Metastability of persistent currents in trapped gases of atoms

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We examine the conditions that give rise to metastable, persistent currents in a trapped Bose-Einstein condensate. A necessary condition for the stability of persistent currents is that the trapping potential is not a monotonically increasing function of the distance from the trap center. Persistent currents also require that the interatomic interactions are sufficiently strong and repulsive. Finally, any off-center vortex state is shown to be unstable, while a driven gas shows hysteresis.

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I. INTRODUCTION

Vapors of ultracold atoms provide an ideal laboratory for testing the superfluid properties of quantum systems, including – among many other things – persistent currents. These phenomena are not only interesting from a theoretical point of view, but may also have very important technological applications \[1\].

As opposed to the traditional studies on liquid Helium that is confined in a box, gases of atoms may be confined in potentials of various form, such as harmonic, anharmonic, etc. In addition, the coupling constant between the atoms is tunable, and it is even possible to change its sign, allowing us to study both repulsive, as well as attractive effective interactions between the atoms.

As we demonstrate below, the two above features allow one to tune the stability of persistent currents in atomic systems by appropriately choosing the functional form of the trapping potential, the size/strength of the scattering length that describes the low-energy two-body collisions between the atoms, or the atom density/atom number.

Numerous theoretical and experimental studies have examined the rotational properties of clouds of trapped atoms, the vortex nucleation and stability, and more generally the superfluid properties of these gases. For a review of the extensive work on all these problems, we refer to the two articles by Leggett, on superfluidity in general \[2\], and in trapped gases \[3\].

In the present study, we examine the metastability of a current-carrying state with one unit of circulation, or equivalently, the energetic stability of a vortex state that is located at the center of the cloud. Our results show that in a two-dimensional trap, at least in the Thomas-Fermi limit of strong interactions, the vortex state, viewed as a particle, feels a force that is proportional to the gradient \(-\nabla n_0(\rho)\), where \(n_0(\rho)\) is the single-particle density distribution of the non-rotating cloud. Here \(\rho\) is the usual radial variable in cylindrical polar coordinates. Therefore, we conclude that a necessary condition for metastability is that \(n_0(\rho)\) is not a monotonically decreasing function. We give an analytic derivation of this result in Sec. VI.

For weak interactions metastability is not possible. The dispersion relation, i.e., the total energy of the cloud \(E\) for a given value of the angular momentum per atom \(l\hbar\), is dominated by the single-particle energy, and therefore local minima cannot appear in \(E(l)\). In the Thomas-Fermi limit of strong and repulsive interactions, metastability is possible, since the interaction energy is much larger than the single-particle energy. In this limit, the density \(n_0(\rho)\) of the non-rotating cloud is a mirror image of the trapping potential \(V(\rho)\). Therefore, we conclude that in the Thomas-Fermi limit a necessary condition for metastability is also that \(V(\rho)\) is not a monotonically increasing function of \(\rho\).

In our discussion so far we have distinguished between \(n_0(\rho)\) and \(V(\rho)\). However, since metastability requires that the interaction energy is at least comparable to the single-particle energy, and in this case a monotonically-increasing \(V(\rho)\) implies a monotonically-decreasing \(n_0(\rho)\), a necessary condition for metastability is also that \(V(\rho)\) is not a monotonically increasing function of \(\rho\).

In what follows we first present our model and our method in Sec. II. Section III describes the results we have derived within the mean-field approximation, and Sec. IV the results of numerical diagonalization. Section V examines the case of attractive interactions. In Sec. VI we give some analytic arguments which support our numerical results. Finally, in Sec. VII we consider a driven gas, and conclude that independently of the form of the trapping potential, any single off-center vortex state is unstable, while the gas shows hysteresis.

II. MODEL AND METHOD

In general one has to solve a three-dimensional problem. However, the motion along the axis of rotation introduces an extra degree of freedom, which may give rise to vortex bending. To get rid of this complication, we thus consider a highly-oblate trap, with a very tight, harmonic confinement along the axis of rotation – taken to be the \(z\) axis – and some axially-symmetric trapping potential \(V(\rho)\) perpendicular to the axis of rotation,

\[ V_{\text{ext}}(\mathbf{r}) = V(\rho) + \frac{1}{2}M \omega_z^2 z^2. \] (1)
We assume that the corresponding quantum of energy \( \hbar \omega_z \) for motion along the \( z \) axis is much larger than any other energy scale in the problem. The motion of the atoms is thus quasi-two-dimensional, since their motion along the \( z \) axis is frozen.

The energy of the gas at \( l = 1 \), \( \mathcal{E}(l = 1) \) is higher than \( \mathcal{E}(l = 0) \). The interesting question is whether there is a barrier in the dispersion relation \( \mathcal{E}(l) \) that separates the state with \( l = 1 \) from the state with \( l = 0 \). In the presence of such a barrier, the current-carrying state is metastable, and relatively weak perturbations that do not conserve the energy and the angular momentum cannot destabilize it.

We mentioned above that our study examines the energetic stability of a vortex state that is located at the center of the cloud. To understand the connection between this kind of stability criterion, and the calculation of \( \mathcal{E}(l) \), one should remember that there is an one-to-one correspondence between the angular momentum per atom \( l \hbar \), and the distance \( R_v \) of the vortex state from the center of the trap. An expression for \( l(R_v) \) is derived in Sec. VI. The function \( \mathcal{E}(l) \) may thus be viewed also as a function \( \mathcal{E}(R_v) \), and since \( l(R_v = 0) = 1 \), a local minimum in \( \mathcal{E}(l) \) for \( l \approx 1 \), implies that the vortex state is energetically stable under (at least) infinitesimal displacements of the vortex from the center of the trap.

To calculate the dispersion relation, we use both the mean-field Gross-Pitaevskii approximation, as well as numerical diagonalization of the Hamiltonian. The calculated energies from the two methods agree to leading order in \( N \) [4], i.e., they differ due to finite-size corrections in the small systems that we consider in numerical diagonalization.

### III. MEAN-FIELD APPROXIMATION

Starting with the mean-field, Gross-Pitaevskii approximation, the form of the trapping potential (which is tight along the \( z \) axis) allows us to use the following ansatz for the order parameter,

\[
\Psi(x, y, z) = \Phi(x, y) \phi_0(z),
\]

where \( \phi_0(z) = e^{-z^2/(2a_z^2)}/(\pi a_z^2)^{1/4} \) is the ground state of the harmonic oscillator along the \( z \) axis, with \( a_z \) being the oscillator length along this axis. The corresponding Gross-Pitaevskii equation for the two-dimensional order parameter \( \Phi(x, y) \) is

\[
-\frac{\hbar^2}{2M} (\nabla_x^2 + \nabla_y^2) \Phi + V(x, y) \Phi + \frac{\tilde{g}}{2} |\Phi|^2 \Phi = \mu \Phi,
\]

where \( \mu \) is the chemical potential, and \( \tilde{g} = N V_0 \int |\phi_0(z)|^4 dz = \sqrt{8\pi} \hbar^2 N a/|M a_z| \). Here \( N \) is the number of atoms, and \( V_0 = 4\pi \hbar^2 a/M \), where \( a \) is the s-wave scattering length for elastic atom-atom collisions, and \( M \) is the atom mass. We define for convenience the dimensionless quantity \( g = M \tilde{g}/\hbar^2 = \sqrt{8\pi} N a/a_z \). This parameter may easily get at least as large as \( 10^3 \), if, for example, \( N = 10^5 \), \( a = 50 \text{ Â} \), and \( a_z \sim 10 \mu \text{m} \).

The functional whose minimum value we are looking for, is

\[
\mathcal{E}(\Phi, \Phi^*) = -\frac{\hbar^2}{2M} \int \Phi^* (\nabla_x^2 + \nabla_y^2) \Phi \, dx dy + \int \Phi^* V(x, y) \Phi \, dx dy + \frac{\tilde{g}}{2} \int \Phi^2 \Phi^* \, dx dy,
\]

under the extra constraint of a fixed normalization \( \int |\Phi|^2 \, dx dy = 1 \). Typically one minimizes the above expression at a fixed rotational frequency of the trap \( \Omega \), by introducing the new function \( \mathcal{E}_{\text{rot}} = \mathcal{E} - l \Omega \), where \( l = i \int \Phi^* (y \partial_x - x \partial_y) \Phi \, dx dy \). If the second derivative of the (minimized) function \( \mathcal{E} \) with respect to \( l \) is positive, then one may get the minimized value of \( \mathcal{E}(\Omega) \), as well as \( \mathcal{E}(\Omega) \), at fixed \( \Omega \), and finally derive the dispersion relation \( \mathcal{E}(l) \).

However, if the second derivative of the (minimized) function \( \mathcal{E} \) with respect to \( l \) is negative, within a given range of \( l \), \( l_1 \leq l \leq l_2 \), the only minima occur at the end points \( l = l_1 \) and \( l = l_2 \). To overcome this difficulty, one may minimize the following expression instead [4],

\[
E(\Phi^*, \Phi) = \mathcal{E}(\Phi^*, \Phi) + \frac{C}{2} \hbar \omega (l - l_0)^2,
\]

again under the constraint of a fixed normalization \( \int |\Phi|^2 \, dx dy = 1 \). Here \( C \) and \( l_0 \) are real, dimensionless, and positive constants. The constant \( C \) has to be chosen sufficiently large to ensure that the last term in \( \mathcal{E} \) is the dominant one, which then also gives the corresponding minimized function \( E(l) \) a positive curvature, namely \( E''(l) + C \hbar \omega > 0 \), for all values of the angular momentum \( l_1 \leq l \leq l_2 \), where \( E''(l) \) denotes the second derivative with respect to \( l \). Under the condition of a positive curvature of \( E(l) \), one may minimize \( E(l) \) at any \( l_{\text{min}} \) that satisfies the equation

\[
l_{\text{min}} = l_0 - \mathcal{E}'(l_{\text{min}})/(C \hbar \omega).
\]

Using the method of imaginary-time propagation [6], we minimize the expression of Eq. [4] for three different trapping potentials, namely harmonic, anharmonic, and “Mexican-hat-like”, that are plotted in Fig. 1. In Fig. 2 we consider the harmonic trapping potential of the form

\[
V(\rho) = \frac{1}{2} M \omega^2 \rho^2,
\]

and plot the dispersion relation \( \mathcal{E}(l) \), in units of \( \hbar \omega \), for four values of the parameter \( g = 10, 100, 500, \) and 1000. In this figure we have shifted the zero of the energy, so that for all curves \( \mathcal{E}(l = 0) = 0 \). The actual shifts of the energies are: for \( g = 10 \), \( \mathcal{E}(l = 0) \approx 1.59 \hbar \omega \), for \( g = 100 \), \( \mathcal{E}(l = 0) \approx 3.95 \hbar \omega \), for \( g = 500 \), \( \mathcal{E}(l = 0) \approx 8.51 \hbar \omega \) and for \( g = 1000 \), \( \mathcal{E}(l = 0) \approx 11.97 \hbar \omega \).

As one can see in Fig. 2, the curvature of \( \mathcal{E}(l) \) is negative for all values of \( g \). Although the slope of this curve...
at $l = 1^-$ decreases with increasing $g$, our calculations show that it never becomes zero, and no metastable minimum forms around $l = 1$. Therefore, independently of the value of the coupling, a harmonic trapping potential cannot support persistent currents.

To examine the effect of the functional form of $V(\rho)$, we also consider a more flat potential around the origin, which has the form

$$V = \frac{1}{2}\hbar \omega (\rho / a_\perp)^\alpha,$$  \hfill (8)

where $a_\perp = (\hbar / M \omega)^{1/2}$ is the oscillator length along the plane of motion of the atoms, for $\alpha = 32$, and $g = 30, 100$, and 1000. Actually, this high value of $\alpha$ corresponds to a trap which is almost like a hard-wall potential, with a radius $a_\perp$.

Again, we plot $\mathcal{E}(l)$ in Fig. 3 shifting the zero of the energy in each case, so that $\mathcal{E}(l = 0) = 0$. These shifts are: for $g = 30$, $\mathcal{E}(l = 0) \approx 7.41\hbar \omega$, for $g = 100$, $\mathcal{E}(L = 0) \approx 67.15\hbar \omega$, and for $g = 1000$, $\mathcal{E}(L = 0) = 124.72\hbar \omega$.

This almost hard-wall potential does not allow the gas to expand radially, as in the case of harmonic confinement. The slope of the dispersion relation $\mathcal{E}(l)$ for $l \to 0$ increases with increasing $g$; in contrast for a harmonic trapping potential, the slope decreases. This observation probably implies that there is a critical power-law dependence of the trapping potential, for which this slope does not depend on $g$. Also, the slope of $\mathcal{E}(l)$ for $l \to 1^-$ tends to zero for high values of $g$, due to the almost homogeneous density of the cloud close to the center of the trap. Apart from these observations, $\mathcal{E}(l)$ has the same qualitative features as in the case of harmonic trapping, with no metastable minimum forming around $l = 1$. Persistent currents are not possible in this case, either. More generally, our calculations imply that this is also true even for a hard-wall potential, $\alpha \to \infty$.

We turn now to another functional form of $V(\rho)$, which does not increase monotonically with $\rho$, i.e., we consider a “Mexican-hat” shape,

$$V(\rho) = \frac{1}{2} M \omega^2 \rho^2 + V_0 e^{-\rho^2 / a_\perp^2},$$  \hfill (9)

with $V_0 > \hbar \omega / 2$. Such a potential can be realized experimentally if one applies a Gaussian, narrow laser beam on top of the ordinary harmonic trap $\hat{a}$.

Figure 4 shows the corresponding dispersion relation, again after shifting the zero of the energy at $l = 0$, for $V_0 / \hbar \omega = 4$, and $g = 2$, 20 and 100. The shifts are: for $g = 2$, $\mathcal{E}(l = 0) \approx 2.44\hbar \omega$, for $g = 20$, $\mathcal{E}(l = 0) \approx 2.94\hbar \omega$, and for $g = 100$, $\mathcal{E}(l = 0) = 4.50\hbar \omega$. In this case $\mathcal{E}(l)$ does develop a local minimum around $l = 1$ for sufficiently strong interactions, $g \approx 20$. Persistent currents are possible in this case. In Ref. $\hat{a}$ we have shown that in a strictly one-dimensional trap with periodic boundary conditions, a similar picture emerges for $\mathcal{E}(l)$ as the
strength of the interaction increases. This is not a surprising result, since, as shown in Fig. 2, the trapping potential is — roughly speaking — toroidal-like in this case.

IV. NUMERICAL DIAGONALIZATION

We have also diagonalized numerically the many-body Hamiltonian, for small systems, of \( N \) atoms and \( L \) units of angular momentum. Again we assume tight confinement along the axis of rotation and essentially consider two-dimensional motion. We use the eigenstates of the harmonic oscillator in two dimensions to build the Fock states, which are eigenstates of the operators \( \hat{N} \) and \( \hat{L} \), and then diagonalize the resulting Hamiltonian matrix.

Clearly one has to truncate, since the dimensionality of the matrix becomes very large if one considers highly-excited states. In the present calculation for each \( L \) and \( N \), we include in the Hilbert space as many single-particle states as are necessary, so that the lowest eigenvalue of the Hamiltonian has converged up to the third decimal point.

The calculated energies that we obtain agree with those of the mean-field approximation, apart from finite-size corrections [3]. The dots in the lower plots of Figs. 2, and 4 show the corresponding dispersion relation (i.e., the lowest eigenenergy divided by \( N \)), as function of the angular momentum per atom \( L/N \), for \( 0 \leq L \leq 4 \), \( N = 4 \), and \( g = 2 \).

V. ABSENCE OF METASTABILITY FOR ATTRACTIVE INTERACTIONS

Another interesting question is the possibility of metastable currents in the case of an effective attractive interaction between the atoms. Our calculations show that metastability is not possible in this case, in agreement with the arguments of Leggett [3].

In two interesting studies, Wilkin, Gunn, and Smith [9], as well as Mottelson [10] have shown that in a harmonic trap, for an effective interaction that is very weak and attractive, within the lowest Landau level approximation, the angular momentum is carried by the center of mass motion [11]. The reason is that in a harmonic trap, the center of mass and relative motions decouple, and as a result the least energetically-expensive way to give angular momentum to the gas, is via excitation of the center of mass. The relative distance between the atoms is thus unaffected, and the interaction energy does not depend on the angular momentum.

More generally, when the effective interaction is attractive, but not infinitesimally weak, the lowest, non-rotating state is already an interesting and non-trivial question. The absolute minimum of the energy of the gas for negative \( g \) corresponds always to a collapsed...
As cases localized for small values of the parameter $g$, the single-particle density of the (non-rotating) cloud is axially-symmetric, but it shrinks towards the origin of the trap, because of the attractive interaction. If the trapping potential does not increase monotonically, the gas may have a homogeneous density along the axially symmetric minimum of the potential, or it may form a symmetry-breaking localized blob.

Depending on the lowest state in the absence of rotation, the current-carrying states may involve vortex excitation, or center of mass excitation. Our results indicate that, independently of the form of the trapping potential, and of the single-particle density distribution, the dispersion relation is a smooth function of $l$, with a non-negative curvature.

Figure 5 shows a specific example, where we calculate $\mathcal{E}(l)$ for a trapping potential that has a “Mexican-hat” shape, with $V_0/h\omega = 4$, and for $g = -2$ (higher curve), and $g = -3$ (lower curve).

VI. ANALYTICAL ARGUMENTS

The results of Secs. III, IV and V show that metastability of superflow is possible for sufficiently strong and repulsive interactions. Furthermore, when the single-particle density $n_0(\rho)$ of the non-rotating cloud decreases monotonically, $\mathcal{E}(l)$ is a monotonically-increasing function and local minima in the dispersion relation are not possible. We give here a simple derivation of this result.

The dispersion relation $\mathcal{E}(l)$ consists of the single-particle energy and of the interaction energy, $\mathcal{E} = \langle H_{\text{sp}} \rangle + \langle V_{\text{int}} \rangle$. The contribution of the single-particle part of the Hamiltonian $H_{\text{sp}}$ is a smooth, and increasing function of $l$, with $\partial \langle H_{\text{sp}} \rangle / \partial l > 0$. We thus focus on the interaction energy $\langle V_{\text{int}} \rangle$, i.e., on the quantity $\langle V_{\text{int}} \rangle = (g/2) \int |\Phi|^4 \, dx dy$.

We consider the derivative

$$\frac{\partial \langle V_{\text{int}} \rangle}{\partial l} = \hat{g} \int |\Phi|^2 \frac{\partial |\Phi|^2}{\partial l} \, dx dy. \quad (10)$$

Clearly, the sign of the above derivative is determined by the sign of $\partial |\Phi|^2 / \partial l$. The density that enters in the above expression is the local density of the cloud $n(\rho, \phi) = |\Phi|^2$. In the limit of strong interactions, $g \gg 1$, the coherence length $\xi$ is much smaller than the radius of the cloud $R_0$, with $\xi/R_0 \sim g^{-1/2}$. The distortion of the cloud (due to the vortex) is localized around a region of radius $\approx \xi$. For this reason, in the calculation of the integral in Eq. (10) one may use the density profile neglecting the density depression due to the vortex, and also the weak dependence on the density of the gas on the polar angle $\phi$. Denoting the corresponding density as $n(\rho)$ [which is qualitatively the same as $n_0(\rho)$],

$$\frac{\partial \langle V_{\text{int}} \rangle}{\partial l} \approx \hat{g} \int n(\rho) \frac{\partial n(\rho)}{\partial l} \, dx dy. \quad (11)$$

Then, using the chain rule

$$\frac{\partial n}{\partial l} = (\hat{\rho} \cdot \nabla n) \frac{\partial R_v}{\partial l}, \quad (12)$$

where $R_v$ is the distance of the vortex from the center of the cloud, we observe that when $n(\rho)$ decreases monotonically, the inner product $\hat{\rho} \cdot \nabla n_0$ is always negative.

Turning to the derivative $\partial R_v / \partial l$, this is negative. The function $R_v(l)$ is monotonically-decreasing, with $R_v = 0$ for $l = 1$, and $R_v = \infty$, when $l = 0$. Generalizing the result of Ref. [10] that is given for a homogeneous system, we derive an approximate expression for $l(R_v)$. More specifically the angular momentum of the gas around the center of the trap is (in units of $\hbar$),

$$l = \frac{1}{\hbar} \int M \rho v n(\rho) \rho d\rho d\phi. \quad (13)$$

However, the circulation

$$\oint v \cdot dw = \frac{\hbar}{M}, \quad (14)$$

provided that the vortex is inside the area that is defined by the corresponding line $w$. Considering a circle of radius $\rho$,

$$\int v \rho d\phi = \frac{\hbar}{M}, \quad (15)$$
for \( \rho > R_c \) and zero for \( \rho < R_c \). From Eqs. (13) and (15) we get that,

\[
\tilde{l}(R_c) = 2\pi \int_{R_c}^{\infty} n(\rho)\rho d\rho = \int_{R_c}^{\infty} n(\rho) d^2\rho,
\]

which is the fraction of the atoms that reside outside a circle of radius \( R_c \). Equation (15) implies that \( \tilde{l}(R_c) \) is a decreasing function, and therefore \( \partial R_c/\partial l < 0 \). An analytic expression for \( \tilde{l}(R_c) \) may be derived for weak interactions (i.e., within the lowest-Landau level approximation), which is \( \tilde{l}(R_c) \approx 1 - R_c^2/(2\alpha_0^2) \) [14], when the vortex state is close to the center of the trap (for small values of \( R_c \)).

We conclude from Eqs. (11), (12) and (13), that when \( n_0(\rho) \) decreases monotonically, \( \partial(V_{\text{int}})/\partial l > 0 \), and thus

\[
\frac{\partial E}{\partial l} = \frac{\partial(H_{\text{sp}})}{\partial l} + \frac{\partial(V_{\text{int}})}{\partial l} > 0,
\]

which means that indeed metastability is not possible in this case.

As mentioned also earlier, in the Thomas-Fermi limit one may go even further with this argument, since \( n_0(\rho) \) is roughly the mirror image of the trapping potential \( V(\rho) \). Therefore, in the Thomas-Fermi limit, a necessary condition for metastability of superflow is that \( V(\rho) \) does not increase monotonically with \( \rho \). This condition holds even for more weak interactions, i.e., in the cross-over region, when the single-particle energy is comparable to the interaction energy.

VII. THE BEHAVIOR OF A DRIVEN GAS AND SOME GENERAL CONCLUSIONS

In addition to the question of metastability of superflow, the calculated \( E(l) \) for the various forms of \( V(\rho) \) also allow us to make some general statements for the behavior of a driven gas. Remarkably these statements are independent of \( V(\rho) \).

More specifically, one may define three critical rotational frequencies, namely the slope \( \Omega_1 \) of \( E(l) \) at \( l = 1^- \), the frequency \( \Omega_2 \) at which \( h\Omega_2 = E(l = 1) - E(l = 0) \), and the slope \( \Omega_3 \) of \( E(l) \) at \( l = 0 \). According to our calculations, in all cases, \( \Omega_1 < \Omega_2 < \Omega_3 \). In a harmonic, and highly-oblate trap, it has been shown that in the Thomas-Fermi limit, \( \Omega_2 = (5/3)\Omega_1 \) [16]. As we explain below, the fact that \( \Omega_1 < \Omega_2 < \Omega_3 \) has some important implications.

Experimentally one may either cool down the gas to very low temperatures and then rotate, or first rotate above the condensation temperature, and then cool down. In the first case, as one starts rotating the trap (at a fixed \( g \)), the cloud undergoes a discontinuous transition from the non-rotating state to the state with one vortex that is located at the center of the trap, at the frequency \( \Omega = \Omega_3 \). In the reverse process, the vortex leaves the cloud discontinuously at an \( \Omega = \Omega_1 \), and therefore, there is hysteresis. In addition, for \( \Omega_1 < \Omega < \Omega_2 \), the vortex state is metastable, i.e., it becomes locally stable before it becomes thermodynamically stable (at \( \Omega = \Omega_2 \)). Finally, because of the negative curvature of \( E(l) \), any single off-center vortex state is unstable.

In the second case, if one first rotates and then cools down, a (meta)stable vortex state will appear at the center of the cloud at a rotational frequency \( \Omega = \Omega_1 \). Again, any single off-center vortex state is unstable.

The physical picture that underlies the above arguments for the metastability, the hysteresis, and the fact that any off-center vortex state is unstable, is that the vortex state creates a node at the density of the gas. As long as the density \( n_0(\rho) \) decreases monotonically, this node cannot produce any energy barrier [3, 17]. On the other hand, if the density is not a monotonically-decreasing function of \( \rho \), there may be an energy barrier in the dispersion relation, provided that the interaction is repulsive and sufficiently strong.

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