

***Wave function anatomy of ultracold fermions in a double well: Wigner-molecules, attractive-pairing, and entanglement***

**Benedikt B. Brandt, Constantine Yannouleas and Uzi Landman  
School of Physics, Georgia Institute of Technology**



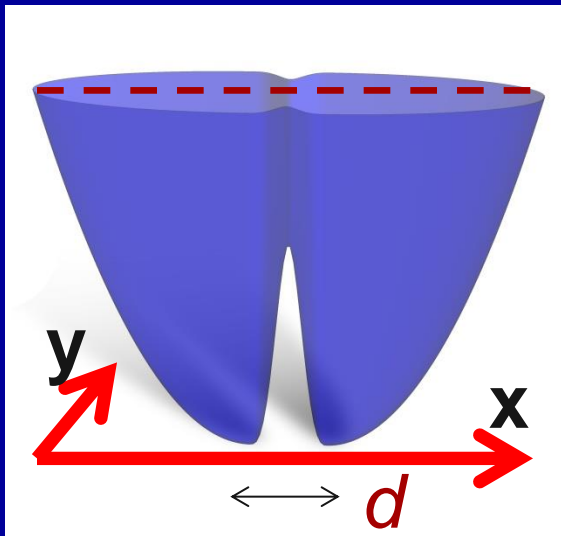
**Nano Lett. 2015, 15, 7105–7111**

APS, March 2016

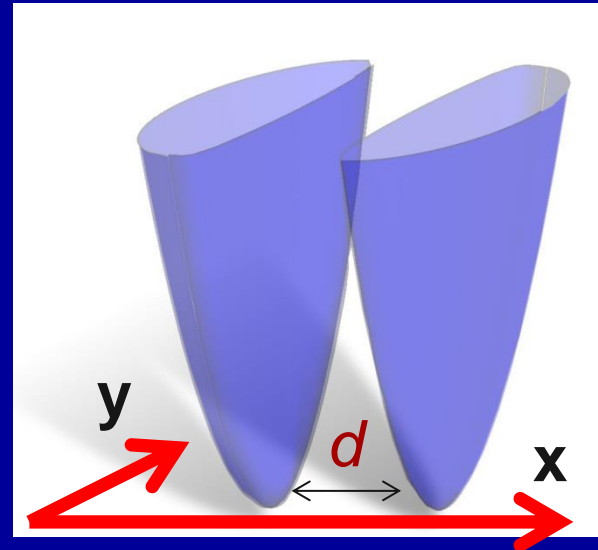
Supported by the AFOSR (FA9550-15-1-0519)

# 2 ${}^6\text{Li}$ ATOMS IN A DOUBLE OPTICAL TRAP

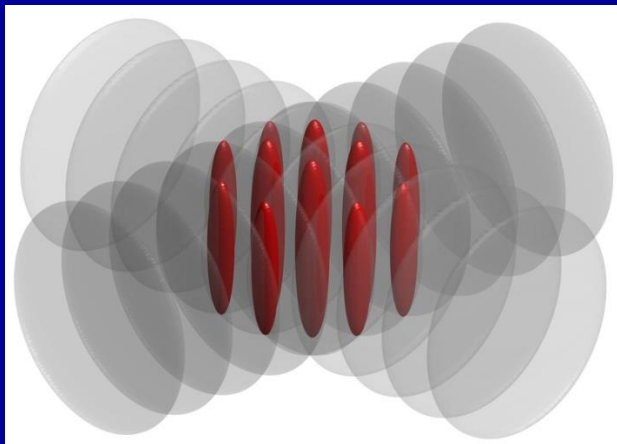
Linear arrangement (LI) Parallel arrangement (PA)



Strictly 1D



2D aspects



Experimental  
depictions of  
1D  
optical traps



# 2D Many-Body exact diagonalization/ Configuration Interaction (CI)

$$\mathcal{H}_{\text{MB}} = \sum_{i=1}^N H(i) + \sum_{i=1}^N \sum_{j>i}^N g_{2\text{D}} \delta(\mathbf{r}_i - \mathbf{r}_j)$$

$$\Phi_{N,q}^{\text{CI}}(\mathbf{r}_1, \dots, \mathbf{r}_N) = \sum_I C_I^q \Psi_I^N(\mathbf{r}_1, \dots, \mathbf{r}_N)$$

Slater determinants:

$$\Psi_I^N = \frac{1}{\sqrt{N!}} \begin{vmatrix} \chi_{j_1}(\mathbf{r}_1) & \dots & \chi_{j_N}(\mathbf{r}_1) \\ \vdots & \ddots & \vdots \\ \chi_{j_1}(\mathbf{r}_N) & \dots & \chi_{j_N}(\mathbf{r}_N) \end{vmatrix}$$

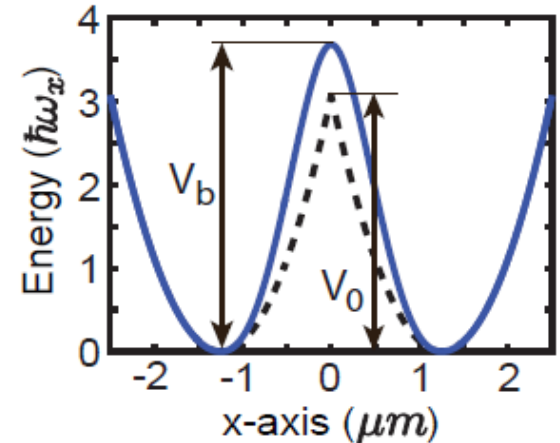
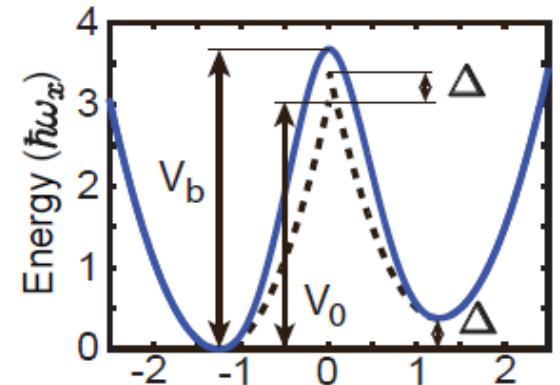
Spin orbitals:  $\chi_j(x, y) = \varphi_j(x, y) \alpha(\beta)$

$$g_{2\text{D}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\mathbf{r}_1 d\mathbf{r}_2 \varphi_i^*(\mathbf{r}_1) \varphi_j^*(\mathbf{r}_2) \delta(\mathbf{r}_1 - \mathbf{r}_2) \varphi_k(\mathbf{r}_1) \varphi_l(\mathbf{r}_2)$$

Beyond Hubbard

Single particle term

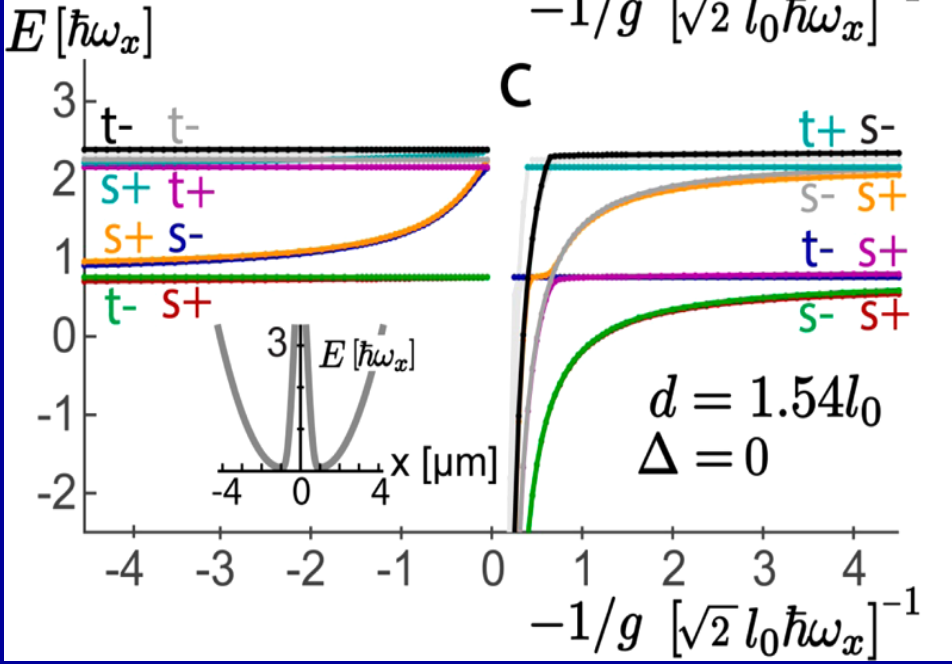
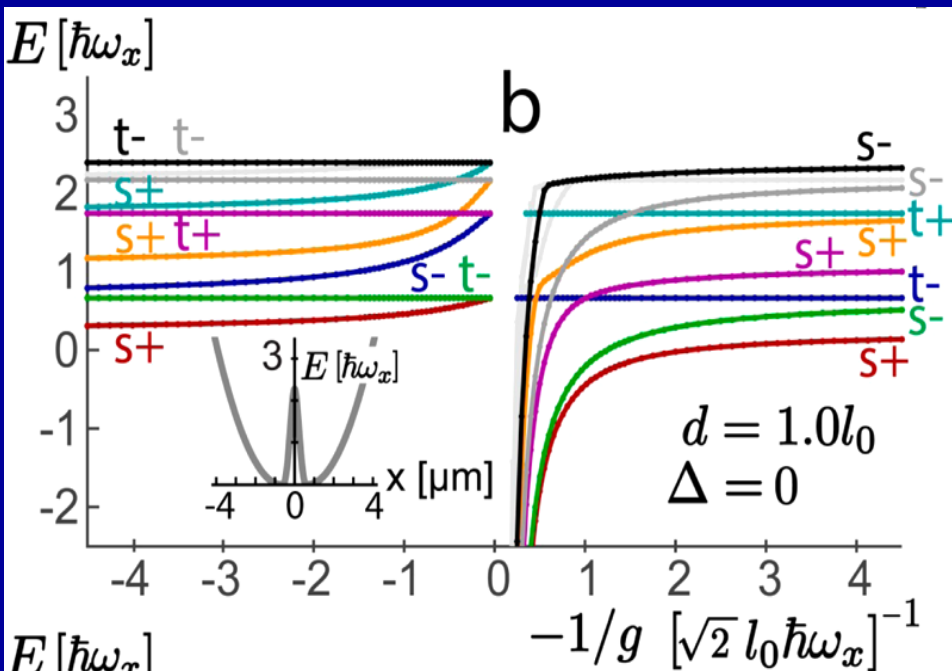
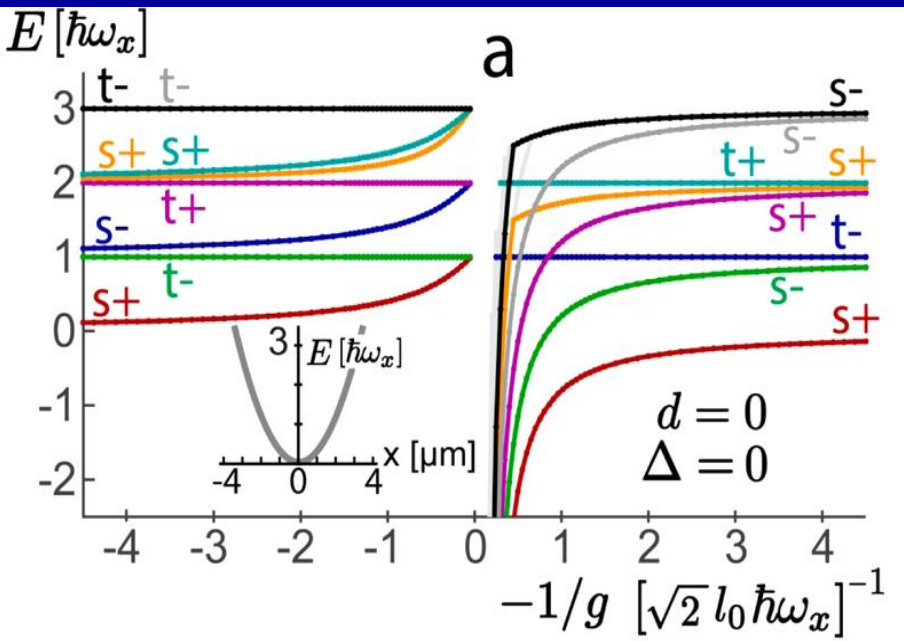
$H(i) \rightarrow \text{TCO in } x$



$H(i) \rightarrow \text{HO in } y$

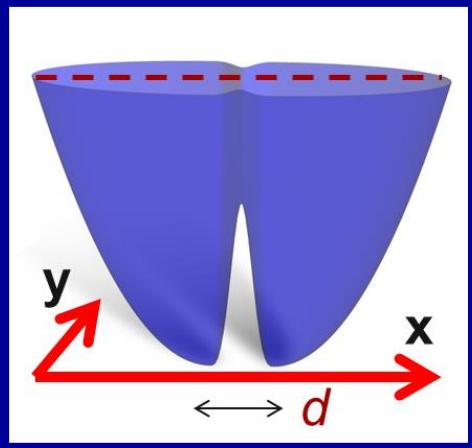
1D

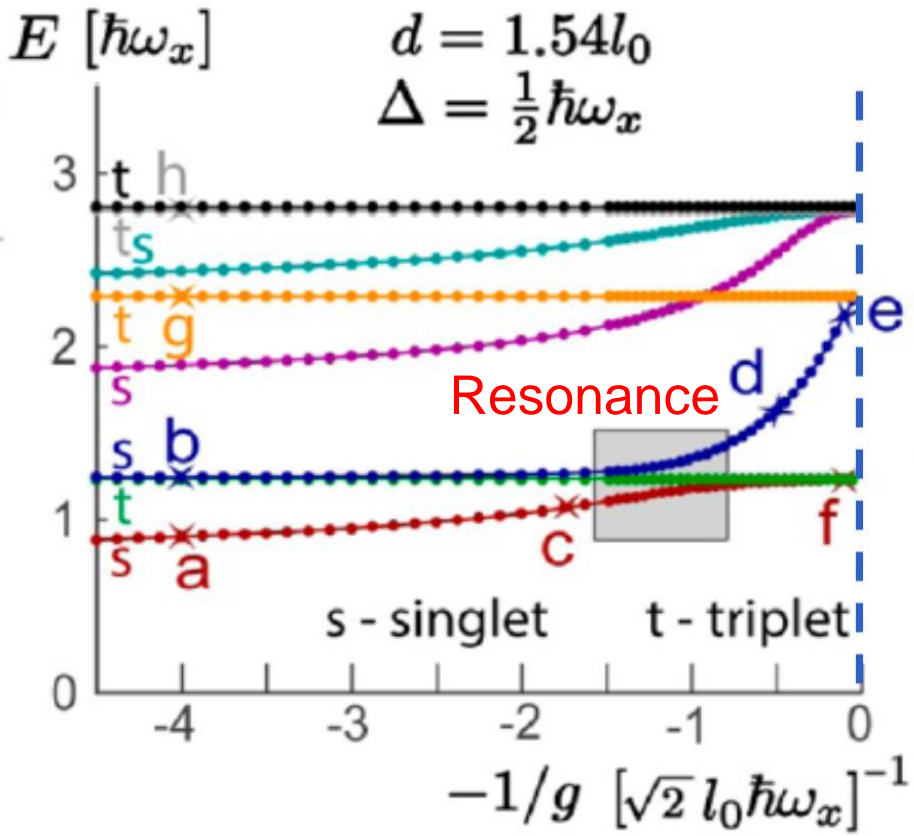
$$g = g_{2\text{D}} \int_{-\infty}^{\infty} du [W(u)]^4$$



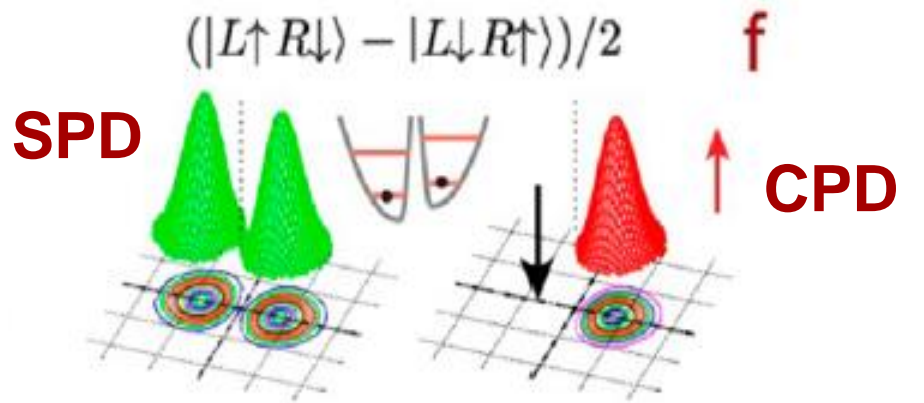
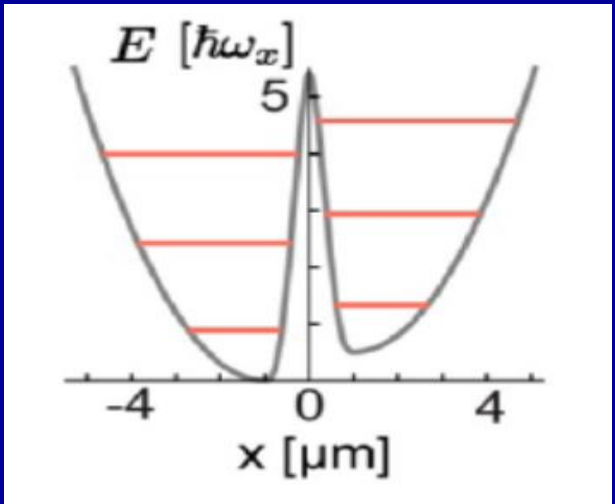
Linear arrangement (LI)

**LIN**  
**No Tilt**  
 **$\Delta=0$**

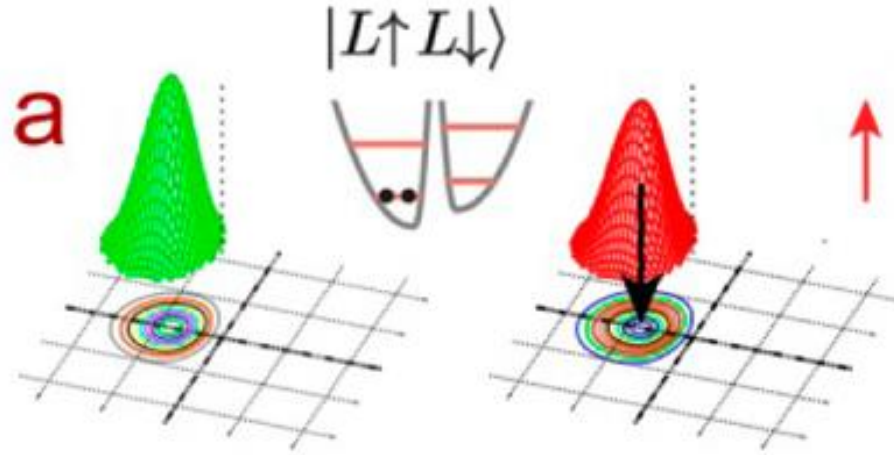
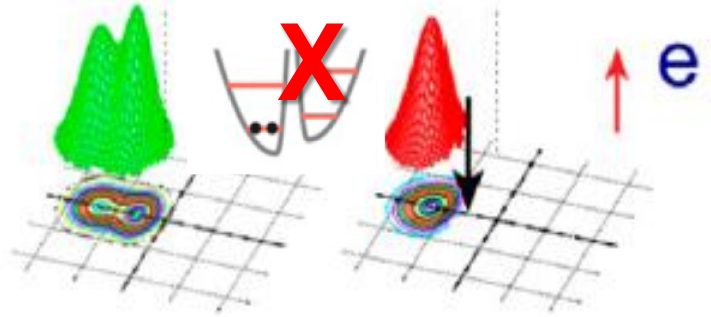




**LIN**  
**Tilt**  
 $\Delta$

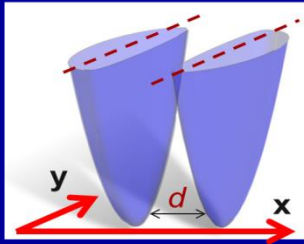


Wigner molecule  
 $|UCWM\rangle \sim (|L_l\uparrow L_r\downarrow\rangle - |L_l\downarrow L_r\uparrow\rangle)/(2\sqrt{1+s^2})$

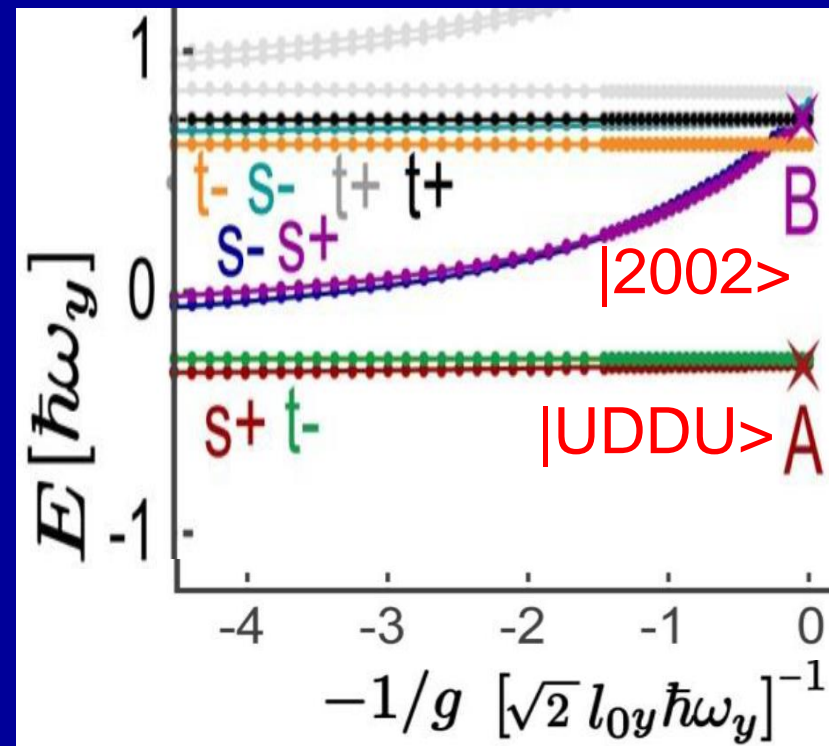
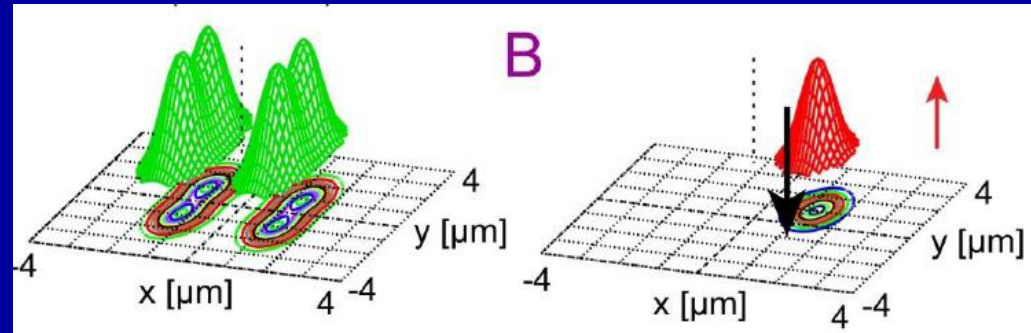


# PARALLEL

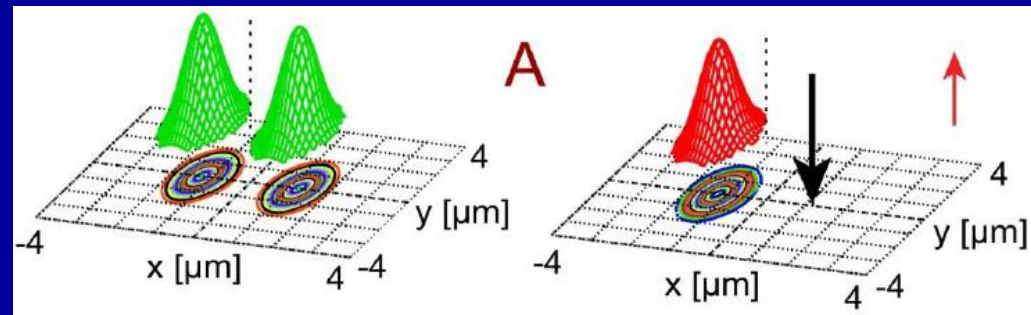
## No tilt $\Delta=0$



Ultracold Wigner molecule (UCWM)  
 $|2002\rangle$  state  $|N00N\rangle$ / Entanglement



Heitler –London/ Hydrogen molecule  
 $|UP-DN-DN-UP\rangle$  spin/ Bell state

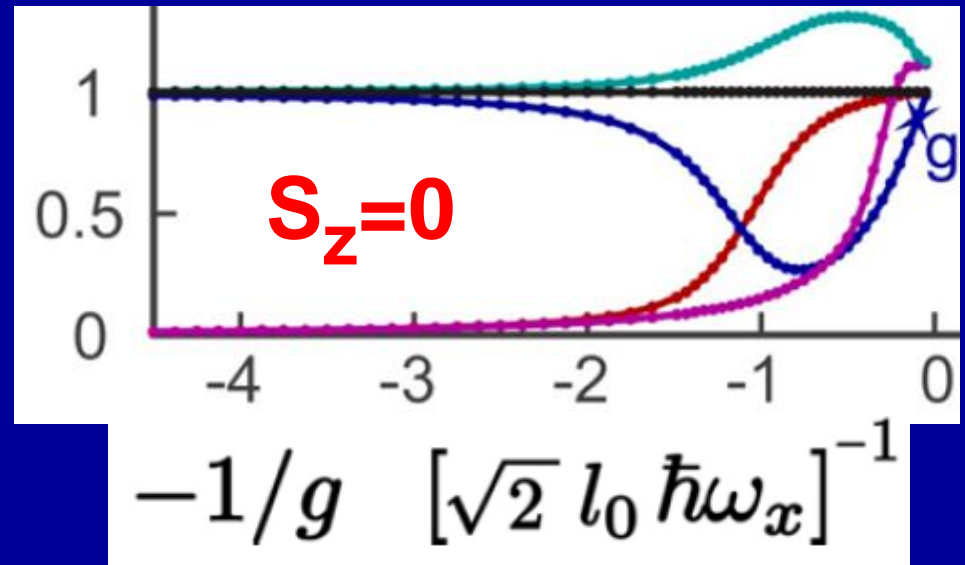
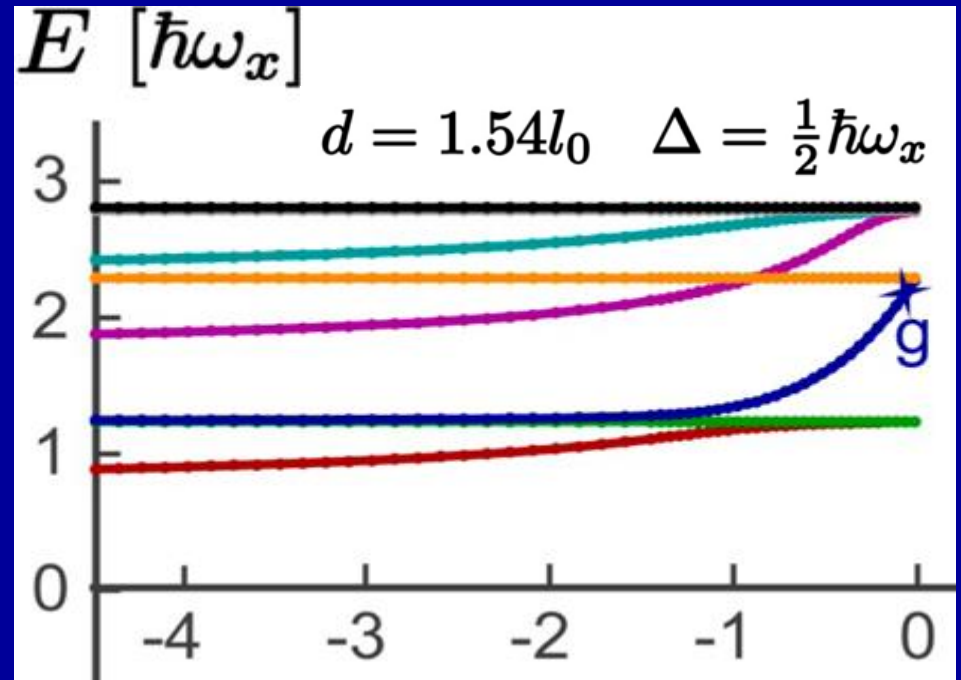
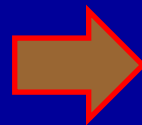


# Quantifying Entanglement

LIN Tilt  $\Delta$

$$S_{\text{vN}} = -\text{Tr}(\rho \log_2 \rho) + C$$

Von Neumann Entropy

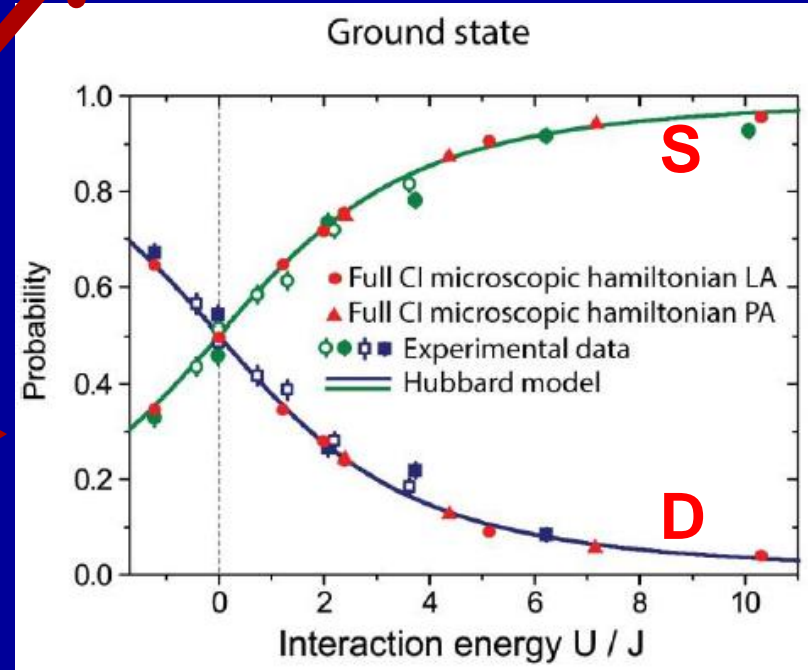
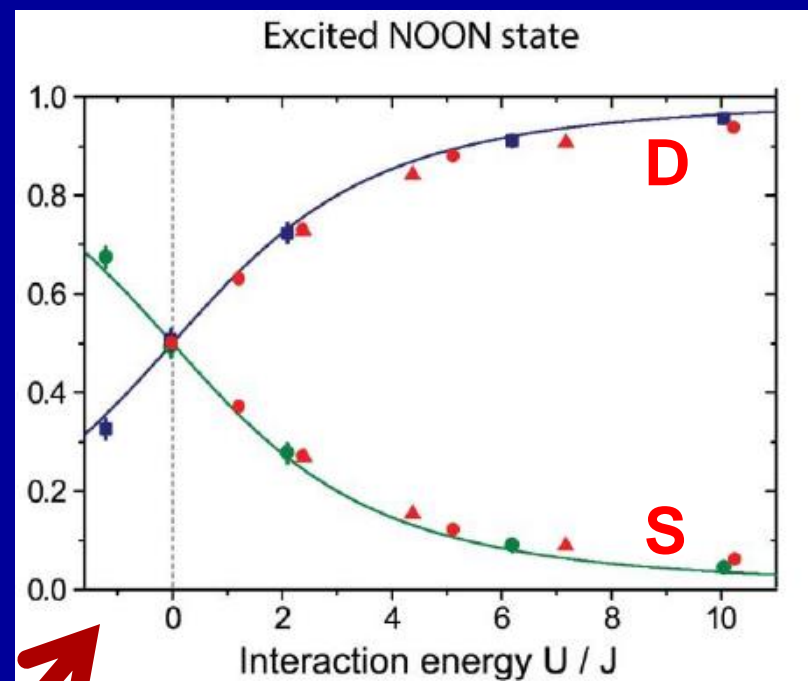
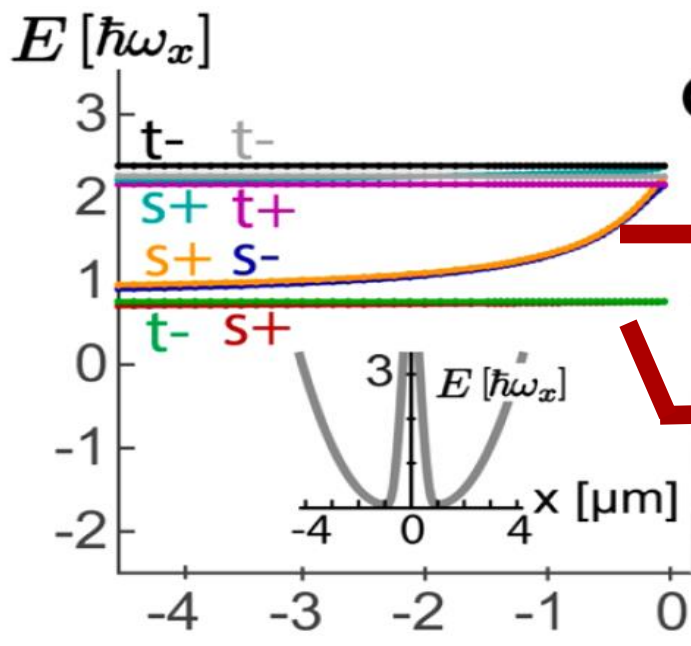


A comparison with experiment:  
 S. Murmann et al.,  
 PRL 114, 080402 (2015)

Probability for Single (S)/Double (D)  
 occupancy in either well

Hubbard limit

LIN No tilt  $\Delta=0$





# Summary

We report **exact benchmark configuration–interaction** microscopic solutions of the many-body Hamiltonian, uncovering the **full spectral evolution, wave function anatomy**, and **entanglement** properties of the interacting fermions **in the entire parameter range**, including **crossover from an Single Well to a Double Well confinement** and a controllable **energy imbalance tilt between the wells**.