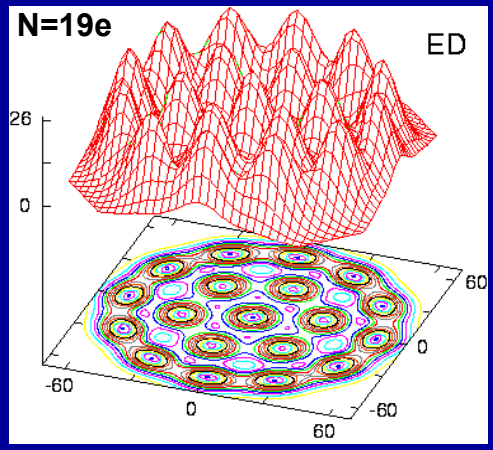
Symmetry breaking and restoration for trapped electrons, ions, and neutral atoms

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

R_W=5, B=0



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)

$$R_W = (e^2/\kappa l_0)/\hbar\omega_0 \sim 1/(\hbar^3\omega_0)^{1/2}$$

e-e Coulomb repulsion — kinetic energy

$$l_0 = (\hbar/m^*\omega_0)^{1/2}$$ } Spatial Extent of 1s s.p. state

κ : dielectric const. (12.9)

m^* : e effective mass ($0.067\ m_e$) GaAS

$\hbar\omega_0$ (5 - 1 meV) => 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)

$$R_\delta = gm/(2\pi\hbar^2)$$

Neutral bosons

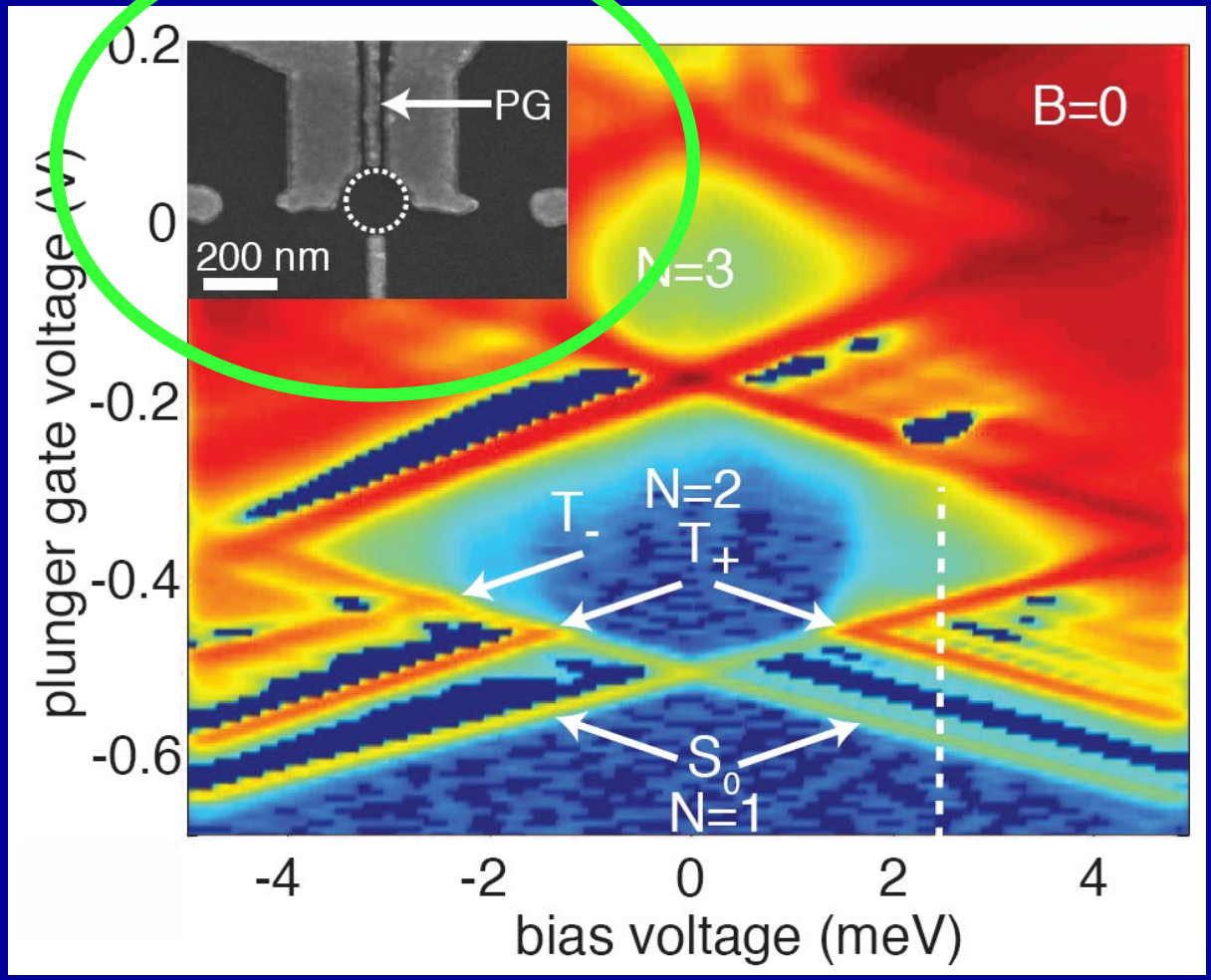
Towards controlling symmetry breaking and symmetry restoration in both space and time in manmade nanosystems (SMALL IS DIFFERENT)

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)**

ETH (Zurich) single QD



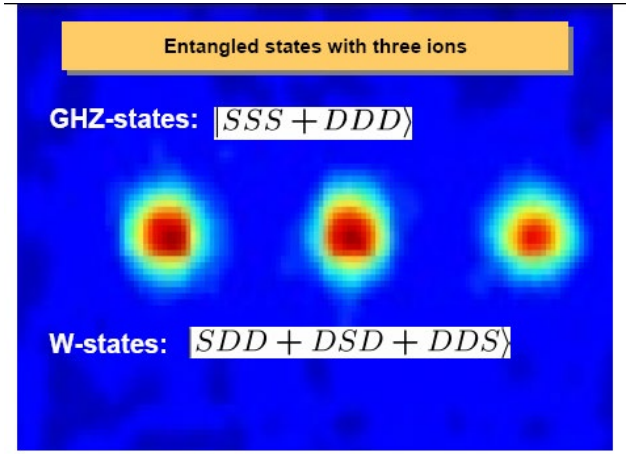
Ellenberger, Ensslin, Yannouleas, Landman et al.,
Phys. Rev. Lett. **96,** 126806 (2006)

Control and measurement of three-qubit entangled states

C. F. Roos[1], Mark Riebe[1], H. Häffner[1], W. Hänsel[1], J. Benhelm[1], G. P. T. Lancaster[1], C. Becher[1], F. Schmidt-Kaler[1] & R. Blatt[1,2]

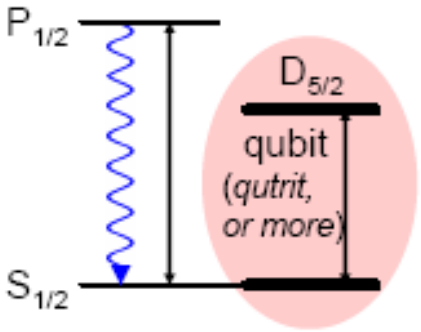
[1]Institut für Experimentalphysik, Universität Innsbruck, Technikerstraße 25, A-6020 Innsbruck, Austria
[2]Institut für Quantenoptik und Quanteninformation, Österreichische Akademie der Wissenschaften

- 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



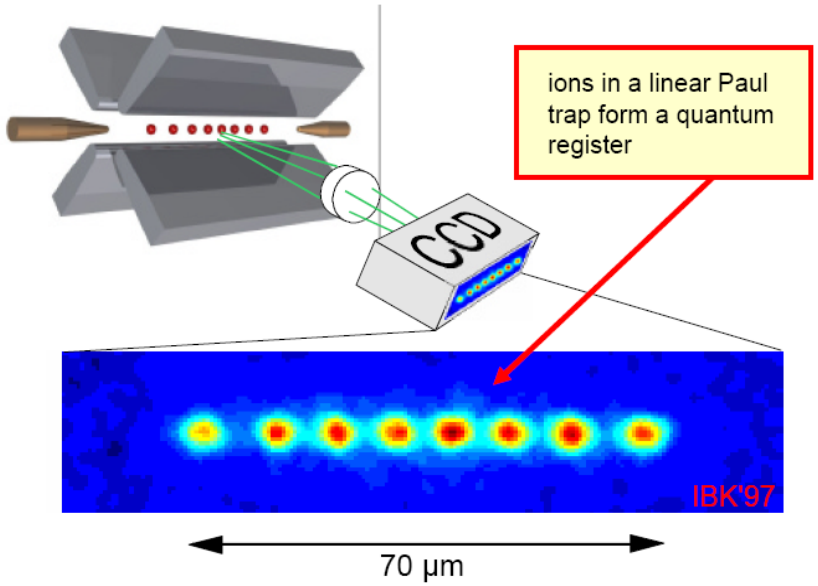
H. Haeffner et al., Nature 438, 643 (2005)

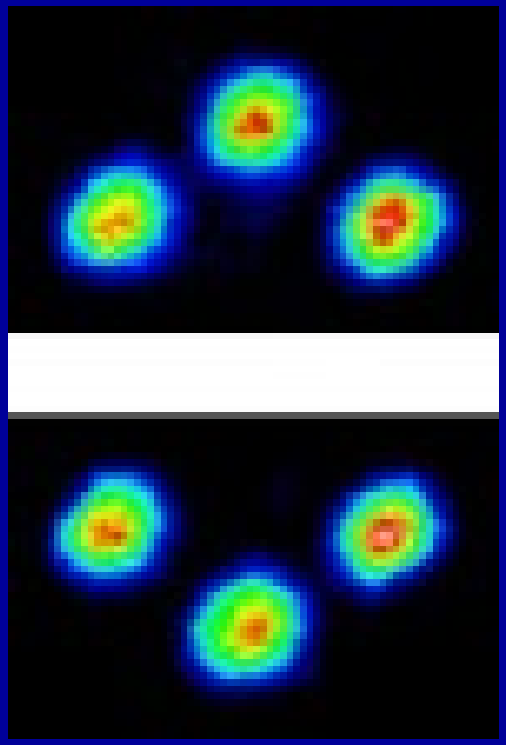
Qubits with trapped ions

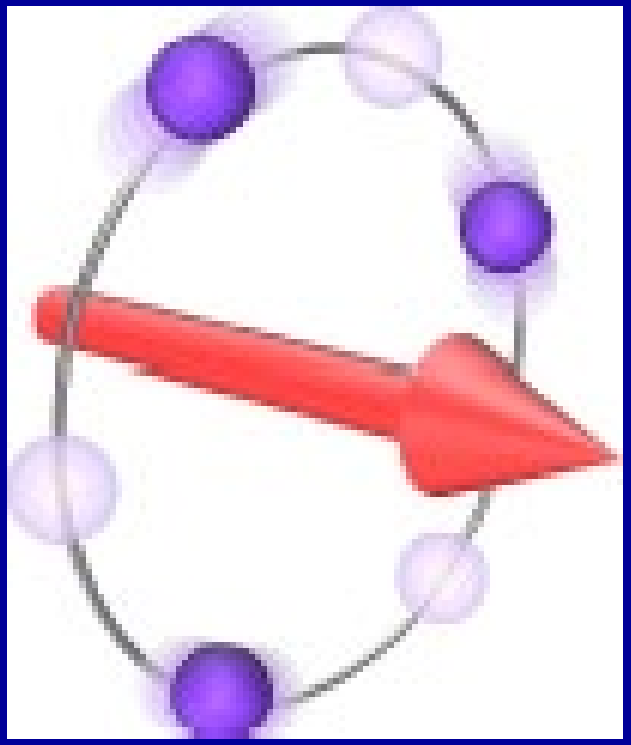


S – D transitions in alkaline earths:
Ca^+, Sr^+, Ba^+, Ra^+, (Yb^+, Hg^+) etc.

The system: String of $^{40}Ca^+$ ions in a linear Paul trap



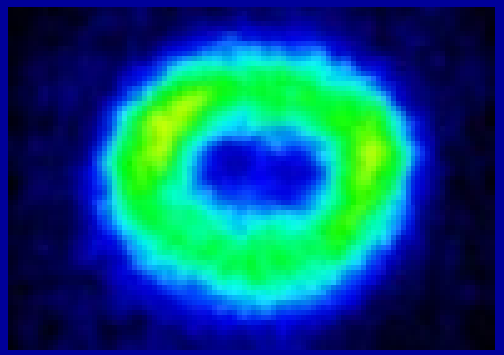


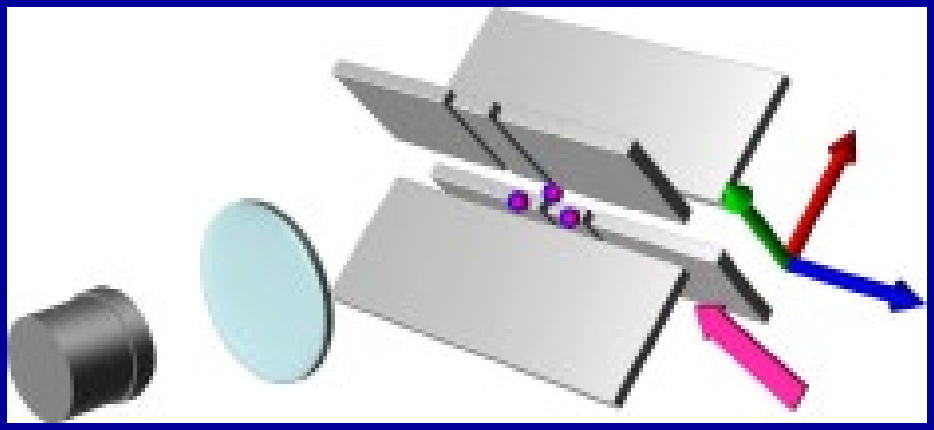


$^{40}Ca^{+}$

Fermion

B





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

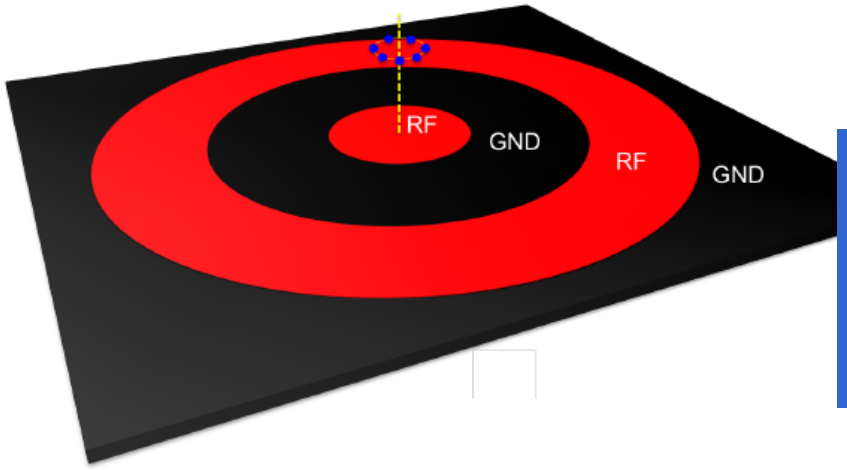
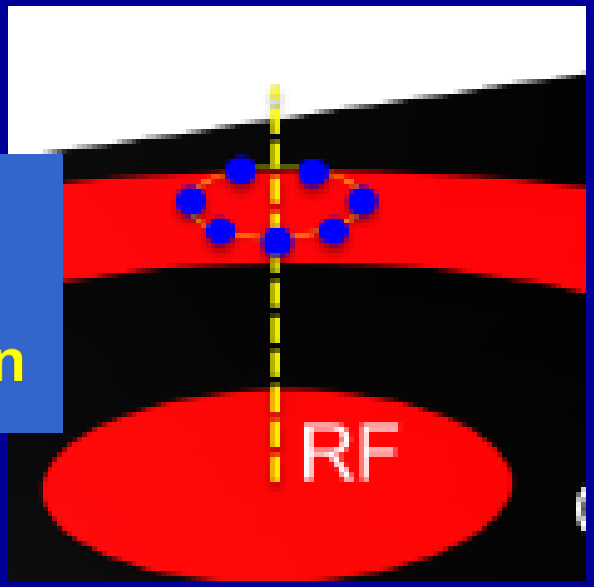


Figure 4.7: Concept for symmetric ring trap. RF electrodes are shown in red, ground in black. Ions trapped above the surface shown in blue.

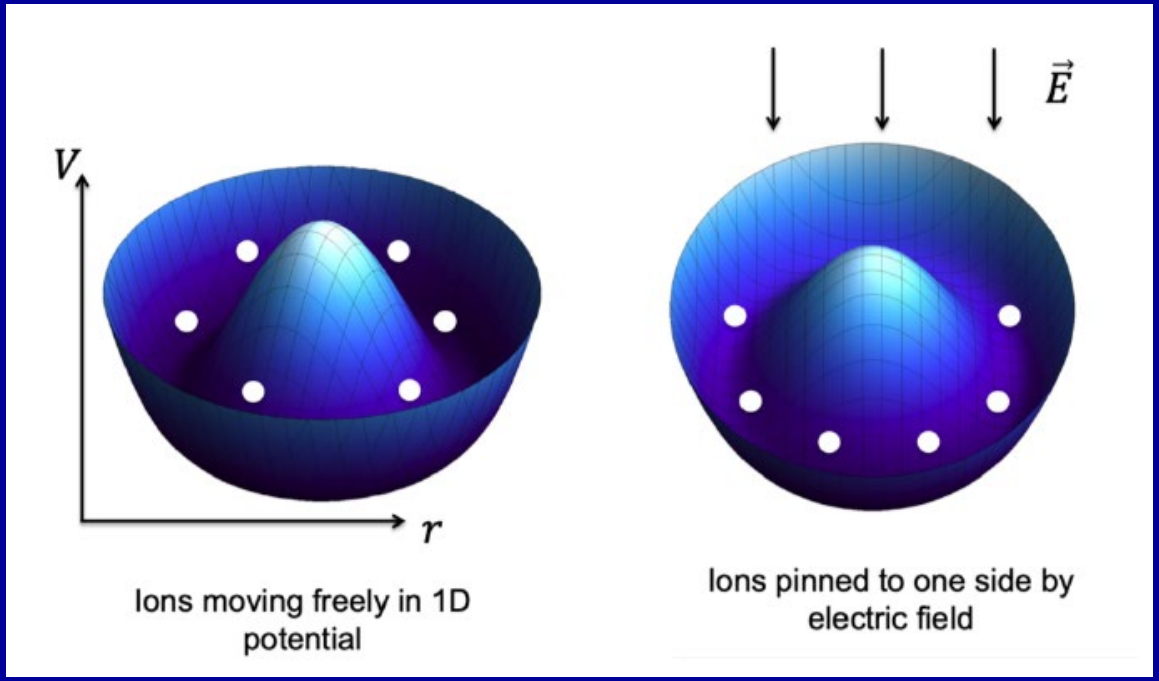
$^{40}Ca^{+}$

Fermion



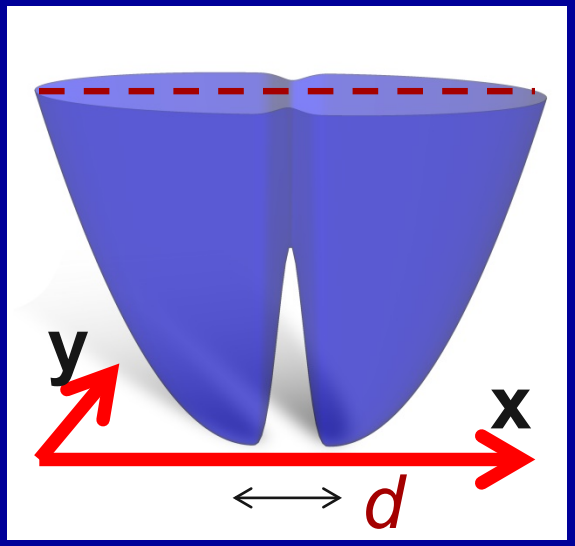
Erik Urban, Ph.D. Thesis, Univ. of California, Berkeley, 2019

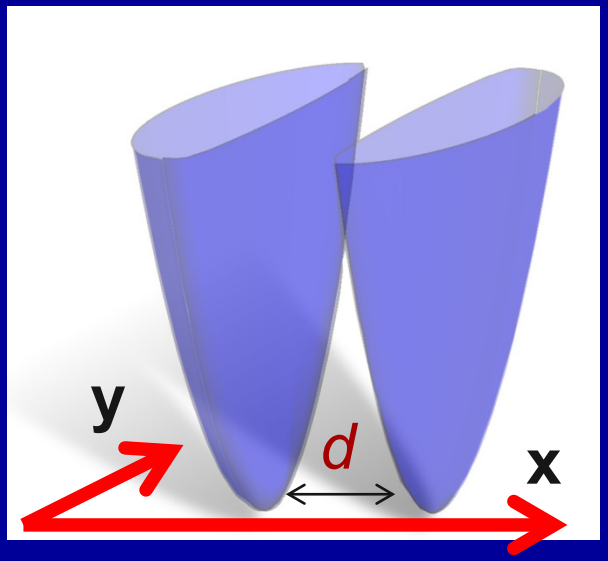
Urban et al., Coherent Control of the Rotational Degree of Freedom of a Two-Ion Coulomb Crystal, arXiv:1903.05763



2 ^{6}Li ATOMS IN A DOUBLE OPTICAL TRAP

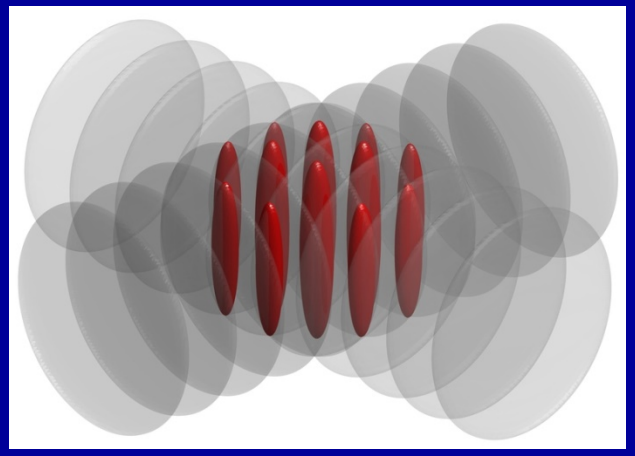
Linear arrangement (LI) **Parallel arrangement (PA)**





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

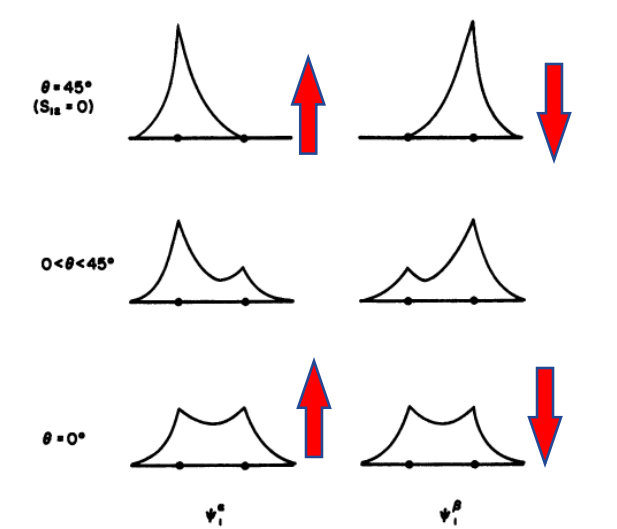
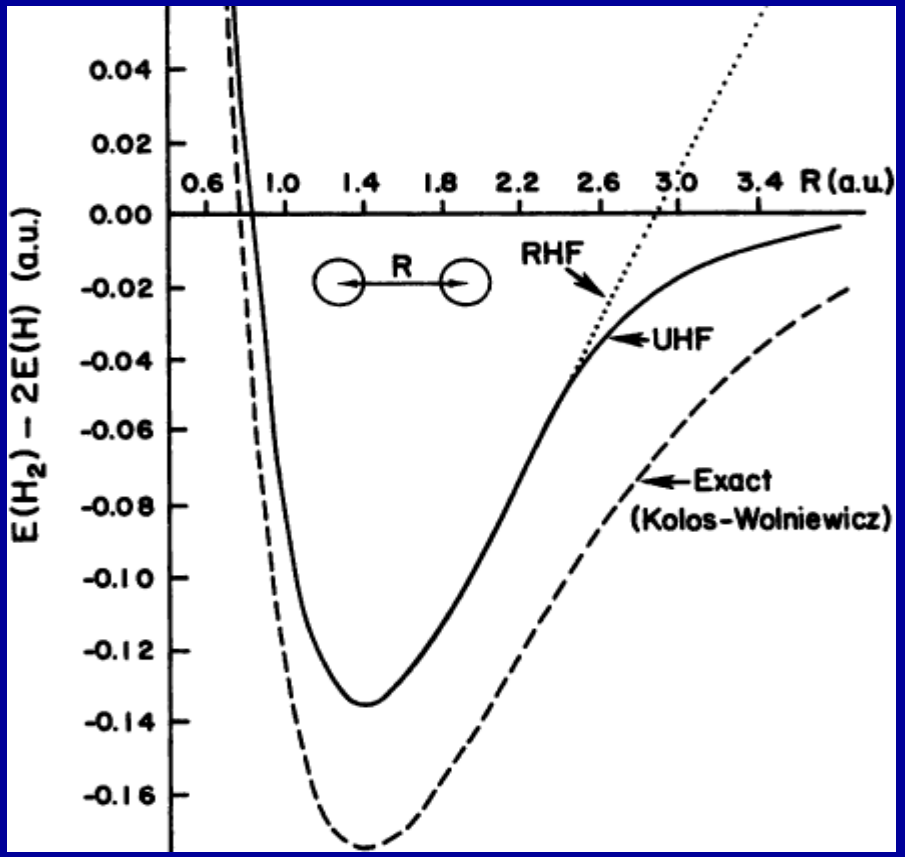
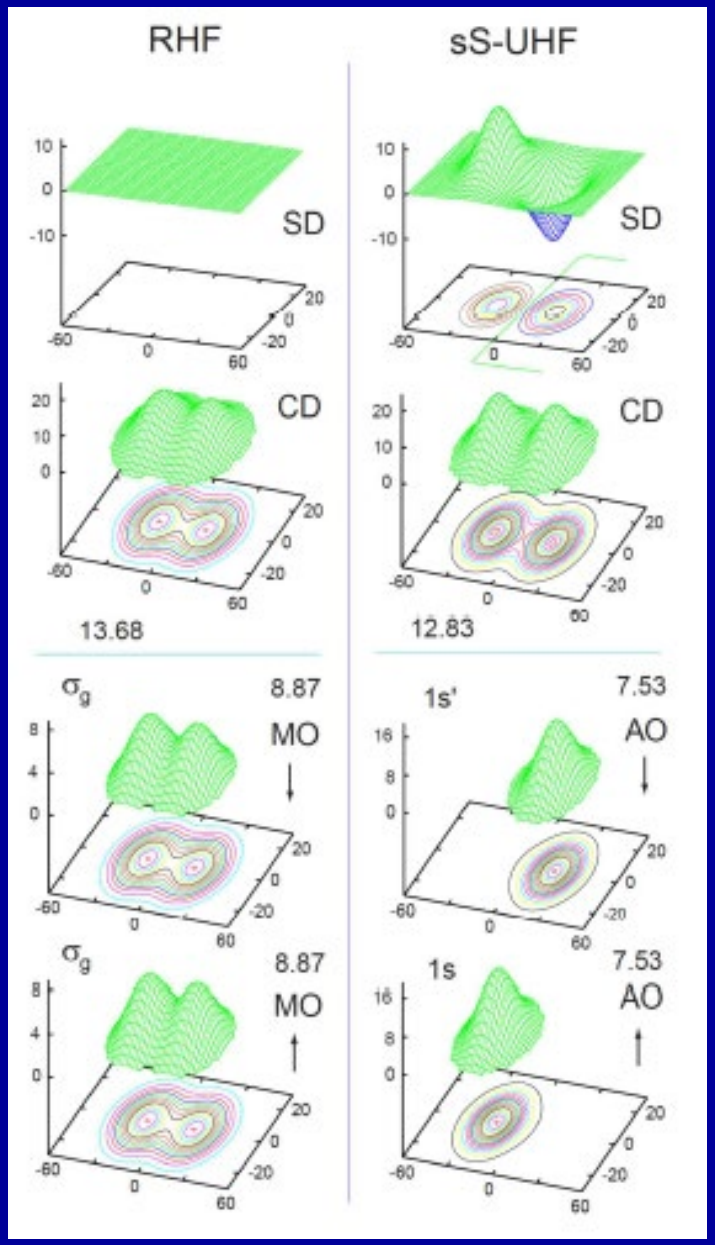


Figure 3.16 Qualitative behavior of unrestricted molecular orbitals ψ_1^α a function of θ.



Next step: Heitler-London

H_2-QDM DOUBLE-WELL



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

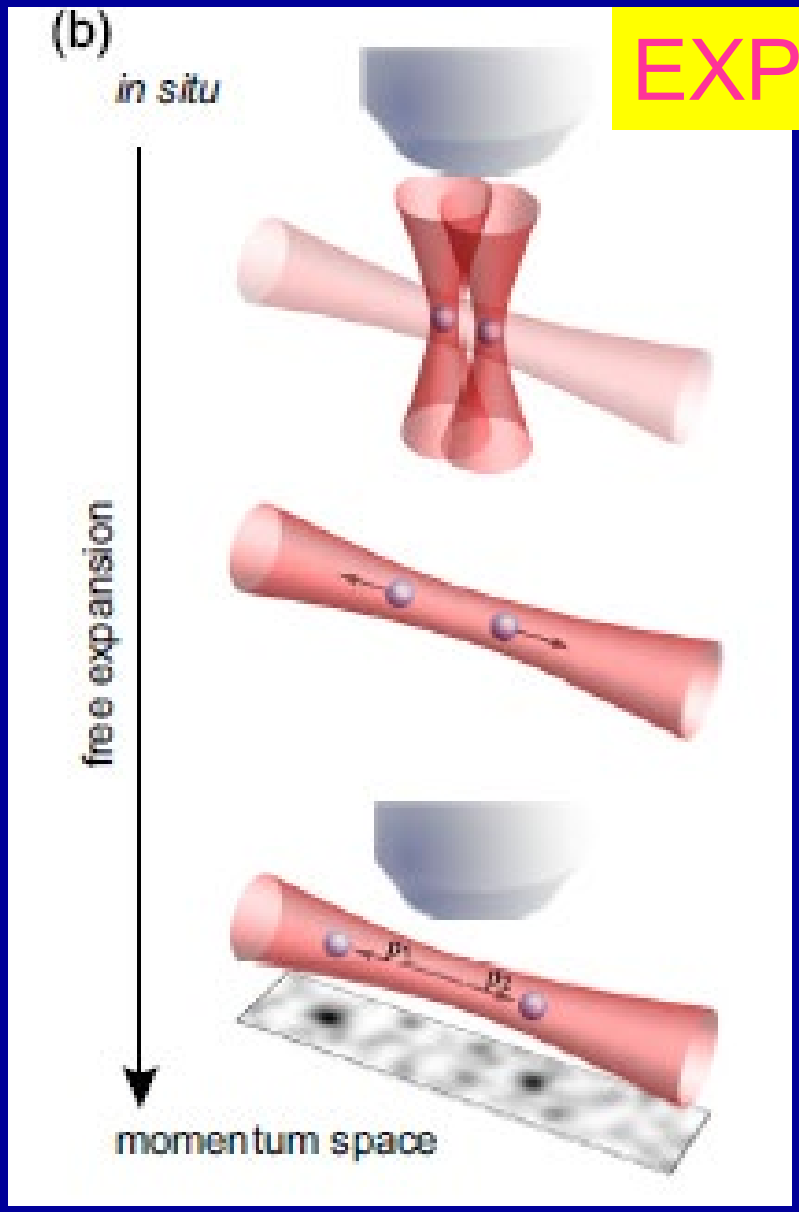
$$\mathcal{P}^{s,t}_{\rm spin} = 1 \mp \varpi_{12}$$

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

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

Heitler-London/ EPR-Bohm-Bell

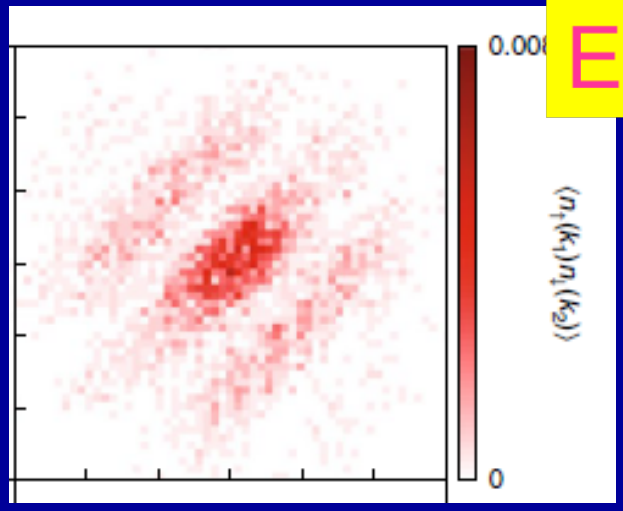
Energy gain vs ENTANGLEMENT



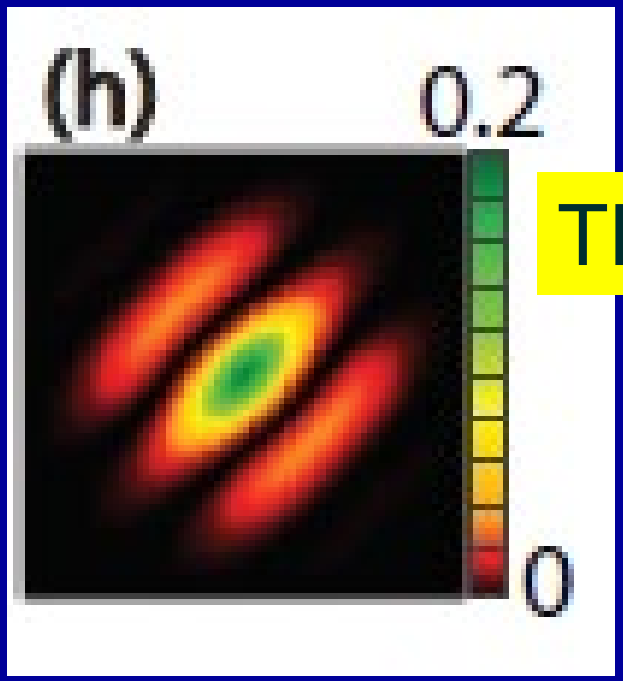
EXP

^{6}Li

Fermion



EXP



THE

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

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

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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

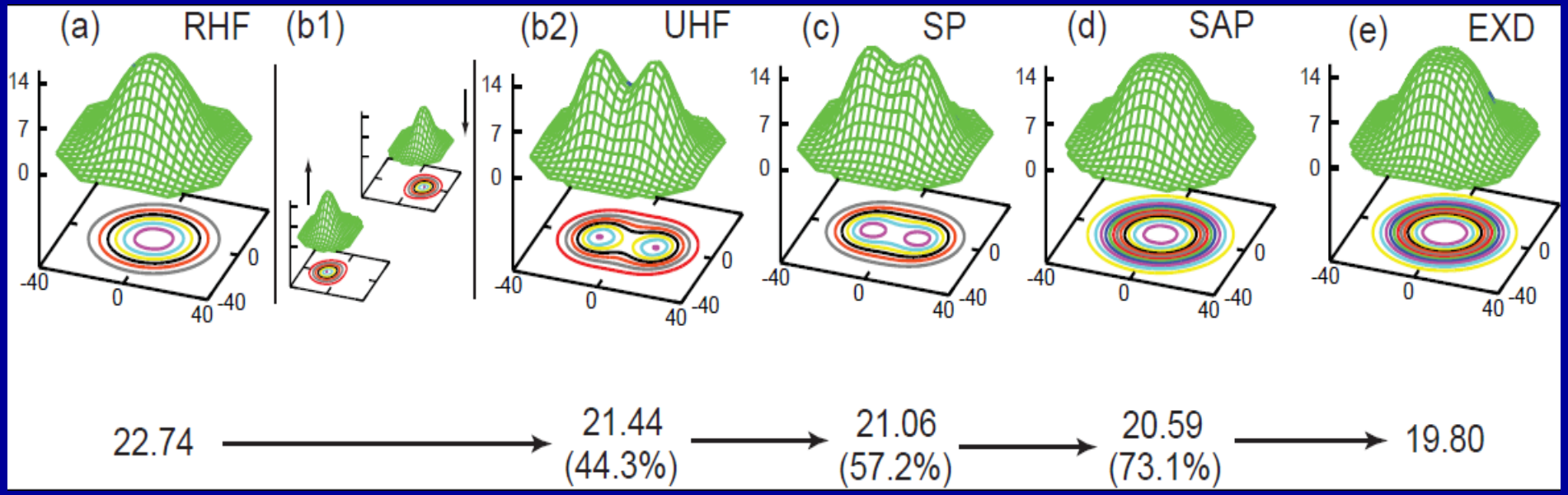
Rajibul Islam[1], Ruichao Ma[1], Philipp M. Preiss[1], M. Eric Tai[1], Alexander Lukin[1], Matthew Rispoli[1] & Markus Greiner[1]

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.

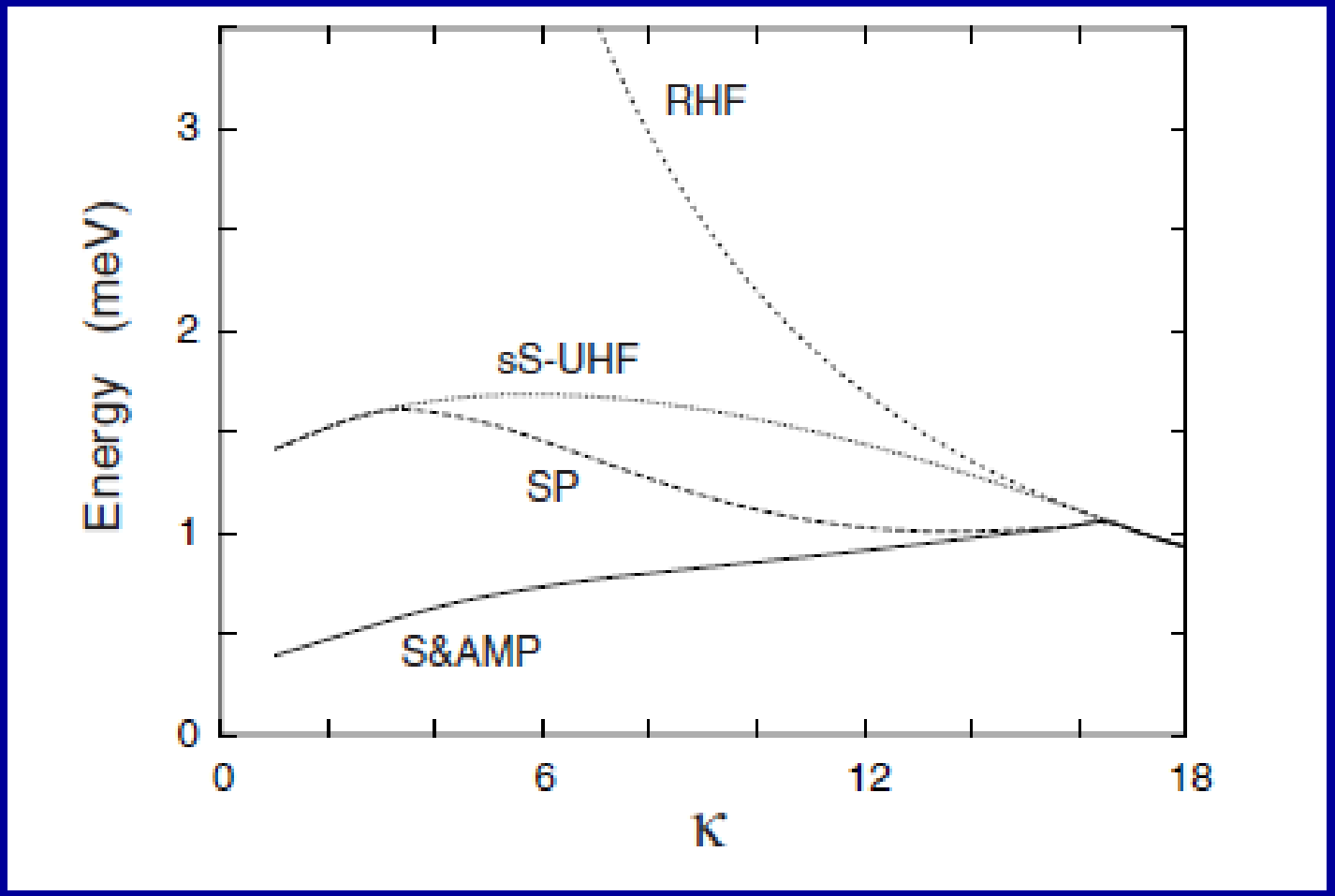
We know what you're thinking. For one thing, this whole idea is ridiculous: Things are what they are regardless of whether you're looking at them. For another, nothing can go faster than light, so how can two particles communicate across the universe in an instant? Einstein thought the same thing, derisively 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 $R_W = 2.40$ $B = 0$

N=2e

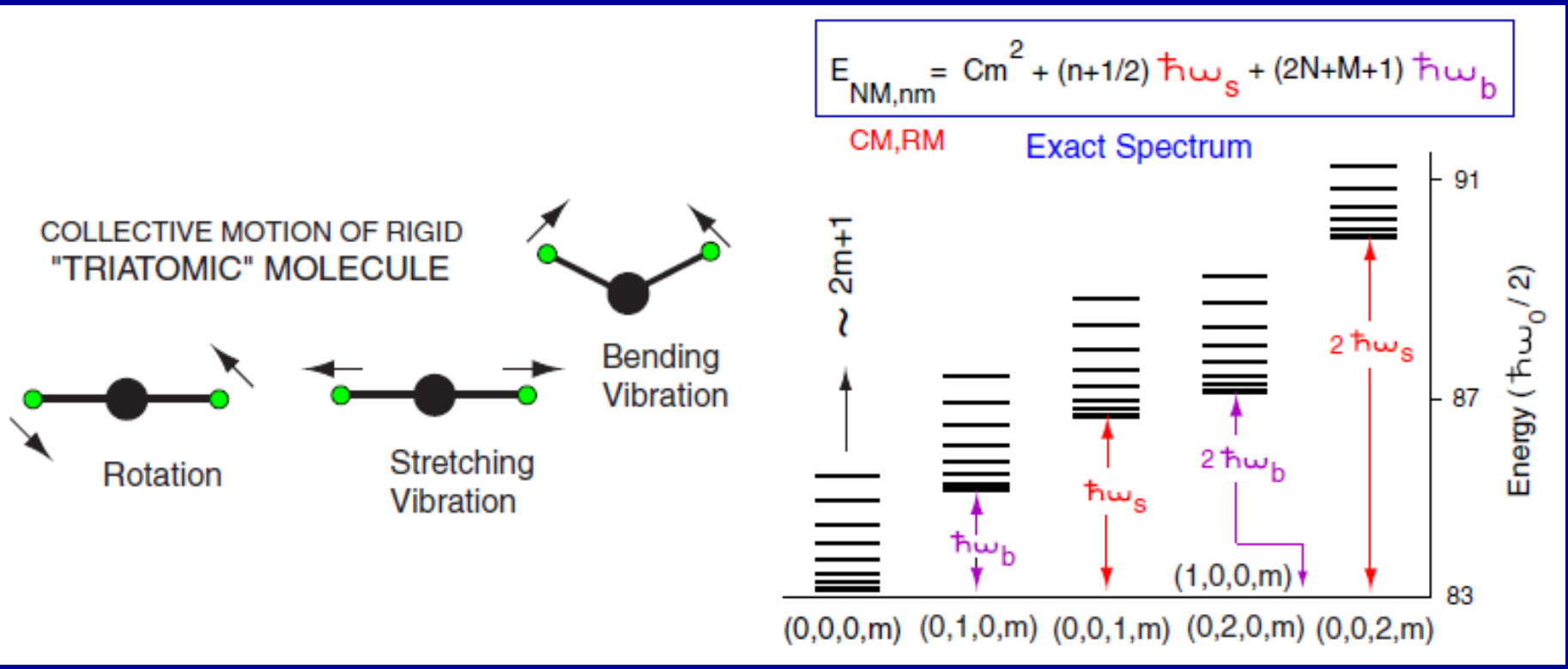


COMBINE PROJECTIONS/
SPIN/ ANGULAR MOMENTUM


RHF
sS-UHF
SP
S&AMP
Energy (meV)
0
1
2
3
0
6
12
18
κ

N=2e QD, R_W=200; EXACT

RIGID ROTOR



Y&L, PRL **85**, 1726 (2000)

PROJECTION/ ANGULAR MOMENTUM

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

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

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

where

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

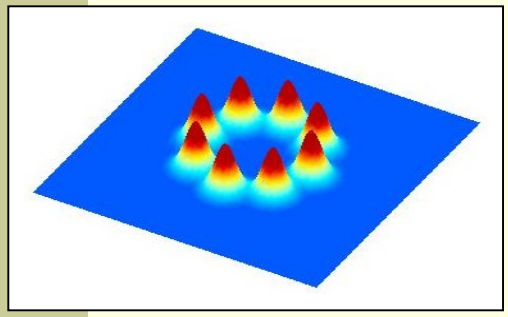
and the norm overlap

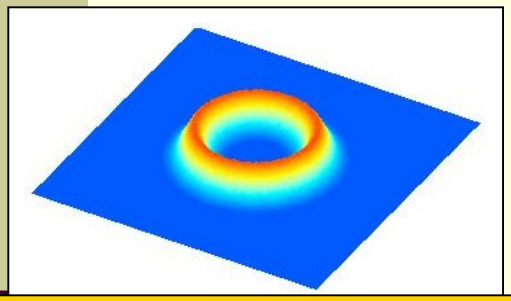
$$n(\gamma) = \langle \Psi^{\mathrm{SB}}(0)|\Psi^{\mathrm{SB}}(\gamma)\rangle$$

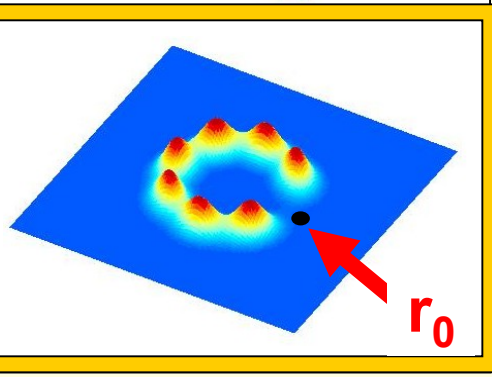
Bosons in the ring trap.

Energy, angular momentum and probability densities.

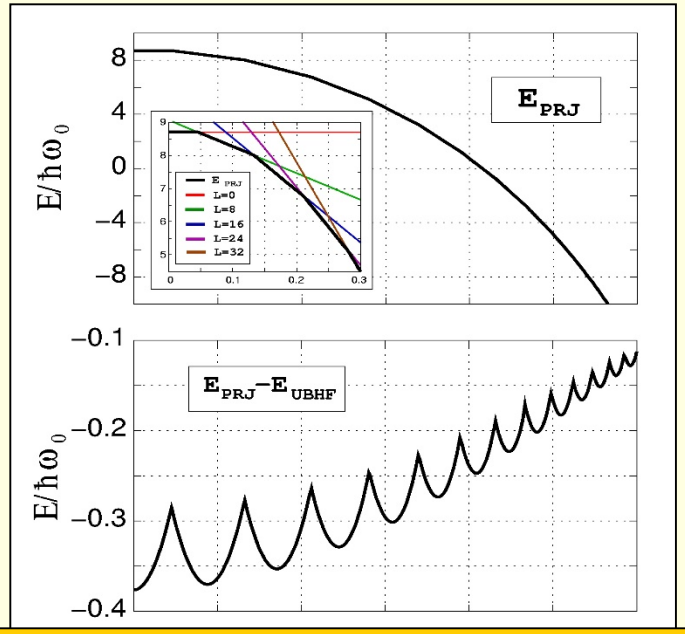
Probability densities



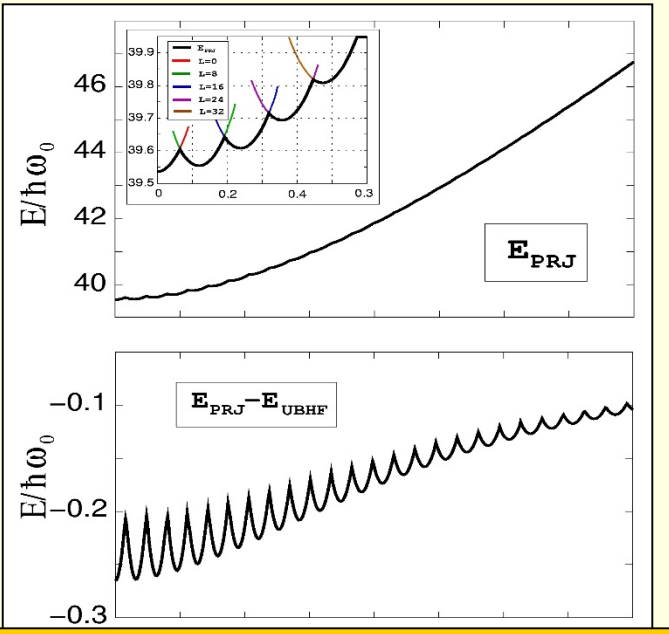




Rotating Frame



Magnetic Field



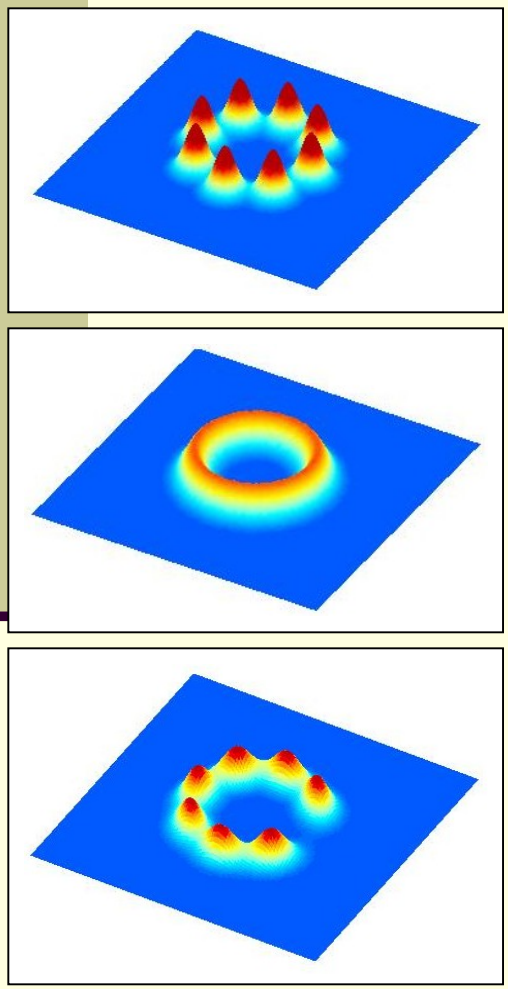
The hidden crystalline structure in the projected function can be revealed through the use of conditional probability density (CPD).

$$\rho(\mathbf{r}|\mathbf{r_0}) = \langle\Phi|\sum_{i\neq j}\delta(\mathbf{r}_i-\mathbf{r})\delta(\mathbf{r}_j-\mathbf{r}_0)|\Phi\rangle/\langle\Phi|\Phi\rangle$$

Bosons in the ring trap.

Energy, angular momentum and probability densities.

Probability densities



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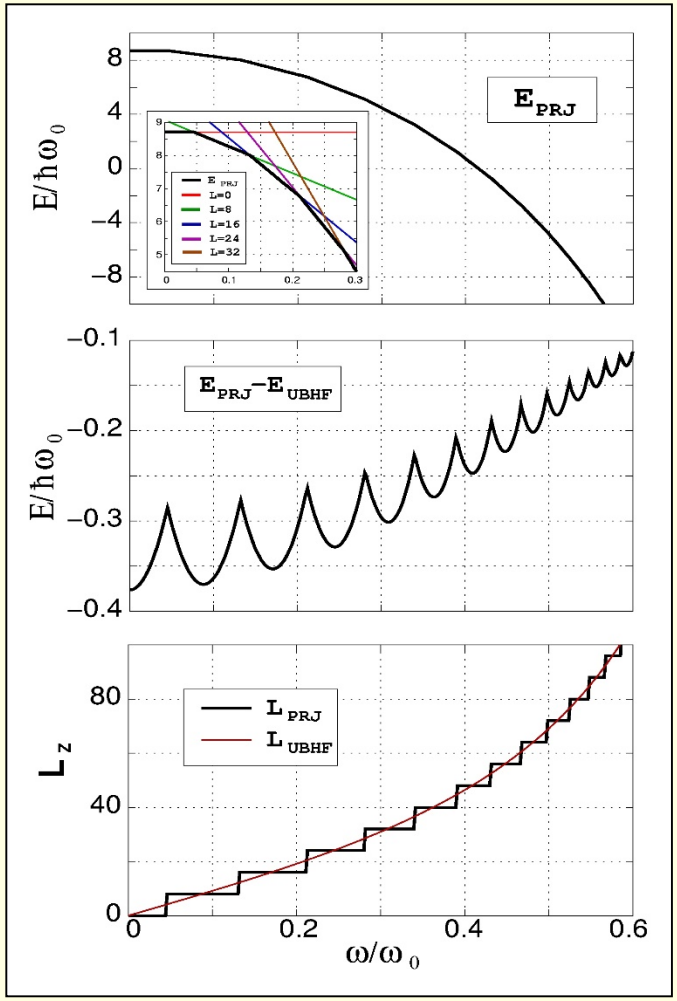
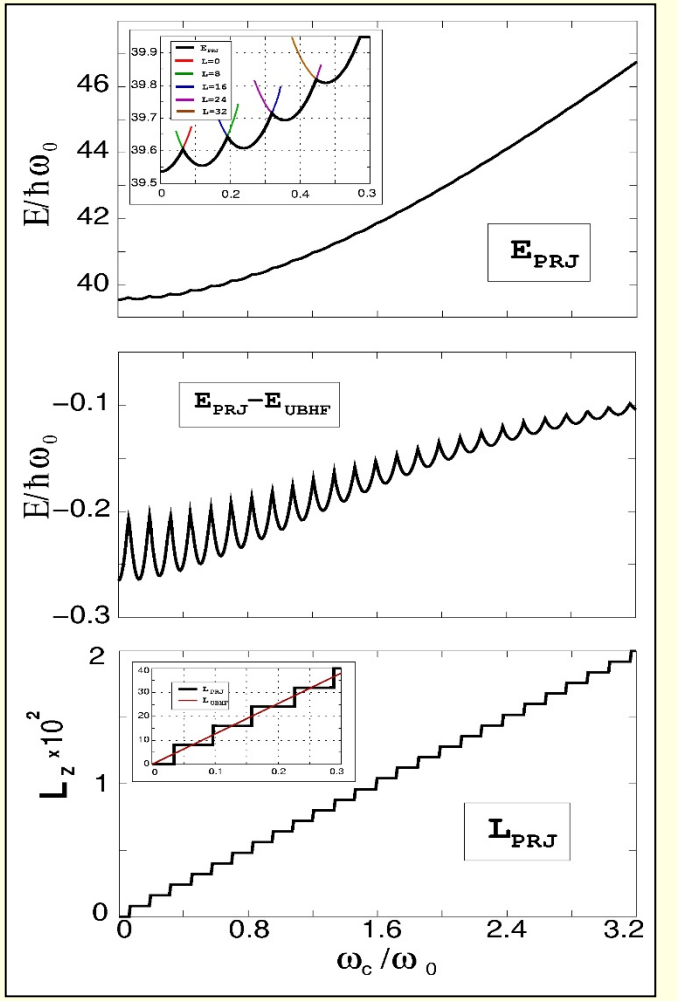


Magnetic Field



A HIERARCHY OF APPROXIMATIONS

TOTAL ENERGY

Restricted Hartree-Fock (RHF)

All spin and space symmetries are preserved

Double occupancy / e-densities: circularly symmetric

Single Slater determinant (central mean field)

Correlations

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)

Non-linear equations
Bifurcations

EMERGENT PHENOMENA

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

TIME EVOLUTION
ENTANGLEMENT

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

$$\mathcal{H} = \sum_{i=1}^{N_e} H(i) + \sum_{i=1}^{N_e} \sum_{j>i} \frac{e^2}{\kappa r_{ij}}$$

$$H(i) = H_0(i) + H_B(i)$$

$$\frac{\vec{p}_i^{\,2}}{2m^*} + V(x_i, y_i)$$

External confinement

Parabolic, single QD

Two-center oscillator with V_b control } QDM

$$[(\vec{p}_i - e\vec{A}_i/c)^2 - \vec{p}_i^{\,2}]/2m^* + g^* \mu_B \vec{B}\cdot\vec{S}_i/\hbar$$

$$\vec{A}_i = B(-y_i, x_i, 0)/2$$

Zeeman

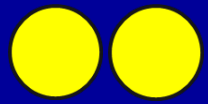
$\mathcal{H}$ can be generalized to:
Multi-component systems

External Confinement

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

2D RING TRAP

2D TRAP



TWO WELLS

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

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

$$\mathcal{H} = \sum_{i=1}^{N_e} H(i) + \sum_{i=1}^{N_e} \sum_{j>i} g\,\delta(\mathbf{r}_i - \mathbf{r}_j)$$

$$H(i) = H_0(i) + H_B(i)$$

$$\frac{\vec{p}_i^{\,2}}{2m^*} + V(x_i, y_i)$$

External confinement

Parabolic, single QD

Two-center oscillator with V_b control } QDM

Ω

$$[(\vec{p}_i - e\vec{A}_i/c)^2 - \vec{p}_i^{\,2}]/2m^* + g^* \mu_B \vec{B}\cdot\vec{S}_i/\hbar$$

$$\vec{A}_i = B\,(-y_i, x_i, 0)/2$$

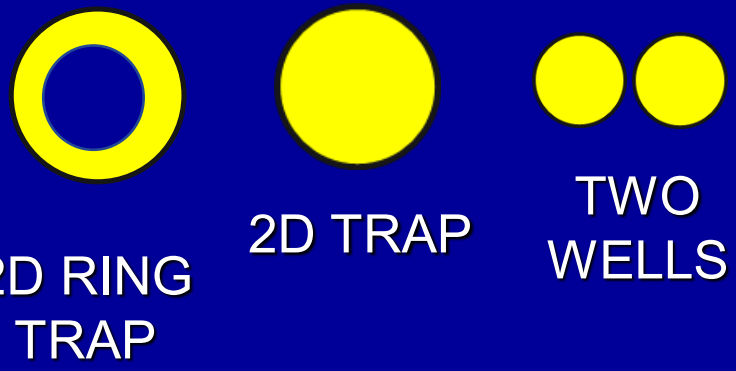
Zeeman

$\mathcal{H}$ can be generalized to Multi-component syste

Neutral Bosonic systems

External Confinement

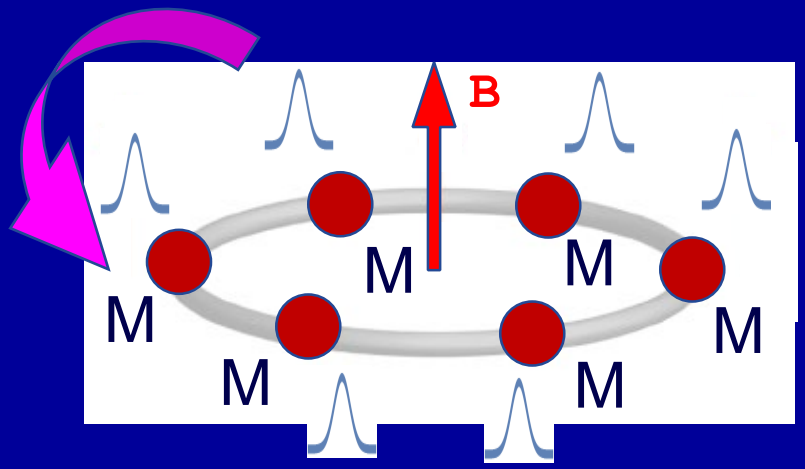
$$\frac{(r_i - R)^2}{2l_0^2/(\hbar\omega_0)}$$



1 hertz [Hz] = 4.135665538535 99E-15 electron-volt [eV]

"ROTATING" QUANTUM-MECHANICAL SP DENSITY SHOULD EXHIBIT PERIODICITY IN BOTH SPACE AND TIME

BREAKING OF TIME TRANSLATIONAL SYMMETRY



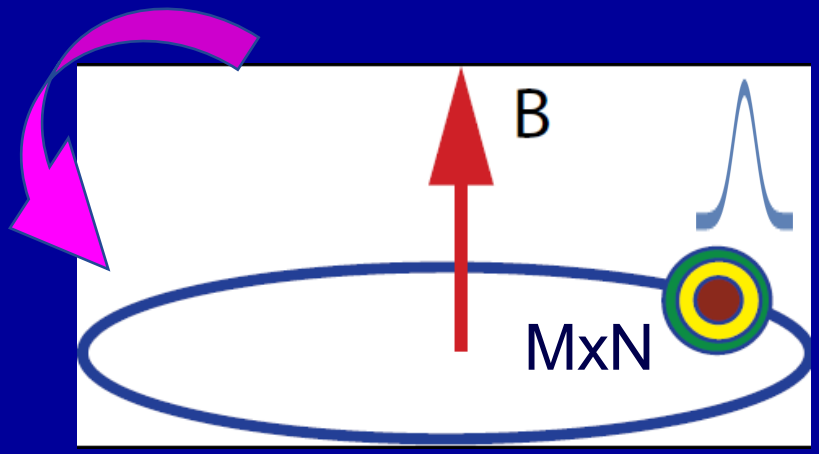
T. Li et al., PRL 109, 163001 (2012)

Ion crystal

Ultracold ions/ Coulomb repulsion

Both fermions ($^{24}Mg^{+}$) and Bosons ($^{9}Be^{+}$)

A different orbital for each particle



F. Wilczek, PRL 109, 160401 (2012)

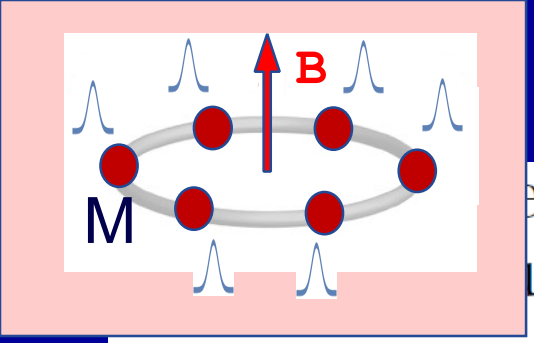
Lump/ Bose-Einstein soliton

Ultracold neutral atoms

Attractive contact interaction

Bosons (^{87}Rb or ^{85}Rb)

The same orbital for all particles



e each particle localized at position $\mathbf{R}_j$ as a ussian 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

$R_W = 1000$

$R_\delta = 50$

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

V_{int} Band head/ where interaction and Correlations show up

Φ Magnetic flux

$$C_R \approx C_R^{\mathrm{cl}} = \hbar^2/[2\mathcal{I}(R_{\mathrm{eq}})] \qquad \mathcal{I}(R_{\mathrm{eq}}) = NMR_{\mathrm{eq}}^2$$

L => magic (fermions spin polarized)

Repelling, polygon crystal:

$L_m = kN; \quad k = 0, \pm 1, \pm 2, \pm 3, \ldots$ Fermions, N odd; bosons

$L_m = (k + \frac{1}{2})N; \quad k = 0, \pm 1, \pm 2, \pm 3, \ldots$ Fermions, N even

$L_m = 0, \pm 1, \pm 2, \ldots$ Attractive bosons, lump

Floppy rotor (high B)

Analytic approximation to REM (quantum)

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

Total *L*

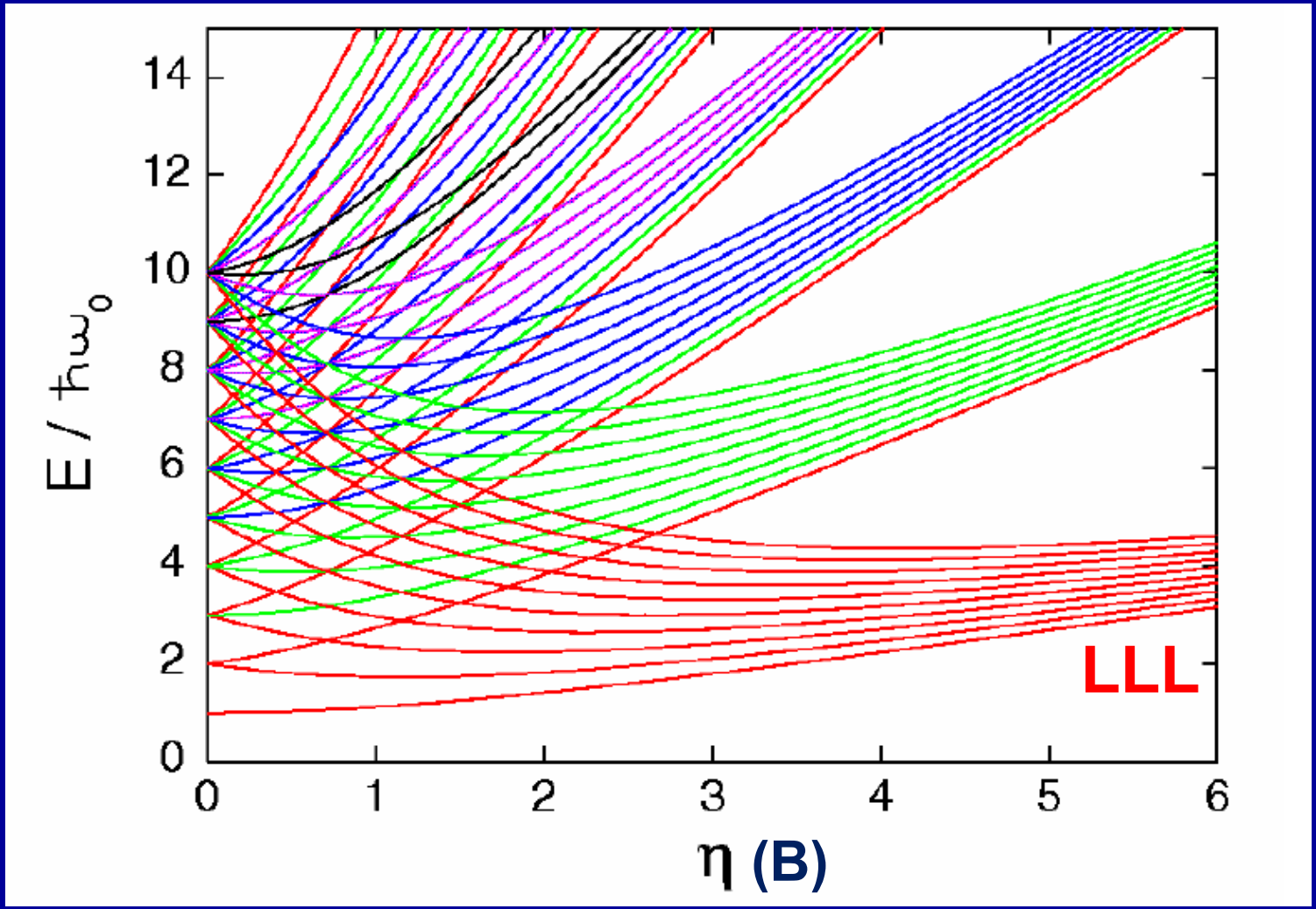
Partial angular momenta (corresponding to rings)

$$V_C(a_q, a_s) = n_q n_s {}_2F_1[3/4, 1/4; 1; 4a_q^2 a_s^2 (a_q^2 + a_s^2)^{-2}] e^2 (a_q^2 + a_s^2)^{-1/2}/\kappa$$

RIGID / Classical

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

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

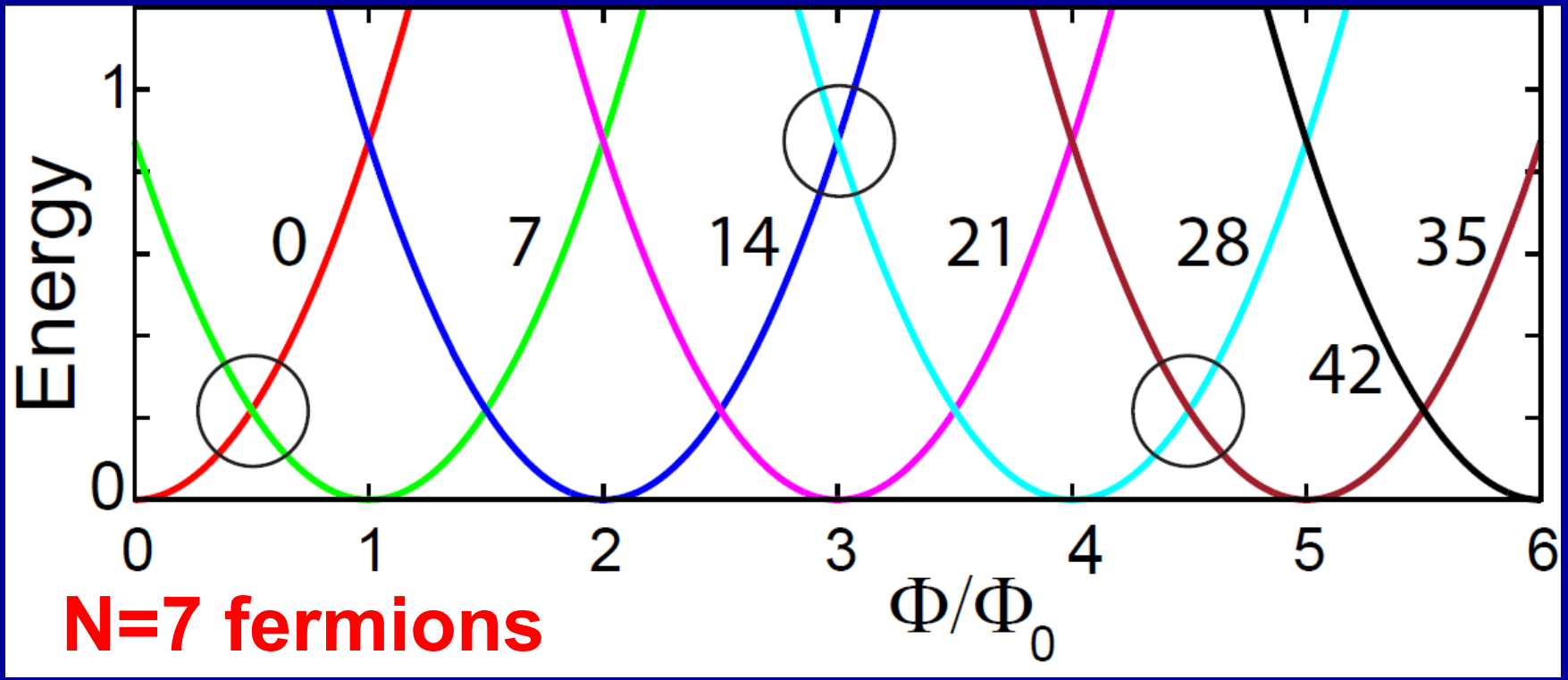


Effect of breaking time reversal symmetry
2D oscillator under a magnetic field
Darwin-Fock spectrum

Rotational spectrum: quantum rigid rotor

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

SECOND TERM/ AHARONOV-BOHM TYPE SPECTRUM



N=7 fermions

GOA/ GCM

Norm overlap/ Time-reversal

KAMLAH expansion

where in such a way that the quotient $h(\alpha)/n(\alpha)$ is a rather smooth tion. 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*

$$n(\alpha) \simeq \exp\left(i\langle \hat{J} \rangle \cdot \alpha - \tfrac{1}{2}\langle \Delta \hat{J}^2 \rangle \alpha^2\right), \tag{11.79}$$

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

nly difference now being that we also allow for time odd components e 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:

$$E^I_{\text{proj}} = \langle H \rangle - \frac{\langle \Delta \hat{J}^2 \rangle}{2\vartheta_Y} + \frac{\langle \hat{J} \rangle}{\vartheta_{sc}}(I - \langle \hat{J} \rangle) + \frac{1}{2\vartheta_Y}(I - \langle \hat{J} \rangle)^2. \tag{11.91}$$

t 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

$$E^I_{\text{proj}} = \langle H - \frac{\hat{J}^2}{2\vartheta_Y} \rangle + \frac{I^2}{2\vartheta_Y}. \tag{11.92}$$

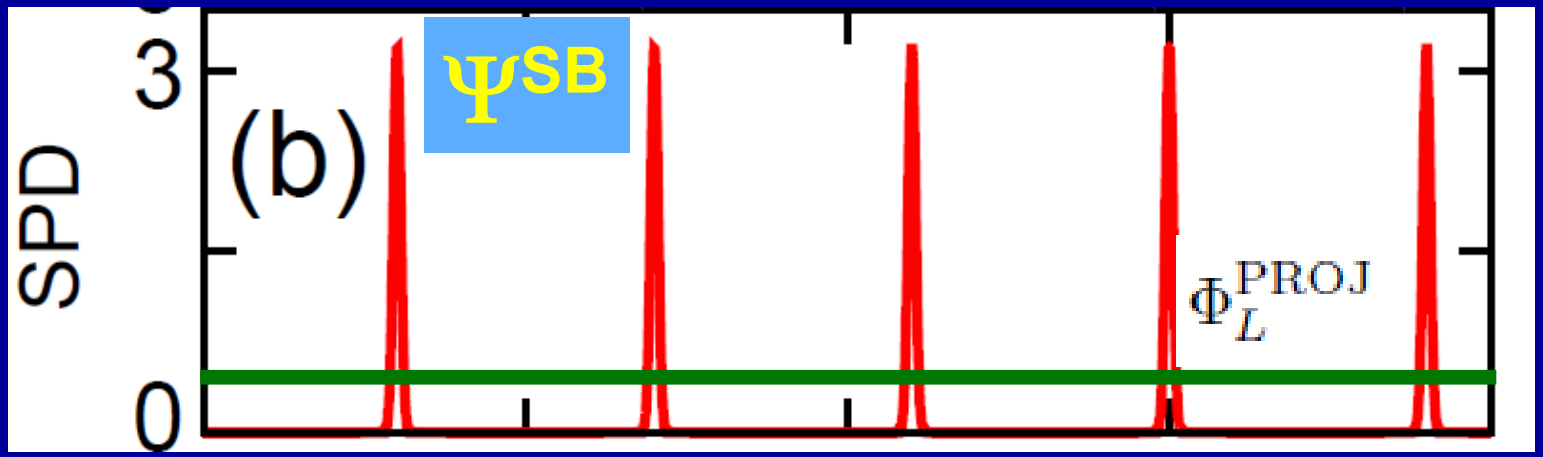
the spectrum of a one-dimensional rotor with the Yoccoz value ϑ_Y for noment of inertia (see Sec. 11.4.5).† The band head is obtained from

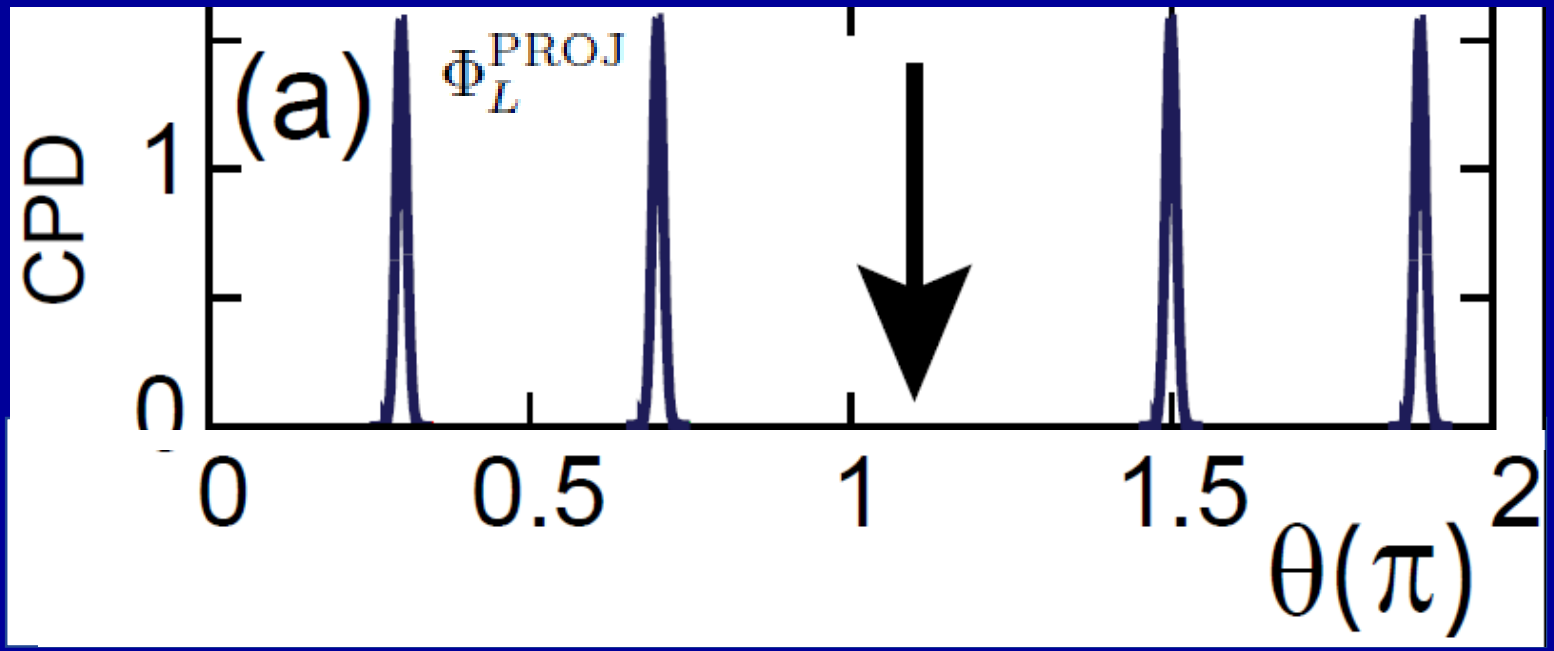
$\langle \hat{J} \rangle$ → Φ/Φ_0

Ring & Schuck, Ch. 11

Structure of many-body wave functions on ring

N=5 ultracold ions (fermions)





Wave packets/ Time evolution

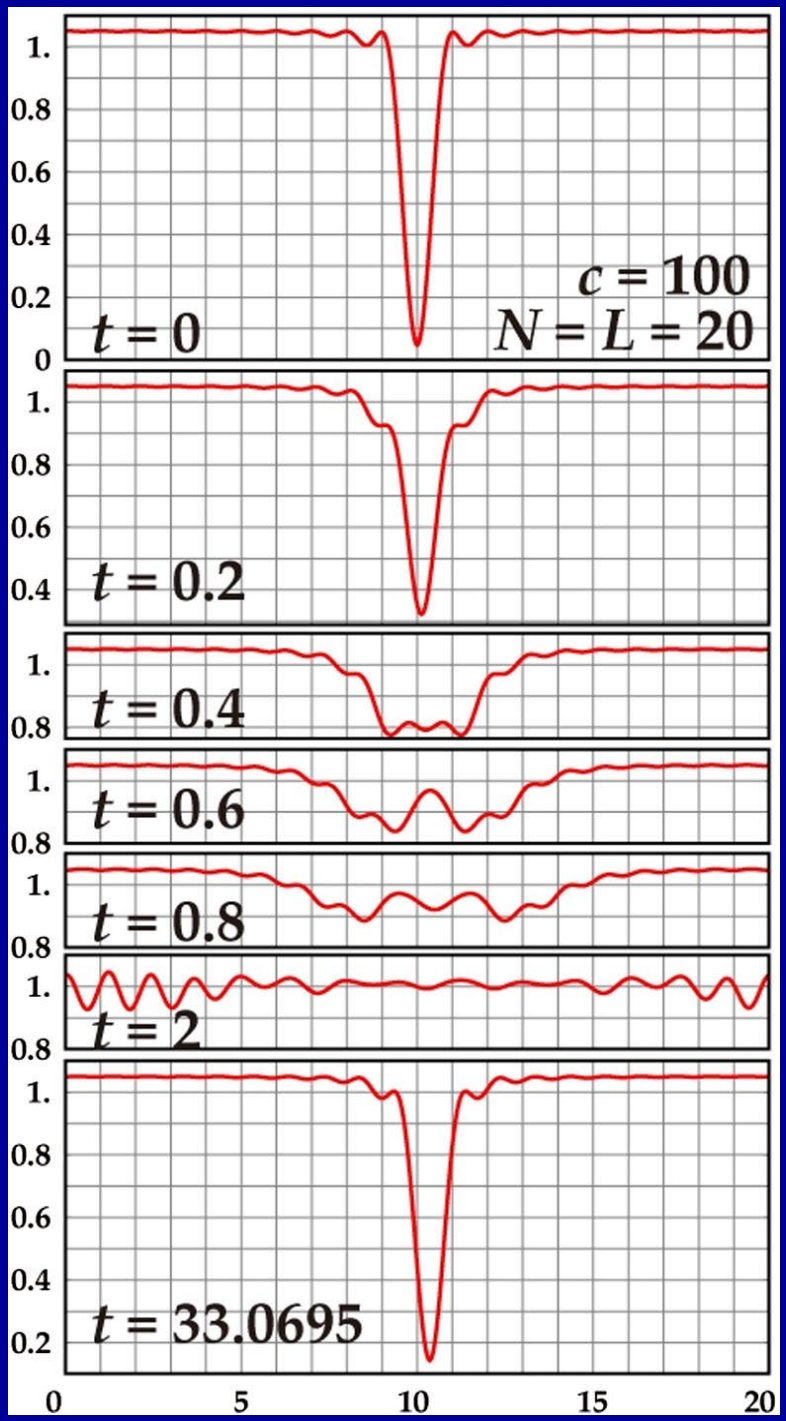
$$\Psi^{\mathrm{SB}} = \sum_L \mathcal{C}_L \Phi_L^{\mathrm{PROJ}}$$

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^{-iE_L}

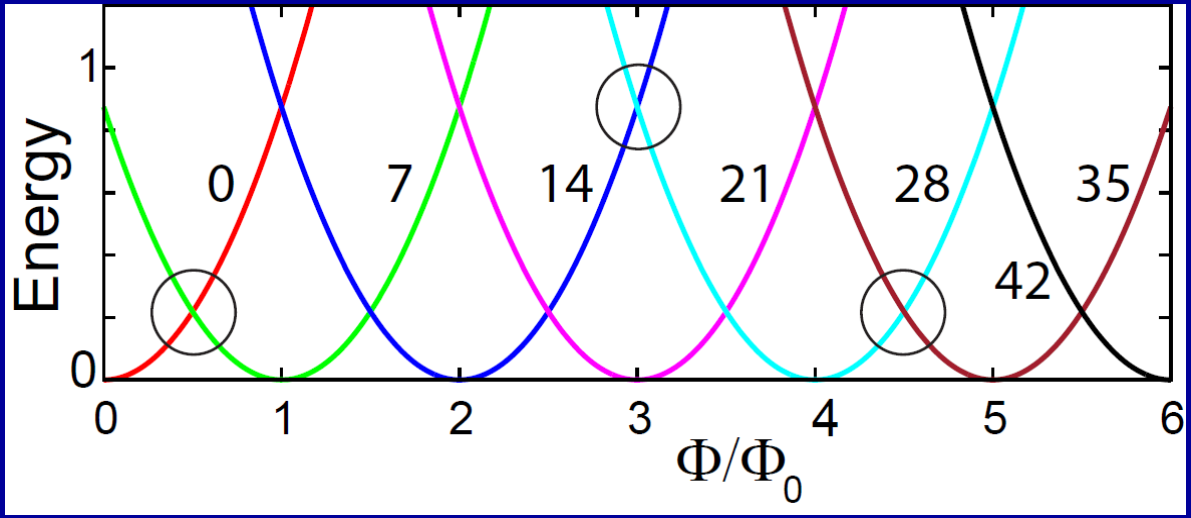
Diffusion and Revival



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

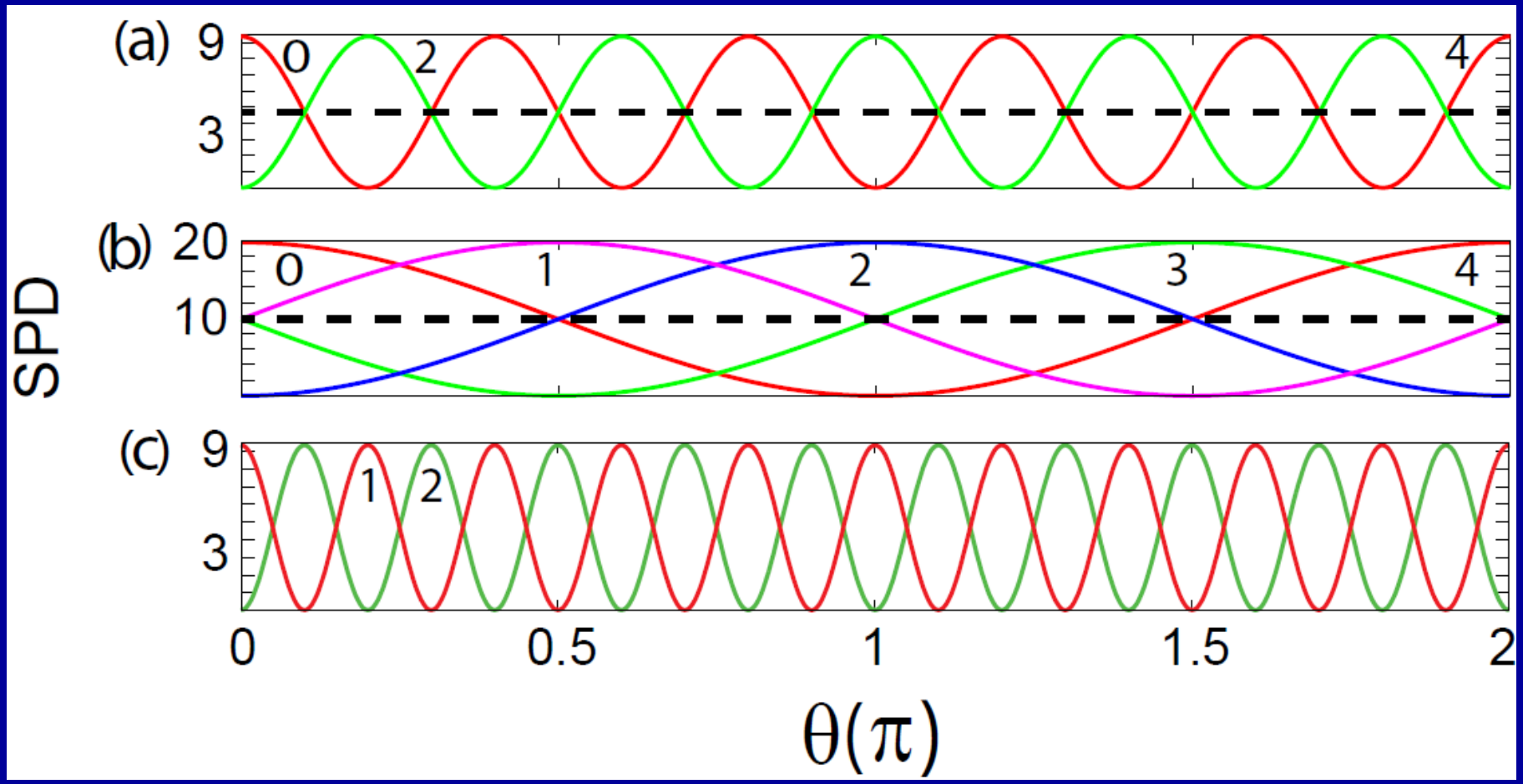
PINNED WIGNER MOLECULE (PWM)/ TWO-PROJECTED-STATE SUPERPOSITION

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



PWM: TIME EVOLUTION OF SPD (snapshots)

$$\tau = 2\pi\hbar/|E_1 - E_2|$$



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

END