. (25)] between the two degrees of freedom in the calculation, which includes this coupling. This graph reveals that the coupling energy $E_c(t)$ ranges between -400 and -550 pK, values that are several hundred times smaller than the center-of-mass energy $E_R(t)$. This substantial energy gap explains why the coupling has minimal influence on the center-of-mass dynamics. This calculation also shows that during the DKC process, the energy gain in the vibrational coordinate is about 100 pK. This value is significantly smaller than the binding energy of the Feshbach

molecule, which can be estimated as $E_b = \hbar^2/(2\mu a^2) \simeq 6$ μK for a scattering length of $a = 1000$ a.u.. This energy gain is approximately 6×10^4 times smaller than the binding energy of the molecule, making it highly unlikely for the molecule to dissociate during the DKC process.

While this study is quantitatively valid for $R(0) = 4.06$ μm , we have performed the same calculations for $R(0) = 40.6$ μm , corresponding to atoms at the edge of the cloud. The results remain unchanged: There is no observable impact on the time evolution of $E_R(t)$ due to the coupling. Similarly, the coupling energy, even if increased up to 15 nK, remains well below E_b , thereby ensuring the stability of the molecule.

It is important to note that these results were obtained under the assumption that the dipolar optical trap operates at a wavelength of $\lambda = 2000$ nm. This could raise questions about the validity of our conclusions regarding the decoupling of the center-of-mass motion and the molecular stability at shorter wavelengths, particularly since wavelengths between 800 and 1100 nm are commonly used for atomic and molecular trapping. Refs. [81,82] illustrate the evolution of the dynamic polarizabilities of Rb and K as a function of wavelength. From these references, it can be concluded that the ratio p of these atomic polarizabilities increases monotonically as the wavelength decreases from 2000 to 800 nm. In addition, according to Eq. (11b), the coupling term decreases as p increases. This trend indicates that the decoupling of the center-of-mass motion and the molecular stability will be further enhanced at shorter wavelengths commonly used in experimental setups, such as those around 1064 nm.

Finally, from Eq. (11b), we can see that the coupling term vanishes when $p = p_{\text{opt}} = m_{\text{Rb}}/m_{\text{K}}$. In this case, Eq. (11a) gives $\omega_r = \omega_{\text{Mol}}$ and since there is no coupling between the two harmonic oscillators for this particular ratio p_{opt} of polarizabilities, the vibrational and translational coordinates oscillate independently at the same frequency ω_{Mol} . Numerically we get $p_{\text{opt}} \simeq 2.12$, and based on Refs. [81,82], this particular ratio of dynamic polarizabilities corresponds to the laser wavelength $\lambda_{\text{opt}} \simeq 808.25$ nm. It is worth noting that this magic wavelength has been reported to cancel the differential gravitational sag in K-41 and Rb-87 mixtures [55]. This magic wavelength is thus also of particular interest in the case of ground-based experiments to allow for an optimal overlap of both species before magnetoassociation.

For an optical trap operating at this so-called “magic” wavelength, there is a complete decoupling between the center-of-mass motion and the relative motion of the atoms. It is worth noting that this decoupling is inherently present in homonuclear Feshbach molecules, as their mass and polarizability ratios are both equal to 1. Therefore, our results naturally extend to the homonuclear case, even though we focus here on heteronuclear molecules, where achieving this decoupling condition is more challenging due to the differing mass and polarizability ratios.

In summary, our findings confirm a strong decoupling between the vibrational and translational degrees of freedom across a broad range of trapping wavelengths. Additionally, three key parameters govern the stability of the molecule during the delta-kick process. The first one is the coupling strength ω_c^2 seen in Eqs. (15a) and (15b). This parameter depends on the relative polarizabilities of the atomic species

forming the molecule and can be tuned by adjusting the trapping wavelength. However, complete suppression of this coupling occurs only at a specific wavelength. For commercially available lasers and the molecule considered in this work, the coupling strength remains nonzero. The second parameter is the initial center-of-mass energy. Indeed, since the coupling is nonzero, the risk of molecular dissociation increases with the initial center-of-mass energy. Given that we are dealing with Feshbach molecules, which have a low binding energy, an initial center-of-mass energy of this magnitude combined with nonzero coupling, could significantly compromise the molecule's stability. Finally, the last parameter is the duration of the delta kick. In our chosen scenario, energy transfer is inefficient because the kick duration (150 μ s) is much shorter than the characteristic timescale required for significant energy transfer between the center-of-mass and the vibrational degrees of freedom. This coupling timescale, on the order of $1/\omega_c$, corresponds to a few milliseconds. Since the delta-kick operates on a far shorter timescale, energy transfer remains negligible, minimizing the impact of coupling and ensuring molecular stability. Nevertheless, for collimation techniques such as in-trap lensing [49,50], the duration of the kick becomes much longer and can exceed 20 ms. Therefore, in such cases, the cumulative effect of the coupling would be much stronger, potentially leading to significant energy transfer between the degrees of freedom, unlike the short pulses studied in this work.

III. DKC PERFORMANCE IN THE DIFFERENT REGIMES

We consider molecular ensembles in both the thermal and BEC regimes. Taking advantage of the quasiseparability of the center-of-mass and relative coordinates, we focus on the DKC dynamics of the cloud with respect to the translational coordinate R , while factorizing out the vibrational dynamics. The molecular ensemble is initially trapped in a dipolar potential [50,83–85]. The DKC sequence, as originally described in Ref. [46], begins with a free expansion phase of duration t_{preTOF} , followed by a brief flashing of the trap for t_{DKC} , and concludes with a final TOF phase of duration t_{TOF} . Finally, if needed, the molecules can be dissociated [70] into two ultracold atomic ensembles with reduced expansion energies compared to the initial atomic ensembles.

While the mathematical structure of the scaling equations used here is shared with atomic systems, their application to weakly bound heteronuclear Feshbach molecules, characterized by enhanced scattering lengths and extremely small binding energies, yields dynamics that differ in both quantitative outcomes and physical constraints. These distinctions justify a dedicated treatment of the DKC protocol.

A. Scaling dynamics across condensed and thermal regimes

To evaluate the dynamics of the molecular ensemble, we use scaling laws of the form $\sigma(t) = \sigma(0)\lambda(t)$, where $\sigma(0)$ represents the initial size of the ensemble, and the equation of motion concerns only the scaling factor $\lambda(t)$.

In the condensed regime, we consider two different scaling approaches. The first approach is based on the Thomas-Fermi approximation, as described in Refs. [86,87], which neglects

the kinetic energy term in the Gross-Pitaevskii equation [88]. The scaling equation for this approach is given by

$$\ddot{\lambda}(t) + \omega_{\text{Mol}}^2(t)\lambda(t) = \frac{\omega_{\text{Mol}}^2(0)}{\lambda^4(t)}. \quad (26)$$

For this model to remain valid, the kinetic term in the Gross-Pitaevskii equation must be negligible. This condition requires either a large number of atoms or a large dimer-dimer scattering length a_{dd} , which implies strong interactions in both cases. If neither of these conditions is met, this approach is no longer applicable, and one must rely on a second approach that uses a variational method [89,90]. This method includes a correction term accounting for the kinetic energy. The scaling equation for this approach is given by

$$\ddot{\lambda}(t) + \omega_{\text{Mol}}^2(t)\lambda(t) = \frac{\omega_{\text{Mol}}^2(0)}{\lambda^4(t)} + \alpha \frac{\omega_{\text{Mol}}^2(0)}{\lambda^3(t)}, \quad (27)$$

where $\alpha = (\pi/2)^{\frac{2}{3}} [a_{\text{Mol}}/(Na_{\text{dd}})]^{\frac{4}{3}}$ and the expression of a_{Mol} is given in Eq. (5). This correction term vanishes in the strong interaction limit, reducing the model to the Thomas-Fermi approximation. In both approaches, the initial size of the ensemble is set to the Thomas-Fermi radius

$$\sigma(0) = \frac{a_{\text{Mol}}}{\sqrt{7}} \left(\frac{15 Na_{\text{dd}}}{a_{\text{Mol}}} \right)^{1/5}. \quad (28)$$

For both the hydrodynamic and thermal regimes, the previous equations cannot be applied, as they are only valid for pure condensates. Instead, we adopt the approach developed in Refs. [91,92] and adapt it to our isotropic case. This leads to the following scaling equation:

$$\ddot{\lambda}(t) + \omega_{\text{Mol}}^2(t)\lambda(t) = (1 - \xi) \frac{\omega_{\text{Mol}}^2(0)}{\lambda^3(t)} + \xi \frac{\omega_{\text{Mol}}^2(0)}{\lambda^4(t)}, \quad (29)$$

where $E_{\text{mf}} = 4\pi \hbar^2 a_{\text{dd}} n_0 / (\sqrt{2} M)$ and $\xi = E_{\text{mf}} / (E_{\text{mf}} + k_B T)$. Here, T is the temperature of the system, and n_0 is the initial average density. It is straightforward to verify that in the limit $k_B T \ll E_{\text{mf}}$, this equation reduces to the Thomas-Fermi scaling equation once again. In the hydrodynamic regime, the initial size $\sigma(0)$ corresponds to the size of a thermal cloud at temperature T , given by

$$\sigma(0) = \sqrt{\frac{k_B T}{m}} \omega_{\text{Mol}} \sqrt{1 - \xi}. \quad (30)$$

B. Performance analysis in condensed regimes

To evaluate the performance of the collimation across the different regimes, we compare the expansion energy gain, defined as $\mathcal{G} = E_i/E_f$, where E_i is the expansion energy without collimation, and E_f is the expansion energy after collimation. We express the expansion energy in units of temperature, using $k_B T = m \dot{\sigma}^2$, where $\dot{\sigma}$ denotes the time derivative of σ .

To facilitate a consistent comparison across the different regimes, we fix the prekick TOF duration to $t_{\text{preTOF}} = 14.9$ ms. At this point in time, the size of the condensed molecular cloud reaches approximately $\sigma(t_{\text{preTOF}}) \simeq 20 \mu\text{m}$, which remains well within the harmonic region of the trap and justifies the continued use of the harmonic approximation. In contrast, thermal clouds under the same conditions expand to sizes roughly ten times larger. While such sizes may still

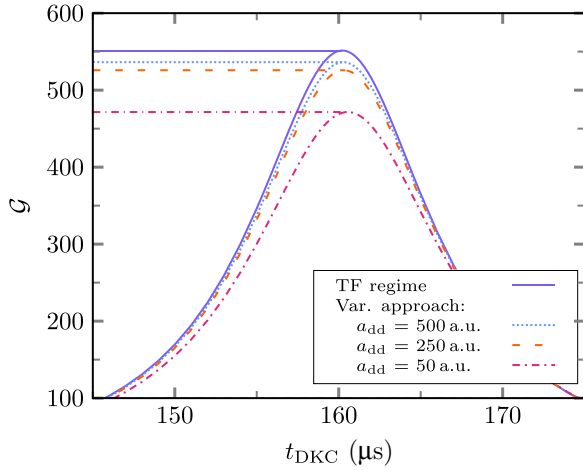


FIG. 2. Expansion energy gain $\mathcal{G} = E_i/E_f$ as a function of the DKC duration for both the Thomas-Fermi regime (purple solid line) and the variational approach at different scattering lengths. While the gain does not depend on the scattering length in the Thomas-Fermi approach, the variational approach shows variations as the scattering length decreases from 500 a.u. (blue dotted line) to 250 a.u. (orange dashed line) and finally to 50 a.u. (red dash-dotted line). As expected, higher interaction strengths bring the gain of the variational method closer to that of the Thomas-Fermi regime.

lie within the harmonic range in the case of time-averaged (painted) dipole potentials, increasing t_{preTOF} further could result in cloud sizes extending to a few millimeters. Maintaining harmonicity over such large distances is experimentally demanding and may limit the practicality of using longer pre-expansion durations.

Starting with the pure BEC case, we first consider the Thomas-Fermi regime. For 5×10^4 molecules trapped in a $2\pi \times 100$ Hz isotropic trap, the expansion energy before the kick is 25.2 nK. The expansion energy gain is shown in Fig. 2 as a function of the DKC duration. We achieve a maximum gain slightly above $\mathcal{G} = 550$ in the Thomas-Fermi high-interaction limit (purple solid line), corresponding to an expansion energy below 50 pK.

For weaker interactions ($a_{\text{dd}} = 500, 250$, and 50 a.u., represented by the blue dotted, orange dashed, and red dash-dotted lines respectively), the maximum gain consistently exceeds $\mathcal{G} = 450$. This implies that the optimal expansion energy is always below 60 pK. Additionally, the gain remains above 100 within the range $t_{\text{opt}} \pm 14 \mu\text{s}$, providing a sufficiently large time window for experimental realization.

Finally, the larger the scattering length, the closer the results of the variational method approach those of the Thomas-Fermi regime. This behavior can be readily understood from the scaling equations: As the interactions increase, the interaction-dependent correction term becomes negligible, causing the equations to reduce to those of the Thomas-Fermi approximation.

C. Hydrodynamic and thermal regime behavior

In the hydrodynamic approach, the key parameter is the temperature of the molecular ensemble. Varying the temperature in this regime is qualitatively analogous to varying the

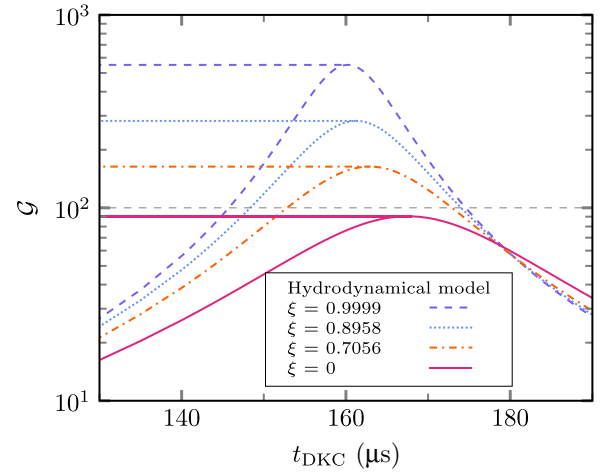


FIG. 3. Expansion energy gain $\mathcal{G} = E_i/E_f$ as a function of the DKC duration for a molecular ensemble at finite temperature, with the molecule-molecule scattering length fixed at $a_{\text{dd}} = 500$ a.u.. Different values of ξ are investigated, corresponding to various thermal regimes. For $\xi = 0.9999$ (2 nK, purple dashed line), the system is in the condensed regime. For $\xi = 0.8958$ (30 nK, blue dotted line) and $\xi = 0.7056$ (50 nK, orange dash-dotted line), the system transitions to the hydrodynamic regime. Finally, $\xi = 0$ (red solid line) corresponds to a purely thermal ensemble. The maximum gains achieved in each case are as follows: 550 for the condensed regime ($\xi = 0.9999$), 282 for $\xi = 0.8958$, 164 for $\xi = 0.7056$, and 90 for the thermal regime $\xi = 0$.

interaction strength in the condensed regime. Specifically, low temperatures are equivalent to high interactions, while high temperatures correspond to low interactions. Finally, at sufficiently high temperatures, where $\xi \ll 1$ (i.e., $k_B T \gg E_{\text{mf}}$), the effect of interactions becomes negligible, and the scaling equation (29) reduces to the noninteracting Ermakov equation [93–95]:

$$\ddot{\lambda}(t) + \omega_{\text{Mol}}^2(t) \lambda(t) = \frac{\omega_{\text{Mol}}^2(0)}{\lambda^3(t)}. \quad (31)$$

In Fig. 3, we analyze the gain for four different temperatures with a molecular scattering length of $a_{\text{dd}} = 500$ a.u.: 2 nK (purple dashed line), 30 nK (blue dotted line), 50 nK (orange dash-dotted line), and 1 μK (red solid line), which correspond to $\xi = 0.9999, 0.8958, 0.7056$, and 0 , respectively. The 2 nK case represents the condensed regime discussed previously, while the 1 μK case corresponds to a purely thermal ensemble. The two intermediate temperatures, 30 nK and 50 nK, lie within the hydrodynamic regime.

The nearly-condensed case at $T = 2$ nK (purple dashed line) reaches a maximum gain $\mathcal{G}$ close to that of the pure BEC case, around $\mathcal{G} = 550$. This outcome is expected, since the hydrodynamic scaling equation (29) reduces to the Thomas-Fermi form (26) in the strong interaction limit, where $E_{\text{mf}} \gg k_B T$ and consequently $\xi \simeq 1$. However, at 2 nK, a slight reduction in $\mathcal{G}$ is observed compared to the zero-temperature case, due to the finite temperature preventing a full recovery of Eq. (26). As the temperature increases and the interaction strength becomes relatively weaker, the gain decreases

accordingly. Specifically, the maximum gain drops to 282, 164, and 90 for $\xi = 0.8958, 0.7056$, and 0, respectively. The case $\xi = 0$ corresponds to the limit $k_B T \gg E_{\text{mf}}$, where the mean-field interactions become negligible. Alternatively, this limit could also be achieved by setting the scattering length $a_{\text{dd}} = 0$.

D. Timescale considerations

These theoretical results, while not surpassing the state-of-the-art collimation achieved experimentally with atoms [52], are of the same order of magnitude. This limitation arises from the conservative value chosen for t_{preTOF} . According to the Heisenberg uncertainty principle, a larger size at the kick results in a smaller momentum width after the kick. Consequently, with larger values of t_{preTOF} , it would be possible to achieve even smaller expansion energies. However, this would increase the cloud size at the kick, with molecules further away from the trap center.

Similarly, by keeping t_{preTOF} constant but increasing the initial trap frequency, a larger size at the kick could be achieved, resulting in a smaller final expansion energy. However, the duration of the DKC is governed by $t_{\text{DKC}} \simeq [\sqrt{2\pi} \omega_{\text{Mol}}^2 t_{\text{preTOF}}]^{-1}$ [46]. Therefore, increasing either t_{preTOF} or the trap frequency would reduce the collimation time, making the procedure possibly more challenging to implement experimentally.

Quantitatively, the above mentioned effect can be estimated by varying either the time-of-flight preceding the kick t_{preTOF} , or the trapping frequency ω_{Mol} , across the different regimes. First, increasing t_{preTOF} leads to an expected enhancement in the gain $\mathcal{G}$. Specifically, in the thermal regime, the maximum gain increases from 40 at $t_{\text{preTOF}} = 9.9$ ms to 90 at 14.9 ms, and reaches 167 at 19.9 ms. In the condensed regime, the corresponding gains are 173, 551, and 1437, respectively. This improvement reflects the larger cloud size at the time of the kick, which, in turn, leads to a narrower final momentum distribution after collimation.

The associated DKC duration t_{DKC} decreases with increasing t_{preTOF} in accordance with the theoretical scaling relation. For instance, t_{DKC} drops from approximately 230 μs at $t_{\text{preTOF}} = 9.9$ ms to about 120 μs at $t_{\text{preTOF}} = 19.9$ ms, effectively halving the kick duration as t_{preTOF} is doubled. The corresponding cloud sizes at the moment of the kick reach about 27 μm for the condensed cloud and 228 μm for the thermal cloud. In the latter case, the large size may begin to probe regions where trap anharmonicities are non-negligible, potentially limiting further gains from increasing t_{preTOF} in practical implementations.

A similar trend is observed when varying the trap frequency. For example, in the condensed regime with t_{preTOF} fixed, increasing ω_{Mol} from $2\pi \times 50$ to $2\pi \times 150$ Hz boosts the gain $\mathcal{G}$ from 81 to 1920, while the kick duration decreases from 598 to 73 μs . This behavior again follows the expected scaling law, as tripling the trap frequency reduces the kick duration by nearly a factor of 9. The higher gain achieved at larger ω_{Mol} is primarily due to the stronger interactions induced by tighter confinement. Although t_{preTOF} is held constant, the cloud expands more rapidly due to the increased initial interaction energy, leading to a larger size at the

moment of the kick and, consequently, a greater collimation gain.

IV. SUMMARY AND CONCLUSION

In this work, we have investigated the extension of the DKC technique to heteronuclear Feshbach molecules, focusing on its performance across different interaction and temperature regimes. We have demonstrated that this technique, applied to molecular ensembles in both condensed and thermal regimes, can achieve substantial reductions in expansion energy, with theoretical predictions in the tens of picokelvin range. Specifically, in the condensed regime, our results reveal expansion energy gains exceeding 550, corresponding to expansion energies below 50 picokelvin. These results highlight the potential of DKC as a robust and efficient tool for controlling ultracold molecular systems.

Nevertheless, challenges remain in bridging the gap between theoretical predictions and experimental realizations, particularly regarding the necessity for long pre-TOF durations. This issue could be solved by experiments conducted in microgravity or space, such as the upcoming BECCAL apparatus [96], where the implementation of dipole traps is planned. Additionally, existing setups that already produce Bose-Einstein condensates of Feshbach molecules [56] offer promising platforms for further investigation. This approach could also be adapted for atom-chip setups that produce mixtures, such as the Cold Atom Laboratory on the International Space Station [68], or for other microgravity facilities [96–99]. However, in the latter case, care must be taken to ensure that the Feshbach field does not interfere with the trapping potential. Additionally, the magnetic traps generated by such atom-chip setups tend to become anharmonic at larger distances, necessitating verification that the molecules do not reach these anharmonic regions. Indeed, in realistic experimental configurations, trap potentials may deviate from perfect isotropy and harmonicity. While our model assumes isotropy and harmonic confinement to isolate essential effects, anharmonic corrections can play a significant role for extended holding times or larger cloud sizes. Notably, molecular ensembles could exhibit enhanced sensitivity to such effects if anharmonicities introduce a coupling between center-of-mass and internal motions. Future studies may address perturbative extensions or numerical simulations in anharmonic traps [100] to assess their influence on molecular DKC performance more quantitatively.

Beyond the immediate gains in collimation performance, our findings carry broad implications for precision measurements and quantum technologies. For example, molecular DKC offers a scalable solution for the simultaneous collimation of dual-species ensembles, circumventing the complexities of species-specific lensing. This capability is particularly relevant for beyond-state-of-the-art experiments seeking to test fundamental principles such as the UFF in dual-species atom interferometry [101]. In such experiments, precise control of the kinematics of both species, along with minimizing their expansion energies, is essential [44] to mitigate systematic effects. Moreover, the molecular collimation of a heteronuclear molecule, followed by its dissociation, has been shown to induce position squeezing of the two atomic

ensembles, allowing to better control the positioning precision and enabling various entanglement applications [102]. By reducing systematic uncertainties and enabling extended interrogation times, molecular DKC could significantly enhance the sensitivity and precision of high-precision experiments, offering a new avenue for probing the foundational aspects of general relativity. In addition, our work also sets the stage for future advancements in molecular interferometry [60].

The ability to collimate molecular ensembles with high precision opens doors to observing universal few-body dynamics, exploring Efimov states [61,62], and preparing larger molecular complexes with controlled quantum properties. The scalability of DKC to various molecular systems, coupled with its compatibility with existing trapping and cooling technologies, underscores its versatility for a wide range of applications in quantum physics and ultracold chemistry.

In summary, our study establishes DKC as a promising tool for advancing the control and manipulation of ultracold molecular systems. Its ability to significantly reduce expansion energy highlights its potential for implementation in experiments requiring long observation times, such as precision tests of fundamental physics [103]. Furthermore, if the collimated ensemble can be retrapped using shallow, long-range optical traps such as those generated by painted potentials, it could represent a crucial step toward cooling heteronuclear molecules to quantum degeneracy. As experimental techniques continue to evolve, we anticipate that molecular DKC will play a pivotal role in unlocking

new frontiers in both fundamental research and technological applications.

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DATA AVAILABILITY

The data supporting this study’s findings are available within the article.

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