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Quantum monodromy in trapped Bose condensates

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Abstract. – Bose-Einstein condensation of ultra cold atoms is typically realized in magnetic traps which effectively lead to an axially symmetric harmonic potential. This letter shows that the spectrum of collective vibrational modes of a repulsive condensate in a prolate potential displays a defect known as *quantum monodromy*. The monodromy is analysed on the basis of the dynamics of quasiparticles. In terms of the quasiparticles the regime of collective modes or the so-called *hydrodynamic regime* is characterized through kinetic energies much smaller than the chemical potential. In this limit the classical dynamics of the quasiparticles is integrable. The monodromy is quantitatively described by a monodromy matrix that is calculated from classical actions.

Introduction. – In the context of integrable Hamiltonian systems with two degrees of freedom the notion *monodromy* was first introduced by Duistermaat [1]. It there describes the effect of a global twisting of a family of invariant 2-tori parameterized by a circle of regular values of the energy momentum mapping of the integrable system. A consequence of monodromy is the obstruction in the global definition of single-valued smooth action variables. In this way monodromy carries over to quantum mechanics via *Einstein-Brillouin-Keller* quantization as was first illustrated for the quantum spherical pendulum by Cushman and Duistermaat [2] followed by other systems [3] in atomic physics [4] as well as in molecular physics [5, 6].

This letter reports on the monodromy of the spectrum of collective excitations of a Bose condensate of atoms trapped in a prolate axially symmetric harmonic potential. To describe the monodromy the quantum-mechanical spectrum is related to the underlying integrable classical dynamics of the corresponding quasiparticles.

Classical quasiparticle dynamics. – Bose condensates are most suitably described in terms of quantum field theory (see [7] for a review and for the references). The essential idea due to Gross and Pitaevskii is to separate off the ground-state wave function from the rest and to consider the rest as a kind of perturbation. This way the field operator of the condensate $\hat{\Psi}(\mathbf{x})$ splits into two parts, $\hat{\Psi}(\mathbf{x}) = \psi_0(\mathbf{x}) + \hat{\varphi}(\mathbf{x})$, where the first-order contribution of the residual field operator $\hat{\varphi}(\mathbf{x})$ vanishes if the scalar wave function $\psi_0(\mathbf{x})$ fulfills the Gross-Pitaevskii equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi_0(\mathbf{x}) + (U(\mathbf{x}) - \mu)\psi_0(\mathbf{x}) + V_0|\psi_0(\mathbf{x})|^2\psi_0(\mathbf{x}) = 0, \quad (1)$$

where μ is the chemical potential. The scalar wave function is normalized to the number of condensed atoms, $\int |\psi_0(\mathbf{x})|^2 d^3x = N_0$. $U(\mathbf{x})$ is the outer potential which in case of a magnetic trap is effectively of harmonic type,

$$U(\mathbf{x}) = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2). \quad (2)$$

Usually, the traps are axially symmetric, *i.e.* $\omega_x = \omega_y = \omega_0$ without restriction. The factor V_0 determining the strength of the two-particle interaction is given by $V_0 = 4\pi\hbar^2 a/m$, where a is the s -wave scattering length which is positive for a repulsive condensate. In the Thomas-Fermi approximation the kinetic term in the Gross-Pitaevskii equation is neglected giving

$$|\psi_0(\mathbf{x})|^2 = \frac{1}{V_0}(\mu - U(\mathbf{x})). \quad (3)$$

A quasiparticle interpretation of the excitations is obtained from the Bogoliubov transform of the residual field operator $\hat{\varphi}(\mathbf{x})$,

$$\hat{\varphi}(\mathbf{x}) = \sum_j \left(U_j(\mathbf{x}) \hat{\alpha}_j - V_j^*(\mathbf{x}) \hat{\alpha}_j^\dagger \right), \quad (4)$$

where the creation and annihilation operators $\hat{\alpha}_j^\dagger$ and $\hat{\alpha}_j$ fulfill bosonic commutator relations and the amplitudes obey the normalization condition $\int (|U_j(\mathbf{x})|^2 - |V_j^*(\mathbf{x})|^2) d^3x = 1$.

The field equations become diagonal to second order in the residual operator if the amplitudes U_j and V_j fulfill the coupled Bogoliubov equations

$$\hat{H}_{\text{HF}} U_j - K V_j = E_j U_j, \quad -K U_j + \hat{H}_{\text{HF}} V_j = -E_j V_j \quad (5)$$

with the Hartree-Fock Hamiltonian $\hat{H}_{\text{HF}} = -\hbar^2/(2m)\nabla^2 + U(\mathbf{x}) + 2V_0|\psi_0(\mathbf{x})|$ and the coupling term $K = V_0|\psi_0(\mathbf{x})|$.

Following [8] we obtain a classical Hamiltonian H from replacing the kinetic term $-(\hbar^2/(2m))\nabla^2$ by the classical expression $\mathbf{p}^2/(2m)$ and solving the secular equation corresponding to the Bogoliubov equations (5) for $H = E$. This gives the classical Hamiltonian

$$H(\mathbf{x}, \mathbf{p}) = \sqrt{H_{\text{HF}}(\mathbf{x}, \mathbf{p}) - K(\mathbf{x})} \quad (6)$$

with $H_{\text{HF}}(\mathbf{x}, \mathbf{p}) = \mathbf{p}^2/(2m) + U(\mathbf{x}) + 2V_0|\psi_0(\mathbf{x})|$. For \mathbf{x} within the boundary $U(\mathbf{x}) = \mu$ of the condensate in Thomas-Fermi approximation (see eq. (3)) $H(\mathbf{x}, \mathbf{p})$ can be written as $H(\mathbf{x}, \mathbf{p}) = (T(\mathbf{p})(T(\mathbf{p}) + 2K(\mathbf{x}))^{1/2}$ with $T(\mathbf{p}) = \mathbf{p}^2/(2m)$. The *hydrodynamic regime* is defined as the limit where the kinetic energy is much smaller than the chemical potential μ , *i.e.* the coupling $K(\mathbf{x})$ is much bigger than $T(\mathbf{p}) = \mathbf{p}^2/(2m)$. The classical Hamiltonian which describes the quasiparticle dynamics in this limit is obtained from rewriting H in the form $H = \sqrt{TK} \sqrt{2 + T/K}$ and neglecting T/K in the second square root. This gives the hydrodynamic Hamiltonian

$$H_{\text{hyd}}(\mathbf{x}, \mathbf{p}) = \sqrt{2TK(\mathbf{x})}. \quad (7)$$

Prolate trap potential. – For the harmonic potential $U(\mathbf{x})$ in eq. (2) the equations of motion generated by H_{hyd} are separable [8]. In the following we will concentrate on a potential with harmonic frequencies $\omega_0 > \omega_z$. In this case the boundary of the Thomas-Fermi condensate is the prolate ellipsoid

$$\frac{\varrho^2}{a_\varrho^2} + \frac{z^2}{a_z^2} = 1, \quad \varrho^2 = x^2 + y^2 \quad (8)$$

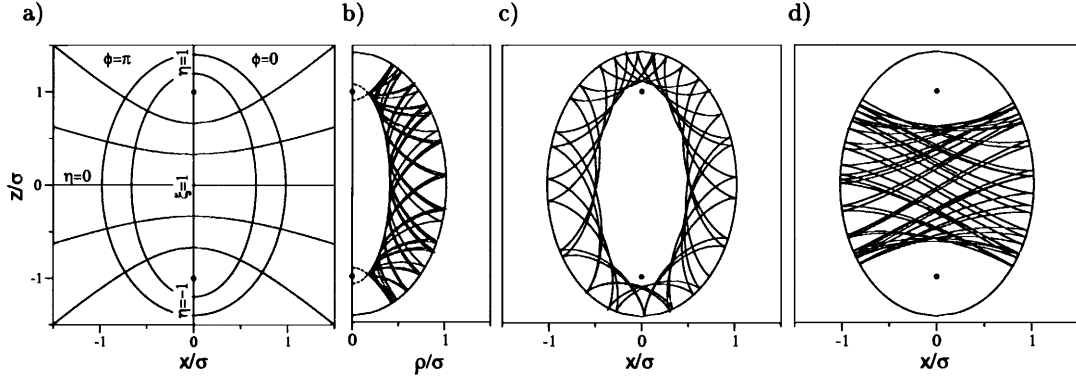


Fig. 1 – a) Ellipsoidal coordinates in the plane (x, z) . b) Trajectory of a generic Liouville-Arnold torus in configuration space (x, ρ) . c) “Whispering gallery” orbit in the plane (x, z) . d) “Bouncing ball” orbit in the plane (x, z) .

with semi-axes $a_\rho^2 = 2\mu/(m\omega_0^2) < a_z^2 = 2\mu/(m\omega_z^2)$, focus points $(x, y, z) = (0, 0, \pm\sigma)$ with $\sigma^2 = 2\mu/m(1/\omega_z^2 - 1/\omega_0^2)$, and eccentricity $\epsilon = (1 - \omega_z^2/\omega_0^2)^{1/2}$. The equations of motion are then separable in prolate ellipsoidal coordinates:

$$(x, y, z) = \sigma(\varrho \cos \phi, \varrho \sin \phi, \eta\xi), \quad \varrho = \sqrt{(\xi^2 - 1)(1 - \eta^2)} \quad (9)$$

with coordinate ranges $\phi \in [0, 2\pi]$, $\eta \in [-1, 1]$ and $\xi \in [1, \infty)$, see fig. 1a. The boundary of the Thomas-Fermi condensate is the coordinate surface $\xi = 1/\epsilon$.

The angle ϕ is a cyclic variable in the transformed H_{hyd} and, accordingly, the angular momentum l about the symmetry axis is a further constant of motion besides the energy $E = H_{\text{hyd}}$. A third constant appears as a separation constant. Ordering terms in the equality $E^2 = H_{\text{hyd}}^2$ yields

$$B = \tilde{E}^2 \frac{1}{1 - \epsilon^2 \eta^2} + (1 - \eta^2) p_\eta^2 + \frac{1}{1 - \eta^2} l^2 = \tilde{E}^2 \frac{1}{1 - \epsilon^2 \xi^2} - (\xi^2 - 1) p_\xi^2 - \frac{1}{\xi^2 - 1} l^2, \quad (10)$$

where p_η and p_ξ denote the momenta conjugate to η and ξ , respectively, and $\tilde{E}^2 = 2E^2/\omega_0^2$. Incorporating in eq. (10) the fact that η varies in the interval $[-1, 1]$ shows that B is always positive, wherefore we write b^2 instead of B . Since the second and the third expression in eq. (10) are identical up to a relabeling of the phase space variables, the squared momenta can be written in the same form,

$$p_s^2 = \tilde{E}^2 \frac{1}{(1 - s^2)^2 (1 - \epsilon^2 s^2)} P_2(s^2), \quad s = \eta, \xi, \quad (11)$$

where P_2 is the binomial $P_2(z) = b^2(1 - z)(1 - \epsilon^2 z) - \tilde{E}^2(1 - z) - l^2(1 - \epsilon^2 z)$. Equation (11) scales with respect to the energy.

The physical ranges of the constants of motion E , B and l are determined from the requirement that they simultaneously must allow for real momenta p_η and p_ξ in eq. (11). This means that there have to exist in both intervals $[-1, 1]$ and $[1, 1/\epsilon]$ subintervals where $P_2(x^2)$ is positive. For $l \neq 0$ the only way for this to occur is that the roots s_1^2 and s_2^2 of P_2 are real and satisfy

$$0 < s_1^2 < 1 < s_2^2 < \frac{1}{\epsilon^2}. \quad (12)$$

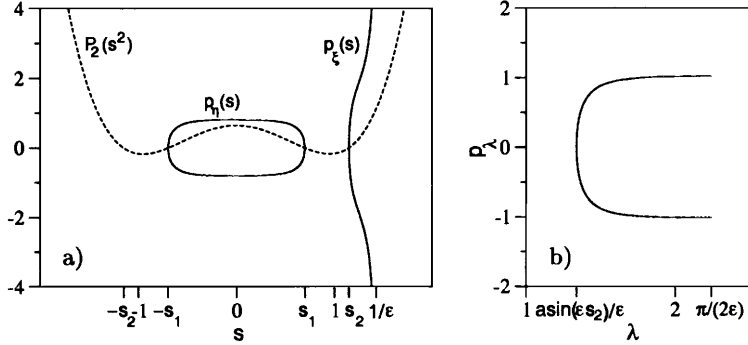


Fig. 2 – a) Phase portraits (η, p_η) and (ξ, p_ξ) and the binomial $P_2(s^2)$. b) Regularization of the singular reflection at the condensate boundary $\xi = 1/\epsilon$ via the canonical transformation $(\xi, p_\xi) \mapsto (\lambda, p_\lambda)$ with $\xi = \frac{1}{\epsilon} \sin(\epsilon\lambda)$ and $p_\lambda = \frac{d\xi}{d\lambda} p_\xi$.

The phase portraits (η, p_η) and (ξ, p_ξ) for a corresponding Liouville-Arnold 3-torus are shown in fig. 2a, *i.e.* η oscillates in $[-s_1, s_1]$ and ξ in $[s_2, 1/\epsilon]$. Similarly, the corresponding trajectory in configuration space is bounded by the η -caustics $\eta = \pm s_1$, the ξ -caustic $\xi = s_2$ and the condensate boundary $\xi = 1/\epsilon$, see fig. 1b.

Critical motions essentially correspond to the boundaries in (12). $s_1 = 0$ or, equivalently, $b^2 = l^2 + \tilde{E}^2$ represents invariant 2-tori of elliptic stability. In configuration space the corresponding motions are restricted to the equatorial plane $z = 0$. In particular, $l = 0$ represents the resonant 2-torus foliated by the one-parameter family of periodic orbits obtained from rotating, *e.g.*, the periodic orbit along the x -axis about the z -axis. $s_2 = 1/\epsilon$ is equivalent to $E = 0$ and represents motion on the surface of the Thomas-Fermi condensate. $s_1 = 1$ and $s_2 = 1$ correspond to $l = 0$. In addition to the critical cases already mentioned, $l = 0$ is critical only for $s_1 = 1$ and $s_2 = 1$, simultaneously, or $b^2 = b^{*2} = \tilde{E}^2/(1 - \epsilon^2)$. The corresponding motion is the unstable periodic orbit running along the z -axis. The non-critical motions with $l = 0$ are resonant 3-tori foliated by invariant 2-tori of planar motions. For $s_1 = 1$ and $1 < s_2 < 1/\epsilon$ or $b^2 > b^{*2}$ the η -caustics have collapsed and the “whispering gallery” type of motion crosses the z -axis outside of the focus points $(x, y, z) = (0, 0, \pm\sigma)$, see fig. 1c. For $s_2 = 1$ and $0 < s_2 < 1$ or $b^2 < b^{*2}$ the ξ -caustic has collapsed and the “bouncing ball” type of motion crosses the z -axis between the focus points, see fig. 1d.

Disregarding the critical case $E = 0$, we represent the critical values of the constants of motion in a bifurcation diagram in terms of the scaled constants $l_{sc} = l/\tilde{E}$ and $b_{sc} = b/\tilde{E}$. The resulting diagram shown in fig. 4a below contains the isolated point $(l_{sc}, b_{sc}) = (0, b_{sc}^*) = (0, (1 - \epsilon^2)^{-1/2})$, wherefore the range of regular values of the constants of motions is not simply connected.

Quantum monodromy. – The quantum-mechanical spectrum of the Bose condensate, *i.e.* the spectrum of the quasiparticles in our approximation, is obtained from the EBK quantization of classical actions. For the integration of actions we have to decide on a triple of fundamental loops γ_i on the 3-tori in phase space along which the differential $\mathbf{p}d\mathbf{q}$ is integrated. A natural choice is a triple that is related to the separating coordinates giving the actions

$$I_\varphi = l, \quad I_\eta = \frac{2}{\pi} \int_0^{s_1} p_\eta d\eta, \quad I_\xi = \frac{1}{\pi} \int_{s_2}^{1/\epsilon} p_\xi d\xi. \quad (13)$$

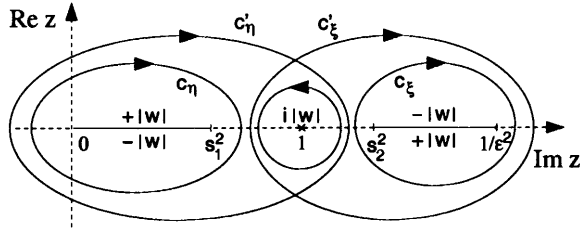


Fig. 3 – Complex plane $\mathbb{C}(z)$ with slits between the pairs of branch points $(0, s_1^2)$ and $(s_2^2, 1/\epsilon^2)$, respectively, and integration paths c_s and c'_s for the calculation of actions and their derivatives with respect to the angular momentum, respectively. The square root w is defined so that its values along the real axis are as indicated in the figure.

This way $2\pi I_\eta$ and $2\pi I_\xi$ are the areas enclosed by the respective phase portraits in fig. 2. The quantum spectrum is defined from the EBK quantization conditions $(I_\varphi, I_\eta, I_\xi) = \hbar(n_\varphi, n_\eta + \alpha_\eta/4, n_\eta + \alpha_\xi/4)$ with quantum numbers $n_\varphi \in \mathbb{Z}$ and $n_\eta, n_\xi \in \mathbb{N}_0$ and Maslov indices $\alpha_\eta = 2$ for a simple oscillation and $\alpha_\xi = 3$ for an oscillation involving a reflection at the condensate boundary $\xi = 1/\epsilon$. The quantum spectrum is a point set $(E, l, b)_{(n_\varphi, n_\eta, n_\xi)}$ in the three-dimensional space of the constants of motion. It has a natural lattice structure due to the EBK quantum numbers. As we will see in the following, this lattice has a defect known as quantum monodromy due to the isolated point of the bifurcation diagram in fig. 4a below.

In order to recover the quantum monodromy let us first have a look at the analytical nature of the action integrals. For this purpose it is convenient to substitute $z = s^2$ and write them as

$$I_s = \frac{n_s}{4\pi} \oint_{c_s} \frac{P_2(z)}{1-z} \frac{dz}{w}, \quad s = \eta, \xi, \quad (14)$$

where n_s are integer coefficients, c_s are integration paths in the complex plane, and w is the square root of the fourth-order polynomial $z(1-\epsilon^2z)P_2(z)$ indicating that the action integrals are of elliptic type. The square root w can only be defined properly if the complex plane is slit twofold between two pairs of branch points of w , see fig. 3. With the integration paths c_η and c_ξ defined as in fig. 3, the expressions for the actions I_η and I_ξ in eqs. (13) and (14) become identical if $(n_\eta, n_\xi) = (2, 1)$.

Despite the fact that the half-line $l = 0$, $b_{sc} > 1$ in fig. 4a represents critical motions only for $b_{sc} = b_{sc}^*$, the actions I_η and I_ξ are continuous but nowhere differentiable across this half-line. To see this, note that I_η and I_ξ are symmetric functions of l , wherefore their derivatives with respect to l would have to vanish along $l = 0$ if the actions were smooth. The derivatives

$$\frac{\partial I_s}{\partial l} = l \frac{n_s}{4\pi} \oint_{c_s} \frac{1-\epsilon^2z}{z-1} \frac{dz}{w}, \quad s = \eta, \xi, \quad (15)$$

contain the vanishing pre-factor l but, in addition, either the η -integral or the ξ -integral becomes singular for $l \rightarrow 0$ because of the collision of the branch point s_1^2 with the pole at $z = 1$ for $b > b^*$ or of s_2^2 with $z = 1$ for $b < b^*$. To evaluate the integrals for $l \rightarrow 0$ it is best to modify the integration paths c_s as shown in fig. 3, *i.e.* the c_s are wrapped across the pole $z = 1$ to give the paths c'_s , where the capture of the pole is subtracted by the small integration path encircling the pole in the opposite direction. Noticing that the integrals (15) along the c'_s are not critical and that the differential $(1-\epsilon^2z)/((z-1)w) dz$ has residue $-i/|l|$ at $z = 1$, we find

$$\lim_{l \rightarrow 0^+} \left(\frac{\partial I_\eta}{\partial l}, \frac{\partial I_\xi}{\partial l} \right) = \begin{cases} (-1, 0), & b > b^* \\ (0, -1/2), & b < b^* \end{cases}. \quad (16)$$

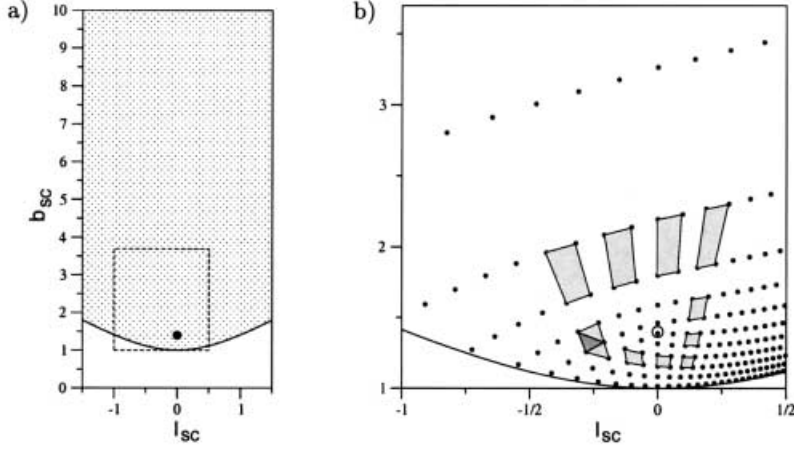


Fig. 4 – a) Bifurcation diagram in the plane of the scaled constants of motion l_{sc} and b_{sc} . The shaded region represents regular motions. b) Magnification of the dashed rectangle in a) with the eigenvalues of quantum states with $\tilde{n}_2 = -20$. The open circle marks the isolated point of the bifurcation diagram.

From the Liouville-Arnold theorem we know that there exist smooth actions for regular values of the constants of motion. To find them we retain the actions $\mathbf{I} = (I_\varphi, I_\eta, I_\xi)^t$ for $l > 0$ and define new actions $\mathbf{J} = \mathbf{T} \mathbf{I}$ for $l < 0$ related to the old actions by a unimodular matrix \mathbf{T} . Since the actions \mathbf{I} are continuous along $l = 0$, the matrix \mathbf{T} can differ from the identity only in its first column which we write as $(1, t_\eta, t_\xi)^t$. The integers t_η and t_ξ are obtained from the requirement of a continuous derivative of the action with respect to l ,

$$\lim_{l \rightarrow 0^+} \frac{\partial I_s}{\partial l} = \lim_{l \rightarrow 0^-} \frac{\partial J_s}{\partial l} \Leftrightarrow t_s = 2 \lim_{l \rightarrow 0^+} \frac{\partial I_s}{\partial l}. \quad (17)$$

But as we have seen above the limits $\lim_{l \rightarrow 0^\pm} \partial I_s / \partial l$, $s = \eta, \xi$, depend on whether $b > b^*$ or $b < b^*$. We therefore obtain two matrices \mathbf{T}_{wg} and \mathbf{T}_{bb} derived from \mathbf{T} with $(t_\eta, t_\xi) = (2, 0)$ and $(t_\eta, t_\xi) = (0, 1)$, respectively, where the “whispering gallery” matrix \mathbf{T}_{wg} leads to smooth actions across $l = 0$ for $b > b^*$ and the “bouncing ball” matrix \mathbf{T}_{bb} leads to smooth actions across $l = 0$ for $b < b^*$. Upon a full counterclockwise circle about the isolated point of the bifurcation diagram in fig. 4a the actions map by the monodromy matrix

$$\mathbf{M} = (\mathbf{T}_{bb} \mathbf{R}_1)^{-1} \mathbf{T}_{wg} \mathbf{R}_1 = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix}, \quad (18)$$

where \mathbf{R}_1 is the reflection matrix $\text{diag}(-1, 1, 1)$ introduced to map actions to one another which differ only in the sign of l . The fact that the matrix \mathbf{M} is not the identity is the reason for monodromy. If the actions related to the separating coordinates for $l > 0$ are smoothly continued about the isolated point there results a multivalued action function whose different leaves are related by powers $n \in \mathbb{Z}$ of the monodromy matrix. Equivalently, we could have started with any other choice of actions $\tilde{\mathbf{I}} = \tilde{\mathbf{T}} \mathbf{I}$ with $\tilde{\mathbf{T}}$ unimodular. This would have given another monodromy matrix $\tilde{\mathbf{M}}$, *i.e.* the monodromy matrix is well defined up to conjugation with unimodular matrices. The special choice

$$\tilde{\mathbf{T}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & -2 \\ 0 & 0 & -1 \end{pmatrix} \text{ leads to } \tilde{\mathbf{M}} = \tilde{\mathbf{T}} \mathbf{M} \tilde{\mathbf{T}}^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}. \quad (19)$$

From this representant of the monodromy matrix we see that there exists a choice of actions with the first two of its components remaining invariant under the monodromy. In terms of quantum mechanics this means that there exist two “good” quantum numbers in the sense that they correspond to smooth single-valued action components.

To illustrate the quantum monodromy graphically we start from the actions \tilde{I} with EBK quantization $\hbar(\tilde{n}_1, \tilde{n}_2 - (\alpha_\eta + 2\alpha_\xi)/4, \tilde{n}_3 - \alpha_\xi/4)$ and quantum numbers $\pm\tilde{n}_1, -\tilde{n}_2, -\tilde{n}_3 \in \mathbb{N}_0$. The eigenvalues with fixed “good” quantum number \tilde{n}_2 lie on a smooth hypersurface in the three-dimensional space of the constants of motion (E, l, b) . Projecting out the energy gives the planar eigenvalue lattice in fig. 4b. This lattice has a defect, as becomes apparent if a lattice cell is transported on a loop about the isolated point. As expected from the monodromy matrix (19), the lattice cell returns distorted by one lattice site.

Conclusions. – Relating the quasiparticle dynamics back to the collective excitations of a condensate in a prolate harmonic trap, we conclude that there exists only a single *generic* type of modes with amplitudes confined to a region kept away from the poles and the symmetry axis of the condensate by the caustics of the classical motion. For vanishing angular momentum the excitations degenerate to two types of modes with amplitudes either concentrated about a surface layer of the condensate (*whispering-gallery modes*) or about its equatorial plane (*bouncing-ball modes*) as indicated by the two types of collapses of the classical caustics. The quantum operator analog of the classical separation constant B can be deduced from rewriting B in Cartesian coordinates giving $B = \mathbf{L}^2 + \sigma^2 p_z^2 + 2H_{\text{hyd}}^2/\omega_0^2 - 2\epsilon^2 m T z^2$. It has a simple interpretation only in the limit of an isotropic trap where it becomes the square of the total angular momentum \mathbf{L} plus the total energy with a pre-factor. More important than the form of the operator is its existence. Since we have three commuting observables, the collective excitations can be assigned by three quantum numbers allowing to unzip the energy spectrum. As a consequence of the quantum monodromy a smooth continuation of quantum numbers across the two types of modes for vanishing angular momentum leads to ambiguous assignments. One might also speculate on a dynamical signature of the monodromy which, *e.g.*, could be displayed by an excitation made up of a superposition of modes with eigenvalues in the neighborhood of the isolated critical point of the classical motion. This remains to be clarified. The monodromy discussed here is similar to the monodromy in prolate ellipsoidal billiards [9].

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