Symmetry breaking and restoration for trapped

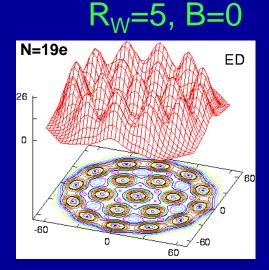
electrons, ions, and neutral atoms

Constantine Yannouleas and Uzi Landman School of Physics, Georgia Institute of Technology

Rep. Prog. Phys. 70, 2067 (2007);

PRA 96, 043610 (2017)





Symmetry breaking and symmetry preserving schemes : how to efficiently grasp collective correlations in mesoscopic many-body systems? CEA-Saclay, May 13-17, 2019

Supported by the U.S. AFOSR (FA9550-15-1-0519)

CONTROL PARAMETERS FOR SYMMETRY BREAKING

IN SINGLE QD'S: WIGNER CRYSTALLIZATION

• Essential Parameter at B=0: (parabolic confinement)

$$R_{W} = (e^{2}/\kappa I_{0})/\hbar\omega_{0} \sim 1/(\hbar^{3}\omega_{0})^{1/2}$$

e-e Coulomb repulsion kinetic energy
$$I_{0} = (\hbar/m^{*}\omega_{0})^{1/2} \} Spatial Extent$$
of 1s s.p. state
$$\kappa : dielectric const. (12.9)$$
$$m^{*}: e effective mass (0.067 m_{e}) GaAS$$
$$\hbar\omega_{0} (5 - 1 meV) \implies R_{W} (1.48 - 3.31)$$

In a magnetic field, essential parameter is B itself

IN QDM'S: DISSOCIATION (Electron puddles, Mott transition)

Essential parameters: Separation (d) Potential barrier (V_b) Magnetic field (B) $R_{\delta} = gm/(2\pi\hbar^2)$

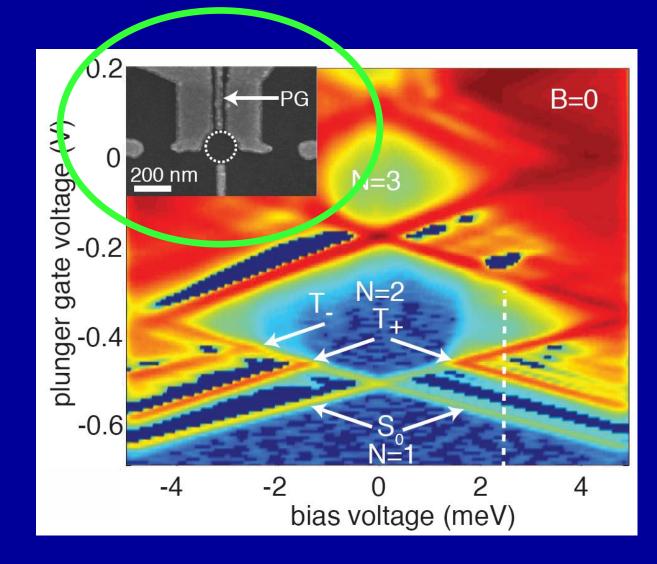
<u>Neutral</u> bosons Towards controlling symmetry breaking and symmetry restoration in both space and time in manmade nanosystems (SMALL IS DIFFERENT)

Unprecedented experimental control of few-body systems of trapped ultracold ions and neutral atoms, and of few-electron assemblies in quantum dots

Time-evolution phenomena in quantum mechanical finite systems which is not captured by mean-field approaches

Different direction from that in the book: "Basic Notions of Condensed Matter Physics", by P.W. Anderson, 1984 (MORE IS DIFFERENT)





Ellenberger, Ensslin, Yannouleas, Landman et al., Phys. Rev. Lett. **96**, 126806 (2006)

Control and measurement of three-qubit entangled states

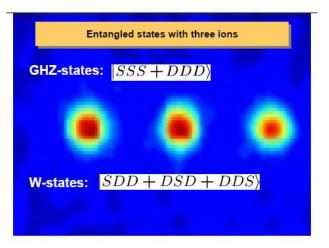
C. F. Roos¹, Mark Riebe¹, H. Häffner¹, W. Hänsel¹, J. Benhelm¹, G. P. T. Lancaster¹, C. Becher¹, F. Schmidt-Kaler¹ & R. Blatt^{1,2}

¹Institut für Experimentalphysik, Universität Innsbruck, Technikerstraße 25, A-6020 Innsbruck, Austria ²Institut für Quantenoptik und Quanteninformation, Östereichische Akademie der Wissenschaften

- Basics of ion trap quantum computers
- Entangling operations (Bell states, CNOT)
- Generation of W- and GHZ-states
- Selective read-out of a quantum register
- Entanglement transformation by condional operations

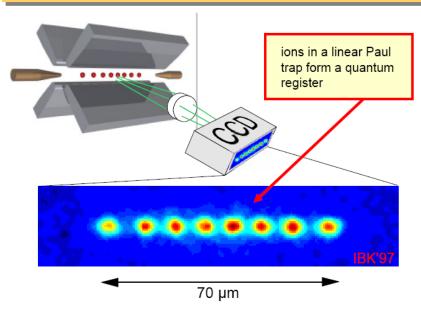


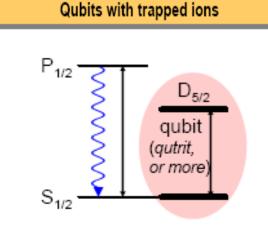




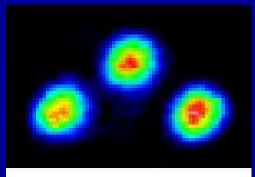
H. Haeffner et al., Nature 438, 643 (2005)

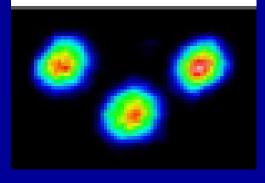
The system: String of ⁴⁰Ca⁺ ions in a linear Paul trap

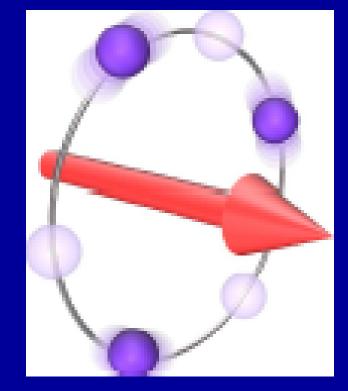




S – D transitions in alkaline earths: Ca⁺, Sr⁺, Ba⁺, Ra⁺, (Yb⁺, Hg⁺) etc.

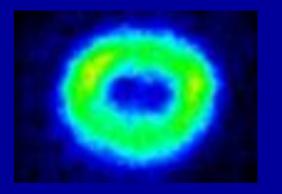


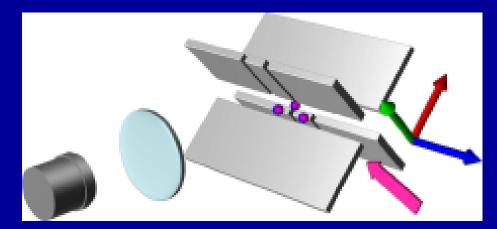




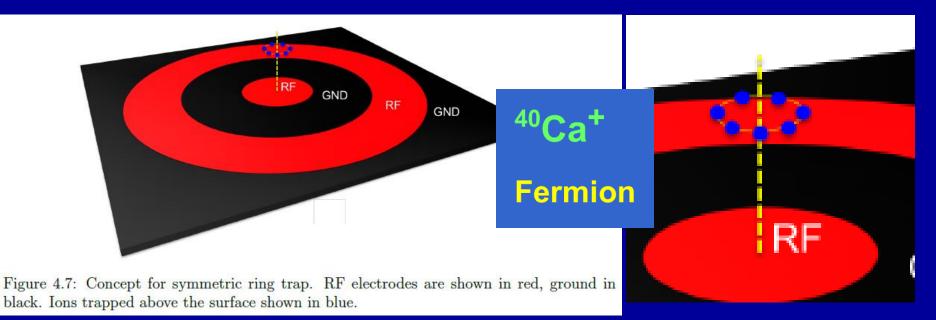






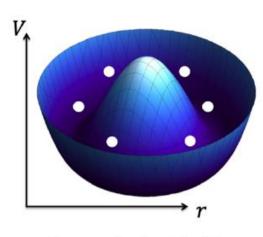


Noguchi, A. et al., Nat. Commun. 5:3868 (2014).



Erik Urban, Ph.D. Thesis, Univ. of California, Berkeley, 2019

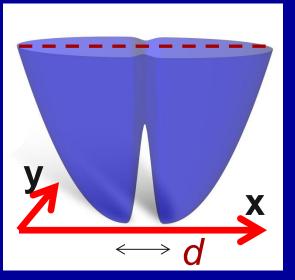
Urban et al., Coherent Control of the Rotational Degree of Freedom of a Two-Ion Coulomb Crystal, arXiv:1903.05763



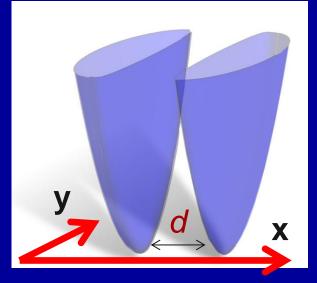
lons moving freely in 1D potential

lons pinned to one side by electric field

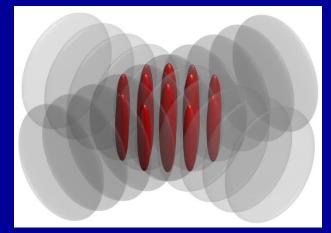
2 ⁶Li ATOMS IN A DOUBLE OPTICAL TRAP Linear arrangement (LI) Parallel arrangement (PA)



Strictly 1D



2D aspects



Experimental depictions of 1D optical traps



LOWERING OF ENERGY AND SYMMETRY BREAKING (SB) IN SELF-CONSISTENT MEAN-FIELD APPROACHES Restricted vs unrestricted and fermions vs bosons

Attraction Restricted approach (RHF)

Same orbital and symmetry breaking (SB):

Nilsson potential (fermions, nucleons)

Gross-Pitaevskii (GP) (attractive bosons, Lump of ultracold neutral atoms)

GP for repulsive bosons: SB raises the energy ! Repulsion Unrestricted approach (UHF)

Different orbitals and symmetry breaking (SB):

Hydrogen molecule, dissociation (electrons, chemistry)

Wigner molecules (electrons, quantum dots)

Space-time crystals on rings (fermion or bosons, ultracold ions)

UNRESTRICTED HF FOR REPELLING FERMIONS (Self-consistent Pople-Nesbet Eqs.)
Different orbitals for different spins
Two coupled equations/ Spin-up coupled to spin-down
Self-consistent solution → orbital localization
[example from chemistry:
dissociation of Hydrogen molecule (next slide)]

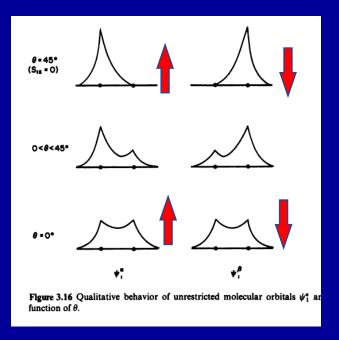
UNRESTRICTED HF FOR REPELLING BOSONS? A different orbital for each particle Self-consistent set of Eqs. is not practical Reason: orbitals for bosons are not orthogonal/ spin-orbitals for fermions are orthogonal

In case of crystals, employ ansatz = permanent of orbitals approximated as displaced Gaussians

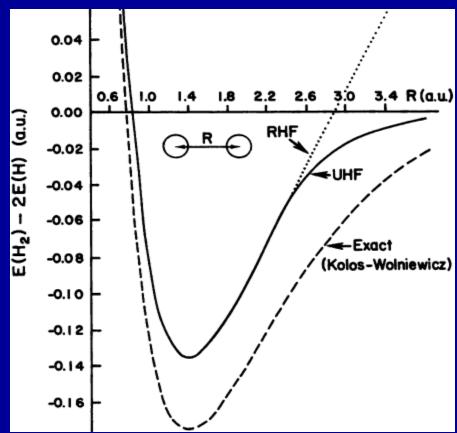
The Hydrogen molecule Szabo and Ostlund, Modern Quantum Chemistry

3.8.7 The Dissociation Problem and Its Unrestricted Solution

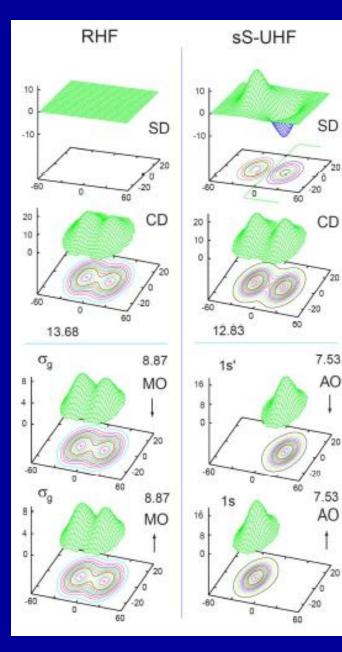
At very large bond lengths, however, one is really trying to describe two individual hydrogen atoms. A proper description will have one electron on one H atom and the other electron on the other H atom, i.e., the two electrons will have quite different spatial distributions. They should not have identical



Next step: Heitler-London



H_2-QDM DOUBLE-WELL O



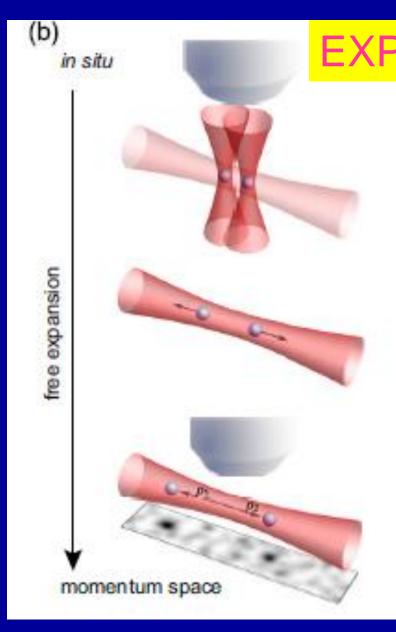
$$\begin{split} \sqrt{2}\Psi_{\text{UHF}}(1,2) &= \begin{vmatrix} u(\mathbf{r}_1)\alpha(1) & v(\mathbf{r}_1)\beta(1) \\ u(\mathbf{r}_2)\alpha(2) & v(\mathbf{r}_2)\beta(2) \end{vmatrix} \\ &\equiv |u(1)\bar{v}(2)\rangle, \end{split}$$

$$\mathcal{P}^{s,t}_{ ext{spin}} = 1 \mp \varpi_{12}$$

$$\sqrt{2}\mathcal{P}_{\rm spin}^s\Psi_{\rm UHF}(1,2) =$$
$$(u(\mathbf{r}_1)v(\mathbf{r}_2) + u(\mathbf{r}_2)v(\mathbf{r}_1))\chi(0,0)$$

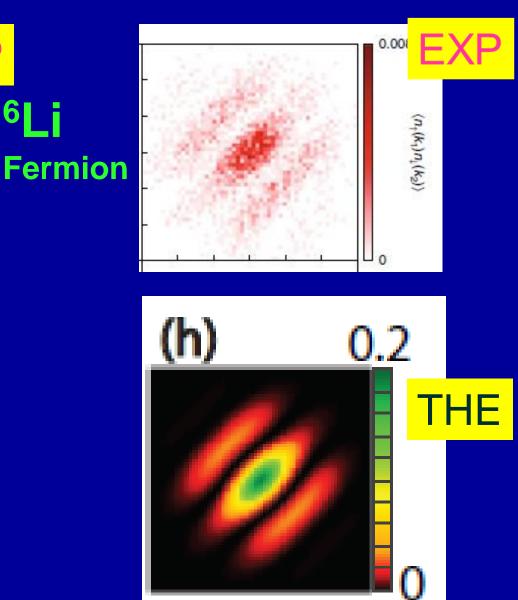
$$\chi(s=0, S_z=0) = (\alpha(1)\beta(2) - \alpha(2)\beta(1))/\sqrt{2}$$

Heitler-London/ EPR-Bohm-Bell Energy gain vs ENTANGLEMENT



6Li

Andrea Bergschneider et al. (Heidelberg), Nature Physics, 22 April 2019



Brandt, Yannouleas, Landman, PRA 97, 053601 (2018)

RESEARCH NEWS & VIEWS

48 | NATURE | VOL 528 | 3 DECEMBER 2015

- Luria, S. E. & Delbrück, M. Genetics 28, 491–511 (1943).
- Vogelstein, B. et al. Science 339, 1546–1558 (2013).
- Craigie, R. & Bushman, F. D. Cold Spring Harb. Perspect. Med. 2, a006890 (2012).
- 11.Wommack, K. E. & Colwell, R. R. *Microbiol. Mol. Biol. Rev.* **64**, 69–114 (2000).
- 12.Reyes, A. et al. Nature 466, 334–338 (2010).
- Barr, J. J. et al. Proc. Natl Acad. Sci. USA 110, 10771–10776 (2013).
- Sharon, I. N. et al. ISME J. 5, 1178–1190 (2011).
 Ruska, H. Naturwissenschaften 28, 45–46 (1940).
- Hu, B., Margolin, W., Molineux, I. J. & Liu, J. Proc. Natl Acad. Sci. USA 112, E4919–E4928 (2015).

QUANTUM PHYSICS

Getting the measure of entanglement

A property called entanglement entropy helps to describe the quantum states of interacting particles, and it has at last been measured. The findings open the door to a deeper understanding of quantum systems. **SEE ARTICLE P.77**

STEVEN ROLSTON

famously bothered by the idea that measuring

To understand what many-particle entanglement means, let's start by considering a non-entangled system. If I create a system that has N particles, each in an identical state independent of their N-1 neighbours, then its many-body description is simple, and measuring one particle or partitioning the sample has little impact on the overall system. Not that such states are uninteresting — this is a good description of a state of matter called a Bose– Einstein condensate, for example. Similarly, if each particle is in its own different state, with no relationship to its neighbours, then measurement or partitioning has no global effect.

But if the particles are entangled with one

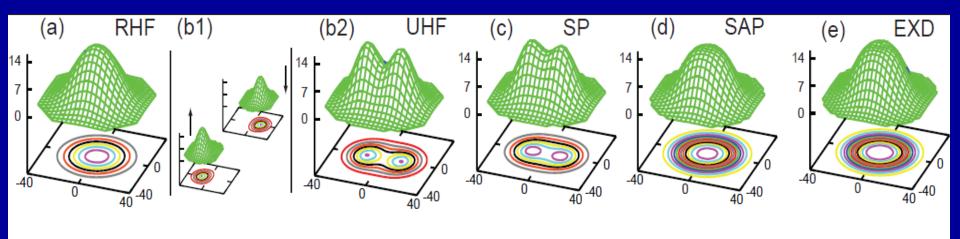
Measuring entanglement entropy in a quantum many-body system

Rajibul Islam¹, Ruichao Ma¹, Philipp M. Preiss¹, M. Eric Tai¹, Alexander Lukin¹, Matthew Rispoli¹ & Markus Greiner¹

3 DECEMBER 2015 | VOL 528 | NATURE | 77

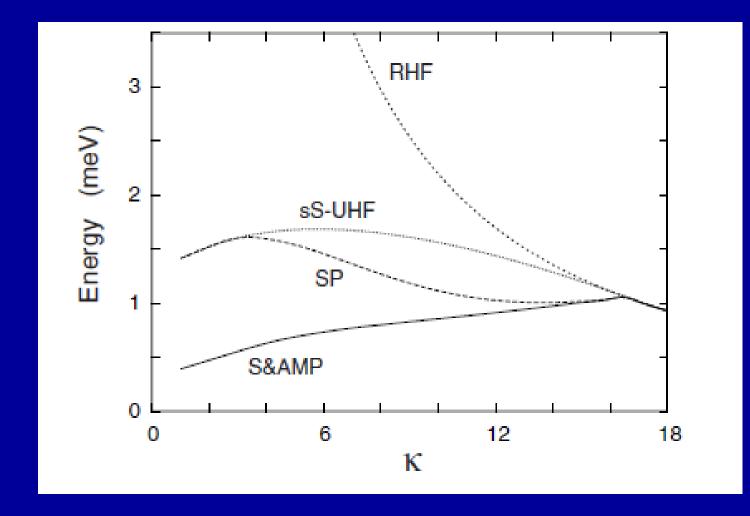
Even weirder, it's possible for two particles to become "entangled," meaning they will retain a sort of causal relationship with each other, no matter their distance in time and space. If you measure one particle and it spins clockwise, for example, then its entangled companion would instantly collapse into a counterclockwise spin, even if it's on the other side of the universe. That either means that one communicated with the other in an instant, or the state of each particle only popped into existence once one was measured. We know what you're thinking. For one thing, this whole idea is ridiculous: Things are what they are regardless of whether you're looking at them. For another, nothing can go faster than light, so how can two particles communicate across the universe in an instant? Einstein thought the same thing, derisively calling the idea "spooky action at a distance." Those in Einstein's camp are in favor of a concept called "local realism." "Locality" says that no signal can travel faster than light, and "realism" says that particles have definite states even before you measure them.

Self-consistent HF Exact $R_W = 2.40$ B = 0N=2e



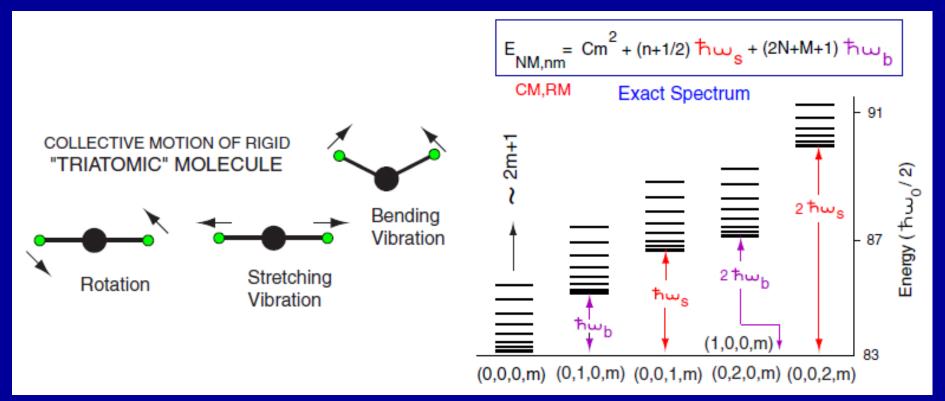


COMBINE PROJECTIONS/ SPIN/ ANGULAR MOMENTUM



N=2e QD, R_W=200; EXACT

RIGID ROTOR



Y&L, PRL 85, 1726 (2000)

PROJECTION/ ANGULAR MOMENTUM

$$\mathcal{P}_L = \frac{1}{2\pi} \int_0^{2\pi} e^{i\gamma(L-\hat{L})} d\gamma$$

$$\Phi_L^{\text{PROJ}} = \frac{1}{2\pi} \int_0^{2\pi} d\gamma \Psi^{\text{SB}}(\gamma) e^{i\gamma L}$$

$$E^{\text{PROJ}}(L) = \int_0^{2\pi} h(\gamma) e^{i\gamma L} d\gamma \Big/ \int_0^{2\pi} n(\gamma) e^{i\gamma L} d\gamma,$$

where

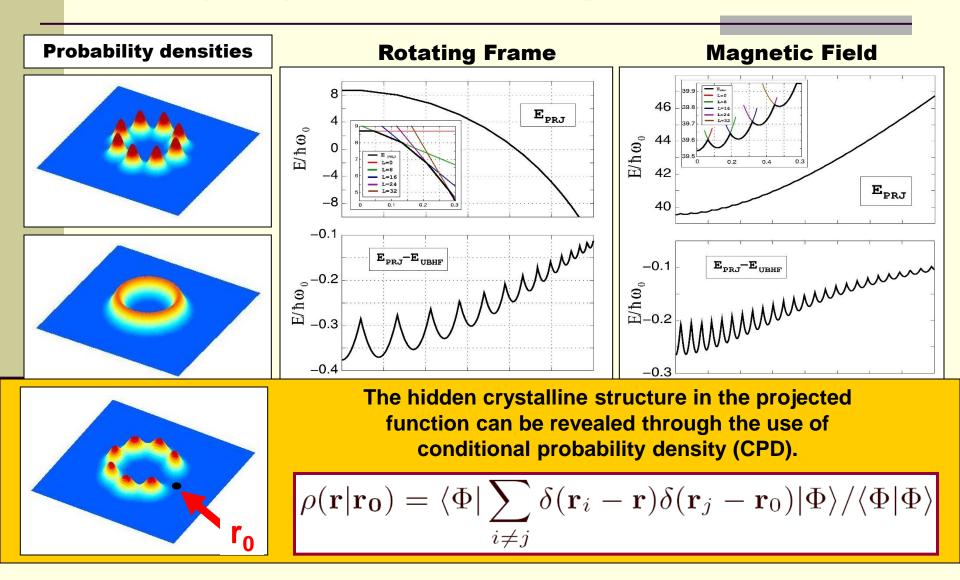
$$h(\gamma) = \langle \Psi^{\rm SB}(0) | \mathcal{H} | \Psi^{\rm SB}(\gamma) \rangle,$$

and the norm overlap

$$n(\gamma) = \langle \Psi^{\rm SB}(0) | \Psi^{\rm SB}(\gamma) \rangle$$

Bosons in the ring trap.

Energy, angular momentum and probability densities.



A HIERARCHY OF APPROXIMATIONS

Restricted Hartree-Fock (RHF)

All spin and space symmetries are preserved Double occupancy / e-densities: circularly symmetric Single Slater determinant (central mean field)

Unrestricted Hartree-Fock (UHF)

Total-spin and space symmetries (rotational or parity) are broken / Different orbitals for different spins Solutions with lower symmetry (point-group symmetry) Lower symmetry explicit in electron densities Single Slater determinant (non-central mean field)

Implementation of UHF: Pople-Nesbet Eqs. 2D harmonic-oscillator basis set Two coupled matrix Eqs. (for up and down spins)

Restoration of symmetry via projection techniques Superposition of UHF Slater det.'s (beyond mean field) e-densities: circularly symmetric Good total spin and angular momenta Lower symmetry is INTRINSIC (or HIDDEN) Detection of broken symmetry: CPDs and rovibrational excitations of quantum dots CPDs and dissociation of quantum dot molecules

Restoration of linearity of many-body equatons

Correlations

Non-linear equations

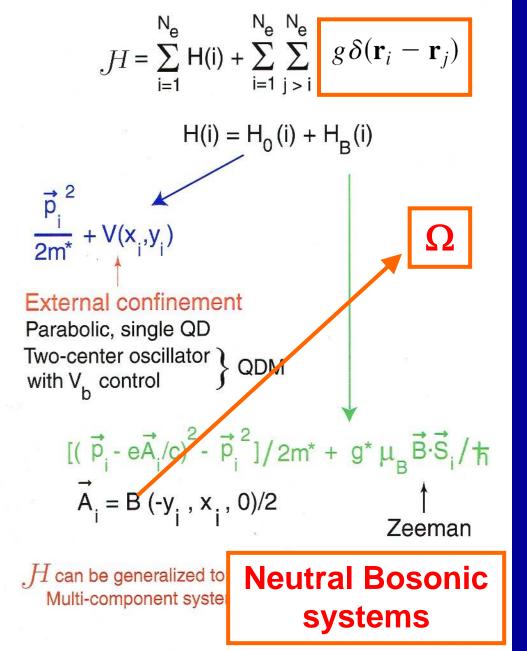
Bifurcations

EMERGENT

PHENOMENA

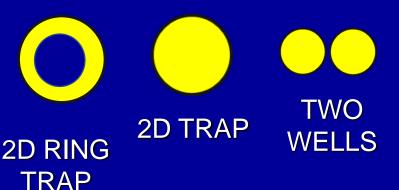
TIME EVOLUTION ENTANGLEMENT

HAMILTONIAN FOR CLEAN 2D QD'S AND QDM'S



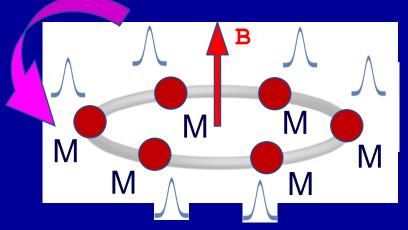
External Confinement

$$\frac{(r_i - R)^2}{2l_0^2/(\hbar\omega_0)}$$



1 hertz [Hz] = 4.13566553853599E-15 electron-volt [eV]

"ROTATING" QUANTUM-MECHANICAL SP DENSITY SHOULD EXHIBIT PERIODICITY IN BOTH SPACE AND TIME BREAKING OF TIME TRANSLATIONAL SYMMETRY

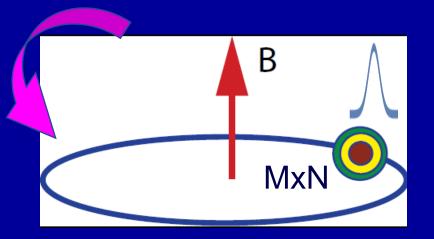


T. Li et al., PRL 109, 163001 (2012)

lon crystal

Ultracold ions/ Coulomb repulsion Both fermions (²⁴Mg⁺) and Bosons (⁹Be⁺)

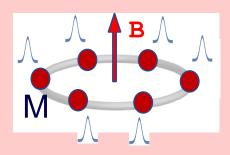
A different orbital for each particle



Lump/ Bose-Einstein soliton Ultracold neutral atoms <u>Attractive</u> contact interaction Bosons (⁸⁷Rb or ⁸⁵Rb)

The same orbital for all particles

F. Wilczek, PRL 109, 160401 (2012)



e each particle localized at position \mathbf{R}_j as a assian function

$$u(\mathbf{r}, \mathbf{R}_j) = \frac{1}{\sqrt{\pi\lambda}} \exp\left(-\frac{(\mathbf{r} - \mathbf{R}_j)^2}{2\lambda^2} - i\varphi(\mathbf{r}, \mathbf{R}_j; B)\right), \quad (3)$$

with $\lambda = \sqrt{\hbar/(M\Omega)}$; $\Omega = \sqrt{\omega_0^2 + \omega_c^2/4}$ where $\omega_c = \eta B/M$ is the cyclotron frequency. The phase in Eq. (3) is due to the gauge invariance of magnetic translations [57, 58]) and is given by $\varphi(\mathbf{r}, \mathbf{R}_j; B) = (xY_j - yX_j)/(2l_B^2)$, with $l_B = \sqrt{\hbar/(\eta B)}$ being the magnetic length. For

$$\varphi(\mathbf{r}, \mathbf{R}_j; B) = (xY_j - yX_j)/(2l_B^2)$$

Construct determinant/ permanent Ψ^{SB} (MF symmetry-breaking ansatz)

Rotational spectrum: quantum rigid rotor

$$R_W = 1000$$

 $R_{\delta} = 50$
 $E^{PROJ}(L) \approx V_{int} + C_R(L - N\Phi/\Phi_0)^2$
Vint Band head/ where interaction and Φ
Vint Correlations show up Magnetic flux
 $C_R \approx C_R^{cl} = \hbar^2 / [2\mathcal{I}(R_{eq})]$
 $\mathcal{I}(R_{eq}) = NMR_{eq}^2$
L => magic (fermions spin polarized)
 $L_m = kN; \quad k = 0, \pm 1, \pm 2, \pm 3, \ldots$
 $L_m = (k + \frac{1}{2})N; \quad k = 0, \pm 1, \pm 2, \pm 3, \ldots$
 $L_m = 0, \pm 1, \pm 2, \ldots$
Attractive bosons, lump

Floppy rotor (high B) Analytic approximation to REM (quantum)

$$E_{\text{app},L}^{\text{REM}}(N) = \hbar(\Omega - \omega_c/2)L + \sum_{q=0}^r \frac{\mathcal{C}_{V,q}}{L_q^{1/2}} + \sum_{q=1}^r \sum_{s>q}^r V_C(\lambda \sqrt{\frac{L_q}{n_q}}, \lambda \sqrt{\frac{L_s}{n_s}})$$

Partial angular momenta (corresponding to rings)

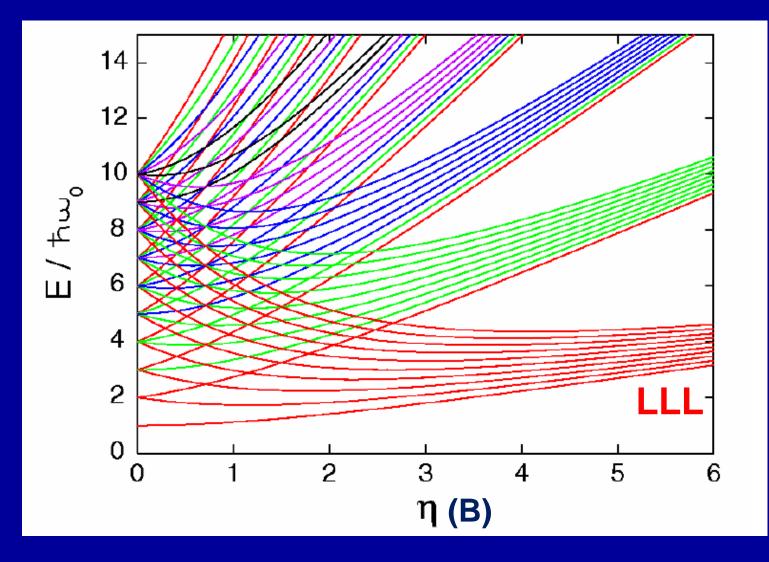
$$V_C(a_q, a_s) = n_q n_{s2} F_1[3/4, 1/4; 1; 4a_q^2 a_s^2 (a_q^2 + a_s^2)^{-2}] e^2 (a_q^2 + a_s^2)^{-1/2} / \kappa$$

RIGIN / Classical

Total L

$$\mathcal{J}_{\rm cl} = \sum_{i=1}^N m^* |Z_i|^2$$

 $E_L^{\text{RCL}} = \hbar^2 L^2 / (2\mathcal{J}_{\text{cl}}) + 0.5 \sum_{i=1}^N m^* \omega_0^2 |Z_i|^2 + \sum_{i=1}^N \sum_{j>i}^N e^2 / (\kappa |Z_i - Z_j|)$



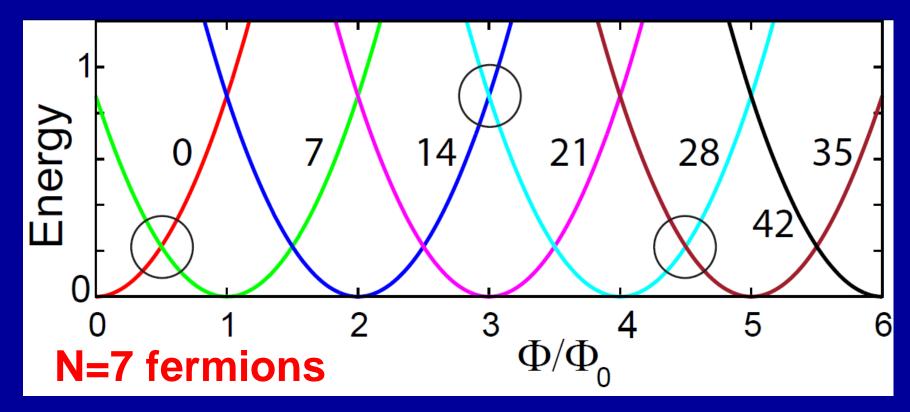


Effect of breaking time reversal symmetry 2D oscillator under a magnetic field Darwin-Fock spectrum

Rotational spectrum: quantum rigid rotor

$$E^{\text{PROJ}}(L) \approx V_{\text{int}} + C_R (L - N\Phi/\Phi_0)^2$$

SECOND TERM/ AHARONOV-BOHM TYPE SPECTRUM



GOA/ GCM

Norm overlap/ Time-reversal

KAMLAH expansion

where in such a way that the quotient $h(\alpha)/n(\alpha)$ is a rather smooth ction. This is a general property of many-body wave functions (which discussed in great detail in Sec. 10.7). Following the arguments of ion 10.7.4, we obtain*

$$n(\alpha) \simeq \exp(i\langle \hat{J} \rangle \cdot \alpha - \frac{1}{2} \langle \Delta \hat{J}^2 \rangle \alpha^2), \qquad (11.79)$$

$$\Delta \hat{J} = \hat{J} - \langle \hat{J} \rangle,$$

only difference now being that we also allow for time odd components be wave functions, which does not give a pure Gaussian, but an ional phase in Eq. (11.79) ($\langle \hat{J} \rangle \neq 0$). The idea of Kamlah is now to he operator

$$\hat{I} := -\langle \hat{J} \rangle + \frac{1}{i} \frac{\partial}{\partial \alpha},$$

projected energy now has the form:

$$E_{\text{proj}}^{I} = \langle H \rangle - \frac{\langle \Delta \hat{J}^{2} \rangle}{2 \mathfrak{G}_{Y}} + \frac{\langle \hat{J} \rangle}{\mathfrak{G}_{\text{sc}}} (I - \langle \hat{J} \rangle) + \frac{1}{2 \mathfrak{G}_{Y}} (I - \langle \hat{J} \rangle)^{2}. \quad (11.91)$$

It us first study the method of variation before projection, which was nally proposed by Peierls and Yoccoz [PY 57, Yo 57]. Here the wave tion $|\Phi\rangle$ is obtained from a minimization of H without constraint. It erefore, time-reversal invariant and has vanishing expectation values and $\langle H\hat{J}\rangle$. The spectrum then has the form

$$E_{\text{proj}}^{I} = \langle H - \frac{\hat{J}^{2}}{2 \mathfrak{G}_{Y}} \rangle + \frac{I^{2}}{2 \mathfrak{G}_{Y}}. \qquad (11.92)$$

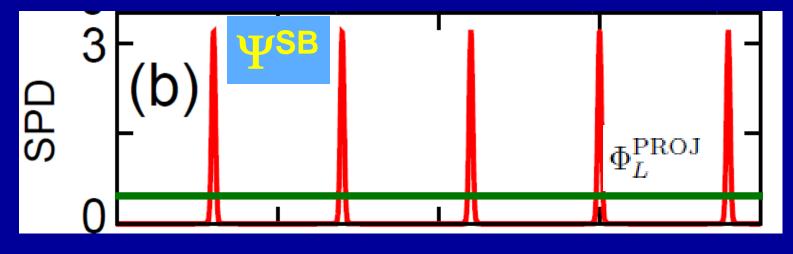
the spectrum of a one-dimensional rotor with the Yoccoz value \mathscr{G}_{γ} for noment of inertia (see Sec. 11.4.5).[†] The band head is obtained from

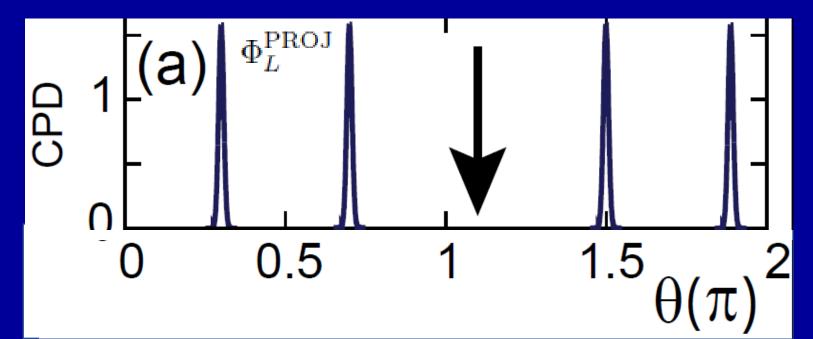
Ring & Schuck, Ch. 11

 $\langle \mathbf{J} \rangle \implies \Phi / \Phi_0$

Structure of many-body wave functions on ring







Wave packets/ Time evolution

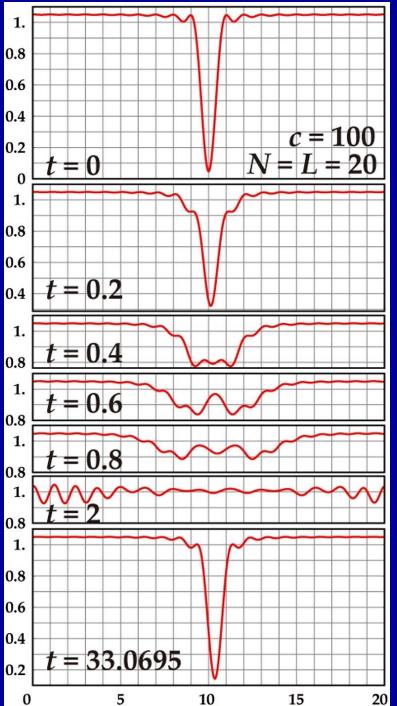
$$\Psi^{\rm SB} = \sum_L \mathcal{C}_L \Phi_L^{\rm PROJ}$$

Invert the projection

$$\mathcal{C}_L = \frac{1}{2\pi} \int_0^{2\pi} d\gamma e^{-i\gamma L} n(\gamma)$$

Many frequencies, terms e^{-iEL}

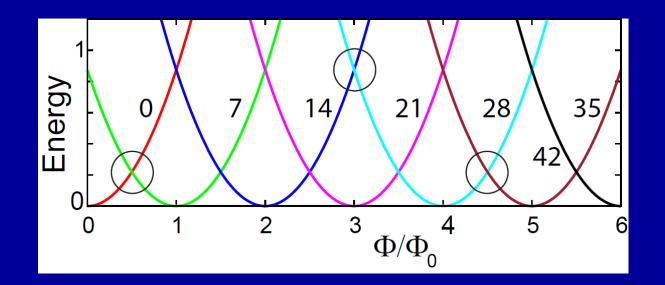
Diffusion and Revival



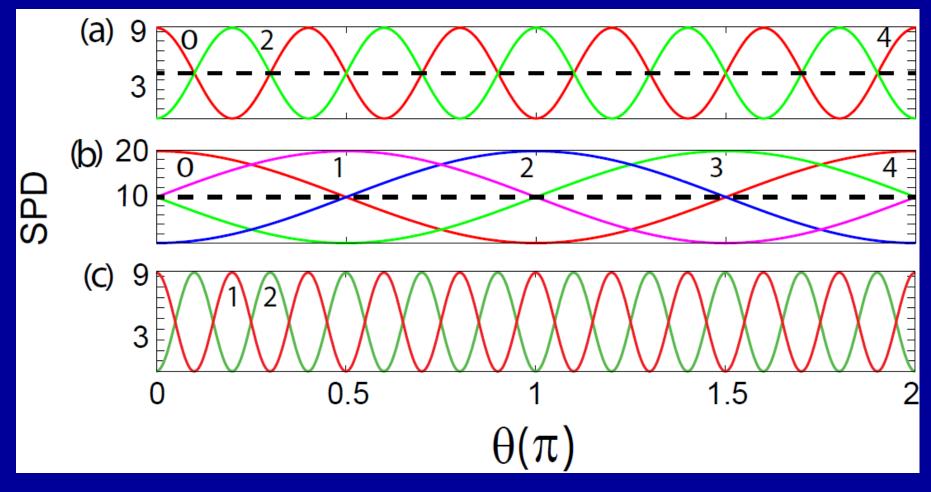
J. Sato et al., PRL **108**, 110401 (2012)

PINNED WIGNER MOLECULE (PWM)/ TWO-PROJECTED-STATE SUPERPOSITION

$\Phi^{\text{PWM}}(L_1, L_2; t = 0) = \alpha \Phi_{L_1}^{\text{PROJ}} + \beta e^{i\phi(t=0)} \Phi_{L_2}^{\text{PROJ}}$



PWM: TIME EVOLUTION OF SPD (snapshots) $au = 2\pi\hbar/|E_1 - E_2|$



BOTH SPACE AND TIME TRANSLATIONAL SYMMETRY ARE BROKEN

CONCLUSIONS:

SYMMETRY RESTORATION IS A NATURAL METHOD TO BE USED IN ADDRESSING THE PHYSICS IN MESOSCOPIC SYSTEMS OTHER THAN NUCLEI



VIEWPOINT

How to Create a Time Crystal

A detailed theoretical recipe for making time crystals has been unveiled and swiftly implemented by two groups using vastly different experimental systems.

by Phil Richerme*

he story of time crystals—whose lowest-energy configurations are periodic in time rather than space—epitomizes the creative ideas, controversy, and vigorous discussion that lie at the core of the scientific process. Originally theorized by Frank Wilczek in 2012 [1] (see 15 October 2012 Viewpoint), time crystals were met with widespread attention, but also a healthy dose of skepticism [2]. This ignited a debate in the literature, culminating in a proof that time crystals cannot exist in thermal equilibrium, as originally imagined by Wilczek [3]. But the

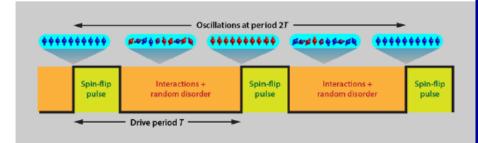


Figure 1: Yao *et al.* [7] have developed a blueprint for creating a time crystal and a method for detecting it, which has been followed by two experimental groups [8, 9]. Quantum spins are subjected to imperfect spin-flip driving pulses and then allowed to interact with each other in the presence of strong random disorder in the local

From Wikipedia

"A time crystal or space-time crystal is a structure that repeats periodically in time, as well in space. Normal three-dimensional crystals have a repeating pattern in space, but remain unchanged with respect to time; time crystals repeat themselves in time as well, leading the crystal to change from moment to moment.

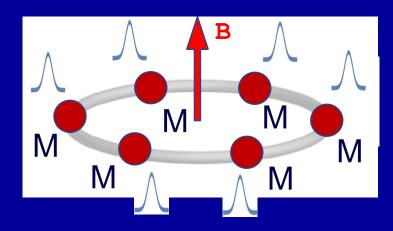
The idea of a time crystal was first described by <u>Nobel laureate</u> and <u>MIT</u> professor <u>Frank Wilczek</u> in 2012"

Time reflection and time translational symmetries are broken Quantum Space Time Crystal (symmetry breaking in all four dimensions: space and time)

Time evolution phenomena in quantum mechanical finite systems

Unprecedented experimental control of few-body systems of trapped ultracold ions and neutral atoms

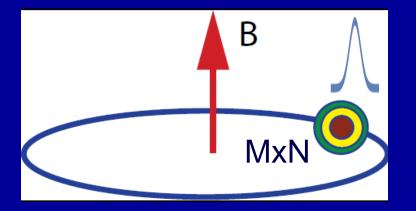




T. Li et al., PRL 109, 163001 (2012)

lon crystal

Ultracold ions/ Coulomb repulsion Both fermions (²⁴Mg⁺) and Bosons (⁹Be⁺)



Lump/ Bose-Einstein soliton Ultracold neutral atoms <u>Attractive</u> contact interaction Bosons (⁸⁷Rb or ⁸⁵Rb)

F. Wilczek, PRL 109, 160401 (2012)



 Per-Olov Löwdin (Chemistry - Spin)

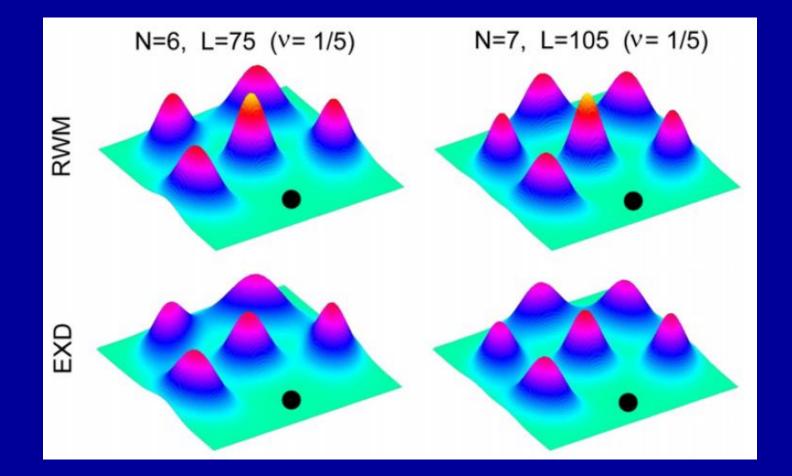


 R.E. Peierls and J. Yoccoz (Nuclear Physics – *L, rotations*)



Ch. 11 in the book by P. Ring and P. Schuck

CPDs for QDs, fully spin polarized



Lowest Landau level $B \rightarrow$ Infinity