

Excited state quantum phase transitions in pairing systems

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New Approaches in Nuclear Many-Body Theory
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Excited state quantum phase transitions

Phenomena analogous to quantum phase transitions (QPT) noted to occur throughout the excitation spectra of certain many-body models:

- Lipkin model

W. D. Heiss, F. G. Scholtz, and H. B. Geyer, J. Phys. A **38**, 1843 (2005).
F. Leyvraz and W. D. Heiss, Phys. Rev. Lett **95**, 050402 (2005).

- Interacting boson model (IBM)

S. Heinze, P. Cejnar, J. Jolie, and M. Macek, Phys. Rev. C **73**, 014306 (2005).
P. Cejnar, M. Macek, S. Heinze, J. Jolie, and J. Dobeš, J. Phys. A **39**, L515 (2006).

Simultaneous singularities in the eigenvalue spectrum, order parameters, and wave function properties

Characteristics of excited state singularities as “phase transitions”?

Numerical and semiclassical analysis

Do these singularities occur in a broader class of many-body models?

M. A. Caprio, P. Cejnar, and F. Iachello, Ann. Phys. (NY) (in press).
arXiv:0707.0325 [quant-ph]

Quantum phase transitions

QPT occurs as a “control parameter” ξ , controlling an interaction strength in the system’s Hamiltonian $\hat{H}(\xi)$, is varied, at some critical value $\xi = \xi_c$.

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

For ground state, QPT characterized by a few distinct but related properties:

- (1) The ground state energy E_0 is nonanalytic.
- (2) The ground state wave function properties, expressed via “order parameters” such as the ground state expectation values $\langle \hat{H}_1 \rangle_0$ or $\langle \hat{H}_2 \rangle_0$, are nonanalytic.

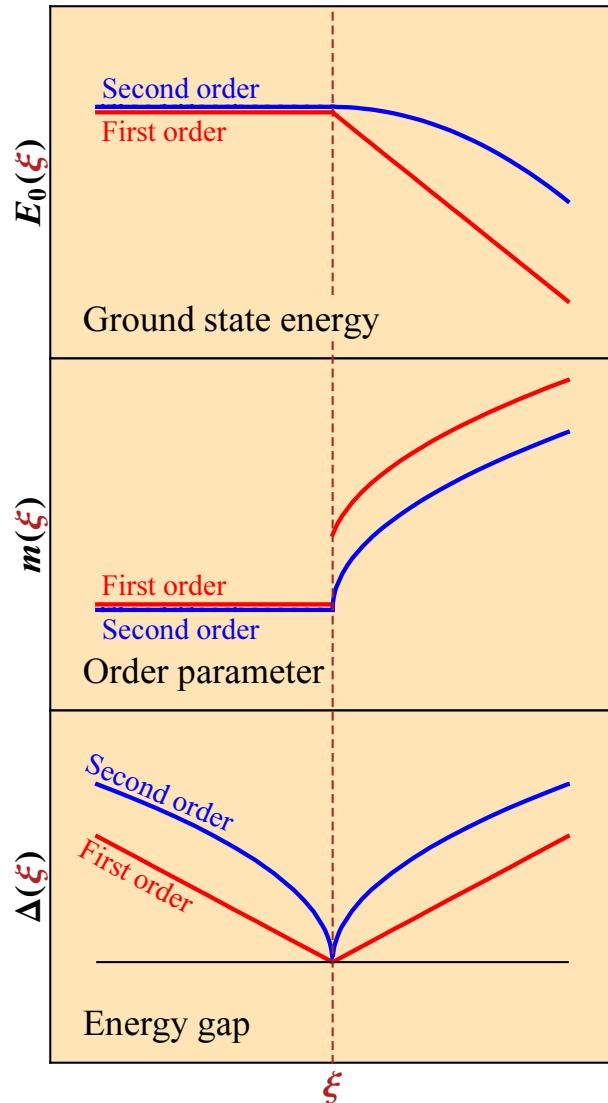
Evolution of E_0 and order parameters related by Feynman-Hellmann theorem:

$$\frac{dE_0}{d\xi} = \langle \hat{H}_2 \rangle_0 - \langle \hat{H}_1 \rangle_0$$

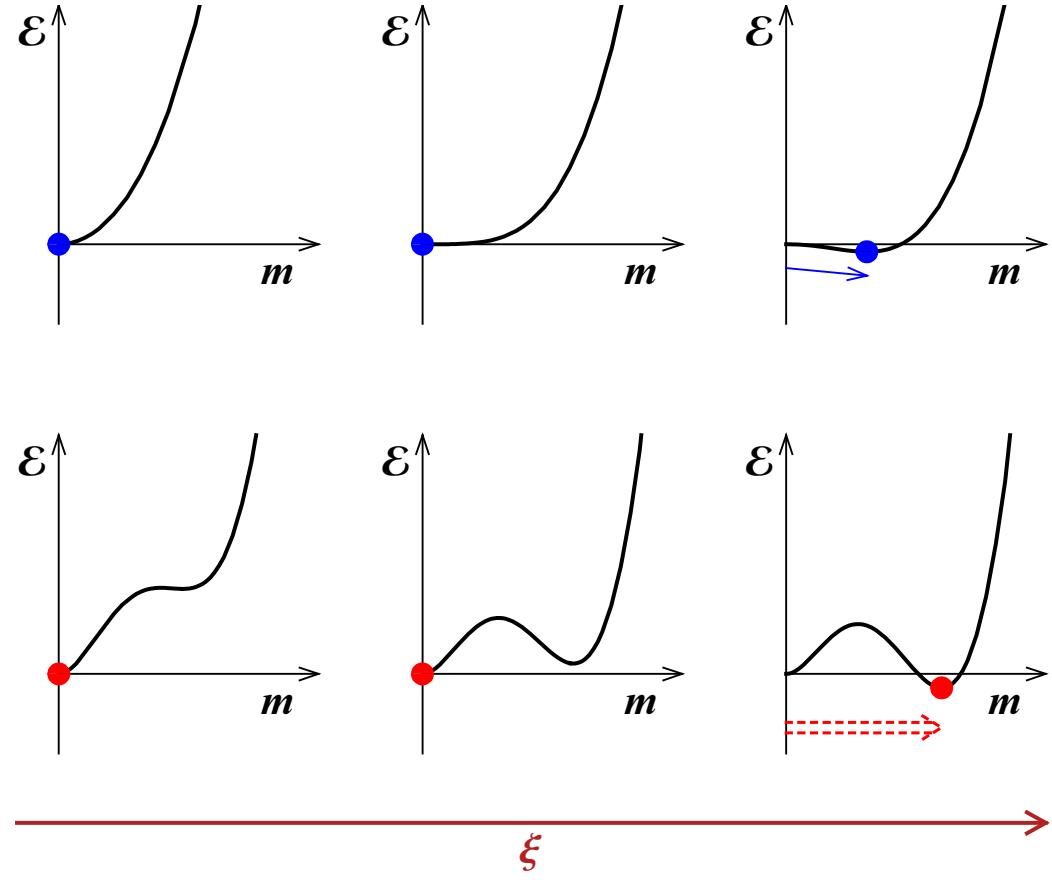
- (3) The gap Δ between the ground state and the first excited state vanishes.

For finite particle number N , the defining characteristic of the QPT is not the presence of a true singularity but rather well-defined scaling behavior of the relevant quantities towards a singular large- N limit.

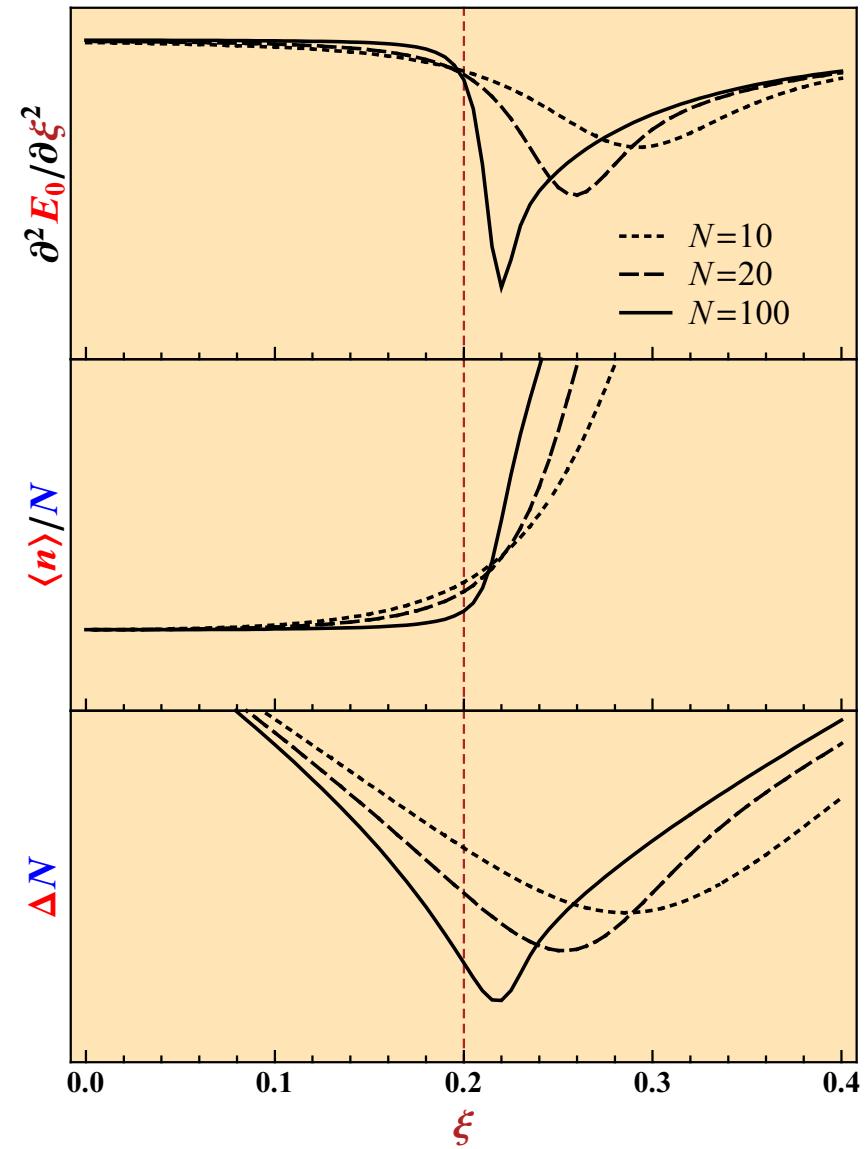
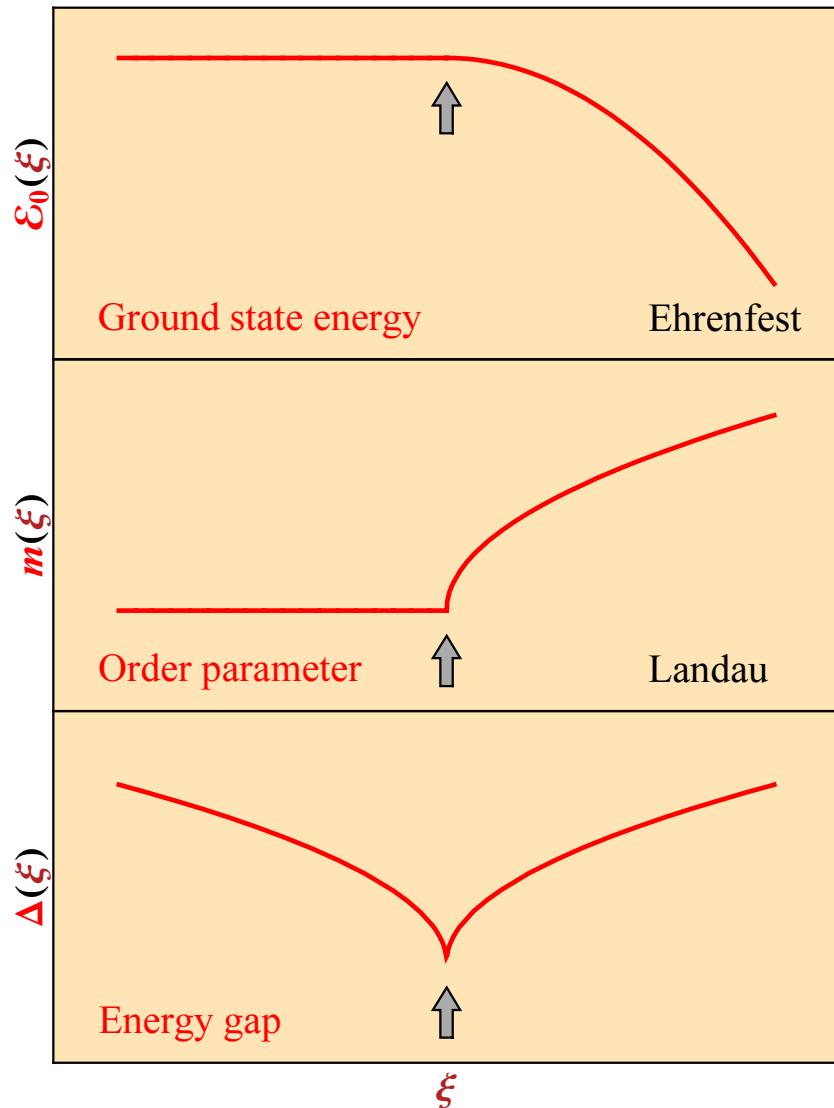
Quantum phase transitions



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



Signatures and finite size precursors



Finite size scaling at the critical point

Numerical studies

R. Botet, R. Jullien, and P. Pfeuty, Phys. Rev. Lett. **49**, 478 (1982).

D. J. Rowe, P. S. Turner, and G. Rosensteel, Phys. Rev. Lett. **93**, 232502 (2004).

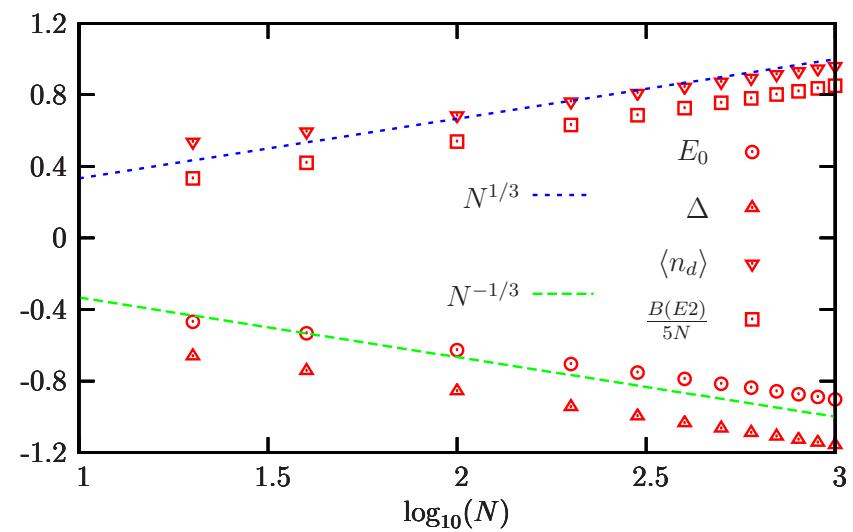
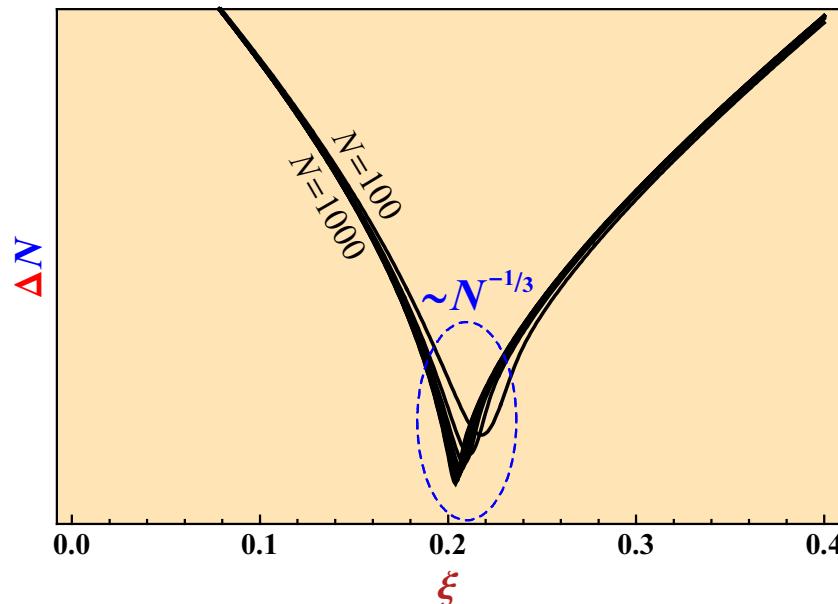
Continuous unitary transformation (CUT)

S. Dusuel and J. Vidal, Phys. Rev. Lett. **93**, 237204 (2004).

S. Dusuel, J. Vidal, J. M. Arias, J. Dukelsky, J. E. García-Ramos, Phys. Rev. C **72**, 064332 (2005).

Exact solution for observables, order-by-order in $1/N$

$$\Phi(N, t) \sim \frac{t^\eta}{N^n} \mathcal{F}(Nt^{3/2}) \sim N^{-(n + \frac{2}{3}\eta)} \quad t \equiv \xi - \xi_c$$



from S. Dusuel *et al.*, Phys. Rev. C **62**, 011301(R) (2005).

Two-level boson models (*s*-*b* models)

$\mathrm{U}(n+1)$ algebra ($n = 2L+1$)

$$s^{(0)} \ b_{-L}^{(L)} \dots b_0^{(L)} \dots b_{+L}^{(L)}$$

$$\mathrm{U}(n+1) \supset \left(\begin{array}{c} \mathrm{SO}(n+1) \\ \mathrm{U}(n) \end{array} \right) \supset \mathrm{SO}(n) \supset \mathrm{SO}(3)$$

$\mathrm{SO}(n)$ -invariant Hamiltonian

$$\hat{H} = \frac{(1 - \xi)}{N} \hat{N}_b - \frac{\xi}{N^2} (s^\dagger \tilde{b} + b^\dagger \tilde{s}) \cdot (s^\dagger \tilde{b} + b^\dagger \tilde{s})$$

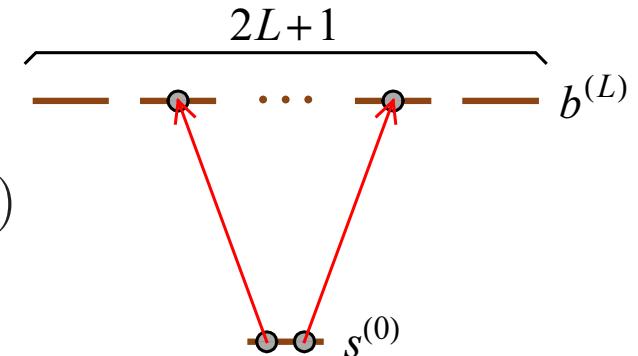
Second order QPT: $\mathrm{U}(n) \Leftrightarrow \mathrm{SO}(n+1)$

$\mathrm{U}(2)$: Lipkin model

*Interacting fermions, interacting spins, interacting bosons
(Schwinger realization)*

$\mathrm{U}(4)$: Molecular vibron model (linear \Leftrightarrow bent)

$\mathrm{U}(6)$: Interacting boson model [$\mathrm{U}(5) \Leftrightarrow \mathrm{SO}(6)$]

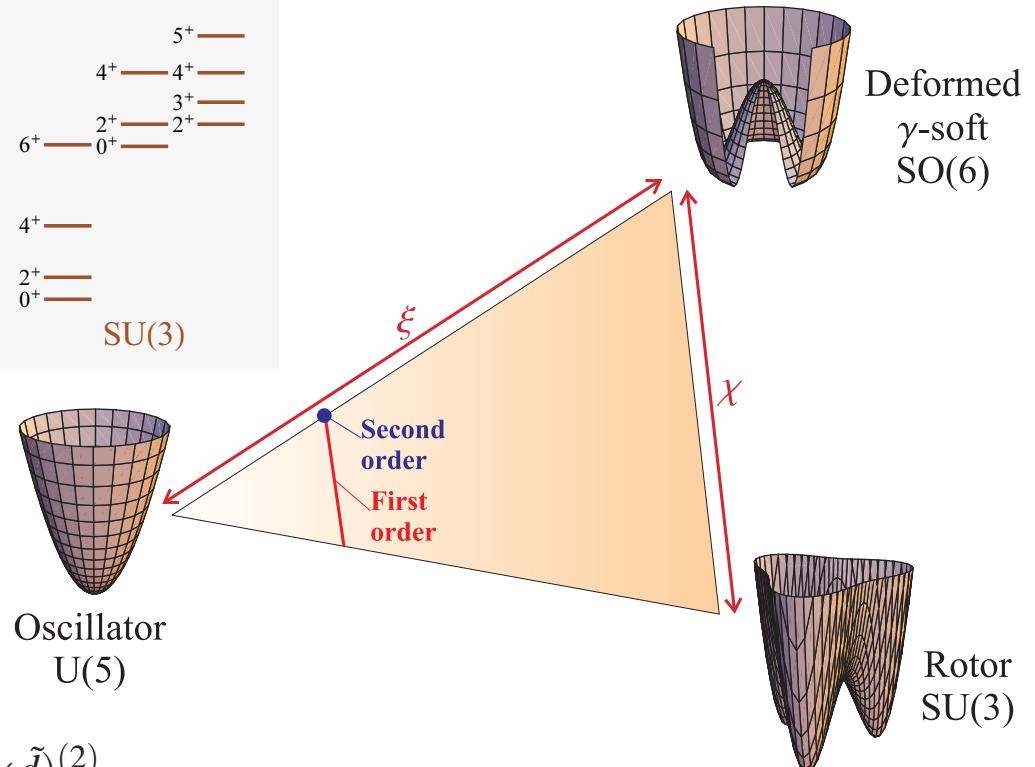


The interacting boson model (IBM)

Truncation to s -wave ($J = 0$) and d -wave ($J = 2$) nucleon pairs

$$U(6) \supset \left(\begin{array}{c} U(5) \\ SO(6) \\ SU(3) \end{array} \right) \supset SO(5) \supset SO(3) \supset SO(2)$$

$\underline{6^+}$	$\underline{4^+}$	$\underline{3^+}$	$\underline{2^+}$	$\underline{0^+}$		$\underline{6^+}$	$\underline{4^+}$	$\underline{3^+}$	$\underline{0^+}$	$\underline{\underline{2^+}}$
$\underline{4^+}$	$\underline{2^+}$	$\underline{0^+}$				$\underline{4^+}$	$\underline{2^+}$			
$\underline{\underline{2^+}}$						$\underline{4^+}$				
$\underline{0^+}$						$\underline{6^+}$	$\underline{4^+}$	$\underline{3^+}$	$\underline{2^+}$	$\underline{0^+}$
U(5)						SO(6)				SU(3)



$$H = \frac{(1 - \xi)}{N} \hat{n}_d - \frac{\xi}{N^2} \hat{Q}^\chi \cdot \hat{Q}^\chi$$

$$\hat{n}_d = d^\dagger \cdot \tilde{d} \quad \hat{Q}^\chi = (s^\dagger \times \tilde{d} + d^\dagger \times \tilde{s})^{(2)} + \chi (d^\dagger \times \tilde{d})^{(2)}$$

The two-dimensional vibron model

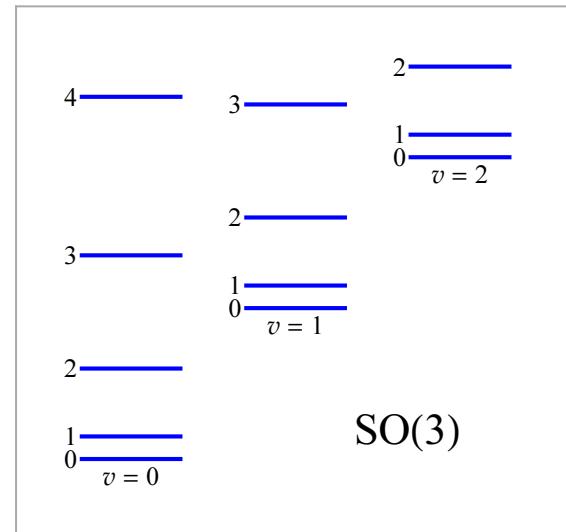
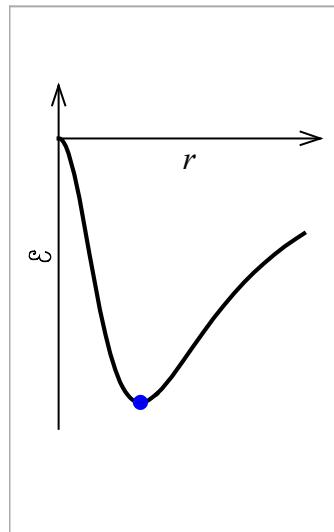
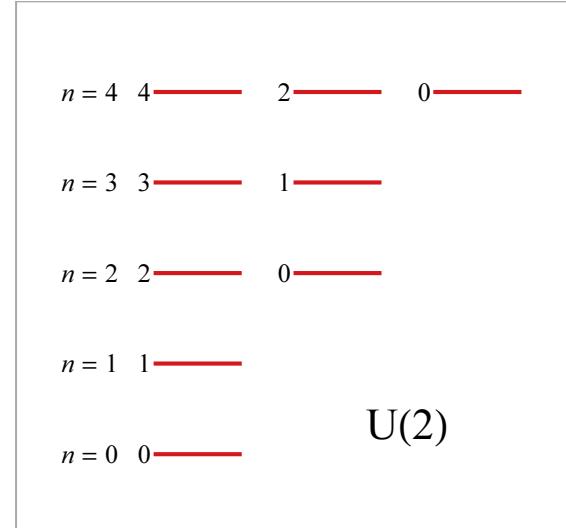
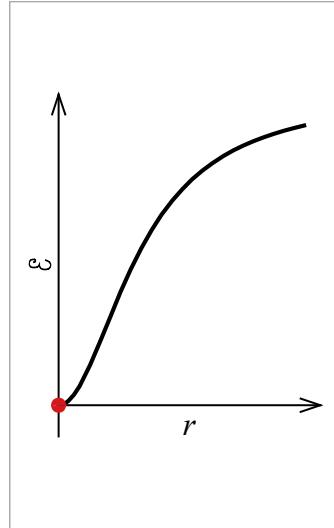
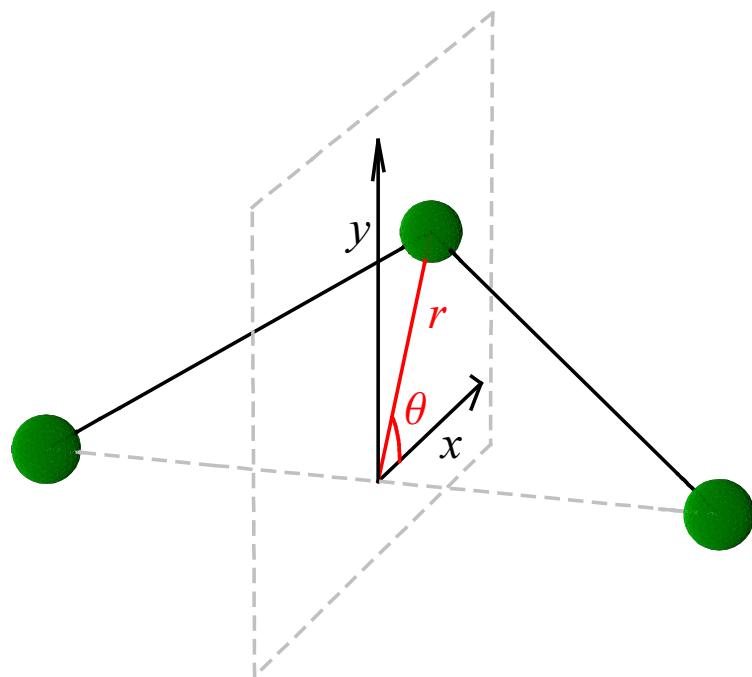
Restriction to planar motion

F. Iachello and S. Oss, J. Chem. Phys. **104**, 6956 (1996).

$U(3)$ algebra

$$s \ b_+ \ b_-$$

$$U(3) \supset \begin{pmatrix} SO(3) \\ U(2) \end{pmatrix} \supset_{\ell} SO(2)$$



Coordinate Hamiltonian

Coherent state analysis yields both *potential* and *kinetic* energy

R. L. Hatch and S. Levit, Phys. Rev. C **25**, 614 (1982).

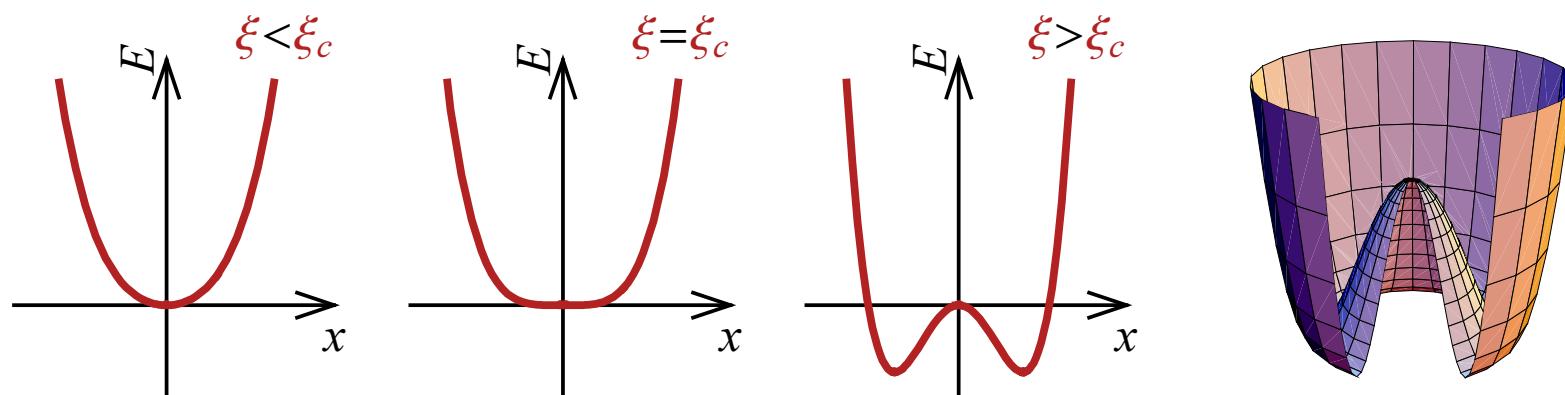
$U(n+1) \Rightarrow n$ coordinates, n momenta

$SO(n)$ -invariant Hamiltonian

- Radial coordinate r (e.g., β in IBM)
- Conjugate momentum p_r
- Conserved angular kinetic energy $T_\vartheta(v) = v(v+n-2)$

$$\hat{H} = \frac{1-\xi}{2N^2}[p_r^2 + r^{-2}T_\vartheta(v)] + \frac{\xi}{N^2}[r^2 p_r^2 + T_\vartheta(v)] + \frac{1-5\xi}{2}r^2 + \xi r^4$$

$$\hat{H} = \frac{1-\xi}{2N^2}p^2 + \frac{\xi}{N^2}x^2 p^2 + \frac{1-5\xi}{2}x^2 + \xi x^4 \quad (\text{Lipkin})$$



Semiclassical relation between spectrum and scaling

Boson number plays role of $1/\hbar$ or \sqrt{m}

c.f., D. J. Rowe, P. S. Turner, and G. Rosensteel, Phys. Rev. Lett. **93**, 232502 (2004).

$$\frac{\hbar^2}{2m} \Rightarrow \frac{1-\xi}{2N^2}$$

Apply semiclassical quantization condition

$$S(\xi; E) = 2\pi\hbar k \Rightarrow \frac{2\pi k}{N} \quad (k = 1, 2, \dots)$$

Specifically...

$$\int_{x_1(E)}^{x_2(E)} dx \sqrt{E - V_\xi(x)} = \frac{(1-\xi)\pi}{2} \frac{k}{N}$$

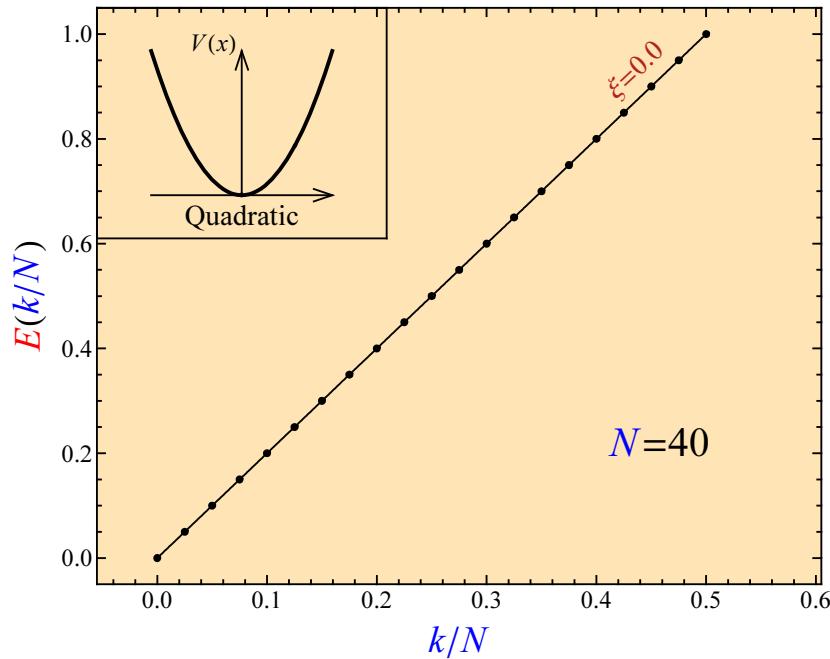
$$\therefore E(N, k) = E\left(\frac{k}{N}\right)$$

Finite size scaling [$E(N)$] and excitation spectrum [$E(k)$] intertwined

Semiclassical scaling for ground state critical point

In WKB approximation, $E(N, k) = E(k/N)$, so *excitation spectrum* [$E(k)$] and *finite size scaling* [$E(N)$] intertwined

$$\hat{H}_{\text{coord}} \approx \frac{1 - \xi}{2N^2} p_r^2 + \left(\frac{1 - 5\xi}{2} r^2 + \xi r^4 \right)$$

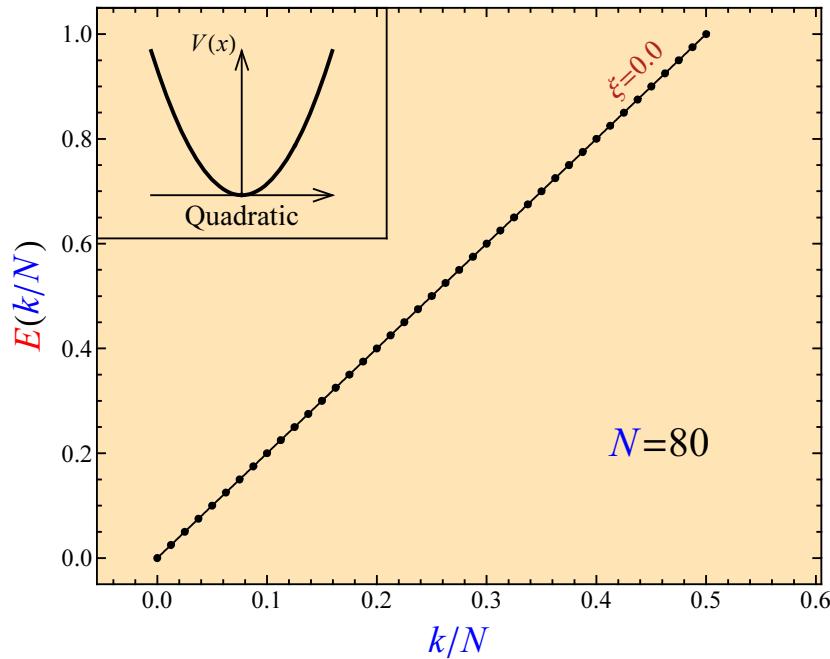


$$E(k/N) \sim (k/N)$$
$$\therefore \Delta \sim N^{-1} \quad \text{i.e., } N\Delta \sim 1$$

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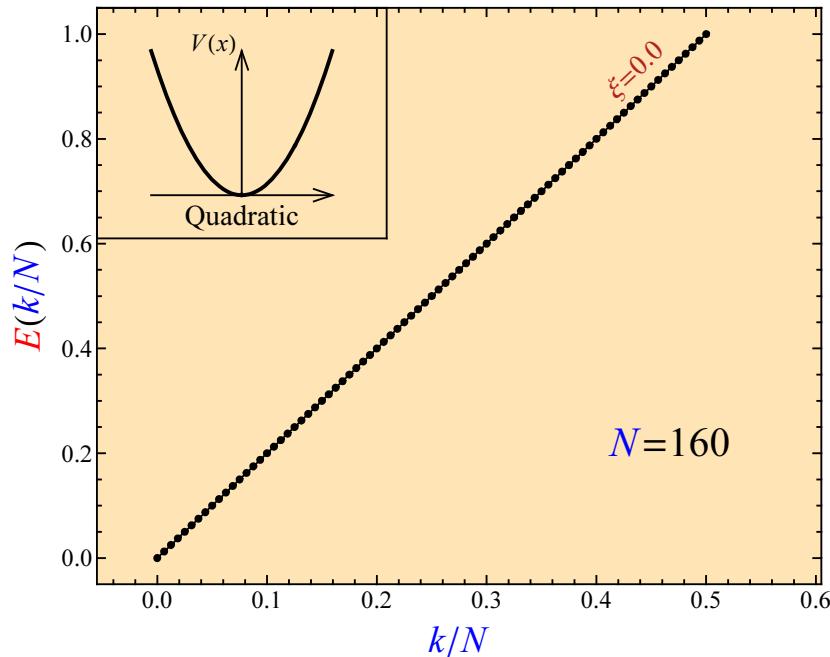


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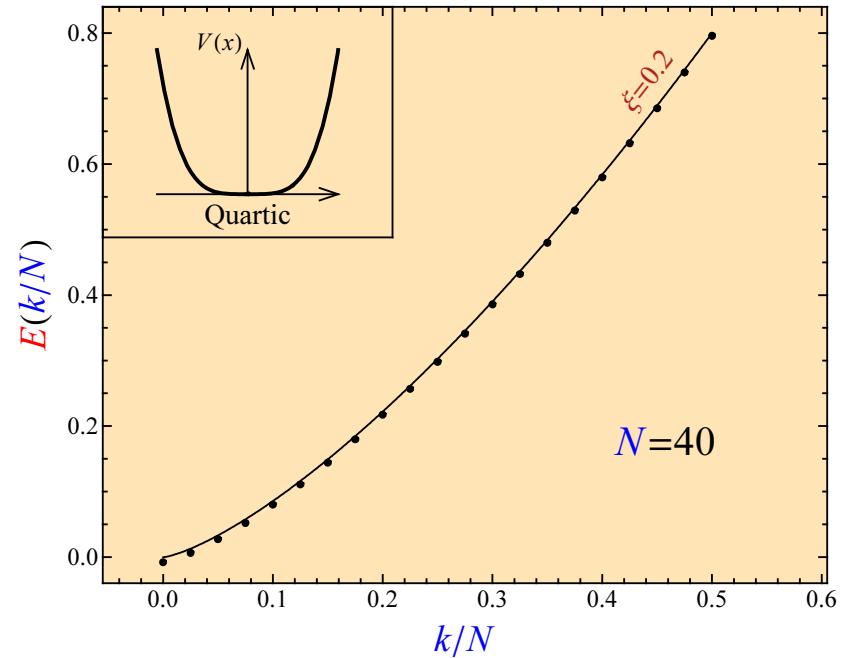
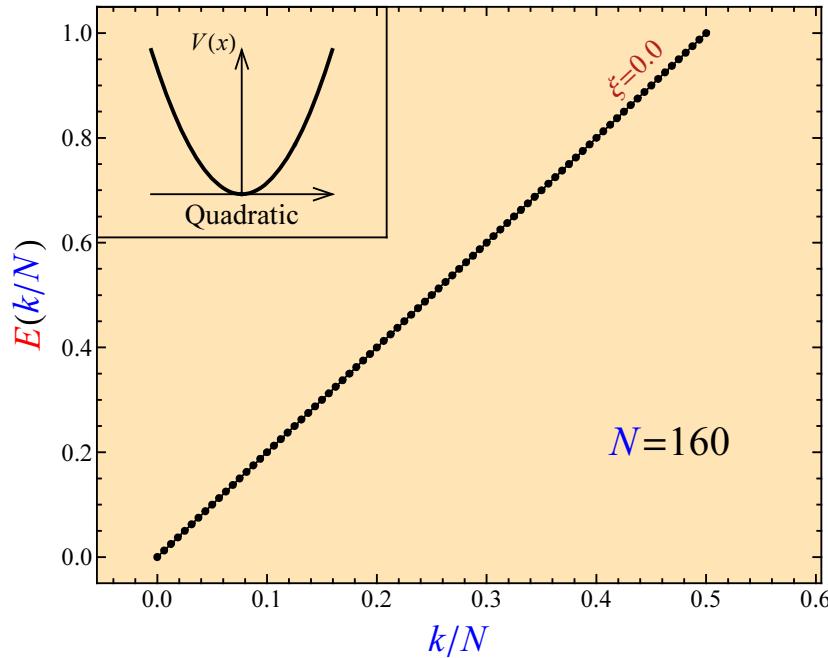


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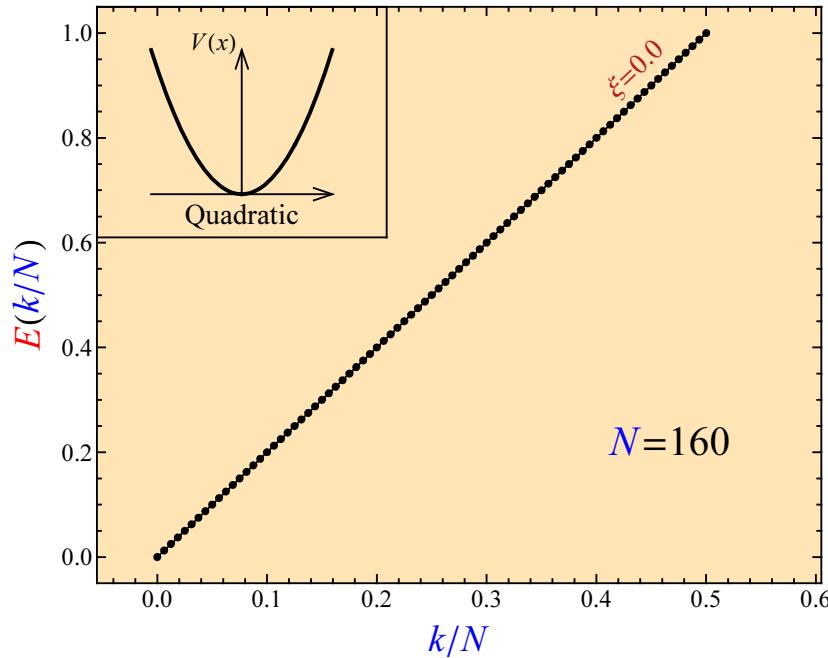
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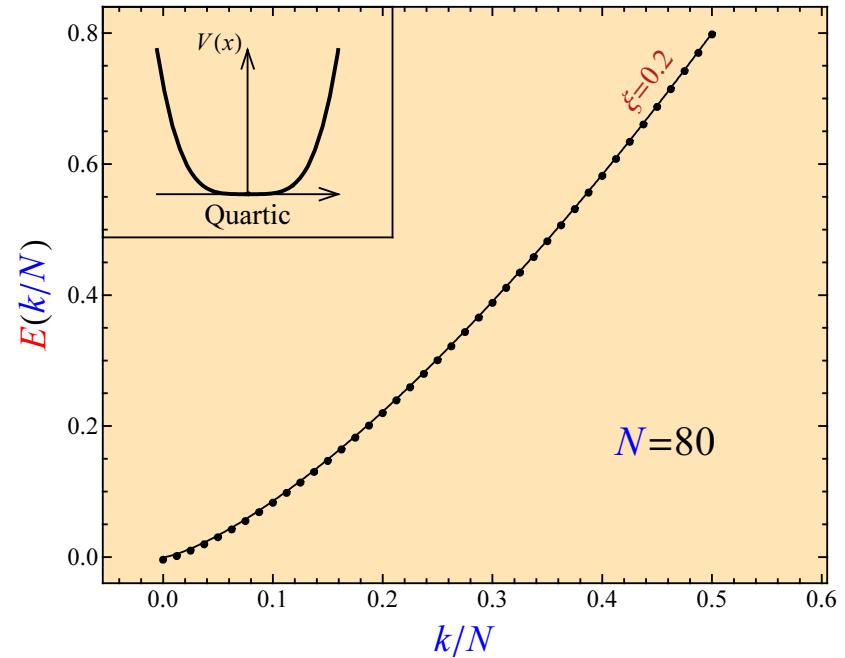
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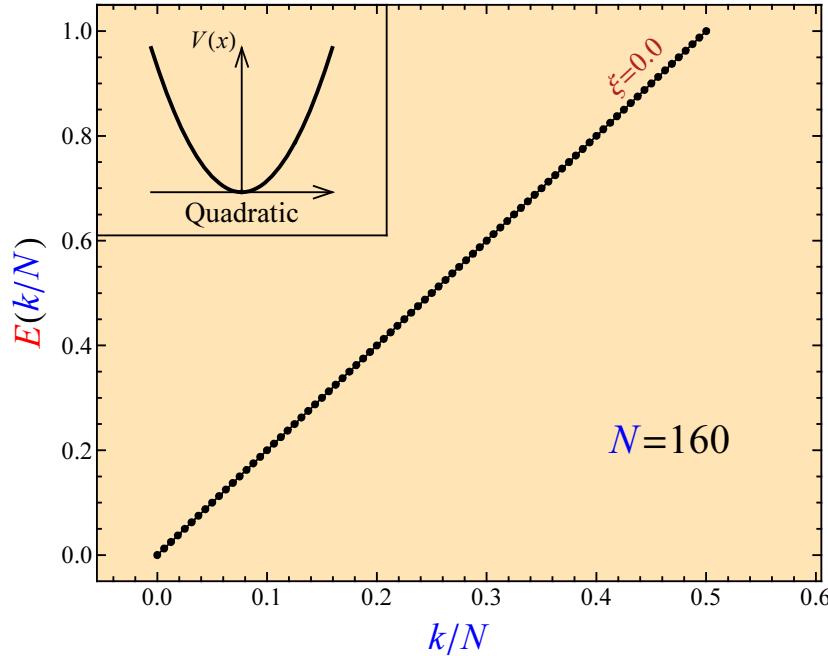
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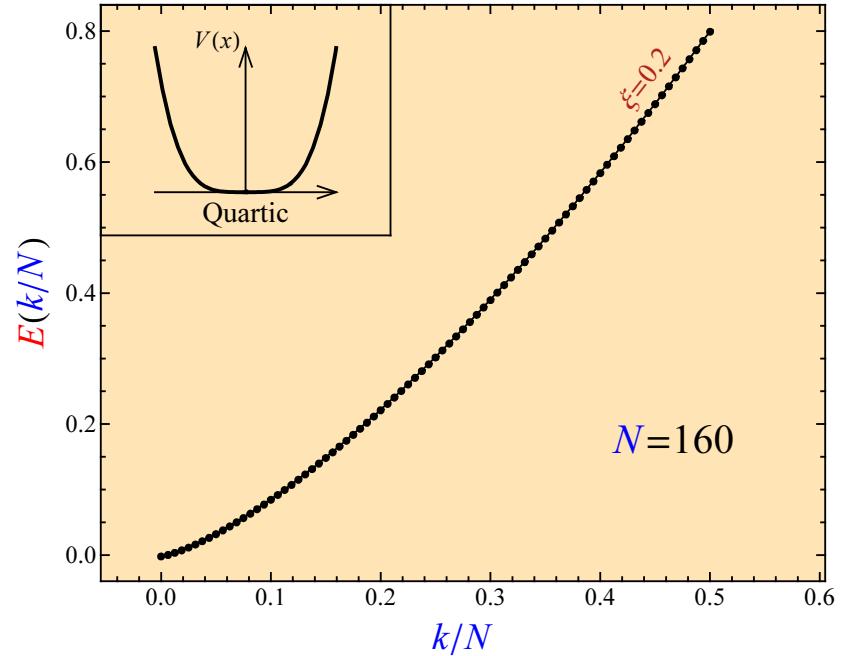
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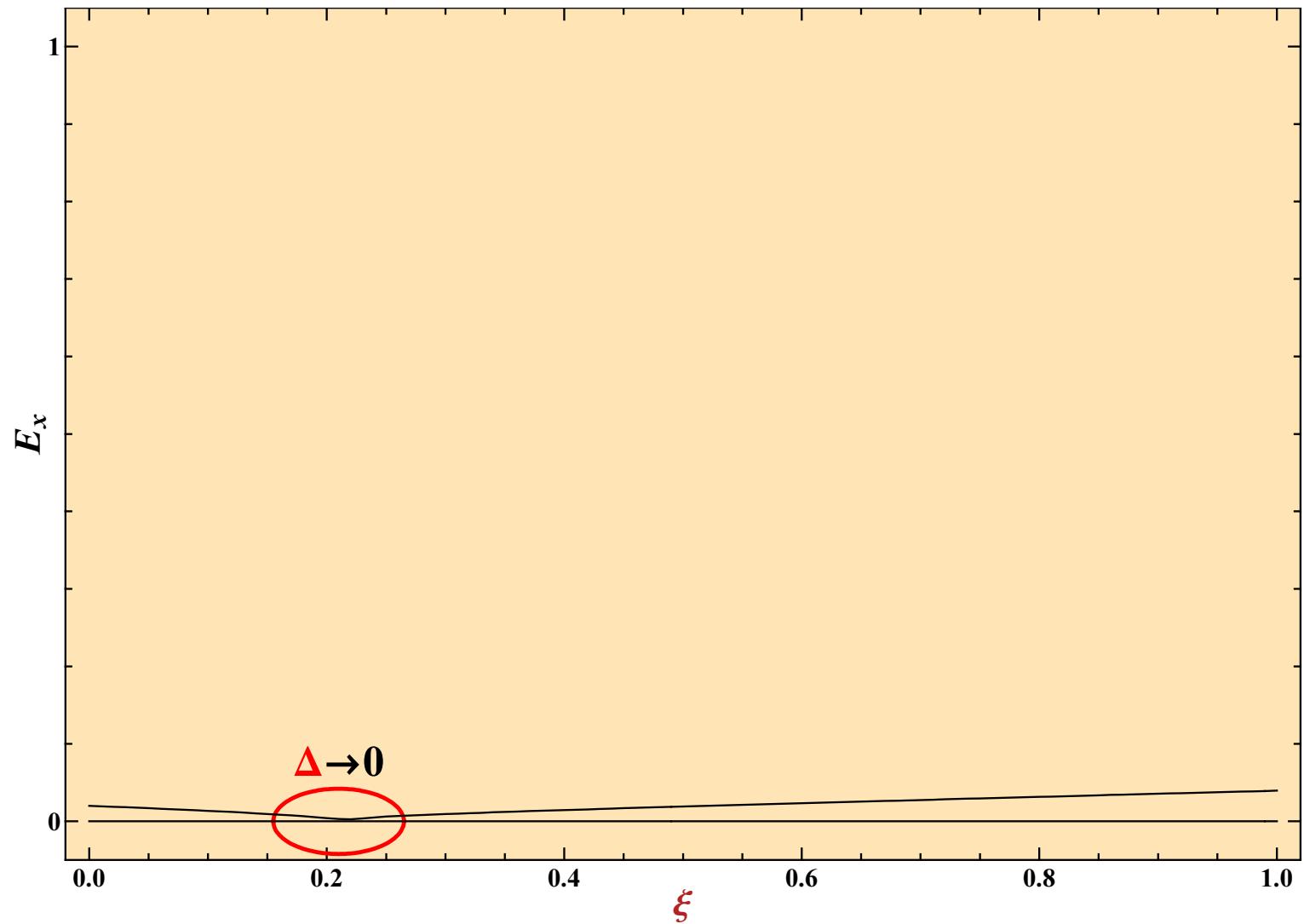


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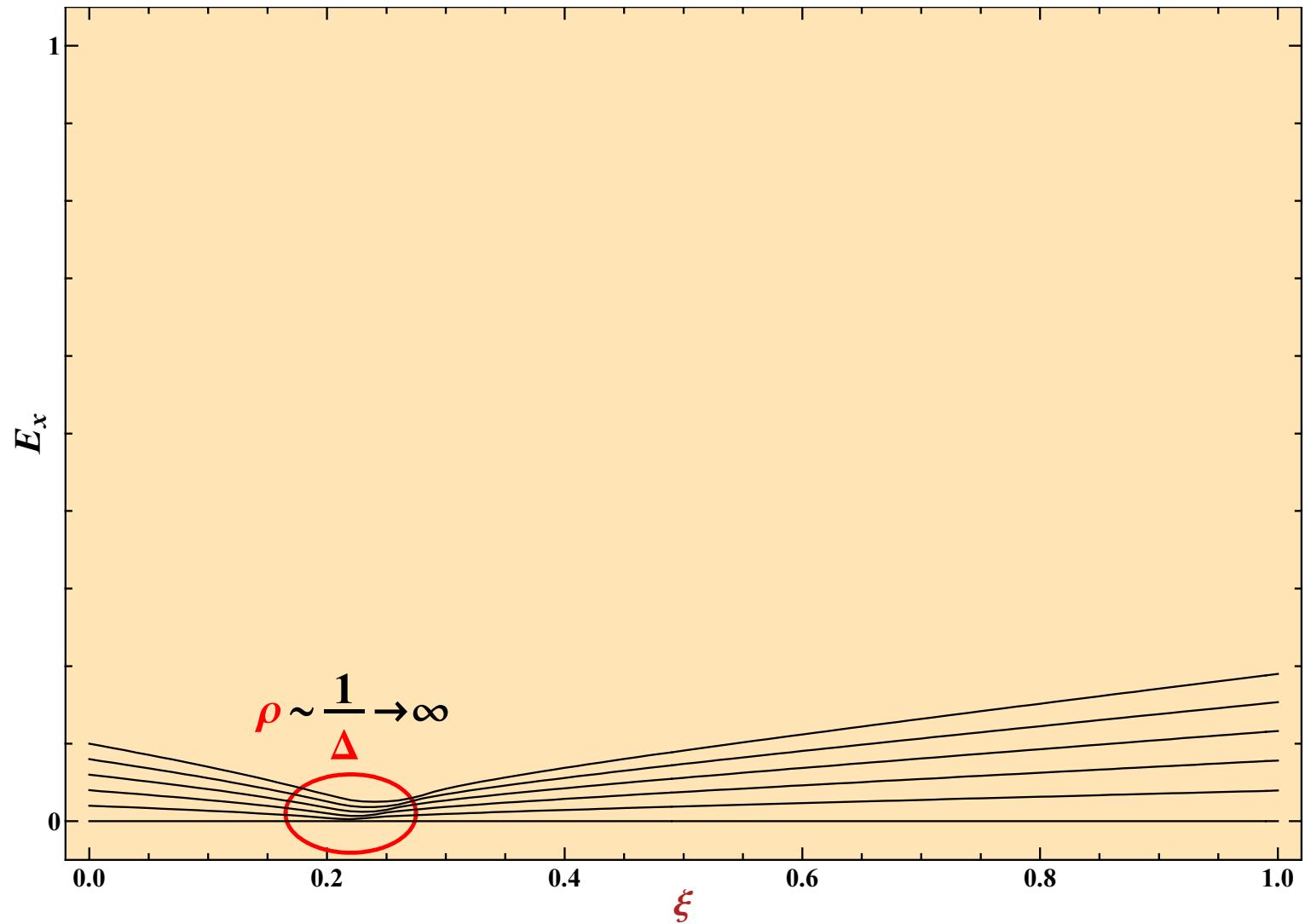
Excited state quantum phase transition

Singularity in level density propagates from ground state QPT



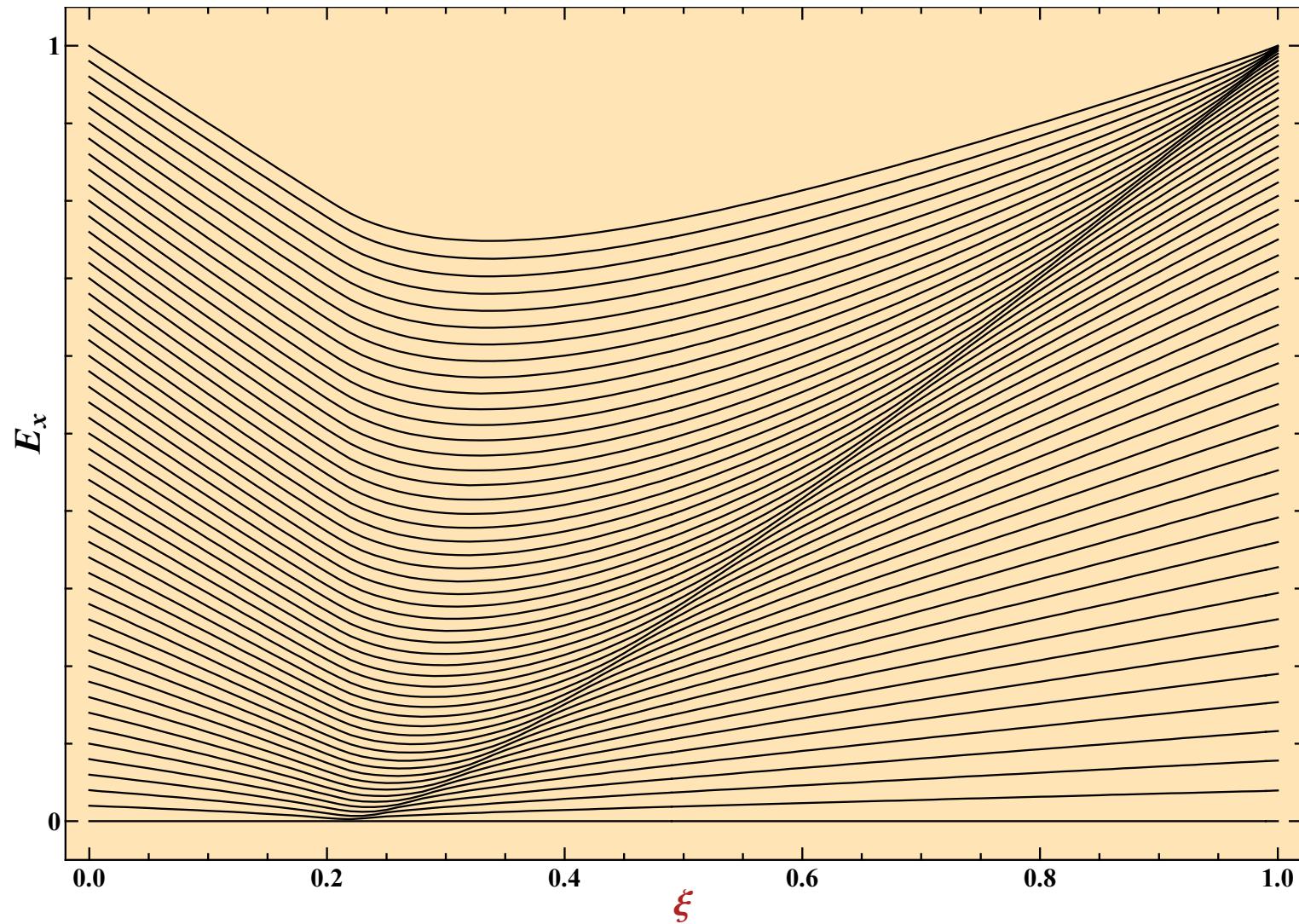
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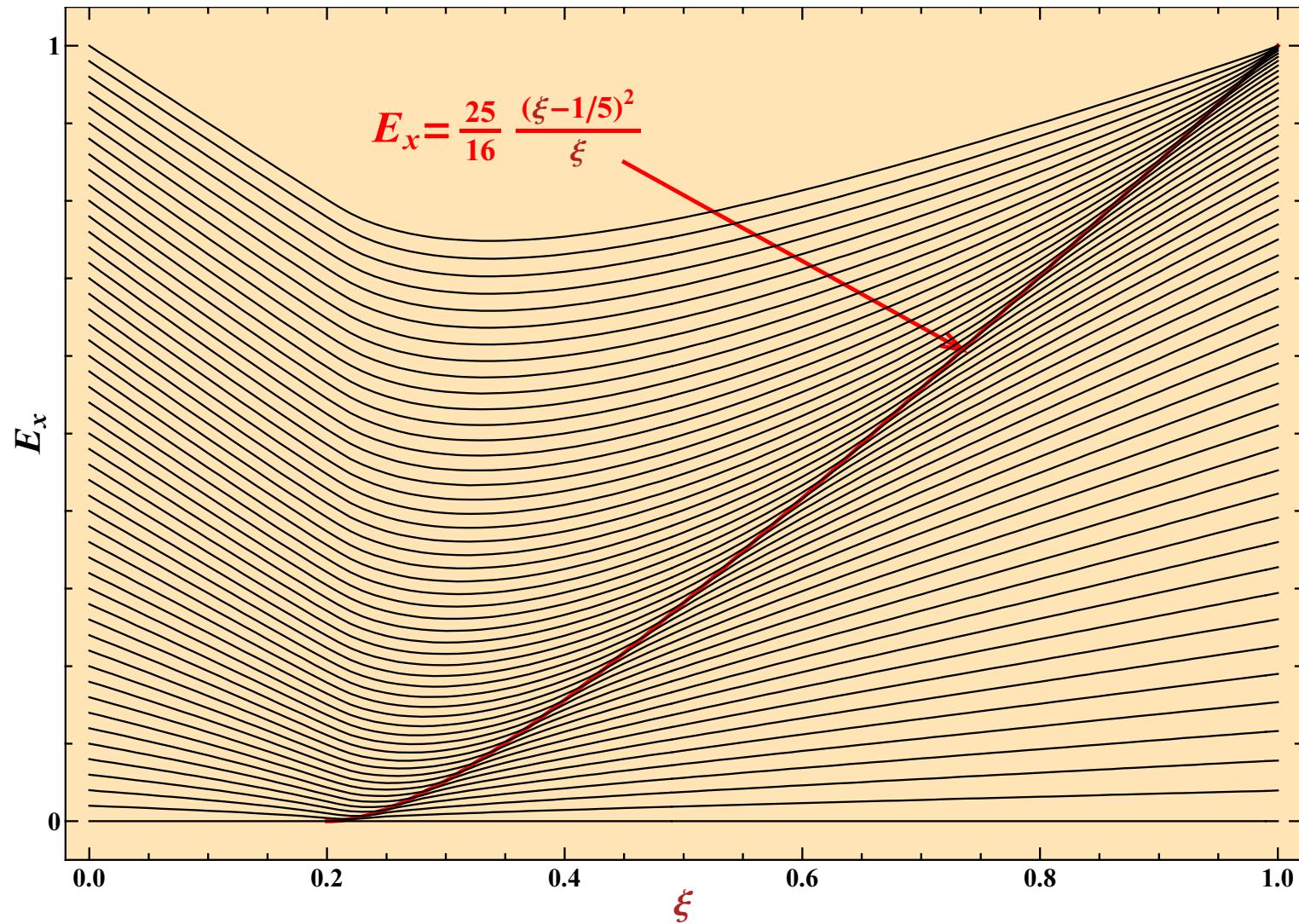
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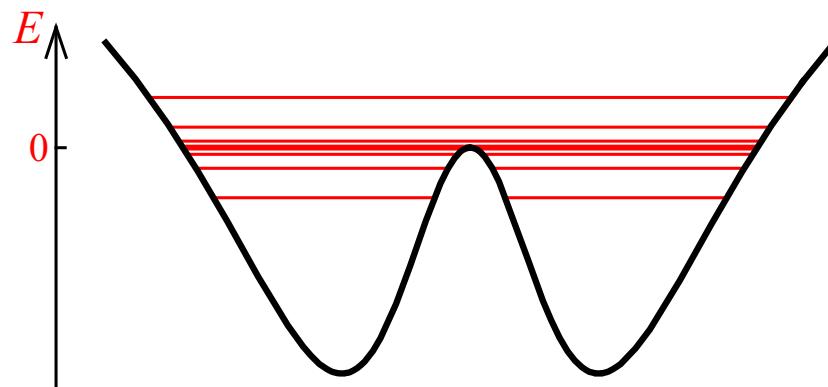
Excited state quantum phase transition

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Semiclassical explanation for excited state QPT

Level density singularity occurs at energy of top of barrier



$$\rho(E) = \frac{1}{\pi\hbar} \int_{x_1(E)}^{x_2(E)} \frac{dx}{v_{\text{cl}}(E, x)} = \frac{T_{\text{cl}}(E)}{2\pi\hbar}$$
$$v_{\text{cl}}(E, x) \equiv \sqrt{\frac{2}{M}[E - V(x)]}$$

Classical velocity $v_{\text{cl}}(x)$ vanishes at top of barrier

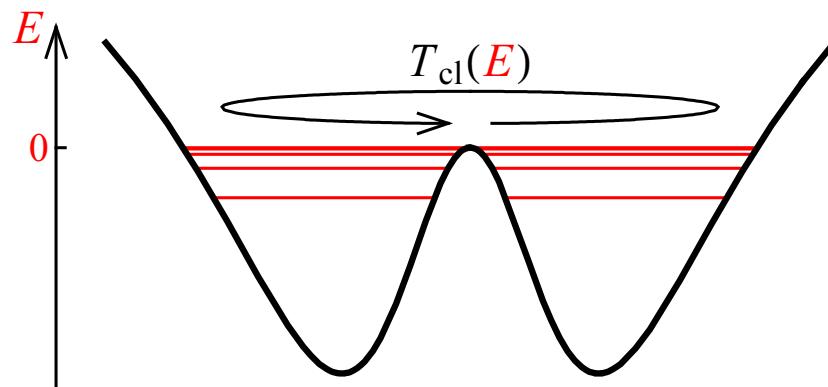
- Classical period $T_{\text{cl}}(E) \rightarrow \infty$
- Level density $\rho(E) \rightarrow \infty$
- Probability density $|\Psi(x)|^2 \sim 1/v_{\text{cl}}(x)$ highly localized at $x = 0$

Excited state QPT demarcates states of qualitatively different nature

- $E < 0$: Trapped in well — $\text{SO}(n+1)$ -like
- $E > 0$: Above barrier — $\text{U}(n)$ -like

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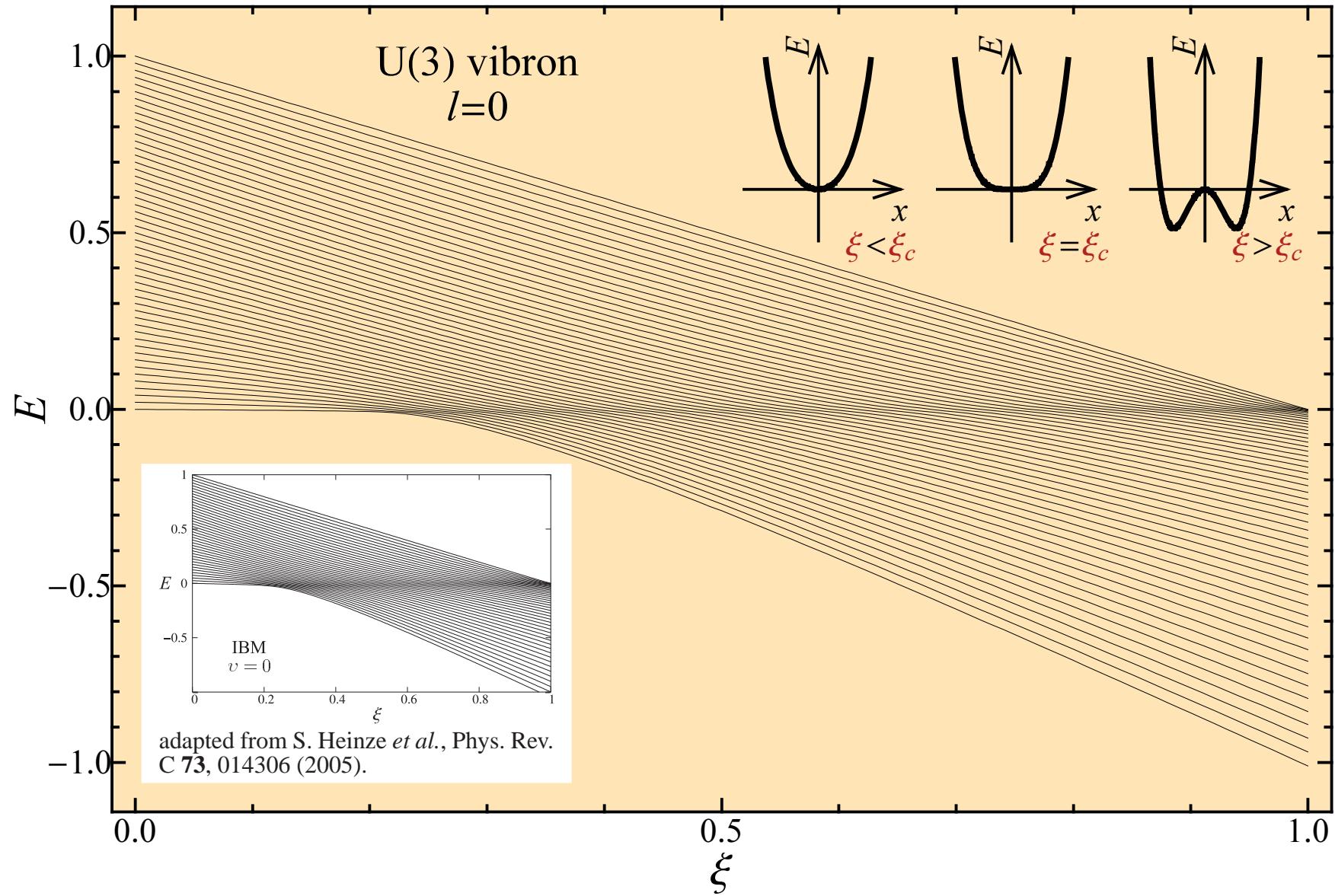
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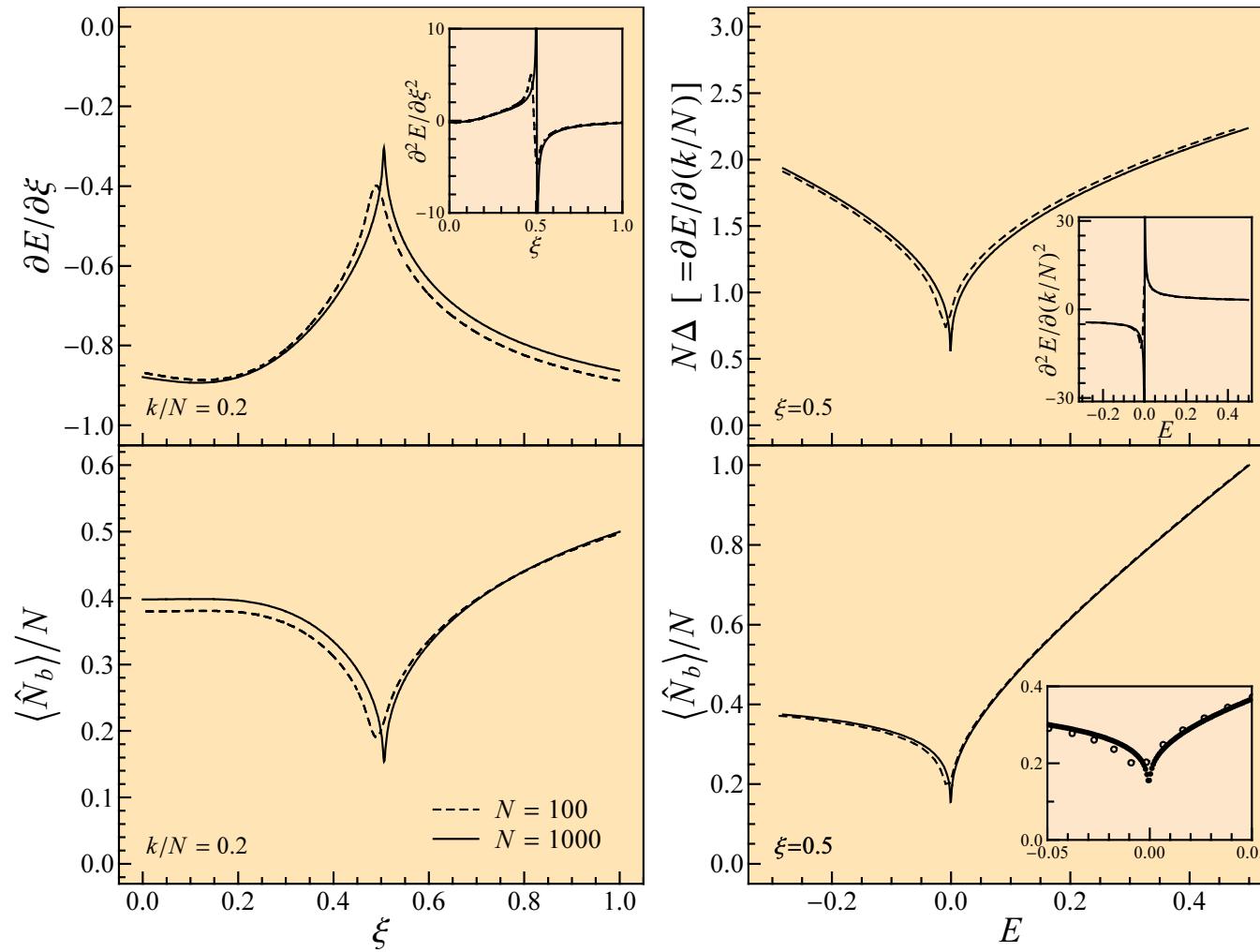
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Evolution of eigenvalues



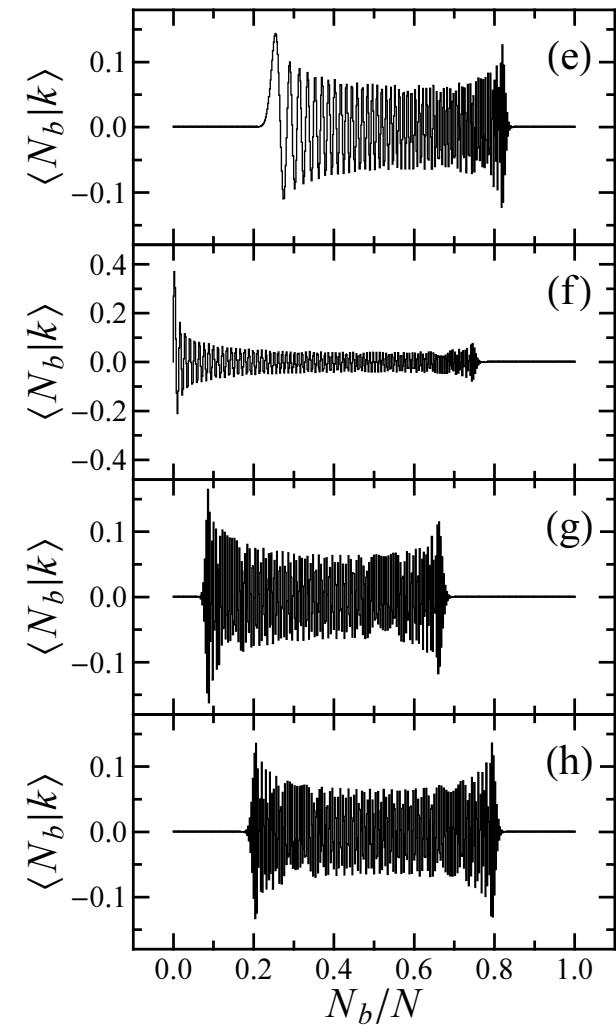
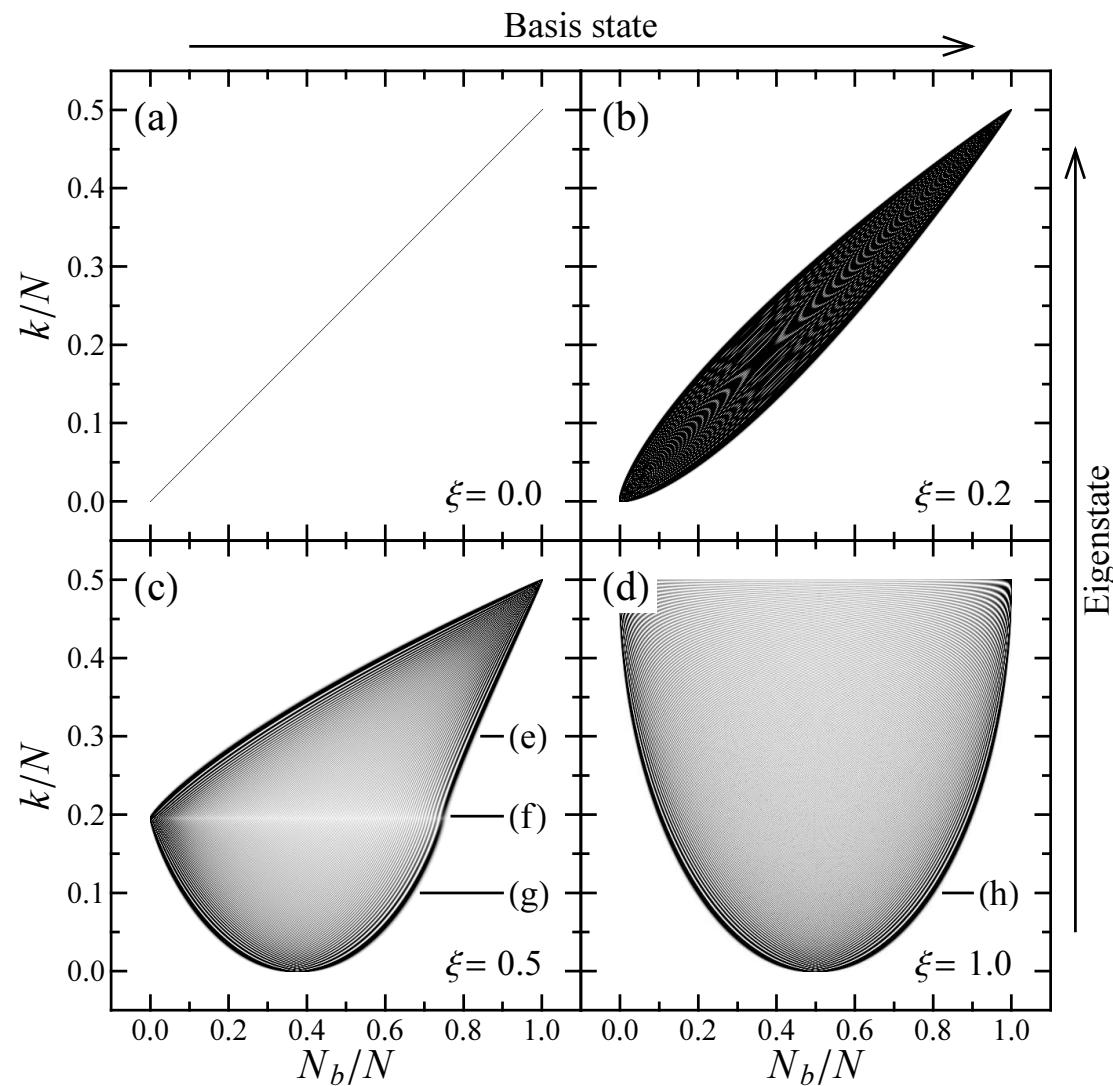
ESQPT eigenvalues and order parameters

Singular evolution with respect to both *control parameter* (ξ) and *energy* (E)



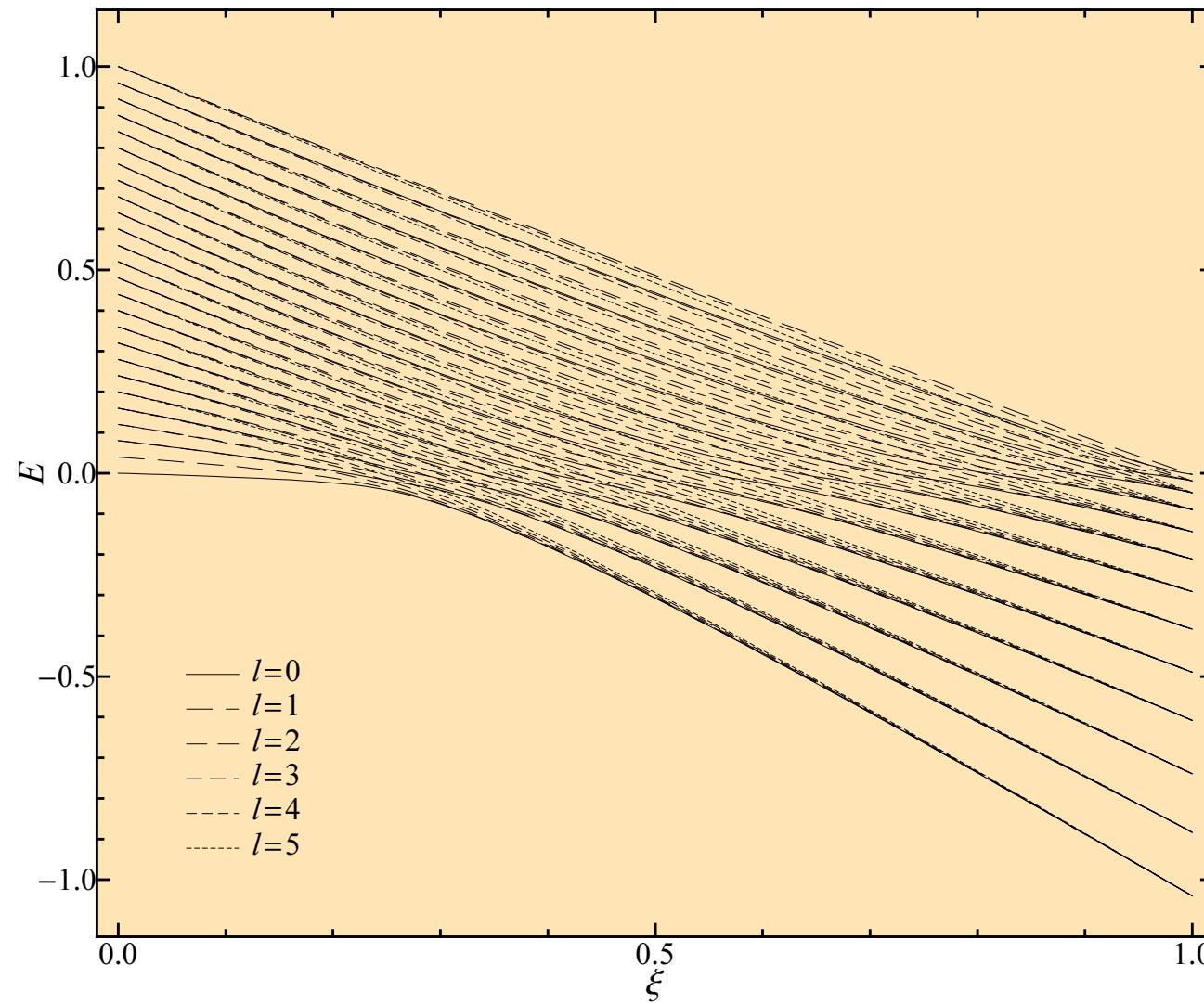
Qualitative changes in wave functions across ESQPT

Decomposition with respect to U(3) basis



Qualitative changes in spectrum across ESQPT

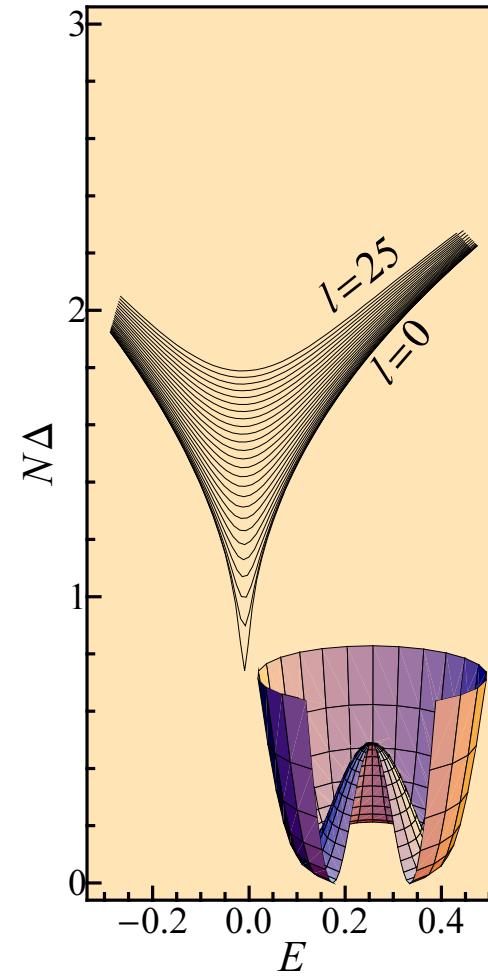
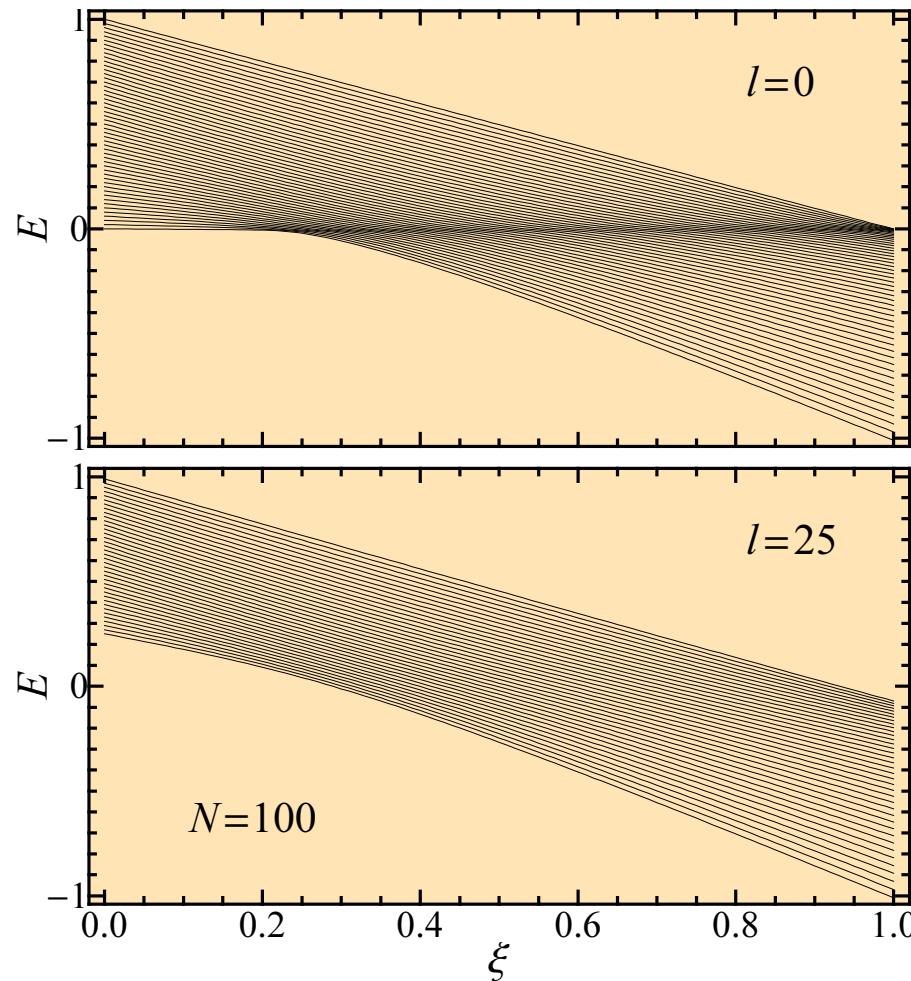
Angular momentum degeneracy patterns



Angular momentum (seniority) dependence

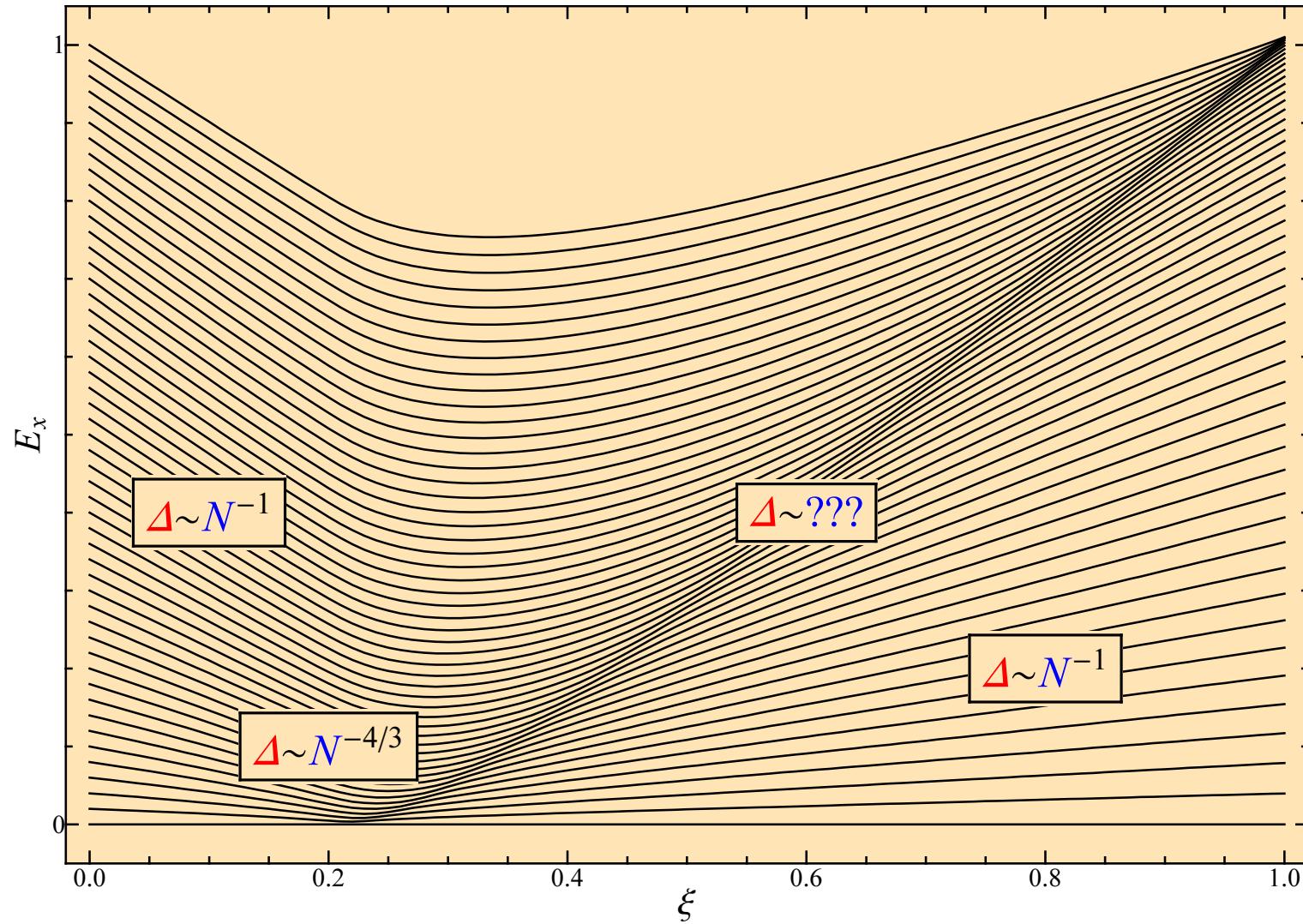
Semiclassically: Centrifugal term suppresses probability near barrier

$$\sim \frac{T_\vartheta(l)}{N^2} \frac{1}{r^2} \sim \left(\frac{l}{N}\right)^2 \frac{1}{r^2}$$



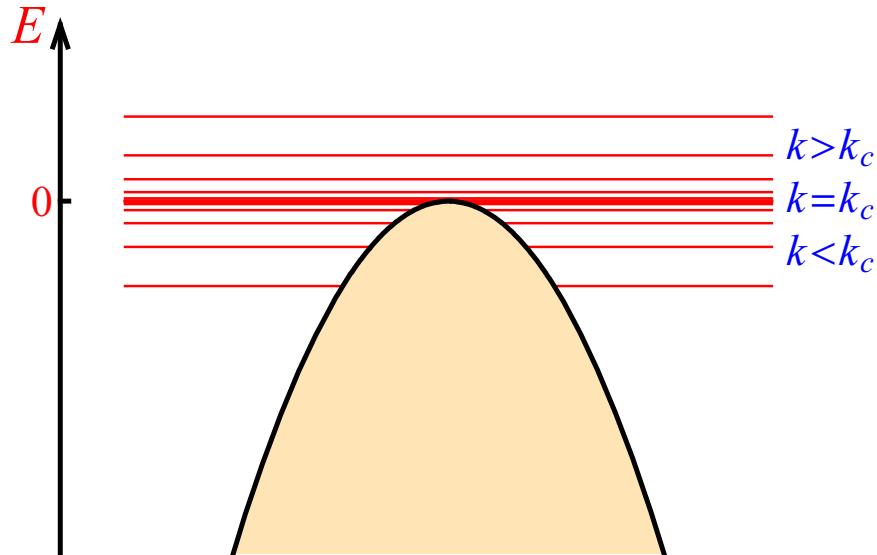
Excited state quantum phase transition

Finite-size scaling behavior?



Semiclassical scaling analysis for excited state QPT

Singular behavior dominated by parabolic barrier?



$$H = \frac{\hbar^2}{2m} p_x^2 - \frac{a}{2} x^2$$

$$\text{“}\hbar\omega\text{”} = \sqrt{\frac{\hbar^2 a}{m}} \Rightarrow \frac{\Xi(\xi)^{1/2}}{N}$$

$$\Xi(\xi) \equiv (1 - \xi)(1 - 5\xi)$$

Semiclassical dynamics studied in depth (phase space separatrix)

K. W. Ford, D. L. Hill, M. Wakano, and J. A. Wheeler, Ann. Phys. (N.Y.) **7**, 239 (1959).

J. R. Cary, P. Rusu, and R. T. Skodje, Phys. Rev. Lett. **58**, 292 (1987).

M. S. Child, J. Phys. A **31**, 657 (1998).

Logarithmic singularity in action at $E = 0$

$$S(E) = 2 \int_0^{x_2} dx [2m(E + \frac{a}{2}x^2)]^{1/2}$$

Semiclassical scaling analysis for excited state QPT

Quantization condition

$$\underbrace{-E \log E}_{\text{Singular}} + \underbrace{\alpha E + \dots}_{\text{Regular}} \approx 2\pi \hbar \omega (\mathbf{k} - \mathbf{k}_c) \quad \hbar \omega = \frac{\Xi(\xi)^{1/2}}{N}$$

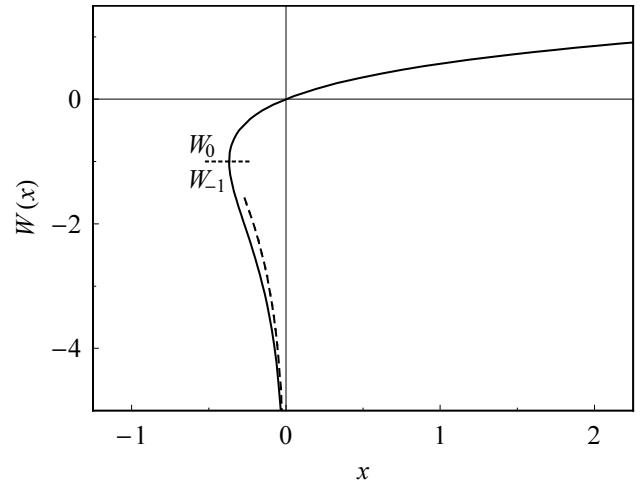
Lambert W function

R. M. Corless, G. H. Gonnet, D. E. G. Hare, D. J. Jeffrey, and D. E. Knuth, Adv. Comput. Math. **5**, 329 (1996).

$$x = ye^y \quad y = W(x)$$

$$W(x) \sim \log(-x) - \log[-\log(-x)]$$

$$y \log y + cy = x \Rightarrow y = x/W(e^c x)$$

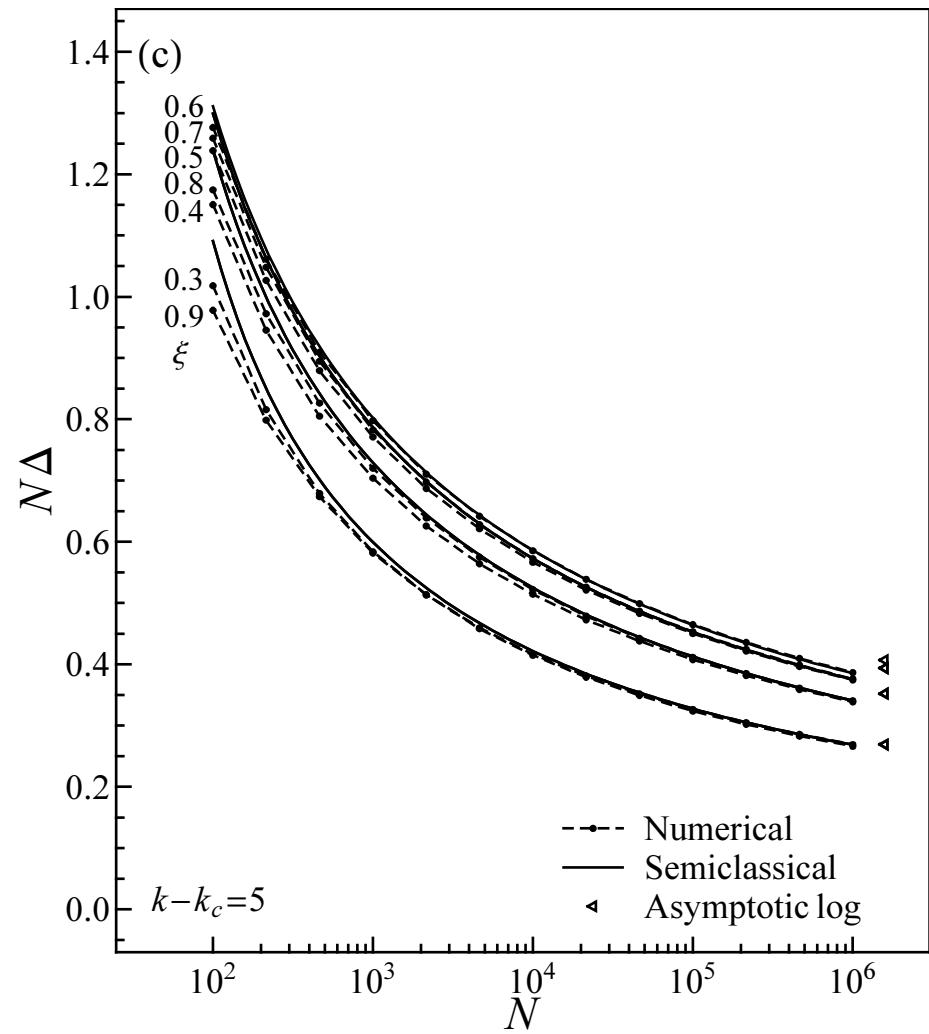
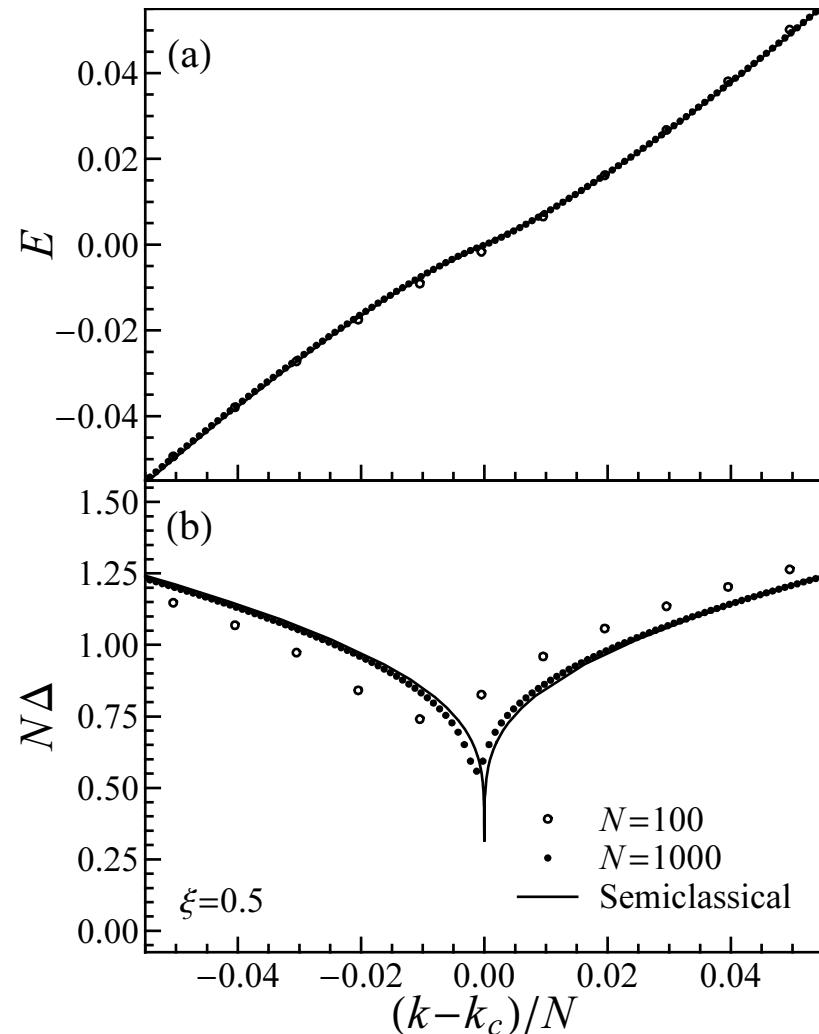


$$E(\xi, N, k) \approx -\frac{2\pi \Xi(\xi)^{1/2} (\mathbf{k} - \mathbf{k}_c)/N}{W[-e^{-\alpha} 2\pi \Xi(\xi)^{1/2} (\mathbf{k} - \mathbf{k}_c)/N]} \sim \frac{2\pi \Xi(\xi)^{1/2}}{\log N}$$

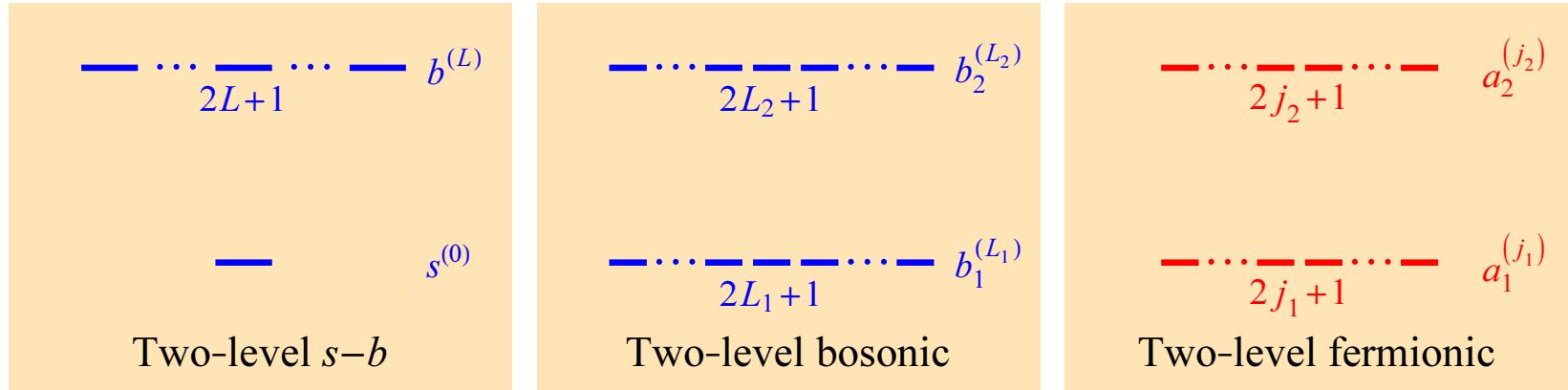
Full asymptotics very accurate ($\sim 1\%$ at $N \sim 10^5$)

Extreme log approximation of limited *quantitative* value

Quantum and semiclassical results for gap Finite-size scaling in the vicinity of the ESQPT



Dual algebraic structures for two-level pairing



Quasipin — $\text{SU}(1, 1)$ or $\text{SU}(2)$

$$\hat{S}_{j+} \equiv \frac{1}{2} \sum_m c_{jm}^\dagger \tilde{c}_{jm}^\dagger \quad \hat{S}_{j-} \equiv \frac{1}{2} \sum_m \tilde{c}_{jm} c_{jm} \quad \hat{S}_{jz} \equiv \frac{1}{4} \sum_m (c_{jm}^\dagger \tilde{c}_{jm} + \tilde{c}_{jm} c_{jm}^\dagger)$$

$$[\hat{S}_{j+}, \hat{S}_{j-}] = \mp 2\hat{S}_{jz} \quad [\hat{S}_{jz}, \hat{S}_{j+}] = +\hat{S}_{j+} \quad [\hat{S}_{jz}, \hat{S}_{j-}] = -\hat{S}_{j-}$$

Second-order QPT — between weak and strong pairing regimes

$$\begin{aligned} \text{SU}_1(1, 1) \otimes \text{SU}_2(1, 1) &\supset \begin{cases} \text{SU}(1, 1) \\ \text{U}_2(1) \otimes \text{U}_2(1) \end{cases} && \text{(bosonic)} \\ \text{SU}_1(2) \otimes \text{SU}_2(2) &\supset \begin{cases} \text{SU}(2) \\ \text{U}_1(1) \otimes \text{U}_2(1) \end{cases} && \text{(fermionic)} \end{aligned}$$

Dual algebraic structures for two-level pairing

Unitary — $\mathrm{U}(n_1 + n_2)$ ($n_i = 2L_i + 1$ or $2j_i + 1$)

$$(c_1^\dagger \times \tilde{c}_1)^{(\lambda)} \quad (c_1^\dagger \times \tilde{c}_2)^{(\lambda)} \quad (c_2^\dagger \times \tilde{c}_1)^{(\lambda)} \quad (c_2^\dagger \times \tilde{c}_2)^{(\lambda)}$$

$$\mathrm{U}(n_1 + n_2) \supset \left(\begin{array}{c} \mathrm{SO}(n_1 + n_2) \\ \mathrm{U}_1(n_1) \otimes \mathrm{U}_2(n_2) \end{array} \right) \supset \mathrm{SO}_1(n_1) \otimes \mathrm{SO}_2(n_2) \supset \mathrm{SO}_{12}(3) \text{ (bosonic)}$$

$$\mathrm{U}(n_1 + n_2) \supset \left(\begin{array}{c} \mathrm{Sp}(n_1 + n_2) \\ \mathrm{U}_1(n_1) \otimes \mathrm{U}_2(n_2) \end{array} \right) \supset \mathrm{Sp}_1(n_1) \otimes \mathrm{Sp}_2(n_2) \supset \mathrm{SU}_{12}(2) \text{ (fermionic)}$$

Associated geometry? $\mathrm{U}(n_1 + n_2)/[\mathrm{U}(n_1) \otimes \mathrm{U}(n_2)]$

Casimir operators simply related to quasispin operators at fixed N

Two-level s - b model as special case of quasispin pairing model

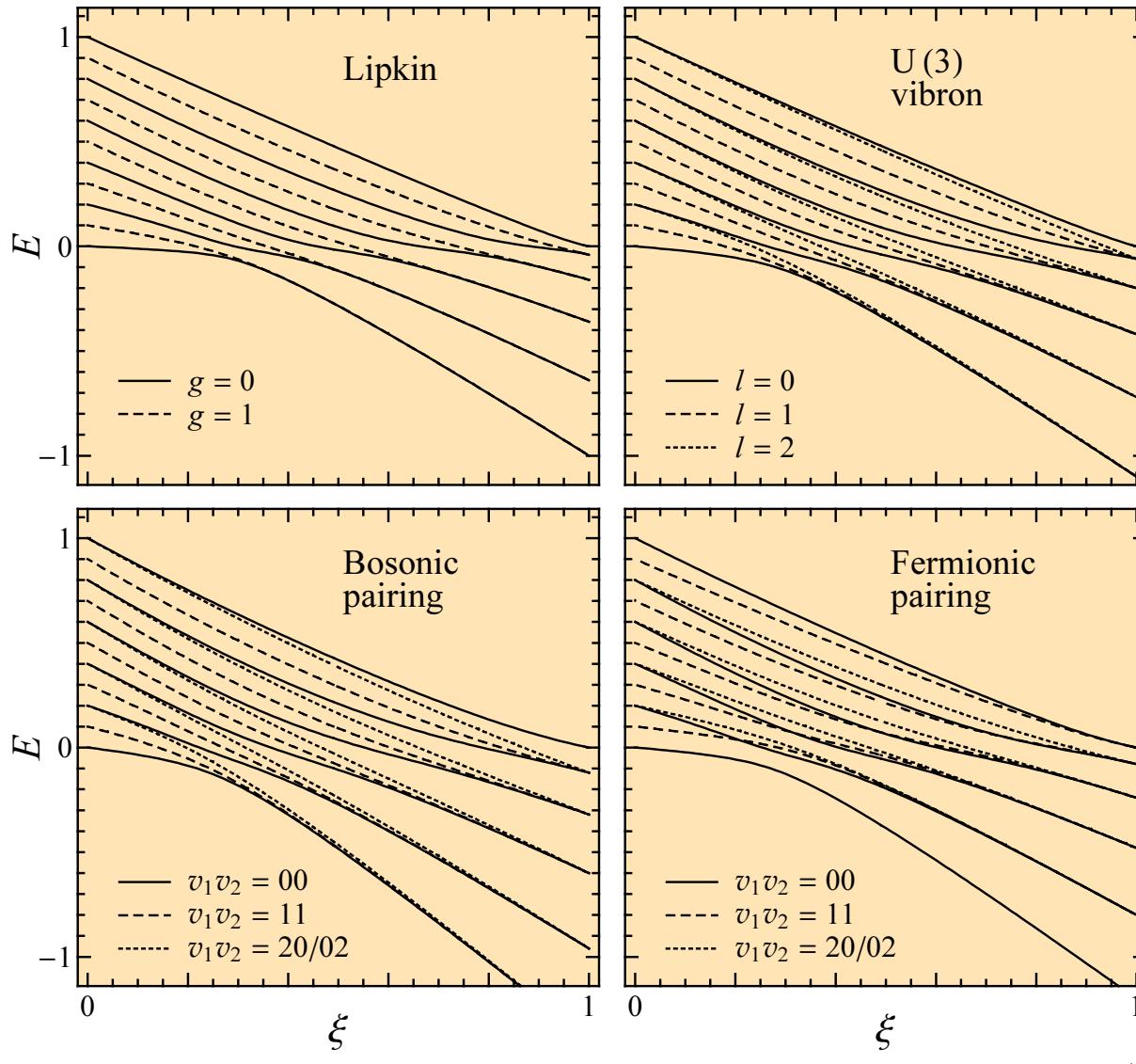
Already applied for IBM U(5)-SO(6):

A. Arima and F. Iachello, Ann. Phys. (N.Y.) **123**, 468 (1979).

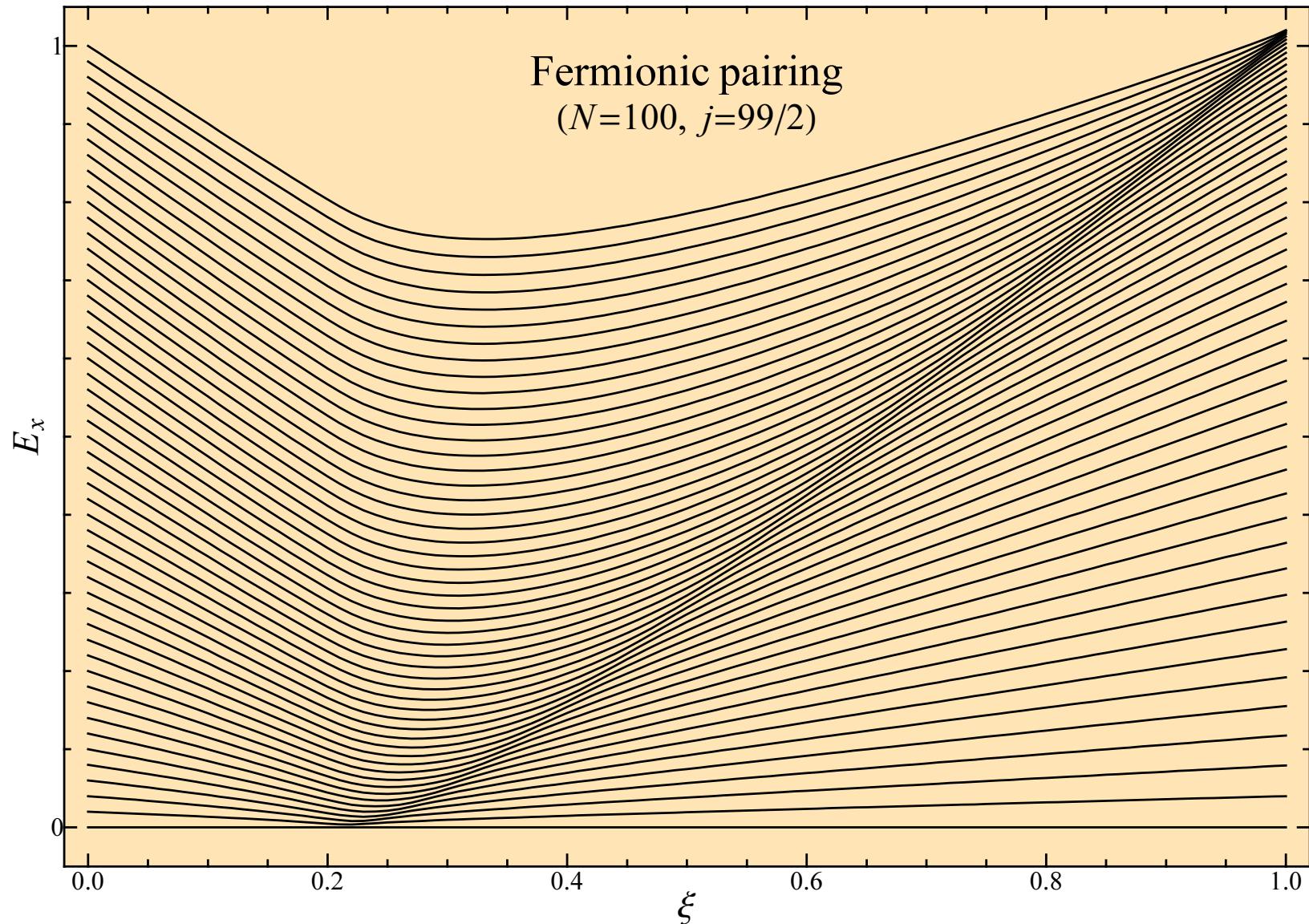
F. Pan and J. P. Draayer, Nucl. Phys. A **636**, 156 (1998).

$$\begin{aligned} \hat{H} &= \frac{(1 - \xi)}{N} \hat{N}_b - \frac{\xi}{N^2} (s^\dagger \tilde{b} + b^\dagger \tilde{s}) \cdot (s^\dagger \tilde{b} + b^\dagger \tilde{s}) \\ &\Rightarrow \frac{(1 - \xi)}{N} \hat{N}_b - \frac{4\xi}{N^2} (-)^{g(L)} (\hat{S}_{s+} \pm \hat{S}_{b+})(\hat{S}_{s-} \pm \hat{S}_{b-}) + f(N, L, v_b) \end{aligned}$$

Spectra of the two-level models



ESQPT for two-level pairing model



Conclusions and...

Excited state quantum phase transition

- Singularity at nonzero excitation energy
- Simultaneously reflected in eigenvalue spectrum (individual levels eigenvalues, level density/gap) and order parameters
- Qualitative difference between distinct “phases” (wave functions) across the ESQPT

Finite-size scaling properties of gap described at semiclassical level

Both parallels with and differences from ground state QPT

Common to bosonic and fermionic pairing models

including the *s-b* models (Lipkin, vibron, IBM)

Open questions

Treatment of scaling beyond semiclassical (“mean field”) scaling

Bridging gap between ground state QPT (power law) and ESQPT

Interactions beyond pure pairing interaction (role of integrability)

$\text{SO}(n_1) \otimes \text{SO}(n_2)$ or $\text{Sp}(n_1) \otimes \text{Sp}(n_2)$ invariance leads to effectively one-dimensional problem (sombrero potential)

System undergoing first-order ground state QPT

How universal are excited state quantum phase transitions?

- Multi-level pairing models (superconducting grains)
- Two-level models as “infinitely-coordinated” limit of Ising-type lattice models... Can ESQPT persist to finite range interaction?

Mapping of pairing model onto Bose-Hubbard type Hamiltonian

F. Pan and J. P. Draayer, nucl-th/0703007.

- Coupled two-level systems

e.g., Dicke model for quantum optical systems