Continuous structural transitions in quasi-one-dimensional classical Wigner crystals

G. Piacente,[1] G. Q. Hai,[1] and F. M. Peeters[2]

[1]*Instituto de Física de São Carlos, Universidade de São Paulo, 13560-970 São Carlos, SP, Brazil*
[2]*Department of Physics, University of Antwerp (Campus Middleheim), Groenenborgerlaan 171, B-2020 Antwerpen, Belgium*

We study the structural phase transitions in confined systems of strongly interacting particles. We consider infinite quasi-one-dimensional systems with different pairwise repulsive interactions in the presence of an external confinement following a power law. Within the framework of Landau's theory, we find the necessary conditions to observe continuous transitions and demonstrate that the only allowed continuous transition is between the single- and the double-chain configurations and that it only takes place when the confinement is parabolic. We determine analytically the behavior of the system at the transition point and calculate the critical exponents. Furthermore, we perform Monte Carlo simulations and find a perfect agreement between theory and numerics.

Recently the static and dynamic properties of low-dimensional ensembles of strongly interacting particles have been attracting much interest both in theoretical and experimental physics. These systems usually consist of particles which interact through a two-body repulsive potential and are held together by an external confinement. Electrons on liquid helium,[1] carriers in quantum dots,[2] and in carbon nanotubes,[3] strongly coupled radio-frequency complex plasmas,[4] laser-cooled ions in Paul and Penning traps,[5] and colloidal suspensions[6] are examples of confined charged particles encountered in modern laboratories. Vortex clusters in isotropic superfluids[7] and in type-II superconductors[8] share similar features with the aforementioned systems. Depending on the particle density and on the relative strengths of interaction and confining potentials, these systems self-organize into ordered structures at low temperature, i.e., they can form a Wigner crystal.

Over the past decade considerable research efforts have focused on quasi-one-dimensional (Q1D) Wigner crystal in the contest of quantum information processing.[9] Among other properties special attention has been devoted to the continuous structural phase transition at zero and (low) finite temperature and to the critical behavior at the transition point.[4,10–12]

Previous studies have manly addressed the case of parabolic confinement.[4,10–13] The reason is that almost any two-dimensional (2D) confinement expanded around its minimum provides a quadratic term as the lowest-order term. However, recent experiments on colloidal suspensions confined between two highly charged plates in a wedge geometry[14] suggest the possibility of a confinement which is not parabolic around its minimum. Motivated by these experimental findings, we study the case of a general power-law confinement for a system at $T=0$ in the classical regime.

We consider 2D infinite systems of particles moving in the x-y plane and interacting through a repulsive pairwise potential V. An external single-particle power confinement in one direction, namely, the y direction, further reduces the dimensionality of the system to quasi-1D. The Hamiltonian for such systems is

$$H = \sum_{i>j} V(r_{ij}) + \beta \sum_i |y_i|^\alpha, \tag{1}$$

where r_{ij} is the interparticle distance, α is a positive real number, and β is a constant that preserves the right dimensions of the Hamiltonian.

As an example, the classical Hamiltonian at $T=0$ of an infinite 2D system of monodisperse charged particles of mass m and charge q interacting through a power-law potential in a y^α external confinement is

$$H = \frac{q^2}{\epsilon R} \sum_{i>j} \frac{R^n}{r_{ij}^n} + \sum_i \frac{1}{2} m\omega_0^2 R^2 \frac{|y_i|^\alpha}{R^\alpha},$$

where ω_0 is the confinement frequency. The exponent n is an integer, R and ϵ are a typical length of the system and the dielectric constant, respectively. By introducing $r_0 = (q^2/\varepsilon\sigma)^{1/(n+\alpha)} R^{(n+\alpha-3)/(n+\alpha)}$ and $E_0 = (q^2/\varepsilon)^{\alpha/(n+\alpha)} \sigma^{n/(n+\alpha)} R^{(2n-\alpha)/(n+\alpha)}$ as units of length and energy, respectively, with $\sigma = m\omega_0^2/2$, the Hamiltonian can be written in the dimensionless form

$$H' = \sum_{i>j} \frac{1}{r_{ij}'^n} + \sum_i |y_i'|^\alpha,$$

where $r' = r/r_0$ and $H' = H/E_0$.

Similar considerations can be made in the cases of pairwise interactions represented both by the Yukawa potential $V(r_{ij}) = (q^2/\varepsilon)\exp(-\kappa r_{ij})/r_{ij}$ with κ the inverse screening length, and by the modified Bessel potential $V(r_{ij}) = u_0 K_0(r_{ij}/\lambda)$ with K_0 the modified Bessel function of the second kind, u_0 the energy unit, and λ a typical distance. The Yukawa potential is suitable to model colloidal suspensions and complex plasmas, while the modified Bessel potential describes vortices in a type-II superconductor, in which case λ is the London penetration depth (for details see, for instance, Refs. 13 and 15).

In general, by choosing proper units of energy and length, the Hamiltonian of a Q1D system of interacting particles can be written in the dimensionless form
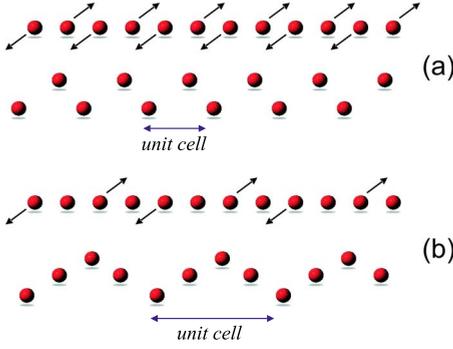
FIG. 1. (Color online) Possible mechanism for continuous structural transitions: (a) zigzag transition from 1 to 2 chains and (b) transition from 1 to 3 inhomogeneous chains.

$$H' = \sum_{i>j} V(r'_{ij}) + \sum_i |y'_i|^\alpha. \qquad (2)$$

The ground-state configuration for a system described by Eq. (2) is the result of competitive effects, that is, the (electrostatic) repulsion and the confining potential that tries to keep the particles close to the x axis. At low temperature the particles crystallize in a chainlike structure. The case of harmonic confinement was studied thoroughly in Ref. 13. For low densities the particles form a single chain, then with increasing density (or increasing repulsion) a continuous "zigzag" transition occurs and the single chain splits into two chains [see Fig. 1(a)]. On further increasing the density multichain structures are formed. The structural transitions are discontinuous, i.e., first order, except for the $1 \rightarrow 2$ chain transition.

Independently of the specific interaction and confinement potentials, from geometrical considerations it is easy to infer that there are only two possible continuous structural transitions: (a) from 1 to 2 chain configuration and (b) from 1 to inhomogeneous 3 chain configuration, as depicted in Fig. 1. In fact, other possible processes for continuous transitions would lead to unstable structures. In the inhomogeneous 3 chain structure, the internal chain is twice denser than the external chains. These configurations are observed in numerical simulations in the case of $\alpha < 2$ for certain values of the parameters while they are never present in the case $\alpha = 2$. Actually, analytical calculations show that in a parabolic confinement the inhomogeneous 3 chain configuration has a higher energy with respect to other homogenous chain structures at the same (linear) density $\tilde{n}_e$, defined as the number of particle per unit cell.

In what follows, we concentrate on the structural transition from 1 to 2 and from 1 to inhomogeneous 3 chains in the case of a general confinement. This problem is not only interesting by itself, but it also carries practical implications: for instance, the performance of atomic clocks based on ion chains depends crucially on trapping many ions and holding them in a linear configuration, so it is important to understand how and when structural transitions from linear to planar configurations occur.[16]

We first notice that for $\alpha \leq 1$ continuous transitions are not allowed because the single chain does not represent an equilibrium configuration. From now on we drop the prime

superscript for dimensionless quantities. From Eq. (2) the equilibrium conditions are obtained as

$$0 = \frac{\partial H}{\partial x_i} = \sum_j \frac{\partial V(r_{ij})}{\partial r_{ij}} \frac{x_i - x_j}{r_{ij}}, \qquad (3)$$

$$0 = \frac{\partial H}{\partial y_i} = \sum_j \frac{\partial V(r_{ij})}{\partial r_{ij}} \frac{y_i - y_j}{r_{ij}} + \alpha |y_i|^{\alpha-1} \text{sgn}(y_i). \qquad (4)$$

The single-chain configuration $x_i = \pm ia$ and $y_i = 0$ with $i = 1, 2, \ldots$ and a the distance between neighboring particles, is always a solution of Eq. (3), while Eq. (4) admits the linear chain as a solution only for $\alpha > 1$.

When continuous structural transitions take place, the system undergoes a transformation from a 1D to a 2D structure, for which the rotational symmetry about the x axis is lost. In this case, one can define a scalar order parameter c, as the displacement of the external chains from the x axis, i.e., the transversal amplitude of the Q1D crystal. The order parameter is 0 in the high-symmetry phase, i.e., the single chain, and $\neq 0$ in the phase with less symmetry, i.e., the multichain structures. Starting from this definition we apply the Landau's theory to the transition, taking as control parameters $\tilde{n}_e$, κ, or λ according to the specific form of the interparticle interactions.

The general form for the energy per particle in a double and in an inhomogeneous three chain configurations as a function of the order parameter are, respectively,

$$E_2 = \sum_{j=1}^{\infty} V\left(\frac{2j}{\tilde{n}_e}\right) + \sum_{j=0}^{\infty} V\left(\frac{2}{\tilde{n}_e}\sqrt{(j+1/2)^2 + c^2}\right) + \frac{c^\alpha}{\tilde{n}_e^\alpha}$$

and

$$E_3 = \frac{1}{2}\sum_{j=1}^{\infty} V\left(\frac{2j}{\tilde{n}_e}\right) + \frac{1}{2}\sum_{j=1}^{\infty} V\left(\frac{4j}{\tilde{n}_e}\right) + \sum_{j=0}^{\infty} V\left(\frac{2}{\tilde{n}_e}\sqrt{(j+1/2)^2 + c^2}\right)$$
$$+ \frac{1}{2}\sum_{j=0}^{\infty} V\left(\frac{4}{\tilde{n}_e}\sqrt{(j+1/2)^2 + c^2}\right) + \frac{1}{2}\frac{(2c)^\alpha}{\tilde{n}_e^\alpha},$$

where c is in units of the unit-cell length. For $c \rightarrow 0$ the energy per particle in the single-chain structure E_1 is recovered. Since we are only interested in the behavior of the system close to the transition, according to the Landau's prescription, we expand the free energy as a function of the order parameter for small values of it. As we are considering $T = 0$, there is no distinction between internal and free energy. Moreover, the order parameter enters quadratically in the interparticle interaction, consequently it is sufficient to consider an expansion to the fourth order of V in order to catch the essential physics of the system. This yields

$$E_{2,3}(c) \simeq E_1 - Ac^2 + Bc^4 + Dc^\alpha, \qquad (5)$$

where $A, B, D > 0$. Coefficients A and B are functions of $\tilde{n}_e$ and, eventually, κ or λ, while coefficient D is a function of $\tilde{n}_e$ only. Notice that coefficient A is preceded by a minus sign. This feature arises either from the fact that the pairwise interactions considered are functions of the inverse distance

between particles or from the properties of the modified Bessel functions.

In order to understand when the 2 or the inhomogeneous 3 chain configurations are stable and energetically favorable, we look for the minimum of $E_{2,3}$. Three conditions have to be fulfilled

$$-2A\tilde{c} + 4B\tilde{c}^3 + \alpha D\tilde{c}^{\alpha-1} = 0, \tag{6a}$$

$$-2A + 12B\tilde{c}^2 + \alpha(\alpha-1)D\tilde{c}^{\alpha-2} \geq 0, \tag{6b}$$

$$-A\tilde{c}^2 + B\tilde{c}^4 + D\tilde{c}^{\alpha} \leq 0, \tag{6c}$$

where Eqs. (6a) and (6b) represents the request of $\tilde{c}$ being a relative minimum while Eq. (6c) translates the condition $E_{2,3} \leq E_1$. With some straightforward algebra one gets

$$8B\tilde{c}^4 + D\tilde{c}^{\alpha}(\alpha-2) \geq 0,$$

$$4B\tilde{c}^4 + D\tilde{c}^{\alpha}(\alpha-2) \geq 0,$$

which are always satisfied for $\alpha > 2$ and $\tilde{c} > 0$.

This leads to the first important result: for an external confinement more than parabolic the single chain is never formed and the multichain structures are always the lowest-energy configurations at low particle density. Of course, this result is strictly valid at $T=0$. At finite temperature, the thermal fluctuations can be of the same order of the chain separation so that it is impossible to distinguish the single from the multichain structure.

Let us discuss now the case $1 < \alpha \leq 2$. From Eqs. (6a)–(6c) it is simple to recover

$$\tilde{c}^2 \geq \frac{A}{2B}\frac{\alpha-2}{\alpha-4},$$

which clearly shows that only for $\alpha=2$ the order parameter can vary continuously from zero. On the other hand, for $\alpha \neq 2$ the order parameter varies abruptly from zero in the single chain to a finite value in the multichain configuration, which produces a jump discontinuity in the derivatives of the energy per particle with respect to the order parameter at the critical point.

This allows us to stress the second important result: only for harmonic confinement second-order transitions are allowed. Furthermore, since inhomogeneous 3 chain structures are never formed in the case of harmonic confinement, we conclude that the $1 \rightarrow 2$ chain transition, i.e., the zigzag transition, is the only continuous structural transition allowed in classical Q1D Wigner crystals.

We are able to study the critical behavior of the system close to the transition point for zigzag transitions in parabolic confining potentials. If we indicate generically with η the control parameters $\tilde{n}_e$, κ, or λ, and expand Eq. (6a) as a function of η around the critical value η_c, where the zigzag transition takes place, retaining the lowest-order term, we obtain

$$c \sim \left[\frac{\partial}{\partial\eta}\left(\frac{A-D}{2B}\right)\bigg|_{\eta=\eta_c}\right]^{1/2}|\eta-\eta_c|^{1/2}, \tag{7}$$

that is, we find that the critical exponent has the value 1/2. This behavior is of general validity: the order parameter in a continuous transition is expected, in the framework of Landau's theory, to possess a square-root dependence as a function of the deviation of the control parameters from the critical values.

Together with the critical exponent, Landau's theory allows the calculation of the transition point. In fact, Eq. (6a) provides the necessary condition for the transition, that is, $A-D=0$. We can write explicitly the latter condition for the different potentials considered:

(1) power potential

$$-2n\tilde{n}_e^n\sum_{j=0}^{\infty}\frac{1}{(2j+1)^{2+n}} + \frac{1}{\tilde{n}_e^2} = 0,$$

(2) Yukawa potential

$$-2\tilde{n}_e\sum_{j=0}^{\infty}\frac{e^{-\kappa(2j+1)/\tilde{n}_e}}{(2j+1)^3} - 2\kappa\sum_{j=0}^{\infty}\frac{e^{-\kappa(2j+1)/\tilde{n}_e}}{(2j+1)^2} + \frac{1}{\tilde{n}_e^2} = 0,$$

(3) modified Bessel potential

$$-\frac{2}{\lambda\tilde{n}_e}\sum_{j=0}^{\infty}\frac{1}{(2j+1)}K_1\left(\frac{2j+1}{\lambda\tilde{n}_e}\right) + \frac{1}{\tilde{n}_e^2} = 0.$$

Solving numerically these equations one finds either the critical density or the critical screening and penetration length at fixed density. The values found are in perfect agreement with other theoretical approaches and numerical simulations.[10,11,13] The critical behavior for the different interaction potential is shown in Fig. 2, where we compare analytical findings to numerical results from Monte Carlo simulations at extremely low temperature.

For continuous structural transitions it is well established that the order parameter is (or is proportional to) a normal mode of the lattice and that one normal mode of the crystal softens. The linear chain becomes mechanically unstable when, by varying the control parameter, the frequency of the soft mode vanishes. In the case of parabolic confinement, independently of the specific interparticle interactions, the soft mode is the transversal mode of the linear chain with wave vector $k=\pi/a$.

This is easily seen by studying the normal modes in the harmonic approximation, as in Refs. 10, 11, and 13. The linearized Hamiltonian for the Q1D crystal about the equilibrium configuration takes the form

$$H_L = H_0 + \frac{1}{2}\sum_{i,j}\mathbf{Q}_i\cdot\mathbf{V}_{ij}\cdot\mathbf{Q}_j + \frac{1}{2}\sum_i w_i\delta y_i^2, \tag{8}$$

where $\mathbf{Q}_i=(\delta x_i, \delta y_i)$ are the displacements from the equilibrium positions, $\mathbf{V}_{ij}$ is the Hessian matrix of the interaction potential calculated at the equilibrium configuration $(\bar{x}_i, \bar{y}_i)$ and
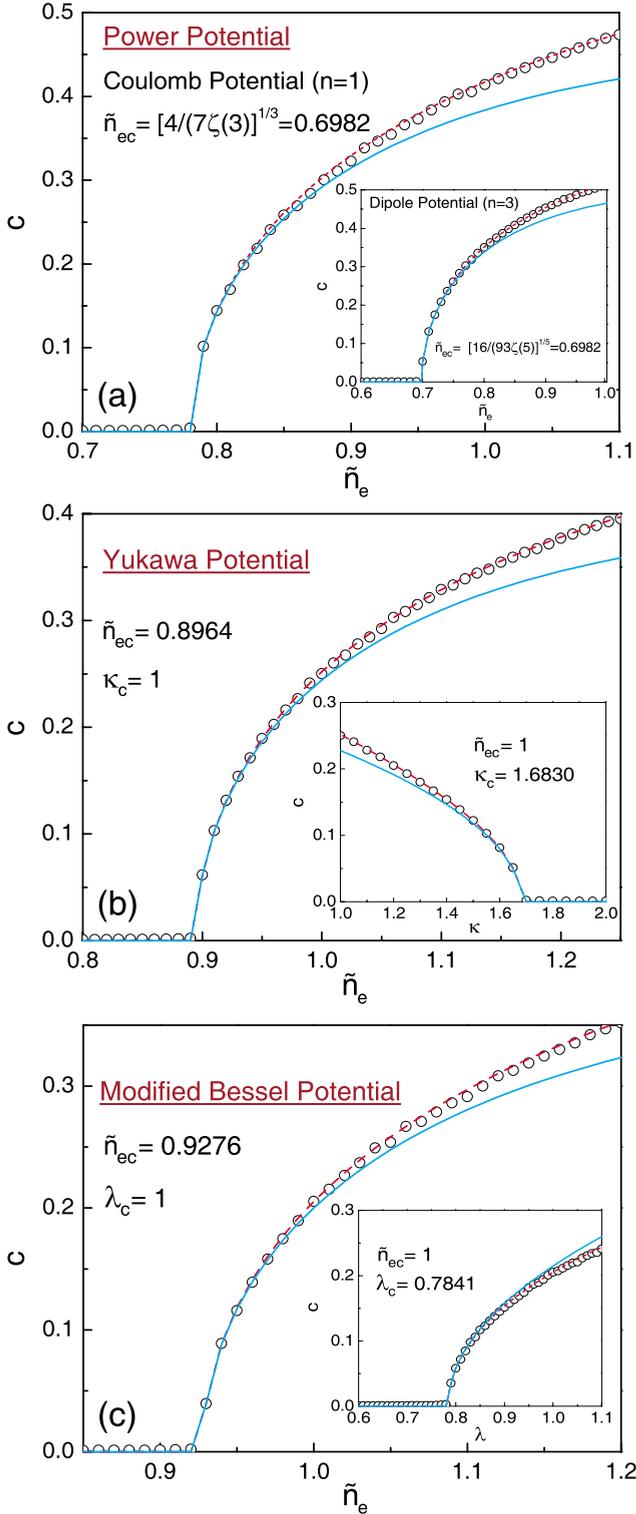
FIG. 2. (Color online) The critical behavior for the different interparticle potentials for the continuous transition. The solid lines are the solutions of Eq. (7) while the dashed line is obtained by minimizing the energy of the 2-chain structure using c as variational parameter. The circles represent the results of Monte Carlo simulations with $N=1000$ particles at a dimensionless temperature $T' = k_B T / E_0 = 10^{-6}$, where k_B is the Boltzmann constant. In the case of Coulomb potential the Ewald technique is used in the calculation of energies.

$$w_i = \left. \frac{\partial^2 |y_i|^\alpha}{\partial y_i^2} \right|_{y_i = \bar{y}_i} = \alpha(\alpha - 1)|\bar{y}_i|^{\alpha-2} + \alpha|\bar{y}_i|^{\alpha-1}\delta(\bar{y}_i)$$

with δ the Dirac delta function. One can notice the similarity of H_L with the Hamiltonian of a lattice model for magnetic systems where at each lattice site i there is a two-component spin variable. It is evident that the Hamiltonian cannot be linearized around the single-chain equilibrium configuration unless $\alpha \geq 2$. For $\alpha < 2$ one has to deal with a dynamical system, whose properties and intrinsically nonlinear oscillations will be studied in a future work. In the case of linear configurations $w_i \equiv w$ and, in particular, $w=2$ for $\alpha=2$, while $w=0$ for $\alpha>2$. From Eq. (8) it is straightforward to calculate the dispersion relations for the normal modes in single-chain arrangements. The frequencies ω_L and ω_T, in units of $\omega_0/\sqrt{2}$, of the longitudinal and transversal modes, respectively, as functions of the wave vectors are

$$\omega_L^2(k) = \sum_{j=1}^{\infty} \left. \frac{\partial^2 V}{\partial x_j^2} \right|_{x_j = \pm ja} [1 - \cos(jk\tilde{n}_e)], \qquad (9)$$

$$\omega_T^2(k) = \frac{w}{2} - \sum_{j=1}^{\infty} \left. \frac{\partial^2 V}{\partial y_j^2} \right|_{y_j=0} [1 - \cos(jk\tilde{n}_e)]. \qquad (10)$$

The longitudinal mode frequencies are independent of the external confinement; ω_L is an increasing function of k, it is zero at $k=0$ and it is maximum at $k=\pi/a$. In the case of harmonic confinement the transversal mode frequency ω_T is a decreasing function of k, with a maximum equal to 1 at the center of the Brillouin zone and minimum at the edge of the Brillouin zone. The condition $\omega_T^2(\pi/a)=0$ returns exactly the equation $A - D = 0$, previously specified for the different kinds of interparticle interactions. This clearly demonstrates that the transversal mode of the linear chain is indeed the soft mode, driving the structural transition from 1 to 2 chains across the critical value of the control parameter. Besides, Eq. (10) shows that ω_T is purely imaginary for $\alpha>2$, which confirms that the single-chain structure is unstable for external confinements more than parabolic.

To conclude, we performed molecular-dynamics and Monte Carlo simulations of the system for different values of α and different interaction potentials. Here we remark some important features, which are common to the different investigated systems. First, we found that for $\alpha < 1$ the system shows instabilities and strong dependence on the initial conditions. For $\alpha \sim 1$ with increasing density the system does not undergo the transition from a single to a multichain configuration but rather tries to expel particles to preserve the single-chain structure. The resulting configurations, which generally are neither translationally invariant nor symmetric with respect to the x axis, consist of a central chain plus few external particles. Moreover, we noticed that for $1 < \alpha < 2$ the amplitudes of transversal oscillations in the single-chain configuration are almost independent of the interparticle interactions, which essentially means that the x and y motion are weakly coupled. Finally, the amplitudes of transversal oscillations around $\alpha \sim 1$ are reduced orders of magnitude with respect to the case of harmonic confinement, which in-

dicate the opportunity of using nonparabolic confinement in those applications for which "unidimensionality" is important.

In summary, using a mean-field approach, namely, the Landau's theory for phase transitions, we have demonstrated that the transition from a single to a double chain structure, in an infinite Q1D system is the only possible second-order phase transition and it only takes place if the external confinement is parabolic. We have also showed that the soft modes in the continuous phase transition are the transversal modes of the linear chain. Our model allows to study the system at the critical point and its vicinity. Our theory is analytical and its predictions agree with numerical simulations. Although our theory is strictly valid at $T=0$ and for infinite systems, it can also be useful for finite systems at low temperature. In particular, confined finite systems far from the edges exhibit characteristics similar to infinite systems, therefore we can conjecture that in this region our analysis provides reliable predictions.

[1] H. Ikegami, H. Akimoto, and K. Kono, Phys. Rev. Lett. **102**, 046807 (2009).

[2] S. M. Reimann and M. Manninen, Rev. Mod. Phys. **74**, 1283 (2002).

[3] V. V. Deshpande and M. Bockrath, Nat. Phys. **4**, 314 (2008).

[4] A. Melzer, Phys. Rev. E **73**, 056404 (2006).

[5] A. Mortensen, E. Nielsen, T. Matthey, and M. Drewsen, Phys. Rev. Lett. **96**, 103001 (2006).

[6] M. Köppl, P. Henseler, A. Erbe, P. Nielaba, and P. Leiderer, Phys. Rev. Lett. **97**, 208302 (2006).

[7] J. R. Abo-Shaeer, C. Raman, J. M. Vogels, and W. Ketterle, Science **292**, 476 (2001).

[8] G. Karapetrov, J. Fedor, M. Iavarone, D. Rosenmann, and W. K. Kwok, Phys. Rev. Lett. **95**, 167002 (2005).

[9] J. M. Taylor and T. Calarco, Phys. Rev. A **78**, 062331 (2008).

[10] S. Fishman, G. De Chiara, T. Calarco, and G. Morigi, Phys. Rev. B **77**, 064111 (2008).

[11] G. E. Astrakharchik, G. Morigi, G. De Chiara, and J. Boronat, Phys. Rev. A **78**, 063622 (2008).

[12] J. P. Schiffer, Phys. Rev. Lett. **70**, 818 (1993).

[13] G. Piacente, I. V. Schweigert, J. J. Betouras, and F. M. Peeters, Phys. Rev. B **69**, 045324 (2004).

[14] H. Löwen, A. Härtel, A. Barreira-Fontecha, H. J. Schöpe, E. Allahyarov, and T. Palberg, J. Phys.: Condens. Matter **20**, 404221 (2008).

[15] B. Partoens and P. S. Deo, Phys. Rev. B **69**, 245415 (2004).

[16] M. G. Raizen, J. M. Gilligan, J. C. Bergquist, W. M. Itano, and D. J. Wineland, Phys. Rev. A **45**, 6493 (1992).