NUCLEAR AND PARTICLE-PHYSICS ASPECTS OF CONDENSED-MATTER NANOSYSTEMS

NUCLEAR MANY-BODY METHODS IN CONDENSED-MATTER NANOSYSTEMS

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Three (among others) major nuclear analogies:

Surface plasmons/Giant resonances

 (via <u>matrix RPA/LDA</u>) in metal clusters
 [see, e.g., Yannouleas, Broglia, Brack, Bortignon,
 PRL 63, 255 (1989)]



 Electronic shells/deformation/fission
 (via <u>Strutinsky/ Shell correction approach</u>) in metal clusters
 [see, e.g., Yannouleas, Landman, Barnett, in "Metal Clusters", edited by W. Ekardt, John-Wiley, 1999]

 Strongly correlated states / Repulsive interaction (Quantum crystals/Wigner molecules/dissociation) in 2D semiconductor quantum dots and ultracold bosonic traps via <u>symmetry breaking/symmetry restoration</u> in conjunction with <u>exact diagonalization (full CI)</u> [see, e.g., Yannouleas, Landman, Rep. Prog. Phys. **70**, 2067 (2007)]





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Strongly correl (Quantum cry in 2D semicor ultracold bosc symmetry bre use multideterminants and in conjunction [see, e.g., Yanno restore symmetries Rep. Prog. Phys.

JO KS-DFT/ due to SIE, open problem of how to

N=7, EXD

Metai Clusters



Electronic shells/ magic numbers/ deformation/ fission in metal clusters
 Surface plasmons/Giant resonances in metal clusters

The physics of free nonrelativistic electrons confined in a central potential, like atomic nuclei (conservation of symmetries/ independent particle model/ delocalized electrons)





 Strongly correlated states (Quantum crystals/Wigner molecules/dissociation) in 2D semiconductor quantum dots

No central potential/ electron localization (relative to each other) due to strong Coulomb repulsion/ mean-filed with broken symmetries



TWO VARIANTS OF SHELL CORRECTION METHOD (SCM) in condensed-matter nanosystems:

1) Fully microscopic (SCM-DFT) / Orbital-free DFT Based on Extended Thomas Fermi (ETF) sp densities and central potentials

Literature: Y&L, PRB 48, 8376 (1993) (multiply anionic metal clusters) Y&L, Ch. 7 in "Recent Advances in Orbital-Free Density Functional Theory," Y.A. Wang and T.A. Wesolowski Eds. (Word Scientific, Singapore, 2013) (metal clusters, nanowires, fullerenes)

2) Semiempirical (SE-SCM) <u>Based on a triaxial H.O. (Nilsson) central potential</u> + liquid drop model for smooth variation
Y&L, PRB 51, 1902 (1995) (deformed metal clusters) Used extensively in nuclear physics

SCM-DFT (based on ETF) 📫 KS-DFT

ETF potentials





Yannouleas & Landman, PRB **48**, 8376 (1993)

$$T_{sh} = \sum_{i=1}^{\text{occ}} \widetilde{\varepsilon}_i - \int \rho_{ETF}(\mathbf{r}) V_{ETF}(\mathbf{r}) d\mathbf{r},$$

Shell correction: Difference of two kinetic energy terms

$$\Delta E_{sh} = T_{sh} - T_{ETF}[\rho_{ETF}]$$

ETF/ Smooth

Applications of DFT-SCM: neutral fullerene C₆₀ Y&L, Chem. Phys. Lett. **217**, 175 (1994)





The Superatom States of Fullerenes and Their Hybridization into the Nearly Free Electron Bands of Fullerites

J. Zhao, M. Feng, J. Yang, H. Petek ACS Nano **3**, 854 (2009) LT-STM



SECOND PART

Strong correlations and symmetry breaking/restoration in 2D finite systems

Constantine Yannouleas and Uzi Landman Phys. Rev. Lett. **82**, 5325 (1999); Rep. Prog. Phys. **70**, 2067 (2007)

Collaborators:

Igor Romanovsky (ultracold bosons & graphene nanostructures) Yuesong Li (electrons in QDs) Ying Li (electrons in Quantum Dot Molecules) Leslie O. Baksmaty (ultracold bosons & electrons in QDs)



and NTT in Japan is fabricated in the shape of a round pillar. The source and drain are doped semiconductor layers that conduct electricity, and are separated from the quantum dot by tunnel barriers 10 nm thick. When a negative voltage is applied to the metal side gate around the pillar, it reduces the diameter of the dot from about 500 nm to zero, causing electrons to leave the dot one at a time.

Vertical QD (Delft)

Electrostatic confinement



FIG. 1. SEM image of the gate geometry forming the quantum dot. This geometry enables a precisely known number of electrons $(N=0,1,2,\ldots,50)$ to be trapped (Ref. 13) and produces a quasiparabolic confinement potential. Sweeping the plunger-gate voltage tunes both the shape and the chemical potential of the quantum dot.

Lateral QD (Ottawa)



Lateral QD Molecule (Delft)

<u>Central common confining potential?</u> Electronic Shells? (B=0; Circular QD)

2D Periodic Table?

4, 9, 16 Hund's Rule

b

C



The current flowing through the quantum dot structure at a temperature of 0.1 K was measured as the gate voltage was varied. (a) The first peak corresponds to the voltage at which the first electron can enter the dot, and the number of electrons increases by one at each subsequent peak. The distance between peaks provide a measure of the addition energies (see inset). (b) The addition of single electrons to the quantum dot can be pictured in terms of circular orbits. The first shell can contain two electrons, the second can contain four and so on. This makes it possible to formulate a periodic table for these artificial two-dimensional atoms (c). Full shells correspond to the magic numbers N = 2, 6, 12, 20 and so on, while half-filled shells (N = 4, 9, 16, etc.) correspond to maximum spin states. (The elements are named after team members from NTT and Delft.)

2, 6, 12, 20 Closed Shells

Kouwenhoven and Marcus, Physics World, June 1998

Wigner Crystals

DECEMBER 1, 1934

PHYSICAL REVIEW

On the Interaction of Electrons in Metals

E. WIGNER, Princeton University (Received October 15, 1934)

The energy of interaction between free electrons in an electron gas is considered. The interaction energy of electrons with parallel spin is known to be that of the space charges plus the exchange integrals, and these terms modify the shape of the wave functions but slightly. The interaction of the electrons with antiparallel spin, contains, fact that the electrons repell each other and try to keep as far apart as possible. The total energy of the system will be decreased through the corresponding modification of the wave function. In the present paper it is attempted to calculate this "correlation energy" by an approximation method which is, essentially, a development of the energy WC: Classical Electron Crystals/ Mean Field/ Broken Symmetry

VOLUME 46

... electrons repell each other and try to keep as far apart as possible. The total energy of the system will be decreased through the corresponding modification of the wave function. ... "correlation energy" ...



"If the electrons had no kinetic energy, they settle in configurations which correspond to the absolute minima of the potential energy. These are **closepacked lattice configurations**, with energies very near to that of the bodycentered lattice ... "

Our work: Quantum Crystals/ Beyond Mean Field/ Full Symmetry

Rotating Wigner molecule

Not a small piece of a classical Wigner crystal (broken symmetries) Quantum crystallite (good symmetries)

 \sim Rigid rotor (L^2) and corrections (as in nuclear physics) B=0

Large B -> ∞ (lowest Landau level - electrons)



Superfloppy, supersolid: a solid flowing like a superfluid (e.g., $aL + b/\sqrt{L}$)

Connection to FQHE

C.Y. & U.L., Physical Review B 69 (2004) 113306



H can be generalized to: Multi-component systems



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





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

Circular external confinement



Wigner molecule in a 2D circular QD. Electron density (ED) from Unrestricted Hartree-Fock (UHF). Symmetry breaking (localized orbitals). Concentric polygonal rings



<u>Concentric rings:</u> (0,6) left, (1,5) right Y&L, PRL 82, 5325 (1999)



<u>Concentric rings:</u> (1,6,12) Y&L, PRB 68, 035325 (2003)

Exact electron densities are circular! No symmetries are broken! (N, small, large?)

Restoration of symmetry A Quantum crystal

Rotating Boson Molecules (Circular trap) Ground states: Energy, angular momentum and probability densities.

 $R_{W} = 10$

 ω_{c}/ω_{0}



Rotating Frame Magnetic Field Probability densities SPD E_{PRJ} L=0 L=5 18 $\mathbf{E}_{_{\mathrm{PRJ}}}$ 70.0 L=10 L=15 90 69.8 $E/\hbar\omega_0$ 14 $E/\hbar \omega_0$ EPRJ 0.2 0.3 0.4 L=080 10 T.=10 L=15 $\mathbf{E}_{_{\mathrm{PRJ}}}$ 0.2 0.4 0.6 70 6 SPD 0.0 E_{PRJ}-E_{UBHF} -0.2 -0.1 $E/\hbar\omega_0$ E/μ®⁰ -0.4 15 E_{PRJ}-E_{UBHE} -0.6 10 -0.3 -0.8 -0.460 \mathbf{L}_{PRJ} 2 Lum \mathbf{L}_{UBHF} L_z×10² 40 L 02 0.3 0.4 20 \mathbf{L}_{PRJ} 0 **CPD** 0 0.2 0.4 0.6 0.8 10 2 8 4 Ω/ω_0

Rotating Boson Molecules (Circular trap) Ground states: Energy, angular momentum and probability densities.

SPD

SPD

CPD

(0



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

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



Quantum Dot Helium

<u>RIGID</u> ROTOR

<u>B=0</u>

Natural Helium Doubly excited States/ Kellman/Herrick Phys. Rev. A **22**, 1536 (1980). Three electron anisotropic QD: pinning Method: Exact Diagonalization (EXD) Anisotropic confinement

Electron Density (ED)

(spin resolved) Conditional Probability Distribution (CPD)





Yuesong Li, Y&L, Phys. Rev. B **76,** 245310 (2007)

EXD wf ~ $| \oint \oint \oint > - | \oint \oint \oint >$ Entangled three-qubit <u>W-states</u>

WAVE-FUNCTION BASED APPROACHES

TWO-STEP METHOD

A HIERARCHY OF APPROXIMATIONS

Bestricted Hartree-Fock (RHF)

otal

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)

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

Non-linear equations Bifurcations

> EMERGENT PHENOMENA

Restoration of linearity of many-body equatons EXACT DIAGONALIZATION (Full Configuration Interaction)

> When possible (small N): High numerical accuracy

Physics less transparent compared to "THE TWO-STEP"

Pair correlation functions, CPDs

Yannouleas and Landman, Rep. Prog. Phys. 70, 2067 (2007)

Restoration of Broken Rotational Symmetry

 To restore the good angular momentum of the wave function one can use the projection operator

$$\hat{P}_{L} = \frac{1}{2\pi} \int_{0}^{2\pi} d\theta e^{i\theta \left(L-\hat{L}\right)} = \delta(L-\hat{L})$$

 Projected wave functions can be written as a Fourier transform of unprojected wave function

$$\Phi_{N,L}^{\mathbf{PRJ}} \rangle = \hat{P}_{L} |\Phi_{N}\rangle = \frac{1}{2\pi} \int_{0}^{2\pi} d\theta |\Phi_{N}(\theta)\rangle e^{i\theta L}$$

Here $|\Phi_N(\theta)\rangle$ is the original UBHF permanent, rotated by an azimutal angle. The wave function $|\Phi_{PRJ}\rangle$ has not only good angular momentum, but also its energy is lower than the energy of $|\Phi_N\rangle$

Romanovsky, Yannouleas, and Landman Phys. Rev. Lett. 93, 230405 (2004) (RBMs) Romanovsky, Yannouleas, Baksmaty, Landman Phys. Rev. Lett. 97, 090401 (2006) (RBMs)

TWO-STEP METHOD

SECOND STEP: RESTORATION OF SYMMETRIES VIA PROJECTION

TOTAL SPIN:

$$P_s \equiv \prod_{s' \neq s} \frac{S^2 - s'(s'+1)\hbar^2}{[s(s+1) - s'(s'+1)]\hbar^2}$$

$$S^{2}\Phi_{\text{UHF}} = \hbar^{2} \left[(N_{\alpha} - N_{\beta})^{2}/4 + N/2 + \sum_{i < j} \overline{\sigma}_{ij} \right] \Phi_{\text{UHF}}$$
interchanges spins

Two electrons in a DQD:

$$\Psi_{\text{GVB}}^{\text{s}}(1,2) = n_{\text{s}}\sqrt{2}P_{0}\Psi_{\text{UHF}}(1,2) - \text{Singlet}$$

 $2\sqrt{2}P_{0}\Psi_{\text{UHF}}(1,2) = (1-\varpi_{12})\sqrt{2}\Psi_{\text{UHF}}(1,2) \\ = |u(1)\bar{v}(2)\rangle - |\bar{u}(1)v(2)\rangle. \text{ two det.'s}$

GVB, Generalized Valence Bond GHL, Generalized Heitler London

> Y&L, Eur. Phys. J. D 16, 373 (2001) Int. J. Quantum Chem. 90, 699 (2002)

localized orbitals

Elongated QD



No circular symmetry

RESOLUTION OF SYMMETRY DILEMMA: RESTORATION OF BROKEN SYMMETRY BEYOND MEAN FIELD (Projection)!

 Per-Olov Lowdin (Chemistry - Spin)



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



Ch. 11 in the book by P. Ring and P. Schuck Note: Example in 2D

Yannouleas, Landman, Rep. Prog. Phys. 70, 2067 (2007)

Excitation Spectrum of Two Correlated Electrons in a Lateral Quantum Dot with Negligible Zeeman Splitting

C. Ellenberger,¹ T. Ihn,¹ C. Yannouleas,² U. Landman,² K. Ensslin,¹ D. Driscoll,³ and A. C. Gossard³ ¹Solid State Physics, ETH Zurich, 8093 Zurich, Switzerland ²School of Physics, Georgia Institutue of Technology, Atlanta, Georgia 30332-0430, USA ³Materials Department, University of California, Santa Barbara, California 93106, USA (Received 16 December 2005; published 30 March 2006)

basis of an avoided crossing with the first excited singlet state at finite fields. The measured spectra are in remarkable agreement with exact-diagonalization calculations. The results prove the significance of electron correlations and suggest the formation of a state with Wigner-molecular properties at low magnetic fields.

<u>ETH single QD</u>

ARTICLES

PUBLISHED ON LINE: 28 JULY 2013 | DOI: 10.1038/NPHYS2692



Observation and spectroscopy of a two-electron Wigner molecule in an ultraclean carbon nanotube

S. Pecker^{1†}, F. Kuemmeth^{2†}, A. Secchi^{3,4‡}, M. Rontani³, D. C. Ralph^{5,6}, P. L. McEuen^{5,6} and S. Ilani^{1*}

1 Weizmann Institute of Science, Israel 2 Niels Bohr Institute, Denmark 5 Physics Department, Cornell University, Ithaca, New York



<u>hwx=4.23 meV; hwy=5.84 meV;</u> <u>m*=0.070; K=12.5; γ=0.86</u> B=3.8 T





Circular 2D QD NO e-e INTERACTION

DARWIN-FOCK S.P. LEVELS AT ANY B



Rotating atomic

<u>B -> Omega</u>





Composite-Fermion (CF) vs. RWM

fractional filling

$$\nu = \frac{N(N-1)}{2L_m}$$

m -> magic

Cusp states -> precursor states of FQHE

(1,5) polygonal ring

EXD, LLL, Coulomb, N=6e



C.Y. & U.L., PRB 68 (2003) 035326

Full LLL spectra (interaction only)

N=3 bosons (delta)

N=4 fermions (Coulomb)





Energy

TRIAL WFs ARE HIGHLY CORRELATED; THEY CAPTURE THE PHYSICS OF CUSP STATES AND CERTAIN SELECTIVE EXCITATIONS (Jastrow-Laughlin, compact CF, Moore-Read, REM)

TO DESCRIBE LARGER PARTS OF LLL SPECTRA: USE TRIAL WFs TO FORM A COMPLETE CORRELATED BASIS Practical: Controlled improvements of variational WF Conceptual: Completeness/ Properties of basis are reflected in exact WFs

EXAMPLE: quantum liquids [J.W. Clark and E. Feenberg, Phys. Rev. 113, 388 (1959)]

EXAMPLE: CF BASIS (mainly the full yrast band) [G.S. Jeon et al, PRB 69, 241304(R) (2004); Eur. Phys. J. B 55, 271 (2007)]

EXAMPLE (this talk): RO-VIBRATIONAL MOLECULAR (RVM) BASIS [Y & L., Phys. Rev. A 81, 023609 (2010)] THE FULL LLL SPECTRUM



RVM trial functions:

RXM -> RBM or REM

$$\Phi_{\mathcal{L}}^{\mathrm{RXM}}(n_1, n_2) Q_{\lambda}^m | 0 >$$

Pure rotations (cusp, vibrationless)

(molecular point-group symmetries)

RBM

$$\Phi_{\mathcal{L}}^{\text{RBM}}(0,3) = \sum_{0 \le l_1 \le l_2 \le l_3}^{l_1 + l_2 + l_3 = \mathcal{L}} C(l_1, l_2, l_3) \operatorname{Perm}[z_1^{l_1}, z_2^{l_2}, z_3^{l_3}]$$

$$C(l_1, l_2, l_3) = \left(\prod_{i=1}^3 l_i!\right)^{-1} \left(\prod_{k=1}^M p_k!\right)^{-1}$$

$$\left(\sum_{i=1}^{l_1 + l_2 + l_3 = \mathcal{L}} C(l_1, l_2, l_3) - \frac{1}{2\pi(l_i - l_i)}\right)$$

 $^{ imes} \left[egin{array}{c} \sum\limits_{1 \leq i < j \leq 3} \cos \left[egin{array}{c} 3 \end{array}
ight]
ight] \mathcal{L} = \mathcal{L}_0 + n_1 k_1 + n_2 k_2$

MAGIC ANGULAR MOMENTA

Vibrations

 $L = \mathcal{L} + \lambda m$

$$Q_{\lambda} = \sum_{i=1}^{N} (z_i - z_c)^{\lambda}$$

$$z_c = (1/N) \sum_{i=1}^N z_i$$

REMs (analytic): Yannouleas and Landman, PRB 66, 115315 (2002); Rep. Prog. Phys. 70, 2067 (2007)



N=4 e L=18 v=1/3

RVMs that DOMINATE EXPANSION

EXD-TI

->

	IL- QX			$\begin{bmatrix} 4 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\$, 4
	BVMs [Ed. (1)]	1> 1> 1> 1> 4 0 4 0 -4 (0,4) REM (f=18)	$f_{1} = \frac{15}{100}$	$ 2\rangle$ $\int_{0}^{1} \int_{0}^{1} \int_{0}^{1$	•
$\frac{nv}{11}$		$\Delta D = 11 [1]$	$\frac{\text{EAD-11}\left[2\right]}{0.3420}$	$\frac{\text{EAD-11}\left[4\right]}{0.0002}$	
1 9	~	0.9294 0.1188	-0.3430	0.0903	
2	<	-0.1188	-0.0035	-0.2596	
$ \Delta$	>	0.0007 0.0137	0.0302	-0.0968	
$ _{5}^{++}$	>	0.2540	0.8486	0.1519	
	/			0.1010	
6	>	0.0211	0.0283	0.3097	

LLL, pinned Wigner crystal (broken symmetry) V = 1/3

PRL 105, 126803 (2010)

PHYSICAL REVIEW LETTERS

week ending 17 SEPTEMBER 2010

Observation of a Pinning Mode in a Wigner Solid with $\nu = 1/3$ Fractional Quantum Hall Excitations

 Han Zhu,^{1,2} Yong P. Chen,³ P. Jiang,^{2,1} L. W. Engel,² D. C. Tsui,¹ L. N. Pfeiffer,¹ and K. W. West¹
 ¹Princeton University, Princeton, New Jersey 08544, USA
 ²National High Magnetic Field Laboratory, Tallahassee, Florida 32310, USA
 ³Purdue University, West Lafayette, Indiana 47907, USA (Received 11 June 2010; published 17 September 2010)

Laughlin liquid versus Wigner crystal : different wave functions Crossover between 1/5 to 1/7 -- At 1/3 liquid lower than WC

RVMs, EXD Good symmetry, crystalline correlations are hidden



LLL, quantum Wigner crystal (broken symmetry) V = 1/3



Pinning -> Impurity -> Linear superposition:

$$\Phi^{\text{PIN}}(L_1, L_2; \alpha, \beta) = \alpha \Phi_{L_1} + \beta e^{i\theta} \Phi_L$$

Energy lower than HF (1 det) crystal, Maki & Zotos, etc.

> *C.Y.* & *U.L.,* PRB **84**, 165327 (2011)



SUMMARY (Symmetry Restoration)

Under appropriate conditions, 2D electrons (and ultracold repelling bosons) <u>exhibit localization (hidden or explicit)</u> and organize themselves in geometric shells, forming Rotating (or pinned) Wigner Molecules (Quantum Crystallites) (semiconductor Quantum Dots, Ultracold rotating bosonic traps, Dissociation of natural molecules)

Instead of:

For electrons: organizing in electronic shells associated with a confining central potential (Cluster physics/ jellium model)

For bosons: forming a Bose-Einstein condensate

In the LLL: Rovibrational molecular theory offers alternative description to Laughlin and composite-fermion approaches for the fractional quantum Hall effect