Rotating ground states of trapped atoms in a Bose-Einstein condensate with arbitrary two-body interactions

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Abstract

In a k-dimensional system of weakly interacting Bose atoms trapped by a spherically symmetric and harmonic external potential, an exact expression is obtained for the rotating ground states at a fixed angular momentum. The result is valid for arbitrary interactions obeying minimal physical requirements. Depending on the sign of a modified scattering length, it reduces to either a *collective rotation* or a *condensed vortex state*, with no alternative. The ground state can undergo a kind of quantum phase transition when the shape of the interaction potential is smoothly varied.

The phenomenon of Bose-Einstein condensation [1–3] observed in the magnetically trapped alkali metal vapors cooled to nanokelvin temperatures T, is extremely interesting when the system rotates [3–13]: at some critical angular velocity, the bulky irrotational condensate admits the built-in vortex lines. This signal of superfluidity, already detected in atomic gases [3], has important links to the physics of strongly interacting Bose liquids like ^{4}He where the vortices are seen directly in the density images [4,10]. The problems of vortex nucleation, their life and death (critical rotational velocities, density profiles, condensate depletion *etc*) require the knowledge of *ground states* at given angular momenta L, the so-called *yrast states* [8,12–17]. Using Feshbach resonance [2], the superfluid rotation can now be probed with controllably weak effective interatomic forces, $v \to \pm 0$. The dimensionless parameter $v = \frac{NV}{\hbar\omega} \simeq N a_s / (\frac{\hbar}{m\omega})^{\frac{1}{2}}$ characterizes the effects of the interaction V with scattering length a_s in a system of N atoms of mass m in a harmonic trap of frequency ω. In this limit, opposite to the Thomas-Fermi regime [5,11] metastability against collapse holds even for $a_s<0$ (as far as $|v| \lesssim 0.6$ [11]). The similarity of this rotating ground state problem at $T=0$ to many others (fractional quantum Hall effect [18], rotating nuclei [14], cold Fermi atoms [19]) makes it interesting in a general context.

The exact ground states were usually studied in the contact approximation $V \sim a_s \delta(\vec{r})$. The case $a_s<0$ was solved analytically by Wilkin *et al.* [8], while the case $a_s>0$ was studied numerically by Bertsch and Papenbrock [15]. The conjecture [15] for the ground state was confirmed analytically in [16]. Refs. [16], [17] establish universal properties of the repulsive and attractive cases.

Emerging possibilities to manipulate the strength, sign [2] and range [20] of the effective forces and the dimensionality [21] of the system raise natural questions: What kind of ground states can arise when the form of the interaction is arbitrarily changed? Can one classify all possible patterns, and relate them to the interaction? How do they depend on dimensionality? This Letter answers these questions, solving the ground states *exactly* for *arbitrary* two-body central forces $V(r)$ in k dimensions. The main results are the following. In the functional space $\{V\}$ of all possible interactions $V(r)$, we may restrict our attention to those of physical interest, $\{V_{phys}\}$, of which we require that the force $\frac{-dV}{dr}$ changes sign only once

$$dV/dr < 0, \quad r < R; \quad dV/dr > 0, \quad r \geq R; \quad R < 1. \tag{1}$$

Since the crossover occurs for atomic reasons, R is assumed smaller than the trapping size, $(\frac{\hbar}{m\omega})^{\frac{1}{2}}=1$, in natural units. The entire functional space $\{V_{phys}\}$ is divided into two distinct classes of (effectively) attractive $\{V^-_{phys}\}$ and repulsive $\{V^+_{phys}\}$ interactions (Fig.1). (The meaning of 'effective' in this context involves dimensionality.) Within each class the energies of the yrast states depend in a simple way on the interaction while their wave functions remain the same. The two are qualitatively distinct: $\{V^-\}$ leads to collective rotation, while $\{V^+\}$ yields vortical states. Variation of the interaction *form* can result in a quantum phase transition in the ground state, with the interparticle angular momentum as a vorticity order parameter. These exact analytical results are exemplified by the analysis of Morse potentials with variable scattering length.

The Hamiltonian in a k-dimensional symmetric trap is

$$H = \sum_{i=1}^{N} \left(\frac{\vec{p}_i^2}{2m} + \frac{m\omega^2 \vec{r}_i^2}{2} \right) + \sum_{i>i'}^{N} V(r_{ii'}) \equiv H_0 + V, \tag{2}$$

H_0 describes harmonic trapping, $\vec{r}_i \equiv \{x_i, y_i, \chi_i, ...\}$ and $\vec{p}_i$ are the i-th boson's position and momentum, V is the two-body interaction with $r_{ij} \equiv |\vec{r}_i - \vec{r}_j|$. By $|0_L)$ we denote the ground state with the conserved angular momentum component $L_{xy}=L$ and the total angular momentum $\vec{L}^2 = L(L+k-2)$, and we use the notations $z \equiv x+iy$, $z^* \equiv x-iy$. Finding $|0_L)$ requires the diagonalization of H within the space of symmetrized products

$$S z_1^{l_1} z_2^{l_2} ... z_N^{l_N} |0\rangle, \quad |0\rangle \equiv e^{-\frac{1}{2}\sum \vec{r}_n^2}, \quad \sum l_n = L, \tag{3}$$

S is the symmetrization operator. We set $\hbar=m=\omega=1$ [22]. Admixtures of the states other than $\varphi_l \equiv z^l e^{\frac{-\vec{r}^2}{2}}$ cost energy $\geq \hbar\omega$, they are neglected for $|v| \ll 1$. Within the subspace (3) the Hamiltonian (2) becomes

$$H = L + (Nk)/2 + W, \tag{4}$$

where W is the interaction V, projected onto the subspace (3). With the ladder operators $\hat{a}_i^+ = z_i/2 - \partial/\partial z_i^*$, $\hat{a}_i = z_i^*/2 + \partial/\partial z_i$ we have $L = \sum_i \hat{a}_i^+ \hat{a}_i$, and using the Fourier transform of arbitrary interaction $V(r)$ [23], we get

$$W = S \sum_{i>j} w(\hat{l}_{ij}) S, \quad \hat{l}_{ij} = (\hat{a}_i^+ - \hat{a}_j^+)(\hat{a}_i - \hat{a}_j)/2, \tag{5}$$
$$w(l) \equiv \int_0^\infty V(\sqrt{2t}) \xi(l) dt, \quad \xi(l) \equiv e^{-t} \frac{t^{l+k/2-1}}{\Gamma(l+k/2)},$$

$\hat{l}_{ij}$ is the relative angular momentum of two atoms. The sum $\mu = \frac{1}{N} \sum_{i,j} \hat{l}_{ij} = 0, 2, 3, .., L$ is an additional quantum number $[\mu, H] = [\mu, L] = 0$. The relation $L = \mu + \frac{1}{N} \sum_i a_i^+ \sum_j a_j$ reflects distribution of the angular momentum between the vortical and other internal modes (μ) and the collective surface-type modes (second term). The structure of (5) is universal, dimensionality is hidden in $w(l)$.

As usual in a many-body system, the number of states (3) grows exponentially with L. Complete diagonalization of (5) is hardly possible. Instead, we seek the exact ground state by splitting [16] the interaction into $W{=}W_0{+}W_S$ such that W_0 is simple enough to find its lowest eigenvalue $\mathcal{E}_0$ and its associated eigenstate $|0)$, and such that $|0)$ is destroyed by W_S

$$W_0|0) = \mathcal{E}_0|0), \quad W_S|0) = 0. \tag{6}$$

The state $|0)$ will also be the ground state of $W_0{+}W_S$ with the eigenvalue $\mathcal{E}_0$ if W_S is *non-negative definite*,

$$W_S \equiv S \sum\nolimits_{i>j} v_S(\hat{l}_{ij}) S \geq 0, \tag{7}$$

having no negative eigenvalues. This condition is the most problematic in solving (6,7) as the eigenvalues of W_S cannot be evaluated in general. It will be controlled exactly as follows. First, we write the operator W_0 as

$$W_0 = S \sum_{i>j} v_0(\hat{l}_{ij}) S, \quad v_0(l) = \sum_{0\leq n<m} c_n l^n, \tag{8}$$

where c_n are hitherto unknown coefficients that need to be fixed to satisfy (6) and (7). The operator $v_S(\hat{l}_{ij})$ is diagonalized in the states $z_1^{l_1} z_2^{l_2} ... z_N^{l_N}|0\rangle$ via the substitution $z_i{\to}z_-, z_j{\to}z_+$, $z_\pm{\equiv}(z_i{\pm}z_j)/\sqrt{2}$. Its eigenvalues are $w(l){-}v_0(l)$, with $l{=}0,1,2,...,L$ the eigenvalue of $\hat{l}_{ij}$. Odd-l eigenvectors are antisymmetric ($\propto z_-^l$) and they are annihilated by S [24]. Therefore, a reasonable choice of c_n is to cancel the first m even-l eigenvalues $\lambda_n{\equiv}w(2n){-}v_0(2n)$ keeping $\lambda_n{\geq}0$ for all n. This will be sufficient for (7): a sum of non-negative operators is also non-negative, and a projector S preserves this property. Superpositions of vectors with $l{<}2m$, $|\alpha\rangle$, can be tried to construct the symmetrized state $|0)$ obeying (6). One can start with low m, increasing it if necessary. If $m{=}2$, Eqs.(6,8) give $\mathcal{E}_0{=}c_0\mathcal{N}{-}c_1\theta(-c_1)NL/2$ with $\theta(x){\equiv}\{^{1,x>0}_{0,x\leq 0}$ and $\mathcal{N}{=}(N^2{-}N)/2$. The trial state is $|\alpha\rangle{=}\prod_j^L \sum_{i=1}^N (z_i{-}z_j\alpha_j)|0\rangle$ with

α_j real numbers. If all α_j are 0 or 1, $S|\alpha\rangle$ becomes eigenstate of W_0 with eigenvalue $\mathcal{E}{=}w(0)\mathcal{N}{+}[w(2){-}w(0)]N\sum_j\alpha_j/4$. The minimum of $\mathcal{E}$ with respect to $\{\alpha_j\}$ coincides with $\mathcal{E}_0$, and the corresponding $S|\alpha\rangle$ obeys both conditions (6), if

$$
\begin{gathered}
c_0 = w(0), \qquad c_1 = -\Delta_2\theta(\Delta_2)/2, \qquad c_{n\geq 2} = 0; \\
\Delta_{2n} \equiv w(0) - w(2n) = \int_0^\infty \phi_{2n} f dt, \quad \phi_{2n} \equiv \sum_{i=1}^{2n} \xi(i).
\end{gathered} \tag{9}
$$

With $f{\equiv}{-}dV(\sqrt{2t})/dt$ the "force", Δ_{2n} can be viewed as the work needed to produce vorticity. Now (7) holds for all V_{phys} defined in (1): $\lambda_n{=}n\theta(\Delta_2)\Delta_2{-}\Delta_{2n}$ and

$$
\lambda_n = \int_0^\infty (n\theta(\Delta_2) - h_n)\phi_2 f dt \geq 0, \quad h_n \equiv \phi_{2n}/\phi_2. \tag{10}
$$

Indeed, by (1) the integrand of Δ_2 in (9) is positive at $t{<}\tau{\equiv}R^2/2$ and negative at $t{>}\tau$, see Fig.1b. If negative area prevails in the elementary work Δ_2, then all $\lambda_{n>0}{>}0$, because h_n increase with t monotonously. In the opposite case ($\Delta_2{>}0$) the positive area ($t{<}\tau$) prevails in Δ_2. Positive contribution from this area will then also prevail in $\lambda_{n>1}$ because $\frac{d(n-h_n)}{dt}{<}0$. In fact, the factors $n{-}h_n$ become negative for $t{>}t_n$ with all $t_n{>}1{>}\tau$, thereby reducing the dangerous contribution to λ_n from $t{>}\tau$. Thus the proper choice of $|\alpha\rangle$ gives exact ground state of (4) and its energy E_0 as functions of L ($L{\leq}N$)

$$
\begin{gathered}
|0_L\rangle = e^{-\frac{1}{2}\sum r_i^2} S \prod_{j=1}^{L} \sum_{i=1}^{N} [z_i - z_j\theta(\Delta_2)\epsilon_L], \\
E_0(L) = L + \frac{Nk}{2} + \frac{N^2 - N}{2} w(0) - \frac{\epsilon_L N L \Delta_2 \theta(\Delta_2)}{4},
\end{gathered} \tag{11}
$$

with $\epsilon_L{=}\theta(L{-}1)$. The wave functions depend on $V(r)$ only via the sign of the vortical work quantum

$$
\Delta_2(k) = \frac{2^{1-k/2}}{\Gamma(k/2)} \int_0^\infty \tilde{V} r^{k-1} dr, \quad \tilde{V} = V(r) \frac{1 - \frac{r^4}{k^2+2k}}{e^{r^2/2}} \tag{12}
$$

which has the form of Born scattering length by the potential $\tilde{V}$. The interactions V^0_{phys} satisfying the equation

$$
\Delta_2(k) = 0, \tag{13}
$$

form the *separatrix* manifold: it divides the interactions $V_{phys}(r)$ into the two classes $\{V^-_{phys}\}$ and $\{V^+_{phys}\}$, with qualitatively different ground state: If $\Delta_2 \leq 0$, (11) gives

$$|0^-_L) = e^{-\frac{1}{2}\sum \vec{r}_i^2} Z^L, \qquad \mu|0^-_L) = 0,$$

where $Z \equiv \sum_i^N \frac{z_i}{N}$ [25] while for $\Delta_2 \geq 0$ and $L > 1$ it gives

$$|0^+_L) = e^{-\frac{1}{2}\sum \vec{r}_i^2} S \bar{z}_1 \bar{z}_2 ... \bar{z}_L, \qquad \mu|0^+_L) = L|0^+_L),$$

with $\bar{z}_j = Z - z_j$. Here μ can be viewed as an order parameter; in fact, the major difference between $|0^-)$ and $|0^+)$ is their vortical correlations. The condensation signatures can be studied from the occupancies $\nu^\pm_n$ of the single-particle orbits $\varphi_n \propto z^n$ in the ground states $|0^\pm)$ and the density profiles $\rho(\vec{r}) \equiv \sum_n \nu_n |\varphi_n|^2$. We obtain

$$\nu^+_n = \frac{(N\sigma^2 - \sigma\kappa + N^2 n) p^N_{L-n}(\kappa) + (1 + 2\sigma + \kappa) p^{N+1}_{L-n}(\kappa)}{N^L (N+1)^{n+2-L} n! p^{N+1}_L(-N)},$$

where $\kappa = -N^2/(N+1)$, $\sigma = N(1-n) - L$ and $p^b_a(s) = \Gamma(a-b)\mathcal{L}^{-b}_a(s)$ with $\mathcal{L}^b_a(s)$ the Laguerre polynomial [26]. Similarly, we have $\nu^-_n = \frac{L!(N-1)^{L-n}}{(L-n)!n!N^L}$. In the limit $N \gg 1$ of primary experimental interest, the quantities depend on L and N via the angular momentum per particle $\bar{l} = L/N$

$$\nu^+_n = \frac{\sqrt{\bar{l}}(\frac{s}{2} + n)^2}{v^{1-n} n! e^v}, \quad \rho^+ = \sqrt{\bar{l}} \frac{(u^2 + s^2) I_0(u) + 2su I_1(u)}{4\pi^{k/2} v e^v exp(\vec{r}^2)},$$

where $v = \sqrt{\bar{l}} - \bar{l}$, $s = 2(\bar{l} - 1)$, $u = 2\sqrt{v}|z|$, and I_n is the modified Bessel function [26]; $\rho^- = I_0(2\sqrt{\bar{l}}|z|)/(\pi^{k/2} e^{\bar{l} + \vec{r}^2})$ and $\nu^-_n = e^{\bar{l}} \bar{l}^{\ n}/n!$. This scaling limit works for $N \gtrsim 10$. The density profiles ρ are shown in Fig.2a. The reduced central density at $\bar{l} \to 1$ signals vortex formation in the state $|0^+)$. We call the branch $|0^+_L)$ *condensed vortex* states. As L grows, the atoms leave the state z^0 for z^2, and next z^1 takes over, see Fig.2b. For $L \to N \gg 1$ they condense in the state z^1, forming a vortex. The sum $\nu^+_0 + \nu^+_1 + \nu^+_2$ never drops below 0.97: ν^+_n describes a kind of fragmented [10] condensate. The distribution ν^-_n is systematically broader, see Fig.2c. At high L there are no preferred occupancies. We call $|0^-_L)$ a *collective rotation* state: Its angular momentum is due to the collective factor Z^L corresponding to a rotation of a non-interacting condensate [27]. Indeed, both $|0_L^-)$ and $|0\rangle$ are seen to have the same two-body correlation function $\zeta(\vec{r}){=}\langle\sum_{i\neq i'}\delta(\vec{r}{-}\vec{r}_{ii'})\rangle$.

The expectation value of the contact interaction in the ground state coincides, up to the strength factor $\propto a_s$, with $\zeta(0)$. Both are minimal in the state $|0^+)$ if $a_s{>}0$: repulsion tends to maximize vorticity, producing hole in $\zeta(\vec{r})$ and $\rho_{\bar{l}\to 1}(\vec{r})$. The opposite is typical for attraction ($a_s{<}0$). This sheds light on the universality of the solutions: the wave functions for arbitrary $V(r)$ and k are simple generalizations of the results for $\pm\delta(\vec{r})$ [8], [15] and the corresponding universality classes [16], [17]. The control parameter $\Delta_2(k)$ measures the balance between repulsion and attraction in a realistic interaction $V_{phys}(r)$.

Let the infinitesimally deformed trap rotate in the x,y plane with angular velocity Ω. In the co-rotating frame, we have $H{\to}H{-}\Omega L$ [12]. By (7,9), the minimum of $E_0(L){-}\Omega L$ at $L{=}0$ is shifted to $L{>}0$ for $\Omega{\geq}\Omega_c$ with

$$\Omega_c = 1 - N\theta(\Delta_2(k))\Delta_2(k)/4, \tag{14}$$

the vortex nucleation threshold in terms of $V(r)$ and k. Eq.(14) generalizes the result for contact interaction [13].

Tuning the interaction, one observes a controllable phase transition in the ground state, as is illustrated in Fig.3a,b for the Morse potential $V_M{=}e^{\frac{2(R-r)}{a}}\ {-}2e^{\frac{R-r}{a}}$. For the critical interaction $V^0_{phys}(r)$ ($\Delta_2{=}0$), the ground state becomes multiply degenerate: The states $|\mu\rangle\equiv S|\alpha\rangle$ with $\alpha_j{=}\theta(\mu{+}1{-}j)$ discussed above have the same energy, see Fig.3b [28]. The states $|0_L^-)\equiv|\mu{=}0)$ and $|0_L^+)\equiv\ |\mu{=}L\rangle$ are unique ground states for $\Delta_2{<}0$ and $\Delta_2{>}0$, respectively. For $\Delta_2{\gtrless}0$, $|0_L^{\mp})$ remain exact excited eigenstates. A sudden change of sign of Δ_2 allows to observe them as metastable states. Fig.3c shows $V_M(r)$ and the resulting even part $w_e(l){\equiv}w(l{=}2n)$ of its transform (5)

$$w(l) = \{1/2\}_g[e^{\frac{2R}{a}}d^{(\frac{2}{a})}_{-2g} - 2e^{\frac{R}{a}}d^{(\frac{1}{a})}_{-2g}], \quad g = l + k/2, \tag{15}$$

for two sets a and R. Here $\{\alpha\}_b{=}\frac{\Gamma(\alpha+b)}{\Gamma(\alpha)\alpha^b}$ and $d_l^{(s)}\ {=}e^{\ s^2/4}\ D_l\ (s)$ with $D_l(s)$ the parabolic cylinder function [26]. Near the critical point, $w_e(l)$ behaves like a thermodynamic potential in a second-order phase transition [29]: For $\Delta_2<0$, w_e has a minimum at $l=0$. As repulsion prevails, $\Delta_2>0$, the minimum of w_e is shifted to $l>0$. The factor θ in the solutions (9,11) results from this threshold behavior, generic within V_{phys}. This "phase transition" persists for finite N and in all dimensions $k\geq 2$.

The separatrices $\Delta_2(k)=0$ between $\{V^-\}$ and $\{V^+\}$ define the curves $\gamma_k(a)=\frac{R}{a}$ on the phase diagram for V_M in the parametric space $(a,\frac{R}{a})$, Fig.3d. The relation $\gamma_3(a)>\gamma_2(a)$ reflects the dimensionality effect that is generic within $\{V_{phys}\}$: By the relations similar to Eq.(10), the vortical work quantum $\Delta_2(k)$ decreases as k grows, so the phase space grabbed by the condensed vortex states shrinks. (The long-range attraction works like surface tension, preventing vortex nucleation at higher k.) Thus $|0_L)=|0_L^+)$ for $k<k_c$ and $|0_L)=|0_L^-)$ for $k>k_c$, where k_c is defined by Eq.(13). If $2<k_c<3$, this dimensional destabilization of vortex can be tested experimentally. This condition is met by V_M with the parameters used in [30] for Li atoms, see Fig.3d.

From (15) one can show that (7) holds throughout: $\lambda_n^-\equiv-\Delta_{2n}\geq 0$ for $\frac{R}{a}\leq\gamma(a)$ and $\lambda_n^+\equiv n\Delta_2-\Delta_{2n}\geq 0$ for $\frac{R}{a}\geq\gamma(a)$. Thus *all* Morse potentials are covered by (11) and fall into two classes decided by the sign of Δ_2. Other multiparametric potential families give similar results.

Is this situation generic? The dense functional manifold $\{V_{phys}\}$ is a part of the complete functional space $\{V\}$ (see Fig.1a), in general it cannot be described by a countable number of parameters. Within $\{V\}$, we can still define the subclasses that have $\lambda_n^-\geq 0$ and $\lambda_n^+\geq 0$ with the ground states $|0_L^-)$ and $|0_L^+)$, respectively. Their boundaries Λ^- and Λ^+ can in general be distinct, leaving room marked by "?" when the ground state is not (11). For example, $V=-|a|\theta(R-r)$ with $R>2.8$ gives $|0_{L=N=4})=\sum_{ij}(z_i-z_j)^4|0\rangle$ for $k=2$. While extensions of V_{phys} are possible (like V_M with $R>1$, see also below), no general trends can be readily established beyond (1). The absence of such *nonuniversality gap* within $\{V_{phys}\}$ is a nontrivial consequence of the constraint (1): The coexistence region V_{phys}^0 (the separatrix) divides the interactions $\{V_{phys}\}$ into two classes, with the ground states $|0_L^-)$ and $|0_L^+)$ with no other alternative.

By similar arguments, one can append the class $\{V_{phys}\}$ (1) by potentials with constant sign of f and $\frac{df}{dt}$, like $\delta(\vec{r})$, $1/r$, $log(r)$, $e^{-r/a}$, $e^{-r/a}/r$, e^{-r^2/a^2} *etc.* We obtain $sign[\Delta_2(k)]{=}sign(f)$ and $V^0{=}0$. Thus $k_c{=}\infty$: Dimensional destabilization of vortex is impossible, such potentials do not share this property of V_{phys}.

The above results give complete description of what happens to the rotating ground states of weakly interacting bosons. In the weak coupling limit, which can be easier approached for moderate number of atoms ($N{\sim}10^2{-}10^3$), the system becomes an ideal laboratory to study the rotational features of degenerate quantum gases, since direct comparison with complete theory is available. With minor modifications, the above results are valid for axially symmetric deformed trap. The same techniques allow to obtain universal results for trapped Fermi atoms [31]; they can also be applied to Bose-Fermi mixtures.

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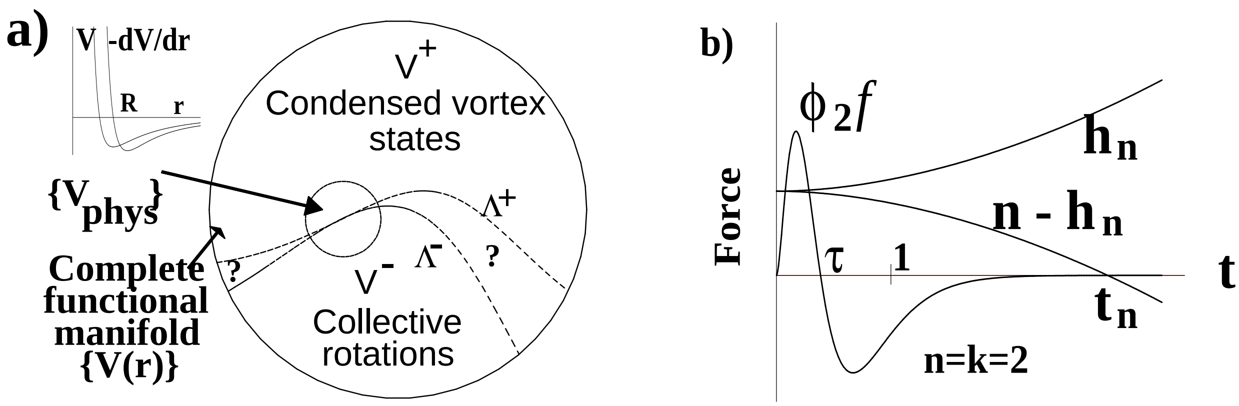

FIG. 1. a) Global phase diagram in the functional space $\{V(r)\}$. b). Vortical work balance (see Eq.(10)).

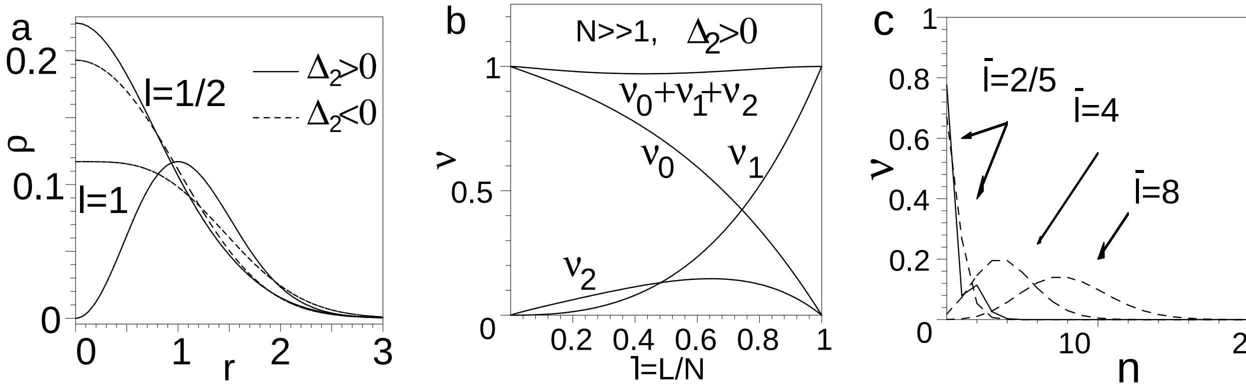

FIG. 2. a) Ground-state matter distributions (k=2). b) Asymptotic condensate occupancies ν_n^+ versus $\bar{l}$. c) ν_n as a function of n for Δ_2>0 (solid) and Δ_2<0 (dashed), N=30.

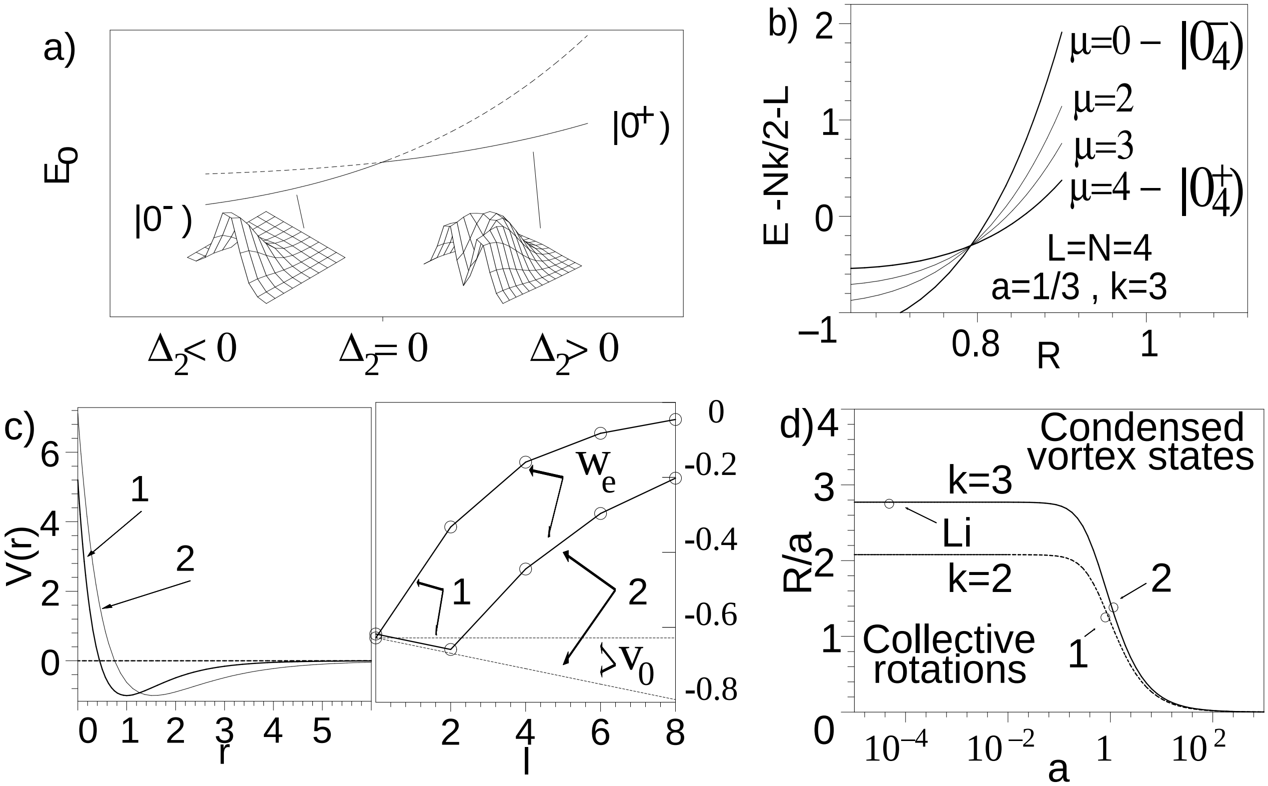

FIG. 3. (a) Energies of $|0^{\pm})$ and the density profiles versus Δ_2. (b) The interaction energy in the states $|\mu\rangle$ versus R for the Morse potential. (c) The Morse potential $V_M(r)$ (left) and $w_e(l)$, $v_0(l)$ (right) in k=3 for two sets of parameters "1" and "2" which are shown on the $\frac{R}{a}$,a-plane of the phase diagram (d). Curves are the separatrices γ_k.