Collision-induced frequency shifts in bright matter-wave solitons and soliton molecules

A. D. Martin

Department of Physics, University of Otago, Dunedin 9016, New Zealand

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A recent experiment has detected collision-induced frequency shifts in bright matter-wave solitons [J. H. V. Nguyen *et al.*, Nat. Phys. **10**, 918 (2014)]. Using a particle model, we derive the frequency shift for two solitons in a harmonic trap, and compare it to the recent experimental results and reported theoretical approximation. We find regimes where the frequency shift is much smaller than previously predicted, and propose experiments to test these findings. We also predict that reducing the experimental trap frequency will reveal soliton molecules or soliton bound states in a cold-atom system. The bound-state dynamics are found to be both highly phase dependent and sensitive to the residual 3D nature of the experiment.

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I. INTRODUCTION

Since the first bright solitons in Bose-Einstein condensates (BECs) [1–3], their suggested uses have included surface-probes [4,5], Bell-state generation [6], and interferometry [7–9]. The longstanding interest in bright solitons has recently been revived by an experiment on soliton collisions [10].

Solitons are solitary waves which pass thorough one another retaining their identity. Since their discovery [11], solitons were found generally to interact during collisions, emerging with a position (and phase) shift [12]. The shift has not been observed in BECs until demonstrated experimentally [10]. In harmonically trapped BECs the system's integrability is broken by the trapping potential, so these are not solitons in the strictest sense. Recent studies have shown that introducing time dependence in the potential and interactions can recover integrability and allows exact (nonautonomous) solitons [13,14]. However, the objects in the experiment behave as solitons despite the broken integrability. The position shifts were manifested in the solitons' increased oscillation frequency. Reference [10] compared the experimental results with an approximate theoretical curve, which agreed reasonably with the experiment in the tested regime.

This paper provides an improved frequency shift prediction based on a particle model that reproduces the exact position shifts for untrapped solitons [15–17]. We identify regimes in which there is a measurable difference between our predictions and the theory of Ref. [10] and propose simple modifications to the experiment to explore these regimes. We also suggest modifications to produce exotic soliton molecules (bound states) [7]. Optical soliton molecules have been produced experimentally [18], using a different scheme with modulation of the system parameters, but until now such states have not been controllably produced to order in cold atoms. We predict that a reduction in the experiment's trap frequency [10] and modifications to control the relative phase will produce soliton molecules in BECs. We investigate the 3-dimensional (3D) corrections to the dynamics, which affect both the stability and the mean-field BEC dynamics, particularly for soliton molecules. Note that the frequency shifts for few-particle systems were investigated numerically in Refs. [19,20].

II. THEORETICAL RESULTS

Bose-Einstein condensates with tight radial trapping are usually well described by the 1-dimensional (1D) Gross-Pitaevskii equation (GPE) [21]:

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + \frac{m\omega^2x^2}{2}\psi + g_{1\mathrm{D}}N|\psi|^2\psi, \tag{1}$$

where $g_{1\mathrm{D}} = 2\hbar\omega_r a_s$, N is the total atom number, ω and ω_r are the axial and radial trapping angular frequencies, and m and a_s are the atomic species' mass and s-wave scattering length. In experiments, a_s may be tuned to vary the interactions' sign and magnitude; negative a_s permits bright soliton solutions [22]. The 1D GPE breaks down when quantum or thermal fluctuations [23] and/or 3D effects become significant [24]. Quantum and thermal effects are not expected to play a role in the situations considered in this paper. However, the system's slightly 3D nature imposes a limit on the interaction strength, beyond which the condensate will collapse [10,25], characterized by critical atom number $|N_c|$. The parameter $N_c = 0.67a_r/a_s$, where $a_r = \sqrt{\hbar/(m\omega_r)}$, is also used here and in Ref. [10] to characterize the interaction strength, since N_s/N_c is proportional to $g_{1\mathrm{D}}N$ ($N_s \approx N/2$ is the particle number per soliton). Adding the quintic nonlinearity $g_2|\psi|^4\psi$ to Eq. (1), where $g_2 = 24\ln(4/3)N^2\hbar\omega_r a_s^2$, yields a 1D equation which approximates the integrability-broken nature of the 3D GPE [26]. We use the GPE equation modified with this quintic term to verify the regimes of validity of our results based on Eq. (1).

Previously [15–17], a soliton-soliton interaction potential was employed to model solitons as individual particles:

$$V = -2\eta_1\eta_2(\eta_1+\eta_2)\mathrm{sech}^2\left[\frac{2\eta_1\eta_2}{\eta_1+\eta_2}\tilde{q}\right], \tag{2}$$

where $\tilde{q} = m|g_{1\mathrm{D}}|Nq/\hbar^2$ is the dimensionless form of the solitons' relative position, q, and η_i are effective soliton mass parameters, where $\eta = 1/8$ for two equally sized solitons [16,17]. This potential produces the exact position shifts for solitons emerging from collisions within Eq. (1) when $\omega = 0$. The interaction potential was shown numerically to provide a good description when combined with an external trapping potential when the solitons were well separated between collisions, particularly when the solitons collided in-phase [17].

Within the particle model, we calculate the solitons' oscillation frequency from dynamics within the potential [Eq. (2)]:

$$\frac{\Omega}{2\pi}=\left[\int_{-\tilde{q}_0}^{\tilde{q}_0}\frac{d\tilde{q}}{\sqrt{\omega\left(\tilde{q}_0^2-\tilde{q}^2\right)/4-4\eta^2(\mathrm{sech}^2(\eta\tilde{q}_0)-\mathrm{sech}^2(\eta\tilde{q}))}}\right]^{-1}. \tag{3}$$

Here, $\pm\tilde{q}_0$ are the turning points of $\tilde{q}$. For solitons initially at rest (as in Ref. [10] and throughout this paper), q_0 is the initial soliton separation. The frequency shift may be written $\Delta\omega=\Omega-\omega$. We have found analytical solutions to Eq. (3), when the solitons are initially close or far apart. In the limit $q_0 m|g_{1\mathrm{D}}|N/\hbar \ll 1$, i.e., where the solitons are extremely close, we find

$$\frac{\Delta\omega}{\omega}=\frac{\sqrt{\omega^2+16|g_{1\mathrm{D}}|^4N^4\eta^4m^2/\hbar^6}}{\omega}. \tag{4}$$

For large initial separation, where $q_0 m|g_{1\mathrm{D}}|N/\hbar \gg 1$ and $\hbar^2\ln(1+16\eta^2|g_{1\mathrm{D}}|^2N^2/\hbar^2\omega^2q_0^2)/2\pi q_0\eta m|g_{1\mathrm{D}}|N \ll 1$, the position shifts generated by Eq. (2) will occur on a time scale much faster than the trap period; hence,

$$\frac{\Delta\omega}{\omega}=\frac{-\chi}{1+\chi}, \tag{5}$$

where

$$\chi=\frac{-2\hbar^2}{q_0\eta m|g_{1\mathrm{D}}|N}\ln\left(1+\frac{16\eta^2|g_{1\mathrm{D}}|^2N^2/\hbar^2}{\omega^2q_0^2}\right). \tag{6}$$

The frequency shift between these limits can be explained qualitatively by considering the effective potential (Fig. 1), which comprises an interaction mode within the harmonic potential. In the limit $q_0m|g_{1\mathrm{D}}|N/\hbar \ll 1$, the solitons are close compared to the interaction potential's width (which becomes large with decreasing interaction strength). The dynamics are small harmonic oscillations, which increase in frequency as the interaction strength increases. Increasing the interactions or solitons' initial separations further, the solitons may still be strongly bound within the interaction potential, but this potential is no longer effectively harmonic, and the frequency increase with interaction strength is slower. For even stronger interactions or wider separations, the intersoliton potential becomes narrow compared with the initial soliton separation, and the solitons effectively "escape" the intersoliton potential each collision. The frequency shift levels off, and starts to decrease as the intersoliton potential's width vanishes in comparison with q_0.

We provide for comparison the approximation derived in Ref. [10] based on the interaction Hamiltonian for Gaussian wave packets:

$$\frac{\Delta\omega}{\omega}=\frac{-g_{1\mathrm{D}}Na_x^2}{2\pi q_0^3\hbar\omega}, \tag{7}$$

where $a_x=\sqrt{\hbar/(m\omega)}$. As opposed to the dynamics in the particle model, within Eq. (7), the shift is linear in the interaction strength. The biggest difference between

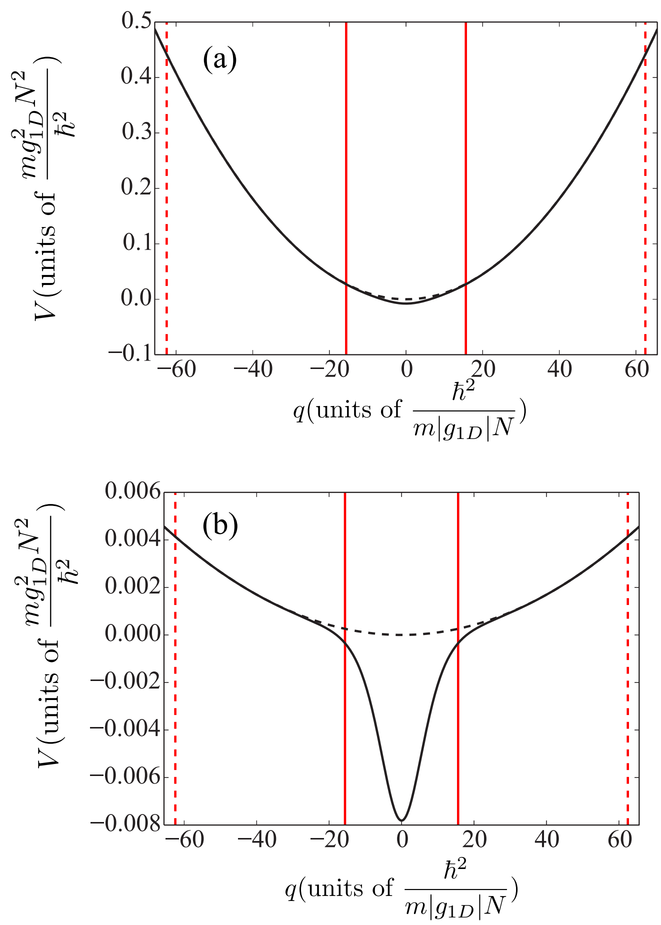

FIG. 1. Effective potential for two solitons in a harmonic trap, with $a_s=-0.57a_0$, $N=56\,000$, and mass parameter for lithium-7. The dashed curved shows the harmonic trapping potential alone. The trap frequencies are (a) $\omega=2\pi\times31$ Hz and (b) $\omega=2\pi\times3$ Hz. The solid (red) vertical lines are at $q_0=26\ \mu$m, and the dashed (red) vertical lines $q_0=106\ \mu$m.

the particle model's prediction and that of Eq. (7) is that the frequency shift in Eq. (7) diverges to infinity, rather than to zero, as the interaction strength goes to infinity. In the opposite limit the particle model goes to zero quadratically, not linearly. However, the important comparison is for experimentally accessible regions ($N_s/N_c>-1$), particularly in regimes where the difference between the predictions is large enough to resolve in experiment. In Ref. [10], the parameters $q_0=26\ \mu$m, $N_s=N/2=28\,000$, $\omega_r=2\pi\times254$ Hz, and $\omega=2\pi\times31$ Hz. The scattering length a_s varied between runs such that N_s/N_c varied between -0.53 and $+0.55$. Note that in the regimes of positive N_s/N_c, the wave packets are not solitons and are not considered in this paper.

Figure 2 shows the frequency shift from numerically evaluating Eq. (3), with the curves for the limits [Eqs. (4) and (5)] and theoretical approximation [Eq. (7)]. The relevant region of the experimental parameters lies within Fig. 2(a), while Figs. 2(b)–2(d) show other regimes—with different initial soliton separations or trap frequencies. The main deviation between the particle model and Eq. (7) is obvious in the large negative N_s/N_c limit, where the frequency in the particle

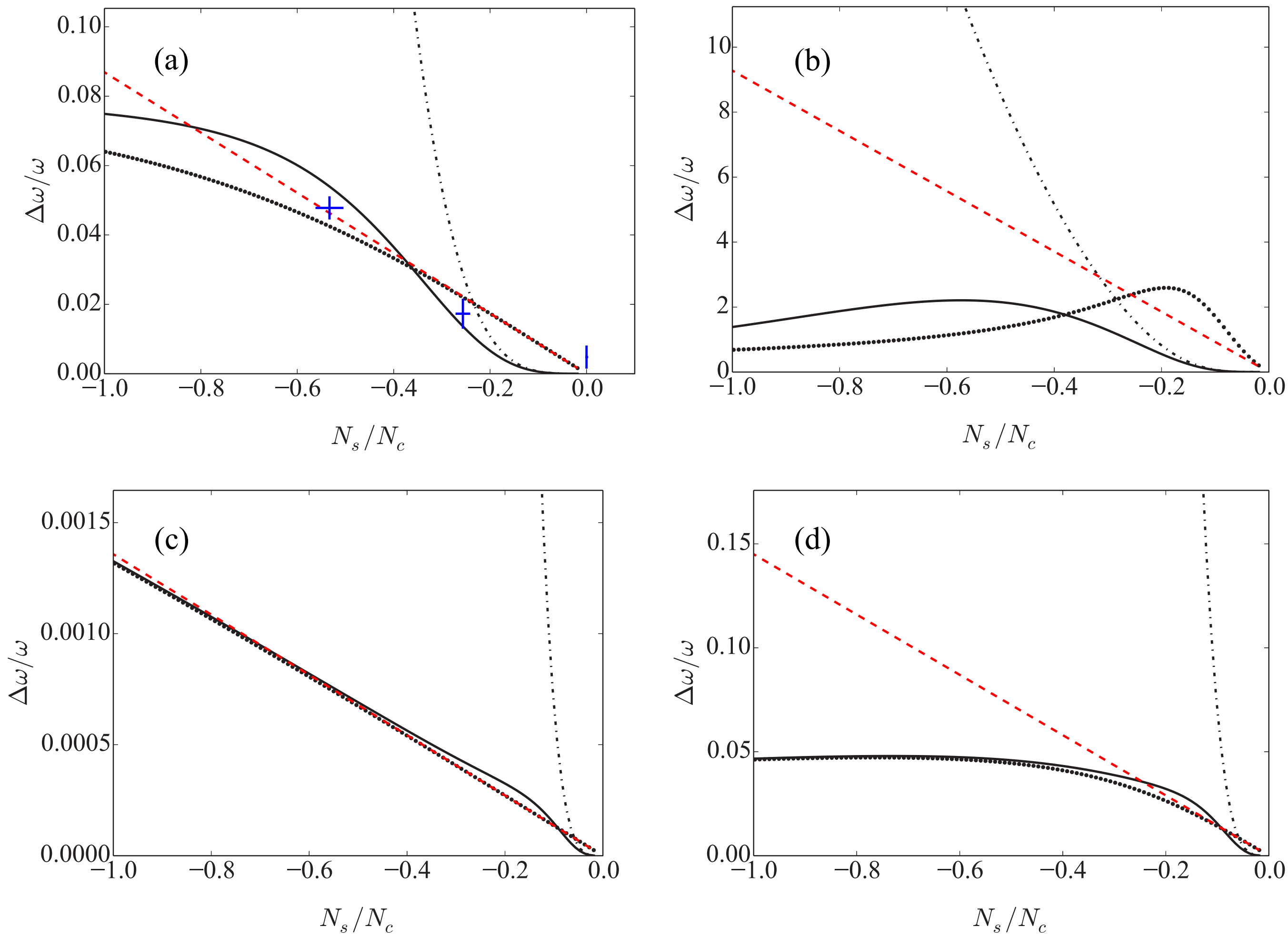

FIG. 2. Relative frequency shifts versus N_s/N_c for (a), (c) $\omega = 2\pi \times 31$ Hz and (b), (d) $\omega = 2\pi \times 3$ Hz. Plots (a), (b) are for $q_0 = 26\ \mu$m and (c), (d) are for $q_0 = 106\ \mu$m. Solid lines were determined by numerical evaluations of Eq. (3). Dot-dashed lines are the small-separation and weak-interaction limit, given by Eq. (4), and the dotted lines are the large-separation and strong-interaction limit, given by Eq. (5). Dashed (red) lines give Eq. (7) and bars give the experimental results [10].

model levels off and then starts to decrease. This is particularly apparent in Figs. 2(b) and 2(d), where the axial trapping frequency is a factor of approximately 10 less than in the recent experiment. However, for the experimental parameters [Fig. 2(a)] the difference between the curves is probably within experimental error; for large initial soliton separation and tight trapping [Fig. 2(c)], the agreement between the curves is extremely close.

III. MODEL VALIDATION AND PREDICTIONS

Before issuing experimental predictions from the particle model results, we must verify the model's performance. The particle model and the theoretical approximation of Ref. [10] assume the solitons separate between collisions, and approach at a sufficient speed such that the relative phase between the solitons plays no effect. It is clear from Ref. [17] that for solitons slow enough that the collision time approaches the order of the trap period, out-of-phase collisions will have smaller frequency shifts than those predicted by the particle model, whereas in-phase collisions are still well described. In the regimes where $q_0 = 26\ \mu$m [10], the ansatz used to derive the particle model comprises initially slightly overlapping solitons, even for the narrowest solitons considered. This obviously contradicts the assumption that the solitons always separate completely between collisions. Also, in some regimes, 3D effects lead to condensate collapse during collisions, especially for $N_s/N_c < -0.5$ and in-phase solitons [10,24].

We first evaluate the position shifts' phase dependence by integrating the GPE without the quintic term. Figures 3(a) and 3(b) show GPE simulations of two solitons for the experimental parameters with $N_s/N_c = -0.53$ for in- and out-of-phase collisions. The in-phase collisions are well described by the particle model, and, as expected, the predicted frequency shift is too large for the out-of-phase collisions.

Interestingly, when the axial trap is weakened to $\omega = 2\pi \times 3$ Hz [Figs. 3(c) and 3(d)], the in-phase solitons form a bound state (soliton molecule) which is surprisingly well described by the particle model (until it dephases at longer time scales). A bound state is also formed when the potential is reduced to zero, showing that the binding is due to the

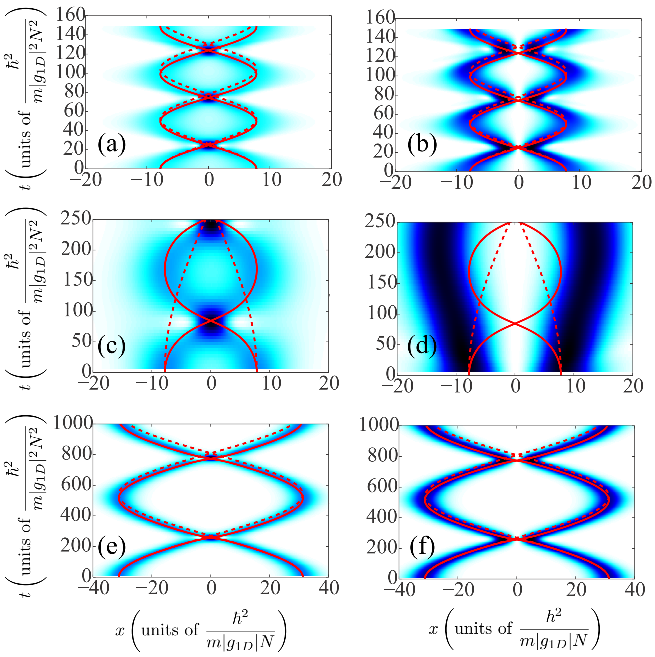

FIG. 3. Atomic density within the GPE for initial separation: (a)–(d) $q_0 = 26$ μm, (e)–(f) $q_0 = 106$ μm; axial trap angular frequency: (a)–(b) $\omega = 2\pi \times 31$ Hz, (c)–(f) $\omega = 2\pi \times 3$ Hz. The relative phase is (a), (c), (e) $\phi = 0$, (b), (d), (f) $\phi = \pi$. The scattering length $a_s = -0.57a_0$, the mass is for lithium-7, and $N = 56\,000$ such that $N_s/N_c = -0.53$. Trajectories within the particle model are given by full (red) lines, and those of noninteracting particles by dashed (red) lines for comparison.

intersoliton force [27], and not a bifurcation of the linear harmonic oscillator modes [28]. The (mutually repulsive) out-of-phase solitons are badly described. Similar solitons with relative phases, ϕ other than 0 and π, will have intermediate behavior. We expect the theoretical models in Refs. [7,29] to describe better the GPE dynamics of soliton molecules—replacing the universally attractive interaction with a short-range interaction force varying as $\cos\phi$. In particular, Ref. [29] predicts a stationary state for $\phi = \pi/2$ (i.e., $\Delta\omega/\omega = -1$). We expect a phase-dependent potential similar to that described in Ref. [7] would provide a better model for bound states.

For larger initial soliton separations than in the recent experiment, the particle model agrees with the GPE for any value of ϕ. We illustrate this by simulating the system for an initial separation four times that of the recent experiment: $q_0 = 106$ μm. For the experimental trap frequency, the frequency shift is too small to detect. We instead consider a weaker trap frequency of $\omega = 2\pi \times 3$ Hz, resulting in slower solitons with easily observable shifts. The agreement between the model and the GPE is illustrated in Figs. 3(e) and 3(f). It is this regime in which there is greatest improvement of the particle model over Eq. (7).

We investigate 3D effects by integrating the 1D GPE with the quintic nonlinearity. We find that for interaction strength $N_s/N_c = -0.53$, the in-phase collisions are unstable to collapse, but not the out-of-phase collisions [see Figs. 4(c) and 4(d)], suggesting that the in-phase collisions [Figs. 3(a), 3(c), and 3(e)] would not be realizable. However,

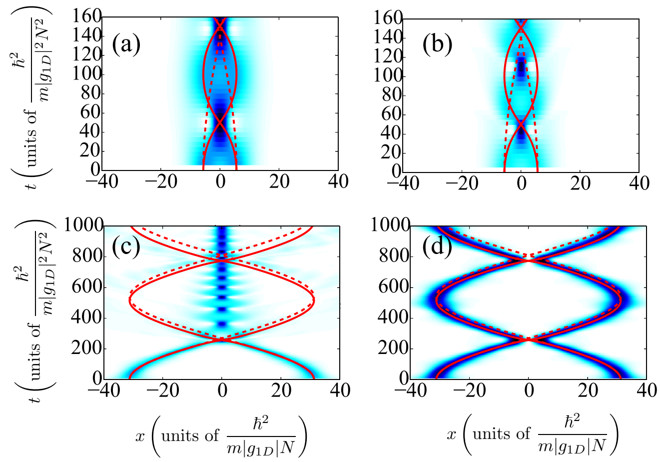

FIG. 4. (a)–(b) Atomic density within the GPE for a bound-state without (a) and with (b) quintic nonlinearity simulating the BEC's 3D nature. Here, $N_s/N_c = -0.41$, $\omega = 2\pi \times 3$ Hz, $q_0 = 26$ μm, and $\phi = 0$. (c)–(d) Atomic density for an unbound state with quintic nonlinearity for in-phase (c) and out-of-phase (d) collisions. Here $q_0 = 106$ μm. Full (red) lines show trajectories within the particle model, and dashed (red) lines show the trajectories of noninteracting particles.

slightly reducing the interaction strength to $N_s/N_c = -0.41$ produces qualitatively similar states which do not collapse. We find that the quintic term increases the bound-state oscillation frequency by a factor of $\sim$1.5 [see Figs. 4(a) and 4(b)]. The increased effective intersoliton binding force caused by the 3D trapping provides a difference with previously studied systems [27,30]. The unbound states' frequency shifts remain unaffected [see Fig. 4(d)], and it is here that the particle model is most useful. Furthermore, we expect these states to be stable to small noise away from the collapse instability, due to the field equations' near integrability, and the two-soliton particle model's exact integrability [16].

IV. CONCLUSIONS

In conclusion, we demonstrated regimes described better by the particle model than the theoretical approximation [10], i.e., those of weak axial trap frequency and stronger interactions. We propose the extension of the recent experiment [10] to verify the particle model predictions. We also suggest that soliton molecules can be created with greater control of the soliton phase, e.g., by applying a light-sheet potential to half the condensate [31–33]. Such states are highly dependent on relative-phase and 3D effects. In future work we propose extending an alternative formalism [7] to include harmonic trapping and 3D effects.

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