


# Arbitrary interaction quench phenomena in harmonically trapped two-body systems

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We consider the evolution of two contact-interacting harmonically trapped particles following an arbitrary quench in interaction strength. We focus on the change in system energy, the work, associated with the quench. When quenching from any nonzero interaction strength to zero interaction strength we observe that the work done and particle separation diverge. In particular, the divergent behavior arises *always* and *exclusively* when quenching *to* the noninteracting regime. We demonstrate that the source of the divergence is its instantaneous nature. This validates and builds upon previous work that found divergent behavior arises when quenching from the strongly interacting limit to the noninteracting limit in both the two- and three-body cases.

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## I. INTRODUCTION

Understanding the nonequilibrium behavior of quantum systems is strongly relevant to a variety of very fundamental problems such as how quantum systems equilibrate [1] and quantum thermodynamics more generally [2]. Ultracold atomic gases are very fertile ground for studying quantum thermodynamics [3–21]. A high degree of experimental control is possible over such systems [22–32], and they exist in a regime where various analytical techniques are highly applicable, e.g., the Fermi pseudopotential [33,34].

We consider two particles in a three-dimensional isotropic harmonic trap interacting via a contact interaction. We are interested in the behavior of the system after a sudden change, a quench, in the interaction strength from one arbitrary value to another. We use known analytic wave functions [35] to calculate the work associated with the quench. Previous calculations of quenched two- and three-body systems in three dimensions find that the system size diverges after a quench from very strong interactions (unitarity) to no interactions [36–38]. This stands in opposition to the one-dimensional case where the divergence occurs when quenching *to* the strongly interacting regime [39]. However, it is unclear how having a finite nonzero interaction strength affects the quench. Additionally, the duration or speed of a quench has been shown to be strongly relevant to a system's behavior [21], and we investigate the effects of quench duration in relation to the divergent behavior.

Additionally, we must note that the physical system of interest, two contact-interacting bodies in a three-dimensional harmonic trap quenched in interaction strength, can be realized with current experimental capabilities. Methods to construct few-atom systems are well understood [25–31], and exploiting Feshbach resonance is a well-known reliable method of controlling the interaction strength [40–43]. In particular the evolution of particle separation of a quenched system has been experimentally measured [44]. However, that experiment considered a quench in trap geometry rather than interaction strength as we consider here.

This paper is structured in the following way. In Sec. II we review the interacting two-body wave function first derived

by Ref. [35]. In Sec. III we calculate the work associated with the quench to determine if the system size diverges. In particular, we examine quenches between the unitary/noninteracting limits and arbitrary interaction strengths, and quenches between two arbitrary interaction strengths. In Sec. IV we investigate the relationship quench duration and the divergent behavior.

## II. OVERVIEW OF THE TWO-BODY PROBLEM

In this paper we consider two distinguishable particles in a three-dimensional isotropic harmonic trap interacting via a contact interaction. We use the Fermi-Huang pseudopotential [33,34] to describe the interaction. The center-of-mass (c.m.) motion separates out as a simple harmonic oscillator Hamiltonian with mass  $M = m_1 + m_2$  and position  $\vec{R} = (m_1\vec{r}_1 + m_2\vec{r}_2)/M$ , where  $m_i$  and  $\vec{r}_i$  are the mass and position of the  $i$ th particle, respectively. However, the relative motion is more complicated due to the interaction term. The relative Hamiltonian is given

$$\hat{H}_{\text{rel}} = -\frac{\hbar^2}{2\mu}\nabla_r^2 + \frac{\mu\omega^2 r^2}{2} + \frac{2\pi\hbar^2 a_s}{\mu}\delta^3(r)\frac{\partial}{\partial r}(r\bullet), \quad (1)$$

where  $\hat{H}_{\text{total}} = \hat{H}_{\text{c.m.}} + \hat{H}_{\text{rel}}$ ,  $\vec{r} = \vec{r}_1 - \vec{r}_2$ ,  $\mu = m_1 m_2 / M$ ,  $\omega$  is the trapping frequency, and  $a_s$  is the  $s$ -wave scattering length which characterizes the interaction. The dot inside the parentheses of the derivative is to indicate that the derivative acts on  $r\psi$  (where  $\psi$  is the wave function) not just  $r$ .

The eigenfunctions of Eq. (1), i.e., the interacting wave functions, were first found by Ref. [35] and are given

$$\psi_\nu(r) = N_\nu \Gamma(-\nu) e^{r^2/2a_\mu^2} U\left(-\nu, \frac{3}{2}, \frac{r^2}{a_\mu^2}\right), \quad (2)$$

$$N_\nu^{-1} = \sqrt{2\pi^2 a_\mu^3 \frac{\Gamma(1-\nu)[\psi^{(0)}(-\nu - \frac{1}{2}) - \psi^{(0)}(-\nu)]}{\nu \Gamma(-\nu - \frac{1}{2})}}. \quad (3)$$

where  $a_\mu = \sqrt{\hbar/\mu\omega}$ , and  $\nu$  is the energy pseudoquantum number with  $E_{\text{rel}} = (2\nu + 3/2)\hbar\omega$ . The values of  $\nu$  are

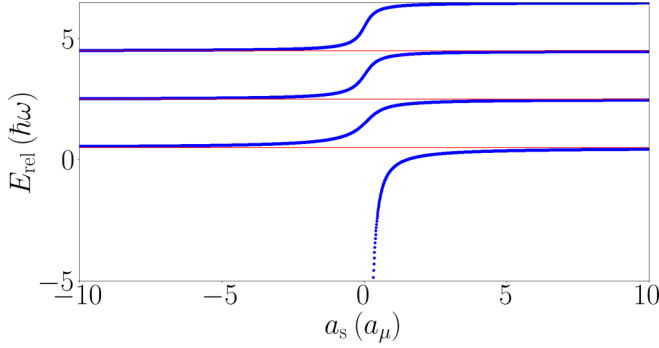


FIG. 1. The energy of the interacting two-body wave function, Eq. (2), as a function of  $s$ -wave scattering length. The red horizontal lines correspond to  $E_{\text{rel}} = (2n + 1/2)\hbar\omega$ , the energies in the unitary limit.

obtained by solving the transcendental equation

$$\frac{a_\mu}{a_s} = \frac{2\Gamma(-\nu)}{\Gamma(-\nu - \frac{1}{2})}. \quad (4)$$

The energy spectrum is presented in Fig. 1. Note the bound state present for small positive  $a_s$ .

### III. QUENCH DYNAMICS

In general, a quench is a sudden change in some variable of the system, e.g., a sudden change in  $\omega$  is a quench in trapping frequency. Here, we are concerned with the effects of a quench in  $a_s$ . In experiment such quenches have been implemented [45] by exploiting Feshbach resonance [41,43].

The wave function of the system,  $\psi(t)$ , as a function of time after the quench can be written

$$\psi(t) = \sum_{j=0}^{\infty} \langle \phi_j | \psi(0) \rangle \phi_j e^{-iE_j t/\hbar}, \quad (5)$$

where  $t = 0$  is the time of the quench,  $\psi(0)$  is the prequench wave function,  $\phi_j$  are the eigenstates of the postquench system, and  $E_j$  are the associated eigenenergies. The overlap terms  $\langle \phi_j | \psi(0) \rangle$  are presented in Ref. [36]. Quenches in  $a_s$  only change the relative Hamiltonian, not the c.m. Hamiltonian. As such, only the relative part of the total wave function is affected. The c.m. wave function simply integrates to one in all calculations, and we do not need to consider it further.

When quenching from the strongly interacting limit to the noninteracting limit the expectation of the particle separation,  $\langle r(t) \rangle$ , diverges [36]. This divergence is also present in the three-body case [37,38]. This divergence arises because a  $1/r^2$  tail forms in the probability distribution of particle separation when  $t \neq n\pi/\omega$ . The first moment of this distribution,  $\langle r(t) \rangle$ , is poorly defined due to the  $1/r$  tail of the integrand. In the three-body case we can only consider quenches between the unitary and noninteracting regimes, but in the two-body case we can consider arbitrary quenches. This naturally leads one to ask if the divergence is present for other quenches and, if so, under what circumstances.

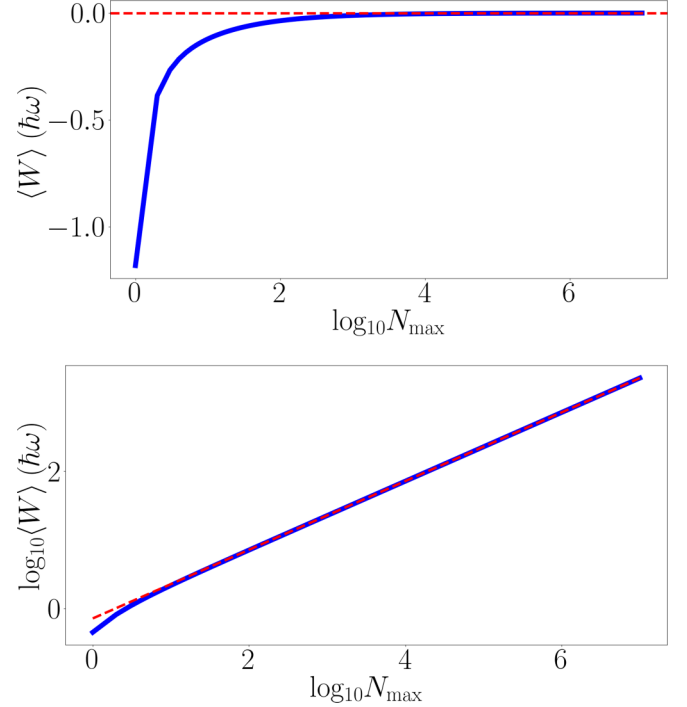


FIG. 2. The work as a function of the number of terms in the expansion in Eq. (6),  $N_{\text{max}}$ . Upper panel:  $\langle W \rangle$  for the forward quench. The dashed red line indicates  $\langle W \rangle = 0$ . Lower panel:  $\langle W \rangle$  for the backward quench. The dashed red line indicates  $\langle W \rangle = 0.7\sqrt{N_{\text{max}}}\hbar\omega$ . In both cases the initial state is the ground state.

#### A. Presence of the divergence

It is not immediately obvious whether the divergence is unique to the unitarity to noninteracting limit (backwards) quench or if there are other quenches with the divergence present. Rather than calculate  $\langle r(t) \rangle$  for a variety of quenches it is more efficient to calculate  $\langle W \rangle$ , the average work associated with the quench,

$$\begin{aligned} \langle W \rangle &= \langle \psi(t) | (\hat{H} - E_i) | \psi(t) \rangle \\ &= \sum_{j=0}^{\infty} (E_j - E_i) |\langle \psi(0) | \phi_j \rangle|^2, \end{aligned} \quad (6)$$

where  $E_i$  is the energy of the initial state and the  $E_j$ 's are the eigenenergies of the postquench Hamiltonian. If  $\langle r(t) \rangle$  is divergent, then so is the potential energy and the work is infinite. It is worthwhile to define the irreversible work,  $\langle W_{\text{irr}} \rangle = \langle W \rangle + E_i - E_{j=0}$ , where  $E_{j=0}$  is the ground-state energy of the postquench system.  $\langle W_{\text{irr}} \rangle$  gives a measure of how the postquench excited states are populated.

In Fig. 2 we display  $\langle W \rangle$  against the number of terms we evaluate up to in Eq. (6),  $N_{\text{max}}$ , for the forward (noninteracting limit to unitarity) and backward quenches. It is clear that the forward quench is convergent and the backward is divergent with  $\langle W \rangle \approx 0.7\sqrt{N_{\text{max}}}\hbar\omega$  for  $N_{\text{max}} \gtrsim 100$ . This is consistent with previous results [36].

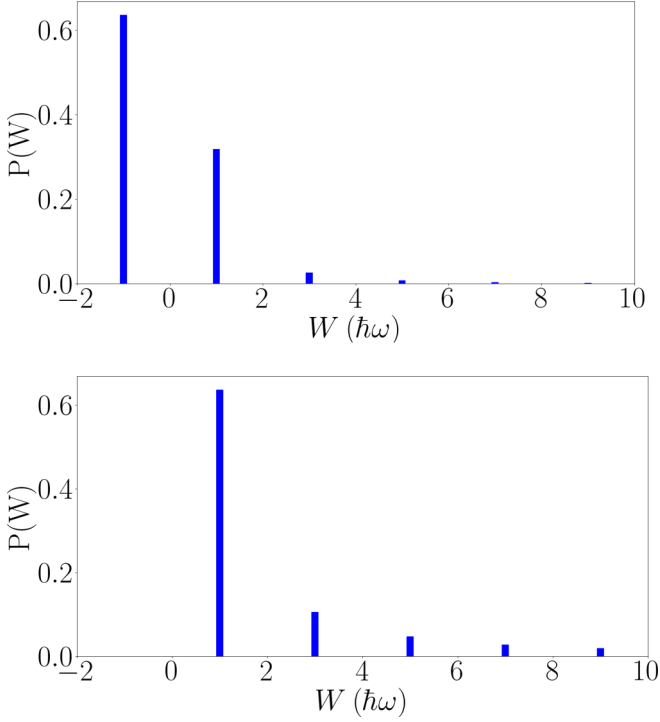


FIG. 3. The probability distribution of work. Upper panel: The work associated with the forward quench. Lower panel: The work associated with the reverse quench. In both cases the initial state is the ground state.

In Fig. 3 we present the probability distribution of the work,

$$P(W) = \sum_{j=0}^{\infty} |\langle \psi(0) | \phi_j \rangle|^2 \delta(W - (E_j - E_i)), \quad (7)$$

for the forward (upper panel) and backward (lower panel) quenches. The work can be negative for the forward quench because the noninteracting ground-state energy is greater than the unitary ground-state energy. Note that the tail decays much more slowly for the reverse quench than the forward quench. This large tail leads to the divergent behavior.

Next, we turn our attention to quenches involving arbitrary scattering length. There are two cases here. There are quenches between two arbitrary scattering lengths, and there are quenches between the unitary/noninteracting limits and arbitrary  $a_s$ . We begin with the former case. In Fig. 4 we plot  $\langle W \rangle$  (upper panel) and  $\langle W_{\text{irr}} \rangle$  (lower panel) for quenches between two arbitrary scattering lengths where the initial state is the ground state. In all cases we find that the quantities converge. Both works peak when quenching from small positive  $a_s$  to small negative  $a_s$ . In this case the initial state is a bound state, and it is being projected onto a basis without bound states. There are significant contributions from higher-order terms with large energies. In Fig. 5 we plot the probability distributions of work for quenches between  $a_s = -0.5a_\mu$  and  $a_s = 0.5a_\mu$ . For the quench towards  $a_s = -0.5a_\mu$  (lower panel) we can see that the tail is much larger, and there is no negative work contribution due to the lack of a bound state in the final Hamiltonian. The presence of the bound state in the

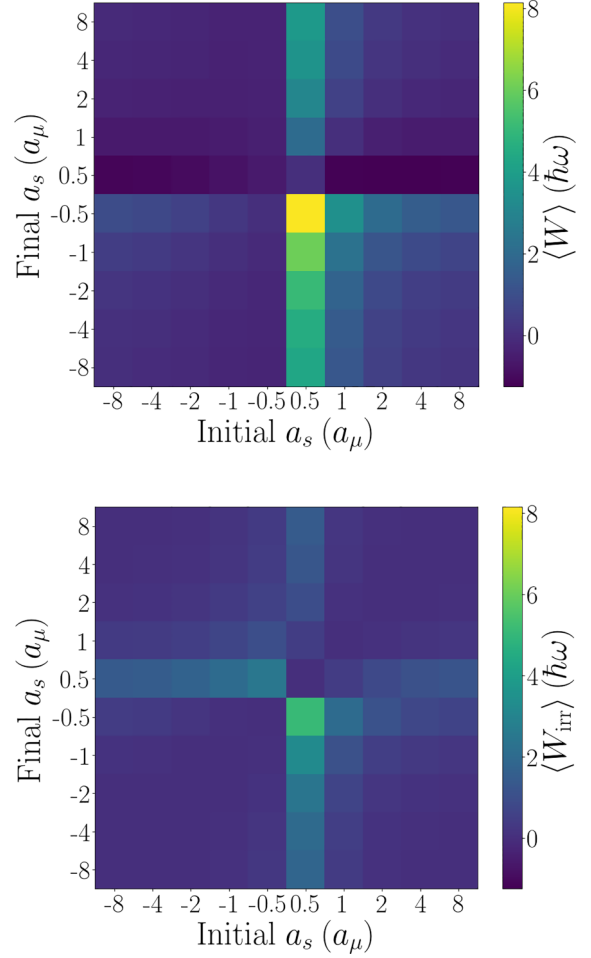


FIG. 4. Work associated with the quench. Upper panel: The average work  $\langle W \rangle$  done by the quench. Lower panel: The average irreversible work  $\langle W_{\text{irr}} \rangle$  done by the quench. Quantities are calculated for a variety of arbitrary  $s$ -wave scattering lengths. In all cases the initial state is the ground state. The main diagonal is where the initial and final scattering lengths are the same. The work and irreversible work associated with these “quenches” is always zero.

postquench system introduces the possibility of negative work leading to less average work.

The irreversible work is maximized when quenching from a bound state or toward a system capable of supporting a bound state. The irreversible work is necessarily positive so there are no negative energy contributions to skew the average. The average irreversible work is then determined by the shape of the tail of the probability distribution. The tail is largest (contributions from excited states are greatest) when quenching between Hamiltonians that can and cannot support bound states. When quenching between regimes that do not support bound states  $\langle W_{\text{irr}} \rangle$  is near zero, as can be seen in the corners of the lower panel of Fig. 4.

Now we turn to quenches between the noninteracting/unitary limits and finite  $a_s$ . In the upper and middle panels of Fig. 6 we present  $\langle W \rangle$  and  $\langle W_{\text{irr}} \rangle$  respectively for quenches between arbitrary  $s$ -wave scattering length and unitarity and from the noninteracting regime to arbitrary  $a_s$ . We find that these quenches are convergent regardless of the values

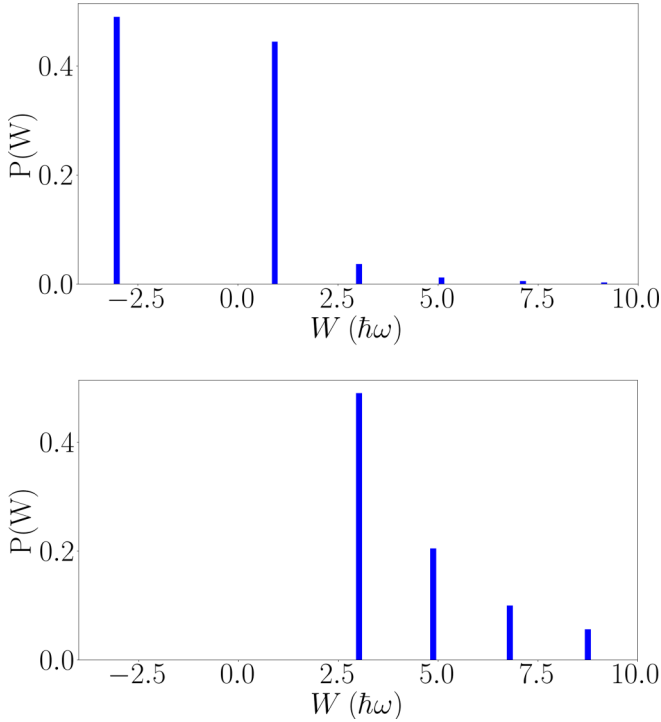


FIG. 5. The probability distribution of work for arbitrary quenches. Upper panel: The work associated with a quench from  $a_s = -0.5a_\mu$  to  $a_s = 0.5a_\mu$ . Lower panel: The work associated with a quench from  $a_s = 0.5a_\mu$  to  $a_s = -0.5a_\mu$ . In both cases the initial state is the ground state.

of  $a_s$ . For the *toward* unitarity quenches  $\langle W \rangle$  and  $\langle W_{\text{irr}} \rangle$  peak near initial  $a_s = 0$ . Small initial  $a_s$  corresponds to values of  $\nu$  which differ significantly from those of the unitary spectrum. When projecting the initial weakly interacting wave function onto the unitary basis there are significant contributions from higher-order terms, because the unitary states are a poor basis for the weakly interacting states. Higher-order terms have larger energies, hence  $\langle W \rangle$  and  $\langle W_{\text{irr}} \rangle$  peak near initial  $a_s = 0$ . For the quenches *from* unitarity we again see the influence of the bound state with the most amount of work (positive or negative) being associated with quenching to/from bound states.

Notably, for the quenches from the noninteracting system the work done is zero. The reason that no work is done for these quenches is explained in more detail in Sec. IV. In brief, in the noninteracting system the probability the two atoms are in the same place and at the same time is zero. When the interaction strength is quenched, the energy of the system does not change because the atoms are not initially in contact. After the quench the system evolves and the atoms come into contact, but at the time of the quench the atoms are not in contact, so a changing contact interaction does not change the energy of the system.

In the lower panel of Fig. 6 we plot  $\langle W \rangle$  against  $N_{\text{max}}$  for a quench from  $a_s = 0.1a_\mu$  to the noninteracting limit. For this quench  $\langle W \rangle$  diverges. In fact, a quench from any nonzero  $s$ -wave scattering length to the noninteracting regime results in a divergence in  $\langle W \rangle$  and  $\langle W_{\text{irr}} \rangle$ . This is not entirely unexpected. After all, the interacting wave function for arbitrary

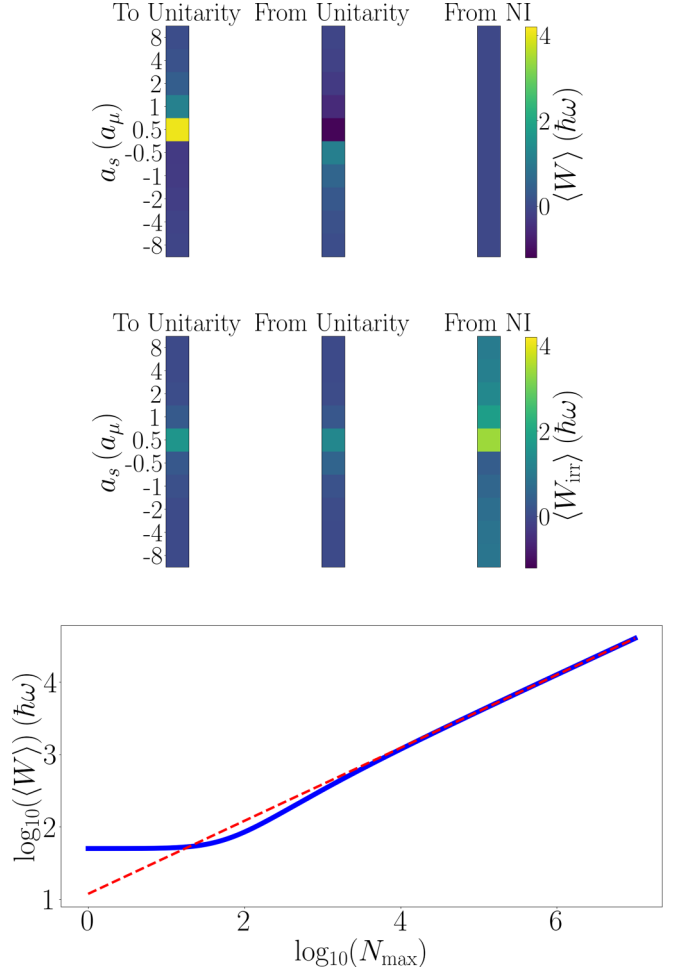


FIG. 6. Quenches between the noninteracting (NI) or unitary limits and arbitrary values of  $a_s$ . Upper panel:  $\langle W \rangle$  for quenches between a variety of  $s$ -wave scattering lengths and unitarity and for quenches from the noninteracting regime to arbitrary  $a_s$ . Center panel:  $\langle W_{\text{irr}} \rangle$  for quenches between a variety of  $s$ -wave scattering lengths and unitarity and for quenches from the noninteracting regime to arbitrary  $a_s$ . Lower panel:  $\langle W \rangle$  for a quench from  $a_s = 0.1a_\mu$  to the noninteracting regime as a function of  $N_{\text{max}}$ . The red dashed line corresponds to  $\langle W \rangle = 11.8\sqrt{N_{\text{max}}}\hbar\omega$ . In all cases the initial state is the ground state.

$a_s$  has the same functional form as the unitary wave function. Importantly, this demonstrates that the divergence behavior is not confined to the backward quench.

#### IV. DYNAMIC SWEEP THEOREM

The results of Sec. III A are consistent with the dynamic sweep theorem [46]. The dynamic sweep theorem relates the work of a quench in scattering length and/or trap geometry to the initial conditions of the system and the properties of the quench. If the trap geometry does not change it can be written

$$\frac{dE}{dt} = \frac{\hbar^2 \Omega C(t)}{8\pi\mu} \frac{d[-a_s(t)^{-1}]}{dt}, \quad (8)$$

where  $\Omega C(t)$  is the integrated contact intensity of the system. It is related to the probability of two particles being in the

same place at the same time. For an instantaneous quench Eq. (8) becomes

$$W = \frac{\hbar^2 \Omega C(0)}{8\pi\mu} \left( \frac{1}{a_i} - \frac{1}{a_f} \right), \quad (9)$$

where  $a_i$  and  $a_f$  are the initial and final scattering lengths. In the static interacting two-body case it is given [47]

$$\Omega C = 16\pi^2 \lim_{r \rightarrow 0} |r\psi_v(r)|^2 = 16\pi^3 a_\mu^2 N_v^2, \quad (10)$$

and in the static noninteracting case  $\Omega C = 0$ . The predictions of the dynamic sweep theorem match our calculations of  $\langle W \rangle$  and  $\langle W_{\text{int}} \rangle$ . That is, Eqs. (6) and (9) are in good agreement. It should be noted that  $\Omega C(0)/a_i$  goes to zero in the limit of  $a_i \rightarrow 0$ . This is why  $\langle W \rangle = 0$  for the quenches from the noninteracting regime.

In prior work it was suggested that the divergent behavior may be caused by the instantaneous nature of the quench and/or the zero-range nature of the interaction [36–38]. Using the dynamic sweep theorem we can show that the divergence is indeed a result of the instantaneous quench. Consider a quench where the scattering length changes as

$$a_s(t) = \frac{a_f - a_i}{\pi} \arctan(xt) + \frac{a_f + a_i}{2}, \quad (11)$$

where  $x$  is a parameter to describe the speed of the quench. We assume that the quench happens on a timescale faster than the dynamical response time such that  $C(t) = C(0)$  and that  $a_s$  changes only between  $t = -t'$  to  $t = t'$ . From Eq. (8) we obtain

$$W = \frac{\hbar^2 \Omega C(0)}{\mu} \left[ \frac{(a_f - a_i) \arctan(xt')}{\pi^2 (a_f + a_i)^2 - 4(a_f - a_i)^2 \arctan(xt')^2} \right]. \quad (12)$$

For a quench to the noninteracting regime Eq. (12) only diverges in the limit of an instantaneous quench ( $x \rightarrow \infty$ ).

A contact-interacting system can be quenched to the noninteracting regime and not diverge provided the quench is not instantaneous. This demonstrates that the divergent behavior is a result of instantaneous quenches.

## V. CONCLUSION

In this paper we consider the postquench evolution of a harmonically trapped system of two contact-interacting bodies with the aim of determining if divergences in particle separation are or are not present. We find that when quenching from finite  $a_s$  to the noninteracting limit the work done diverges. This builds upon previous work that found the system size diverges when quenching from unitarity to the noninteracting limit [36–38]. Importantly, we observe that this divergent behavior is present in *only* these two cases: unitarity to the noninteracting regime and finite  $a_s$  to the noninteracting regime. The divergence is not present in any other quench. Using the dynamic sweep theorem we are able to determine that the divergence arises due to the instantaneous nature of the quench rather than the zero-range nature of the interaction.

Finally, we reemphasize that these predictions are experimentally testable. Modern techniques allow for low atom number systems to be constructed with high fidelity [25–31]. Feshbach resonances are well understood [40–43] and have been implemented in experiment before [45,48]. In particular, the evolution of the postquench particle separation of a two-atom system has been measured before [44], albeit the quench was in trap geometry not  $a_s$ . While particle separation will not diverge in experiments where  $a_s$  is quenched to zero, it is likely that oscillations in system size will still be large.

## ACKNOWLEDGMENTS

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