# An algebraic approach to intertwined quantum phase transitions in the Zr isotopes

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December 14, 2022



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34th International Colloquium on Group Theoretical Methods in Physics Strasbourg, 18-22 July 2022 doi:10.21468/SciPostPhysProc.?

# **3** Abstract

The algebraic framework of the interacting boson model with configuration mixing is employed to demonstrate the occurrence of intertwined quantum phase transitions (IQPTs) in the <sub>40</sub>Zr isotopes with neutron number 52–70. The detailed quantum and classical analyses reveal a QPT of crossing normal and intruder configurations superimposed on a QPT of the intruder configuration from U(5) to SU(3) and a crossover from SU(3) to SO(6) dynamical symmetries.

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## 31 **1 Introduction**

Quantum phase transitions [1–3] are qualitative changes in the structure of a physical system that occur as a function of one (or more) parameters that appear in the quantum Hamiltonian describing the system. In nuclear physics [4], we vary the number of nucleons and examine mainly two types of quantum phase transitions (QPTs). The first describes shape phase transitions in a single configuration, denoted as Type I. When interpolating between two shapes, for example, the Hamiltonian can be written as a sum of two parts

$$\hat{H} = (1 - \xi)\hat{H}_1 + \xi\hat{H}_2 , \qquad (1)$$

with  $\xi$  the control parameter. As we vary  $\xi$  with nucleon number from 0 to 1, the equilibrium shape and symmetry of the Hamiltonian vary from those of  $\hat{H}_1$  to those of  $\hat{H}_2$ . QPTs of this type have been studied extensively in the framework of the interacting boson model (IBM) [4–7]. One example of such QPT is the  $_{62}$ Sm region with neutron number 84–94, where the shape evolves from spherical to axially-deformed, with a critical point at neutron number 90. The second type of QPT occurs when the ground state configuration changes its character,

typically from normal to intruder type of states, denoted as Type II QPT. In such cases, the
Hamiltonian can be written in matrix form [8]. For two configurations A and B we have

$$\hat{H} = \begin{bmatrix} \hat{H}_A(\xi_A) & \hat{W}(\omega) \\ \hat{W}(\omega) & \hat{H}_B(\xi_B) \end{bmatrix},$$
(2)

with  $\xi_i$  (*i* = *A*, *B*), the control parameter of configuration (*i*), and  $\hat{W}$ , the coupling between them with parameter  $\omega$ . QPTs of this type are manifested empirically near (sub-) shell closure, e.g. in the light Pb-Hg isotopes, with strong mixing between the configurations [9, 10].

<sup>49</sup> Recently, we have introduced a new type of phase-transitions in even-even [11, 12] and <sup>50</sup> odd-mass [13] nuclei called intertwined quantum phase transitions (IQPTs). The latter refers <sup>51</sup> to a scenario where as we vary the control parameters ( $\xi_A$ ,  $\xi_B$ ,  $\omega$ ) in Eq. (2), each of the <sup>52</sup> Hamiltonians  $\hat{H}_A$  and  $\hat{H}_B$  undergoes a separate and clearly distinguished shape-phase transi-<sup>53</sup> tion (Type I), and the combined Hamiltonian simultaneously experiences a crossing of config-<sup>54</sup> urations *A* and *B* (Type II).

### **55** 2 Theoretical framework

A convenient framework to study the different types of QPTs together is the extension of the
 IBM to include configuration mixing (IBM-CM) [14–16].

#### 58 2.1 The interacting boson model with configuration mixing

The IBM for a single shell model configuration has been widely used to describe low-lying quadrupole collective states in nuclei in terms of *N* monopole ( $s^{\dagger}$ ) and quadrupole ( $d^{\dagger}$ ) bosons, representing valence nucleon pairs. The model has U(6) as a spectrum generating algebra, where the Hamiltonian is expanded in terms of its generators, { $s^{\dagger}s, s^{\dagger}d_{\mu}, d^{\dagger}_{\mu}s, d^{\dagger}_{\mu}d_{\mu'}$ }, and consists of Hermitian, rotational-scalar interactions which conserve the total number of *s*- and *d*- <sup>64</sup> bosons  $\hat{N} = \hat{n}_s + \hat{n}_d = s^{\dagger}s + \sum_{\mu} d^{\dagger}_{\mu}d_{\mu}$ . The boson number is fixed by the microscopic interpre-<sup>65</sup> tation of the IBM [17] to be  $N = N_{\pi} + N_{\nu}$ , where  $N_{\pi}$  ( $N_{\nu}$ ) is the number of proton (neutron) <sup>66</sup> particle or hole pairs counted from the nearest closed shell.

The solvable limits of the model correspond to dynamical symmetries (DSs) associated with chains of nested sub-algebras of U(6), terminating in the invariant SO(3) algebra. In the IBM there are three DS limits

$$U(6) \supset \begin{cases} U(5) \supset SO(5) \supset SO(3), \\ SU(3) \supset SO(3), \\ SO(6) \supset SO(5) \supset SO(3). \end{cases}$$
(3)

<sup>70</sup> In a DS, the Hamiltonian is written in terms of Casimir operators of the algebras of a given <sup>71</sup> chain. In such a case, the spectrum is completely solvable and resembles known paradigms of <sup>72</sup> collective motion: spherical vibrator [U(5)], axially symmetric [SU(3)] and  $\gamma$ -soft deformed <sup>73</sup> rotor [SO(6)]. In each case, the energies and eigenstates are labeled by quantum numbers <sup>74</sup> that are the labels of irreducible representations (irreps) of the algebras in the chain. The <sup>75</sup> corresponding basis states for each of the chains (3) are

$$U(5): |N, n_d, \tau, n_\Delta, L\rangle, \tag{4a}$$

$$SU(3): |N, (\lambda, \mu), K, L\rangle,$$
 (4b)

$$SO(6): |N, \sigma, \tau, n_{\Delta}, L\rangle,$$
 (4c)

where  $N, n_d, (\lambda, \mu), \sigma, \tau, L$  label the irreps of U(6), U(5), SU(3), SO(6), SO(5) and SO(3), respectively, and  $n_{\Lambda}, K$  are multiplicity labels.

An extension of the IBM to include intruder excitations is based on associating the different shell-model spaces of 0p-0h, 2p-2h, 4p-4h, ... particle-hole excitations, with the corresponding boson spaces with N, N+2, N+4, ... bosons, which are subsequently mixed [15, 16]. For two configurations the resulting IBM-CM Hamiltonian can be transcribed in a form equivalent to that of Eq. (2)

$$\hat{H} = \hat{H}_A^{(N)} + \hat{H}_B^{(N+2)} + \hat{W}^{(N,N+2)} .$$
(5)

<sup>83</sup> Here, the notations  $\hat{\mathcal{O}}^{(N)} = \hat{P}_N^{\dagger} \hat{\mathcal{O}} \hat{P}_N$  and  $\hat{\mathcal{O}}^{(N,N')} = \hat{P}_N^{\dagger} \hat{\mathcal{O}} \hat{P}_{N'}$ , stand for an operator  $\hat{\mathcal{O}}$ , with <sup>84</sup>  $\hat{P}_N$ , a projection operator onto the *N* boson space. The Hamiltonian  $\hat{H}_A^{(N)}$  represents the *N* <sup>85</sup> boson space (normal *A* configuration) and  $\hat{H}_B^{(N+2)}$  represents the *N*+2 boson space (intruder <sup>86</sup> *B* configuration).

#### 87 2.2 Wave functions structure

The eigenstates  $|\Psi; L\rangle$  of the Hamiltonian (5) with angular momentum *L*, are linear combinations of the wave functions,  $\Psi_A$  and  $\Psi_B$ , in the two spaces [*N*] and [*N* + 2],

$$|\Psi;L\rangle = a |\Psi_A;[N],L\rangle + b |\Psi_B;[N+2],L\rangle , \qquad (6)$$

with  $a^2 + b^2 = 1$ . We note that each of the components in Eq. (6),  $|\Psi_A; [N], L\rangle$  and  $|\Psi_B; [N+2], L\rangle$ , can be expanded in terms of the different DS limits with its corresponding boson number in the following manner

$$|\Psi_i; [N_i], L\rangle = \sum_{\alpha} C_{\alpha}^{(N_i, L)} |N_i, \alpha, L\rangle, \qquad (7)$$

where  $N_A = N$  and  $N_B = N + 2$ , and  $\alpha = \{n_d, \tau, n_\Delta\}, \{(\lambda, \mu), K\}, \{\sigma, \tau, n_\Delta\}$  are the quantum numbers of the DS eigenstates. The coefficients  $C_{\alpha}^{(N,L)}$  give the weight of each component <sup>95</sup> in the wave function. Using them, we can calculate the wave function probability of having <sup>96</sup> definite quantum numbers of a given symmetry in the DS bases, Eq. (7), for its *A* or *B* parts

U(5): 
$$P_{n_d}^{(N_i,L)} = \sum_{\tau,n_\Delta} [C_{n_d,\tau,n_\Delta}^{(N_i,L)}]^2$$
, SO(6):  $P_{\sigma}^{(N_i,L)} = \sum_{\tau,n_\Delta} [C_{\sigma,\tau,n_\Delta}^{(N_i,L)}]^2$ , (8a)

SU(3): 
$$P_{(\lambda,\mu)}^{(N_i,L)} = \sum_{K} [C_{(\lambda,\mu),K}^{(N_i,L)}]^2$$
, SO(5):  $P_{\tau}^{(N_i,L)} = \sum_{n_d,n_\Delta} [C_{n_d,\tau,n_\Delta}^{(N_i,L)}]^2$ . (8b)

<sup>97</sup> Here the subscripts i = A, B denote the different configurations, i.e.,  $N_A = N$  and  $N_B = N + 2$ . <sup>98</sup> Furthermore, for each eigenstate (6), we can also examine its coefficients *a* and *b*, which <sup>99</sup> portray the probability of the normal-intruder mixing. They are evaluated from the sum of the <sup>100</sup> squared coefficients of an IBM basis. For the U(5) basis, we have

$$P_a^{(N_A,L)} \equiv a^2 = \sum_{n_d,\tau,n_\Delta} |C_{n_d,\tau,n_\Delta}^{(N_A,L)}|^2; \qquad P_b^{(N_B,L)} \equiv b^2 = \sum_{n_d,\tau,n_\Delta} |C_{n_d,\tau,n_\Delta}^{(N_B,L)}|^2.$$
(9)

where the sum goes over all possible values of  $(n_d, \tau, n_\Delta)$  in the  $(N_i, L)$  space, i = A, B, and  $a^2 + b^2 = 1$ .

#### 103 2.3 Geometry

To obtain a geometric interpretation of the IBM is we take the expectation value of the Hamil tonian between coherent (intrinsic) states [5, 18] to form an energy surface

$$E_N(\beta,\gamma) = \langle \beta,\gamma; N | \hat{H} | \beta,\gamma; N \rangle .$$
(10)

The  $(\beta, \gamma)$  of Eq. (10) are quadrupole shape parameters whose values,  $(\beta_{eq}, \gamma_{eq})$ , at the global minimum of  $E_N(\beta, \gamma)$  define the equilibrium shape for a given Hamiltonian. The values are  $(\beta_{eq} = 0)$ ,  $(\beta_{eq} = \sqrt{2}, \gamma_{eq} = 0)$  and  $(\beta_{eq} = 1, \gamma_{eq} \text{ arbitrary})$  for the U(5), SU(3) and SO(6) DS limits, respectively. Furthermore, for these values the ground-band intrinsic state,  $|\beta_{eq}, \gamma_{eq}; N\rangle$ , becomes a lowest weight state in the irrep of the leading subalgebra of the DS chain, with quantum numbers  $(n_d = 0)$ ,  $(\lambda, \mu) = (2N, 0)$  and  $(\sigma = N)$  for the U(5), SU(3) and SO(6) DS limits, respectively.

<sup>113</sup> For the IBM-CM Hamiltonian, the energy surface takes a matrix form [19]

$$E(\beta,\gamma) = \begin{bmatrix} E_A(\beta,\gamma;\xi_A) & \Omega(\beta,\gamma;\omega) \\ \Omega(\beta,\gamma;\omega) & E_B(\beta,\gamma;\xi_B) \end{bmatrix},$$
(11)

where the entries are the matrix elements of the corresponding terms in the Hamiltonian (2), between the intrinsic states of each of the configurations, with the appropriate boson number. Diagonalization of this two-by-two matrix produces the so-called eigen-potentials,  $E_{\pm}(\beta, \gamma)$ .

### 117 2.4 QPTs and order parameters

The energy surface depends also on the Hamiltonian parameters and serves as the Landau 118 potential whose topology determines the type of phase transition. In QPTs involving a single 119 configuration (Type I), the ground state shape defines the phase of the system, which also 120 identifies the corresponding DS as the phase of the system. Such Type I QPTs can be studied 121 using a Hamiltonian as in Eq. (1), that interpolates between different DS limits (phases) by 122 varying its control parameters  $\xi$ . The order parameter is taken to be the expectation value of 123 the d-boson number operator,  $\hat{n}_d$ , in the ground state,  $\langle \hat{n}_d \rangle_{0_1^+}$ , and measures the amount of 124 deformation in the ground state. 125

In QPTs involving multiple configurations (Type II), the dominant configuration in the 126 ground state defines the phase of the system. Such Type II QPTs can be studied using a Hamil-127 tonian as in Eq. (5), that interpolates between the different configurations by varying its control 128 parameters  $\xi_A, \xi_B, \omega$ . The order parameters are taken to be the expectation value of  $\hat{n}_d$  in the 129 ground state wave function,  $|\Psi; L = 0^+_1\rangle$ , and in its  $\Psi_A$  and  $\Psi_B$  components, Eq. (6), denoted 130 by  $\langle \hat{n}_d \rangle_{0_1^+}$ ,  $\langle \hat{n}_d \rangle_A$  and  $\langle \hat{n}_d \rangle_B$ , respectively. The shape-evolution in each of the configurations A 131 and *B* is encapsulated in  $\langle \hat{n}_d \rangle_A$  and  $\langle \hat{n}_d \rangle_B$ , respectively. Their sum weighted by the probabilities of the  $\Psi_A$  and  $\Psi_B$  components  $\langle \hat{n}_d \rangle_{0^+_1} = a^2 \langle \hat{n}_d \rangle_A + b^2 \langle \hat{n}_d \rangle_B$ , portrays the evolution of the 132 133 normal-intruder mixing. 134

### **3 QPTs in the Zr isotopes**

Along the years, the  $Z \approx 40$ ,  $A \approx 100$  region was suggested by many works to have a ground 136 state that is dominated by a normal spherical configuration for neutron numbers 50–58 and 137 by an intruder deformed configuration for 60 onward. This dramatic change in structure is 138 explained in the shell model by the isoscalar proton-neutron interaction between non-identical 139 nucleons that occupy the spin-orbit partner orbitals  $\pi 1g_{9/2}$  and  $\nu 1g_{7/2}$  [20]. The crossing 140 between configurations arises from the promotion of protons across the Z=40 subsell gap. 141 The interaction energy results in a gain that compensates the loss in single-particle and pairing 142 energy and a mutual polarization effect is enabled. Therefore, the single-particle orbitals at 143 higher intruder configurations are lowered near the ground state normal configuration, which 144 effectively reverses their order. 145

#### 146 **3.1 Model space**

Using the framework of the IBM-CM, we consider  ${}^{90}_{40}$ Zr as a core and valence neutrons in the 50–82 major shell. The normal *A* configuration corresponds to having no active protons above *Z* = 40 sub-shell gap, and the intruder *B* configuration corresponds to two-proton excitation from below to above this gap, creating 2p-2h states. Therefore, the IBM-CM model space employed in this study, consists of  $[N] \oplus [N + 2]$  boson spaces with total boson number N = 1, 2, ... 8 for  ${}^{92-106}$ Zr and  $\bar{N} = \bar{7}, \bar{6}$  for  ${}^{108,110}$ Zr, respectively, where the bar over a number indicates that these are hole bosons.

#### **3.2** Hamiltonian and *E*2 transitions operator

In order to describe the spectrum of the Zr isotopes, we take a Hamiltonian that has a form as in Eq. (5) with entries

$$\hat{H}_{A}(\epsilon_{d}^{(A)},\kappa^{(A)},\chi) = \epsilon_{d}^{(A)}\hat{n}_{d} + \kappa^{(A)}\hat{Q}_{\chi}\cdot\hat{Q}_{\chi} , \qquad (12a)$$

$$\hat{H}_{B}(\epsilon_{d}^{(B)},\kappa^{(B)},\chi) = \epsilon_{d}^{(B)}\hat{n}_{d} + \kappa^{(B)}\hat{Q}_{\chi}\cdot\hat{Q}_{\chi} + \kappa^{\prime(B)}\hat{L}\cdot\hat{L} + \Delta_{p} , \qquad (12b)$$

where the quadrupole operator is given by  $\hat{Q}_{\chi} = d^{\dagger}s + s^{\dagger}\tilde{d} + \chi(d^{\dagger} \times \tilde{d})^{(2)}$ , and  $\hat{L} = \sqrt{10}(d^{\dagger}\tilde{d})^{(1)}$ is the angular momentum operator. Here  $\tilde{d}_m = (-1)^m d_{-m}$  and standard notation of angular momentum coupling is used. The off-set energy between configurations *A* and *B* is  $\Delta_p$ , where the index *p* denotes the fact that this is a proton excitation. The mixing term in Eq. (5) between configurations (*A*) and (*B*) has the form [14-16]  $\hat{W} = \omega [(d^{\dagger} \times d^{\dagger})^{(0)} + (s^{\dagger})^2] + \text{H.c.}$ , where H.c. stands for Hermitian conjugate. The parameters are obtained from a fit, elaborated in the appendix of Ref. [12].

The *E*2 operator for two configurations is written as  $\hat{T}(E2) = e^{(A)}\hat{Q}_{\chi}^{(N)} + e^{(B)}\hat{Q}_{\chi}^{(N+2)}$ , with  $\hat{Q}_{\chi}^{(N)} = \hat{P}_{N}^{\dagger}\hat{Q}_{\chi}\hat{P}_{N}$  and  $\hat{Q}_{\chi}^{(N+2)} = P_{N+2}^{\dagger}\hat{Q}_{\chi}\hat{P}_{N+2}$ . The boson effective charges  $e^{(A)}$  and  $e^{(B)}$  are



Figure 1: Comparison between (a) experimental and (b) calculated energy levels  $0_1^+, 2_1^+, 4_1^+, 0_2^+, 2_2^+, 4_2^+$ . Empty (filled) symbols indicate a state dominated by the normal *A* configuration (intruder *B* configuration), with assignments based on Eq. (9). The symbol[•,  $\blacktriangle$ ,  $\blacklozenge$ ], indicates the closest dynamical symmetry [U(5), SU(3), SO(6)] to the level considered, based on Eq. (8). Note that the calculated values start at neutron number 52, while the experimental values include the closed shell at 50. References for the data can be found in [12].

determined from the  $2^+ \rightarrow 0^+$  transition within each configuration [12], and  $\chi$  is the same parameter as in the Hamiltonian (12).

For the energy surface matrix (11), we calculate the expectation values of the Hamiltonians  $\hat{H}_A$  (12a) and  $\hat{H}_B$  (12b) in the intrinsic state of Section 2.3 with *N* and *N*+2 bosons respectively, and a non-diagonal matrix element of the mixing term  $\hat{W}$  between them. The explicit expressions can be found in [12].

### 172 **4 Results**

<sup>173</sup> In order to understand the change in structure of the Zr isotopes, it is insightful to examine <sup>174</sup> the evolution of different properties along the chain.

#### 175 4.1 Evolution of energy levels

In Fig. 1, we show a comparison between selected experimental and calculated levels, along 176 with assignments to configurations based on Eq. (9) and to the closest DS based on Eq. (8), 177 for each state. In the region between neutron number 50 and 56, there appear to be two con-178 figurations, one spherical (seniority-like), (A), and one weakly deformed, (B), as evidenced by 179 the ratio  $R_{4/2}$ , which is  $R_{4/2}^{(A)} \cong 1.6$  and  $R_{4/2}^{(B)} \cong 2.3$  at at 52–56. From neutron number 58, there 180 is a pronounced drop in energy for the configuration (B) states and at 60, the two configura-181 tions exchange their role, indicating a Type II QPT. At this stage, the B configuration appears 182 to undergo a U(5)-SU(3) Type I QPT, similarly to case of the Sm region [14, 21, 22]. Beyond 183 neutron number 60, the B configuration is strongly deformed, as evidenced by the small value 184 of the excitation energy of the state  $2_1^+$ ,  $E_{2_1^+} = 139.3$  keV and by the ratio  $R_{4/2}^{(B)} = 3.24$  in <sup>104</sup>Zr. At still larger neutron number 66, the ground state band becomes  $\gamma$ -unstable (or triaxial) as 185 186 evidenced by the close energy of the states  $2_2^+$  and  $4_1^+$ ,  $E_{2_2^+} = 607.0$  keV,  $E_{4_1^+} = 476.5$  keV, in 187 <sup>106</sup>Zr, and especially by the results  $E_{4_1^+} = 565$  keV and  $E_{2_2^+} = 485$  keV for <sup>110</sup>Zr of Ref. [23], a 188 signature of the SO(6) symmetry. In this region, the B configuration undergoes a crossover 189 from SU(3) to SO(6). 190



Figure 2: Left panels: percentage of the wave functions within the intruder B-configuration [the  $b^2$  probability in Eq. (6)], for the ground  $0_1^+$  (bottom) and excited  $2_1^+$  (top) states in  $92^{-110}$ Zr. Right panels: evolution of symmetries for the lowest  $0^+$  (bottom) and  $2^+$  (top) state of configuration *B* along the Zr chain. Shown are the probabilities of selected components of U(5) (•), SU(3) ( $\blacktriangle$ ), SO(6) (•) and SO(5) (•), obtained from Eq. (8). For neutron numbers 52–58 (60–70),  $0_B^+$  corresponds to the experimental  $0_2^+$  ( $0_1^+$ ) state. For neutron numbers 52–56 (58–70),  $2_B^+$  corresponds to the experimental  $2_2^+$  ( $2_1^+$ ) state.

### 191 4.2 Evolution of configuration content

We examine the configuration change for each isotope, by calculating the evolution of the 192 probability  $b^2$ , Eq. (9), of the  $0_1^+$  and  $2_1^+$  states. The left panels of Fig. 2 shows the percentage 193 of the wave function within the B configuration as a function of neutron number across the 194 Zr chain. The rapid change in structure of the  $0_1^+$  state (bottom left panel) from the normal *A* configuration in  ${}^{92-98}$ Zr (small  $b^2$  probability) to the intruder *B* configuration in  ${}^{100-110}$ Zr 195 196 (large  $b^2$  probability) is clearly evident, signaling a Type II QPT. The configuration change appears however sooner in the  $2_1^+$  state (top left panel), which changes to configuration *B* 197 198 already in  $^{98}$ Zr, in line with [24]. Outside a narrow region near neutron number 60, where 199 the crossing occurs, the two configurations are weakly mixed and the states retain a high level 200 of purity, especially for neutron number larger than 60. 201

### 202 4.3 Evolution of symmetry content

We examine the changes in symmetry of the lowest  $0^+$  and  $2^+$  states within the B configuration, 203 which undergoes a Type I QPT. In the right bottom panel of Fig. 2 the red dots represent the 204 percentage of the U(5)  $n_d = 0$  component in the wave function,  $P_{n_d=0}^{(N+2,L=0)}$  of Eq. (8). It is 205 large ( $\approx$  90%) for neutron number 52–58 and drops drastically ( $\approx$  30%) at 60. The drop 206 means that other  $n_d \neq 0$  components are present in the wave function and therefore this state 207 becomes deformed. Above neutron number 60, the  $n_d = 0$  component drops almost to zero 208 (and rises again a little at 70), indicating the state is strongly deformed. To understand the 209 type of DS associated with the deformation above neutron number 60, we add in blue triangles 210 the percentage of the SU(3)  $(\lambda, \mu) = (2N + 4, 0)$  component,  $P_{(\lambda,\mu)=(2N+4,0)}^{(N+2,L=0)}$  of Eq. (8) for 60– 211 66. For neutron number 60, it is moderately small ( $\approx$  35%), at neutron number 62 it jumps 212 ( $\approx$  85%) and becomes maximal at 64 ( $\approx$  92%). This serves as a clear evidence for a U(5)-213 SU(3) Type I QPT. At neutron number 66 the SU(3)  $(\lambda, \mu) = (2N+4, 0)$  component it is lowered, 214 and one sees by the green diamonds the percentage of the SO(6)  $\sigma = N + 2$  component, 215  $P_{\sigma=N+2}^{(N+2,L=0)}$  of Eq. (8). The latter becomes dominant for 66–70 ( $\approx$  99%), suggesting a crossover 216 from SU(3) to SO(6). 217



Figure 3: (a) Evolution of order parameters along the Zr chain, normalized (see text). (b) B(E2) values in W.u. for  $2^+ \rightarrow 0^+$  transitions in the Zr chain. The solid line (symbols •, •, •) denote calculated results (experimental results). Dotted lines denote calculated *E*2 transitions within a configuration. The data for  ${}^{94}$ Zr,  ${}^{96}$ Zr,  ${}^{100}$ Zr,  ${}^{102}$ Zr and ( ${}^{104}$ Zr,  ${}^{106}$ Zr) are taken from [25], [26], [27], [28], [29], respectively. For  ${}^{98}$ Zr (neutron number 58), the experimental values are from [30] (•), from [31] (•), and the upper and lower limits (black bars) are from [24, 27].

In order to further elaborate the Type I QPT within configuration B from U(5) to SU(3)218 and the subsequent crossover to SO(6), we examine also the evolution of SO(5) symmetry. 219 The gray histograms in the right panel of Fig. 2 depict the probability of the  $\tau$  =0 component 220 of SO(5),  $P_{\tau=0}^{(N+2,L=0)}$  of Eq. (8), for  $0_B^+$ . For neutron numbers 52–56, the  $0_B^+$  state is composed 221 mainly of a single  $(n_d = 0, \tau = 0)$  component, appropriate for a with state good U(5) DS. For 222 neutron number 58, the larger  $\tau = 0$  but smaller  $n_d = 0$  probabilities imply the presence of 223 additional components with  $(n_d \neq 0, \tau = 0)$ . For neutron numbers 60–64, the  $\tau = 0$  probability 224 decreases, implying admixtures of components with  $(n_d \neq 0, \tau \neq 0)$ , appropriate for a state 225 with good SU(3) DS. For neutron numbers 66–70, the  $\tau = 0$  probability increases towards 226 its maximum value at 70, appropriate for a crossover to SO(6) structure with good SO(5) 227 symmetry. 228

In the top right panel of Fig. 2 we observe a similar trend for the  $2_B^+$  state. For neutron numbers 52–58, it is dominated by a single  $(n_d = 1, \tau = 1)$  component. For neutron number 60,  $P_{n_d=1}^{(N+2,L=2_B^+)}$  is smaller than  $P_{\tau=1}^{(N+2,L=2_B^+)}$ , indicating the onset of deformation. For 62– 64,  $P_{n_d=1}^{(N+2,L=2_B^+)}$  is much smaller than  $P_{\tau=1}^{(N+2,L=2_B^+)}$ , implying admixtures of components with  $(n_d \neq 1, \tau \neq 1)$ . For neutron numbers 66–70,  $P_{n_d=1}^{(N+2,L=2_B^+)}$  remains small but  $P_{\tau=1}^{(N+2,L=2_B^+)}$  increases towards its maximum value at 70.

### 235 4.4 Evolution of order parameters

The configuration and symmetry analysis of Sections 4.2 and 4.3 suggest a situation of si-236 multaneous occurrence of Type I and Type II QPTs. The order parameters can give further 237 insight to these QPTs. Fig. 3(a) shows the evolution along the Zr chain of the order param-238 eters  $(\langle \hat{n}_d \rangle_A, \langle \hat{n}_d \rangle_B$  in dotted and  $\langle \hat{n}_d \rangle_{0_1^+}$  in solid lines), normalized by the respective boson 239 numbers,  $\langle \hat{N} \rangle_A = N$ ,  $\langle \hat{N} \rangle_B = N+2$ ,  $\langle \hat{N} \rangle_{0_1^+} = a^2 N + b^2 (N+2)$ . The order parameter  $\langle \hat{n}_d \rangle_{0_1^+}$  is close 240 to  $\langle \hat{n}_d \rangle_A$  for neutron number 52–58 and coincides with  $\langle \hat{n}_d \rangle_B$  at 60 and above. The clear jump 241 and change in configuration content from 58 to 60 indicates a Type II phase transition [8], 242 with weak mixing between the configurations. Configuration A is spherical for all neutron 243 numbers, and configuration B is weakly-deformed for neutron number 52-58. From neutron 244 number 58 to 60 we see a sudden increase in  $\langle \hat{n}_d \rangle_B$  that continues towards 64, indicating a 245 U(5)-SU(3) Type I phase transition. Then, we observe a decrease from neutron number 66 246 onward, due in part to the crossover from SU(3) to SO(6) and in part to the shift from bo-247



Figure 4: Contour plots in the  $(\beta, \gamma)$  plane of the lowest eigen-potential surface,  $E_{-}(\beta, \gamma)$ , for the <sup>92-110</sup>Zr isotopes.

son particles to boson holes after the middle of the major shell 50–82. These conclusions are stressed by an analysis of other observables [12], in particular, the B(E2) values. As shown in Fig. 3(b), the calculated B(E2)'s agree with the experimental values and follow the same trends as the respective order parameters.

#### 252 4.5 Classical analysis

In Fig. 4, we show the calculated lowest eigen-potential  $E_{-}(\beta, \gamma)$ , which is the lowest eigenvalue of the matrix Eq. (11). These classical potentials confirm the quantum results, as they show a transition from spherical ( $^{92-98}$ Zr), Figs. 4(a)-(d), to a double-minima potential that is almost flat-bottomed at  $^{100}$ Zr, Fig. 4(e), to prolate axially deformed ( $^{102-104}$ Zr), Figs. 4(f)-(g), and finally to  $\gamma$ -unstable ( $^{106-110}$ Zr), Figs. 4(h)-(j).

# **258 5 Conclusions and outlook**

The algebraic framework of the IBM-CM allows us to examine QPTs using both quantum and 259 classical analyses. We have employed this analysis to the Zr isotopes with A=92-110, which 260 exhibit a complex structure that involves a shape-phase transition within the intruder config-261 uration (Type I QPT) and a configuration-change between normal and intruder (Type II QPT), 262 namely IQPTs. This was done by analyzing the energies, configuration and symmetry content 263 of the wave functions, order parameters and E2 transition rates, and the energy surfaces. Fur-264 ther analysis of other observables supporting this scenario is presented in [12]. Recently, we 265 have also exemplified the notion IQPTs in the odd-mass  $_{41}$ Nb isotopes [13] and it would be 266 interesting to examine the notion of IQPTs in other even-even and odd-mass chains of isotopes 267 in the  $Z \approx 40$ ,  $A \approx 100$  region and other physical systems. 268

### **269** Acknowledgments

This work was done in collaboration with F. Iachello (Yale university) and A. Leviatan (Hebrewuniversity).

**Funding information** This work was supported in part by the US-Israel Binational Science Foundation Grant No. 2016032 and the Israel Academy of Sciences for a Postdoctoral Fellowship Program in Nuclear Physics.

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