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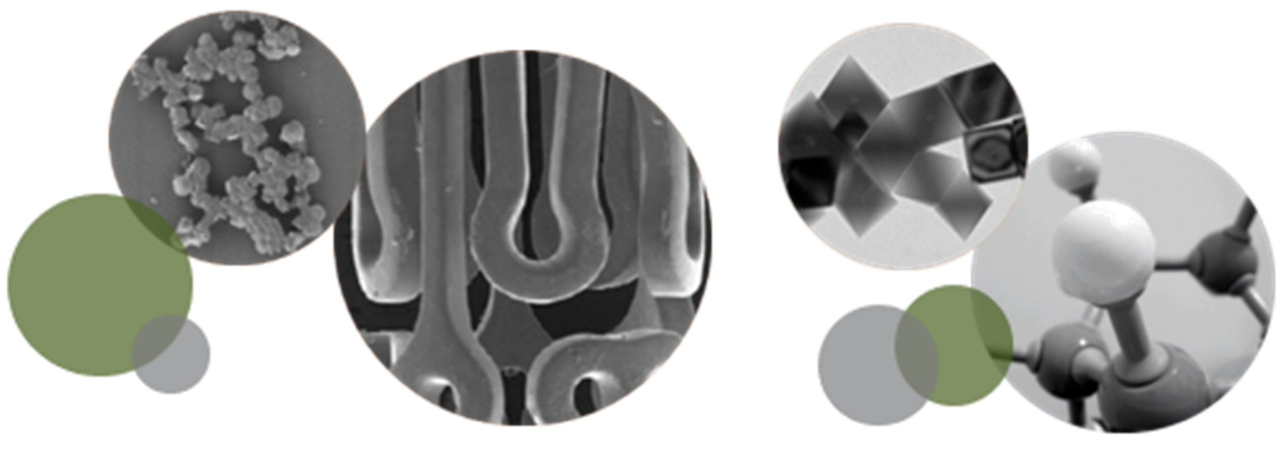

Nanoscience and Nanotechnology International Conference

A CIRCULAR MODEL FOR ELECTRON CONFIGURATIONS IN 2D HETEROSTRUCTURES AT HIGH MAGNETIC FIELD

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Motivation

1. Conduction electrons in circular QD's with parabolic confinement and magnetic field

$$H=\sum_i\left(\frac{p^2}{2m}+\frac{1}{2}m\Omega^2r^2+\frac{\omega_c}{2}\hat{L}_z+g^*\mu_B B S_z\right)_i+\frac{e^2}{\kappa}\sum_{i<j}\frac{1}{r_{ij}}\qquad \Omega=\sqrt{\omega_0^2+(\omega_c/2)^2}$$

Two relevant parameters (interaction – confinement) and magnetic – confinement ratios

parabolic (pu) or magnetoparabolic units (mpu)

$\hbar\omega_0$ and $\ell_0=\sqrt{\hbar/m\omega_0}$ $\qquad$ $\hbar\Omega$ and $\ell_\Omega=\sqrt{\hbar/m\Omega}$

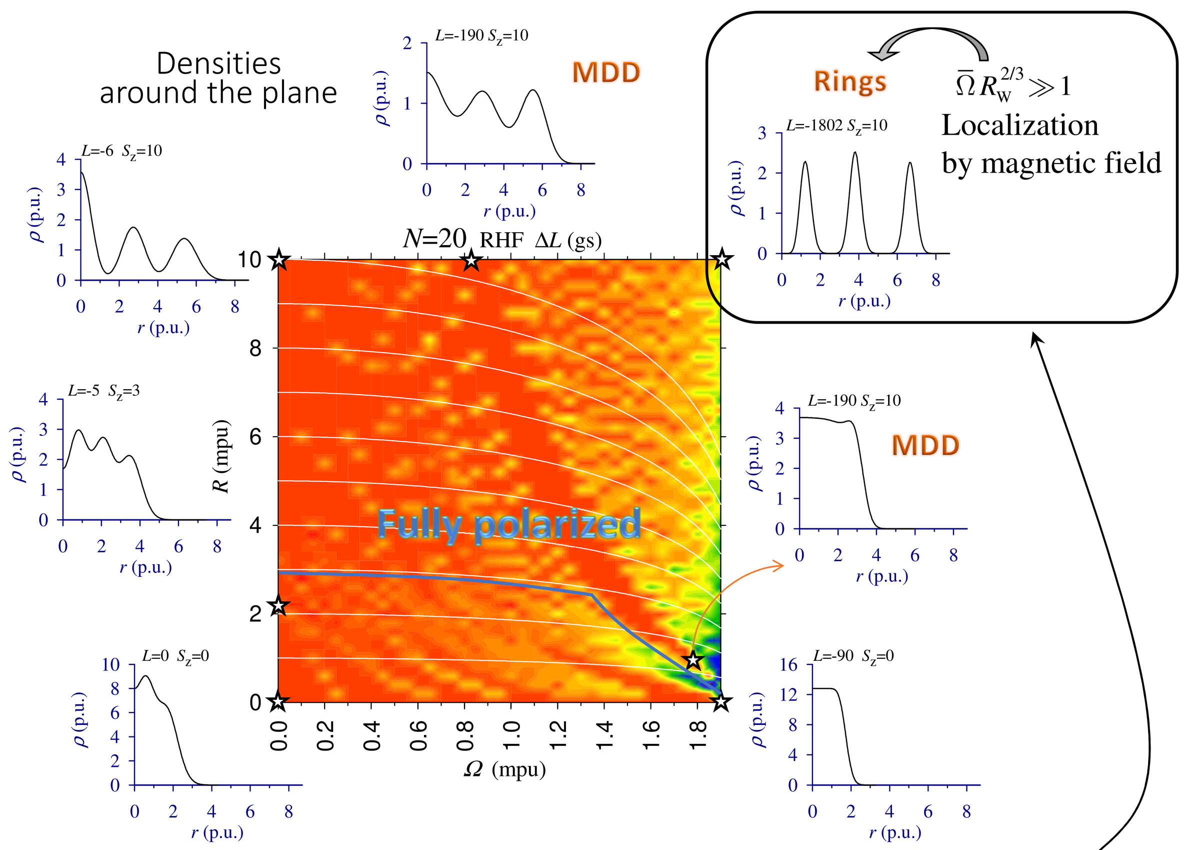
$R_W=\dfrac{e^2/\kappa}{\hbar\omega_0\ell_0}$ $\qquad$ $\tilde{R}=\dfrac{e^2/\kappa}{\hbar\Omega\ell_\Omega}$

$\bar{\Omega}=\omega_c/\omega_0$ $\qquad$ $\tilde{\Omega}=\omega_c/\Omega=0\ldots2$

$\bar{\Omega}=\tilde{\Omega}/(1-(\tilde{\Omega}/2)^2)^{1/2}$
$R_W=\tilde{R}/(1-(\tilde{\Omega}/2)^2)^{1/4}$
$E(\mathrm{pu})=E(\mathrm{mpu})/(1-(\tilde{\Omega}/2)^2)^{1/2}$
$r(\mathrm{pu})=r(\mathrm{mpu})\,(1-(\tilde{\Omega}/2)^2)^{1/4}$

Theoretical studies of electronic wave functions in the plane $\bar{\Omega}-R_W$

$$\mathcal{H}(\hbar\Omega)=\sum_i\left(-\frac{1}{2}\nabla^2+\frac{1}{2}r^2+\frac{\tilde{\Omega}}{2}L_z+\mathcal{H}_z\right)_i+\tilde{R}\sum_{i<j}\frac{1}{r_{ij}}$$



Energy = Zero point + Classical Energy ($\{R_i\}$) + corrections

At high enough magnetic fields, zero point dominates system's energy and the individual electrons "localize" (sharp intrinsic probability distributions) around the classical equilibrium positions

Circular Model (CM)

2. *Total energy of* N point charges uniformly distributed over p concentric rings

$$\varepsilon=\sum_{i=1}^{p}n_i V_{\mathrm{ext}}(r_i)+\sum_{i=1}^{p}E_{n_i}(r_i)+\sum_{i<j}^{p}E_{n_in_j}(r_i,r_j,\varphi_i-\varphi_j)$$

external confinement — intra-ring — inter-ring

Basic entities: rings

$\boxed{p,\{n_i,r_i,\varphi_i\}}$

Ring's partition, radius and angular offset

$$\boxed{\varepsilon_{\mathrm{avg}}(\boldsymbol{n},\boldsymbol{r})=\sum_{i=1}^{p}n_i V_{\mathrm{ext}}(r_i)+\alpha\sum_{i=1}^{p}\frac{n_i S_{n_i}}{4r_i}+\frac{2\alpha}{\pi}\sum_{i<j}^{p}n_in_j\frac{K\left[(r_j/r_i)^2\right]}{r_i}}\qquad \alpha=e^2/\kappa$$

GS configuration ➡ minimize wrt $p,\boldsymbol{n},\boldsymbol{r}$

- Far fewer variables than in Molecular Dynamics (MD)
- Unique solution ($\boldsymbol{r}$) for a given partition $p,\boldsymbol{n}$
- Easier scan of shell structure for increasing N

It can be shown (cyclic symmetry)

$$E_n(r)=\alpha\frac{nS_n}{4r}\quad\text{with}\quad S_n=\sum_{k=1}^{n-1}\frac{1}{\sin\frac{k\pi}{n}}$$

$$E_{n_in_j}(r_i,r_j,\psi)=\alpha\,G\sum_{k=1}^{L}\epsilon(r_i,r_j,\psi_k+\psi)$$

with $G=GCD(n_i,n_j)$, $L=lcm(n_i,n_j)$ and $\epsilon(r_i,r_j,\theta)=\left(r_i^2+r_j^2-2r_i\,r_j\cos\theta\right)^{-1/2}$

Ring-Ring interaction is an even periodic ($2\pi/L$) function

$$E_{n_in_j}(r_i,r_j,\psi)=\langle E_{n_in_j}\rangle+\sum_{\ell=1}^{\infty}C_{\ell n_in_j}(r_i,r_j)\cos(\ell L\psi)$$

average

$$\langle E_{n_in_j}\rangle=2\alpha\,n_in_j\frac{K(t^2)}{\pi\,r_>}\qquad O\left(t\equiv\frac{r_<}{r_>}\right)^{\ell L}\ll1$$

3. Results for Hard (infinite wall) and Soft (harmonic) confinement

***N* that open new Shell (particle at center in CM) Hard confinement**

N	CM configuration	Energy	MD configuration	Energy
12	[11,1]	59.57568	[11,1]	59.57568
30	[23,6,1]	479.0854	[23,6,1]	479.0796
56	[37,12,6,1]	1862.734	[37,12,6,1]	1862.650
92	[53,20,12,6,1]	5358.578	[53,20,12,6,1]	5358.353
136	[70,28,19,12,6,1]	12181.755	[70,28,19,12,6,1]	12181.345
187	[87,37,26,18,12,6,1]	23652.947	[87,37,26,18,12,6,1]	23652.188
248	[106,46,34,25,18,12,6,1]	42447.440	[107,46,34,25,17,12,6,1]	42446.278
317	[126,55,42,32,25,18,12,6,1]	70418.854	[126,56,42,33,22,19,12,6,1]	70416.883
395	[147,65,50,40,32,24,18,12,6,1]	110667.59	[147,66,51,40,26,26,19,13,6,1]	110664.44

; length and energy units (Hard conf): R (Disk radius), $e_0\equiv\dfrac{e^2/\kappa}{R}$

***Examples for* Soft confinement**

N	CM configuration	Energy	MD configuration	Energy
6	[5,1]	9.280127	[5,1]	9.280127
16	[10,5,1]	84.49102	[10,5,1]	84.44850
33	[15,11,6,1]	306.9034	[15,11,6,1]	306,8574
53	[19,16,11,6,1]	701.8207	[18,17,11,6,1]	701.7045
80	[24,21,17,11,6,1]	1429.075	[22,22,17,12,6,1]	1428.827
112	[28,26,22,17,12,6,1]	2545.141	[27,27,21,18,12,6,1]	2544.754
149	[32,31,27,23,17,12,6,1]	4143.661	[31,31,26,24,18,12,6,1]	4143.077
187	[37,36,32,27,22,17,11,5]	6099.538	[34,34,34,24,24,18,12,6,1]	6098.766
191	[36,36,32,28,23,17,12,6,1]	6322.955	[34,34,34,28,24,18,12,6,1]	6322.128

; length and energy units (Soft conf): $R=R_W^{1/3}\ell_0$ and $e_0\equiv R_W^{2/3}\hbar\omega_0$

Universal solutions (everything scales with corresponding units)

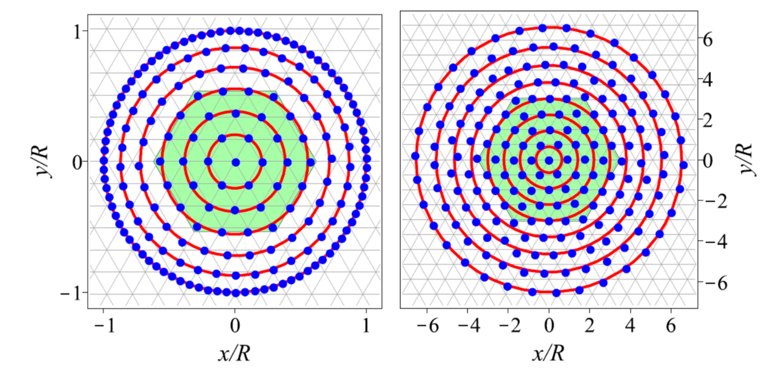
- **As N increases the number of rings does too, progresively changing the internal occupation from 1 to 5 and back again to 1 with an additional ring**
- **For big N internal shells develop a hexagonal lattice, which gradually transform to a well defined circular ring structure approaching the boundary**

- **Fits from systematic CM results provide good estimates for number of rings and external Shells fillings**

$$p^H=\left[\frac{\sqrt{N+7}}{2}\right]\qquad p^S=\left[\frac{\sqrt{6N+7}}{4}+\frac{1}{2}\right]$$

$$n_1^H=\left[2.795\,N^{2/3}-3.184\right]\qquad n_2^H=\left[1.351\,N^{2/3}-6.566\right]$$

$$n_1^S=\left[0.2423\,N^{2/3}+6.229\,N^{1/3}-6.375\right]$$



The CM (rings) and MD results (dots) for N = 187 particles confined in disk (left) or harmonic (right) potentials. The *core* (green) region with {**1,6,12,18,(24)**} particles exhibits a clear hexagonal pattern. The external *valence* shells show an almost perfect circular structure.

4. Quenched Molecular Dynamics (exact classical configurations)

Equilibrium configurations of interacting classical particles

$$m\ddot{\vec{r}}_i=-\nabla_i\Big(V_{\mathrm{ext}}+\alpha\sum_{j\neq i}1/r_j\Big)-\big(b_i\,\dot{\vec{r}}_i\big)$$

Friction quenched dynamics

- **Need to find GS (minimun energy)**
  Many simulations with different initialization
- **Lots of isomers with increasing N**
  Sometimes *hard to visit* GS configurations

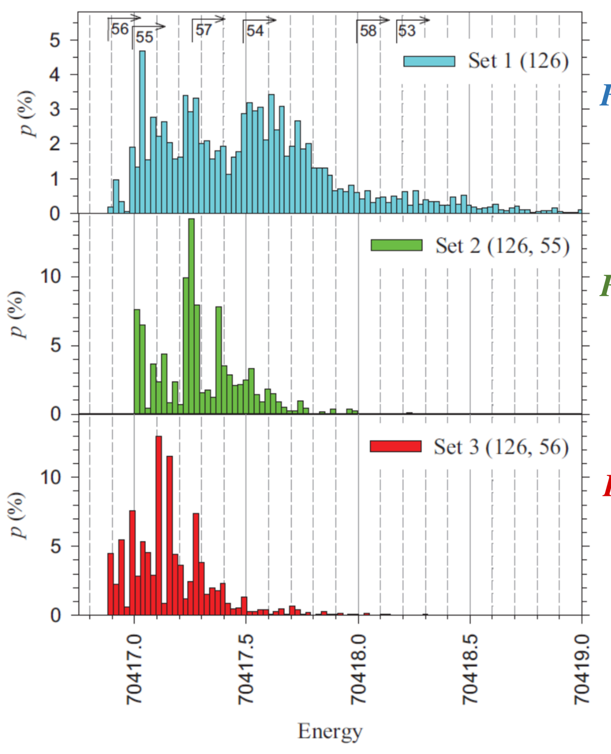
CM can help MD (or Montecarlo) with sensible starting configurations

⇩

Set 3: with $n_1,n_2=n_1^H,n_2^H(317)$
25 factor increase in visits to GS

N=317 MD histograms (Hard conf.)

CM guided start



Fix $n_1=126$ < 0.2% → GS

Fix $n_1=126,n_2=55$ *only excited*

Fix $n_1=126,n_2=56$ 4.5% → GS

5. Clustering algorithm in MD: how good is the Circular Model ?

How to define MD partitions? – Group particles in Rings

$r_1\le r_2\le\cdots\le r_N\ \to\ \delta_i=r_{i+1}-r_i$ and sort: $\delta_{i_1}\ge\delta_{i_2}\ge\cdots\ge\delta_{i_{N-1}}$

⇨ Maximize average radial separation between groups $\quad F_{\mathrm{MD}}(p)=\dfrac{r_1+\sum_{k=1}^{p-1}\delta_{i_k}}{p}$

additionally

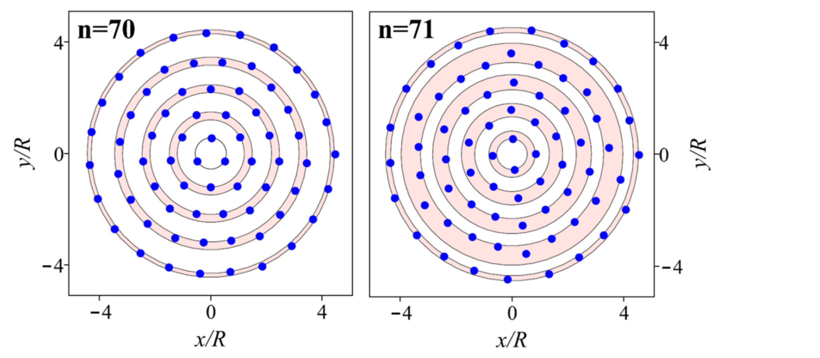
- impose $0\le p(N)-p(N-1)\le1$
- detect new particle at center $r_1\approx0$ (new shell)

With optimal p, define measure (proximity to Ring structure)

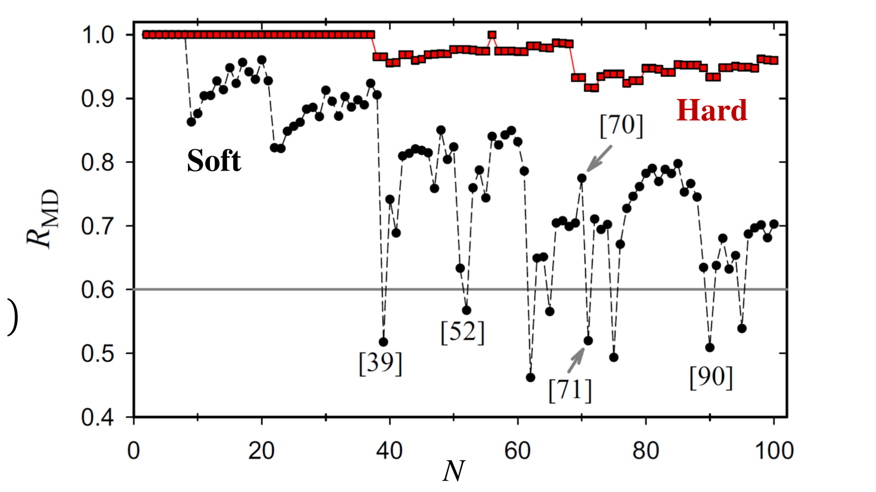
$$R_{\mathrm{MD}}(N)=\frac{p\,F_{\mathrm{MD}}(p)}{r_N}\le 1$$

Perfect rings (as in CM)

- Remarkable description for hard confinement $\left(n_1^H(N)\gg n_1^S(N)\right)$
- Not so accurate for harmonic trap, but still
- Very reasonable model of self-organization in finite 2D



Results of the clustering algorithm applied to two MD ground state configurations for harmonic confinement. The obtained MD (CM) ring structures are [23,20,15,9,3] (same) for N=70 and [21,21,15,10,4] ([23,20,15,9,4]) for N=71.



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