

# Theory of STM Imaging of Fullerene Peapods

*C.L. Kane and E.J. Mele*



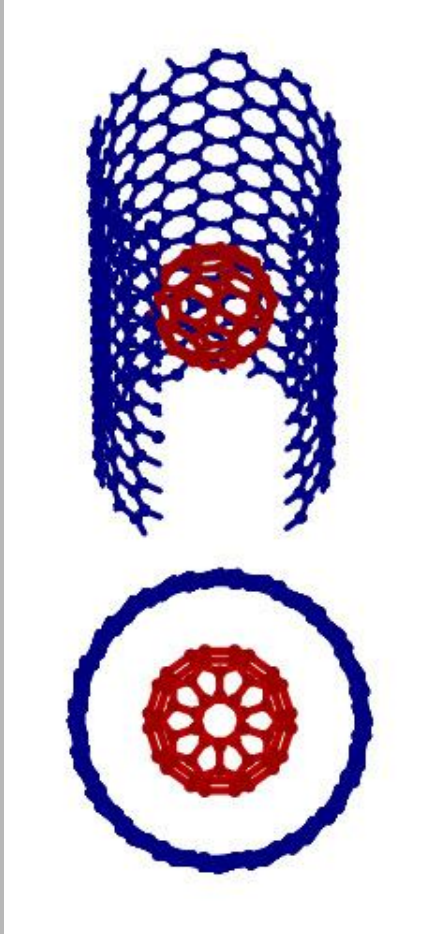
*D. Hornbaker, A. Yazdani,  
A.T. Johnson, D.E. Luzzi*



- Tube states hybridize with  $C_{60}$  orbitals
- “Strongest” mixing in  $t_{1u}$  channel
- Coupling sensitive to tube chirality and ball setting

**LRS**M the University of Pennsylvania's  
Materials Research Science  
and Engineering Center

$$H = H_{\text{tube}} + H_{\text{ball}} + H_{\text{mixing}}$$



$$H_{\text{tube}} = \hbar v_F \begin{pmatrix} 0 & q_x - i\Delta_m \\ q_x + i\Delta_m & 0 \end{pmatrix}$$

crystal momentum:  $q_x$

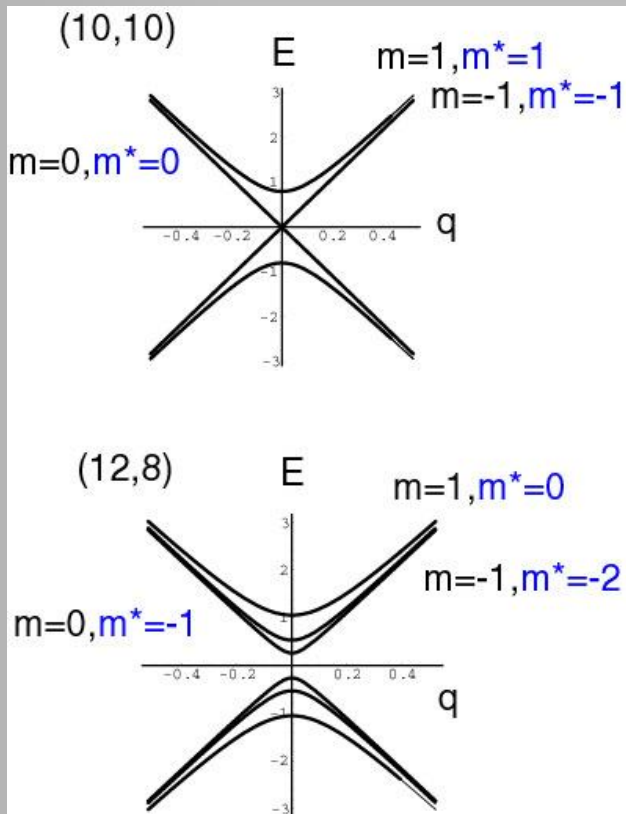
$$m^* = m - \underline{\text{int}} \left( \frac{M-N}{3} \right)$$

$$H_{\text{ball}} = \sum_{\alpha=h_u, t_{1u}, t_{1g}} E_{\alpha} \Phi_{\alpha}^{\dagger} \Phi_{\alpha}$$

$$L=5 \Rightarrow h_u + t_{1u} + \dots$$

$$L=6 \Rightarrow t_{1g} + \dots$$

Tube states are indexed by  $m^* = m - \text{int}[(M-N)/3]$



M	N	$\Delta$	$(m^*)$
10	10	-1(-1)	0(0) 1(1)
10	11	-4/3(-1)	-1/3(0) 2/3(1)
10	12	-2/3(0)	1/3(1) 4/3(2)
11	8	-1(-2)	0(-1) 1(0)
11	9	-4/3(-2)	-1/3(-1) 2/3(0)
12	8	-2/3(-2)	1/3(-1) 4/3(0)
⋮	⋮	⋮	⋮
⋮	⋮	⋮	⋮
17	0	-4/3(-7)	-1/3(-6) 2/3(-5)

**Table: m distributions for  $h_u$ ,  $t_{1u}$ ,  $t_{1g}$  orbitals  
(quantized about a fivefold symmetry axis)**

$$\left. \begin{array}{c} \alpha \\ \downarrow \\ -L \leq m \leq L \rightarrow \end{array} \right\} C_{\alpha m} = \left| \langle \Phi_\alpha | Lm \rangle \right|^2$$

$$h_u: \left\{ \begin{array}{cccccccccc} \cdot & \cdot & \cdot & 0.46 & \cdot & \cdot & \cdot & \cdot & 0.54 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 0.65 & \cdot & \cdot & \cdot & \cdot & 0.35 & \cdot \\ 0.5 & \cdot & \cdot & \cdot & \cdot & 0 & \cdot & \cdot & \cdot & \cdot & 0.5 \\ \cdot & 0.35 & \cdot & \cdot & \cdot & \cdot & 0.65 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 0.54 & \cdot & \cdot & \cdot & \cdot & 0.46 & \cdot & \cdot & \cdot \end{array} \right\} \begin{array}{l} L=5 \\ \text{“pseudotensor”} \end{array}$$

$$t_{1u}: \left\{ \begin{array}{cccccccc} \cdot & \cdot & \cdot & 0.25 & \cdot & \cdot & \cdot & 0.75 & \cdot \\ 0.11 & \cdot & \cdot & \cdot & 0.78 & \cdot & \cdot & \cdot & 0.11 \\ \cdot & 0.75 & \cdot & \cdot & \cdot & 0.25 & \cdot & \cdot & \cdot \end{array} \right\} \begin{array}{l} L=5 \\ \text{“vector”} \end{array}$$

$$t_{1g}: \left\{ \begin{array}{cccccccc} 0.14 & \cdot & \cdot & \cdot & 0.62 & \cdot & \cdot & \cdot & 0.24 & \cdot & \cdot \\ \cdot & 0.5 & \cdot & \cdot & \cdot & 0 & \cdot & \cdot & \cdot & 0.5 & \cdot \\ \cdot & \cdot & 0.24 & \cdot & \cdot & \cdot & 0.62 & \cdot & \cdot & \cdot & 0.14 \end{array} \right\} \begin{array}{l} L=6 \\ \text{“pseudovector”} \end{array}$$

## Electrons hop from the tube to the $\alpha$ -th ball orbital

$$H_{\text{mixing}}(m) = T_{i,\alpha} \psi_i^\dagger \Phi_\alpha + T_{i,\alpha}^* \Phi_\alpha^\dagger \psi_i \quad ; \quad i = a, b$$

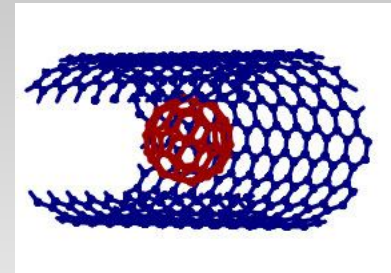
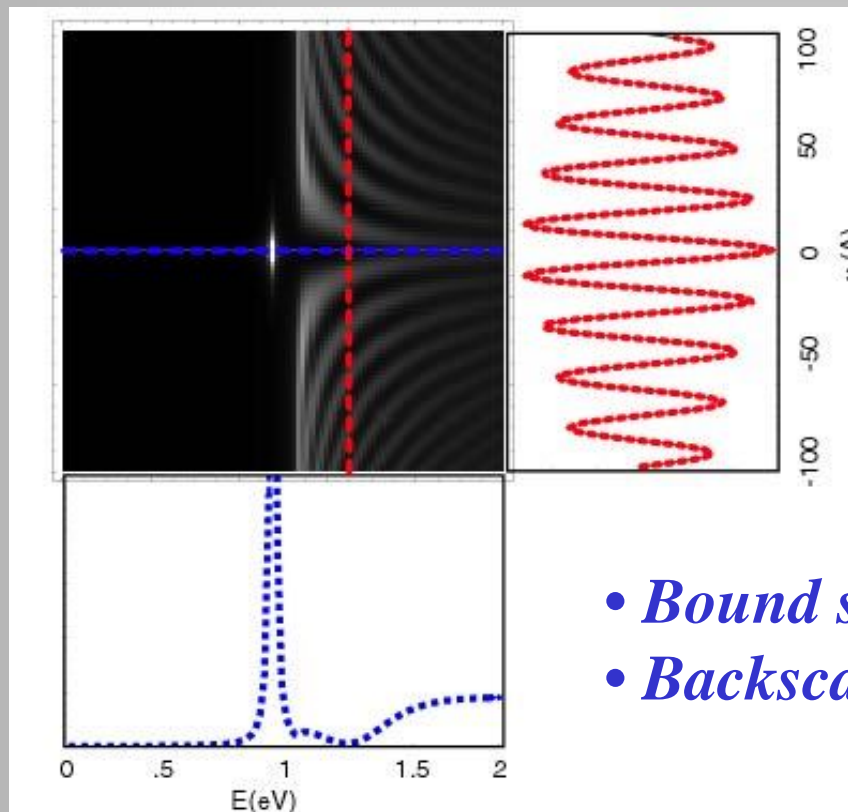
## Eliminating the buckyball degrees of freedom using...

$$\hat{\Sigma}_{ij}(x, E) = \psi_i^\dagger(x) \frac{T_{i\alpha} T_{j\alpha}^*}{E - E_\alpha} \psi_j(x) a \delta(x - na)$$

## ..gives the effective Hamiltonian as seen from the tube

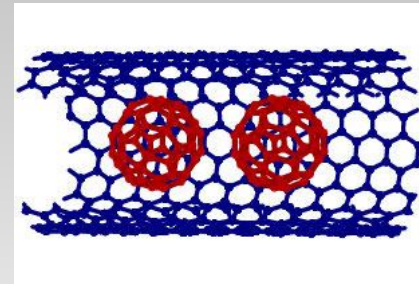
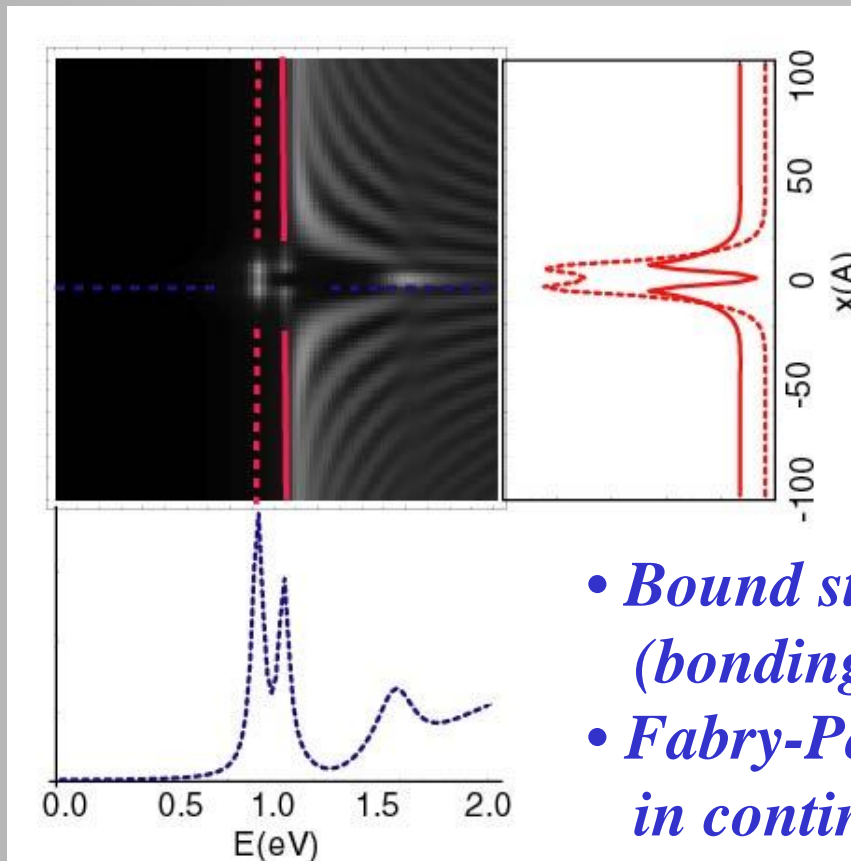
$$\tilde{H}_{\text{tube}} = \int \frac{dx}{a} \Psi^\dagger(x) (-i\hbar v_F \hat{\sigma} \cdot \vec{\nabla}) \Psi(x) + \Psi^\dagger(x) \hat{\Sigma}(x, E) \Psi(x)$$

# Spectrum for an Isolated Scatterer



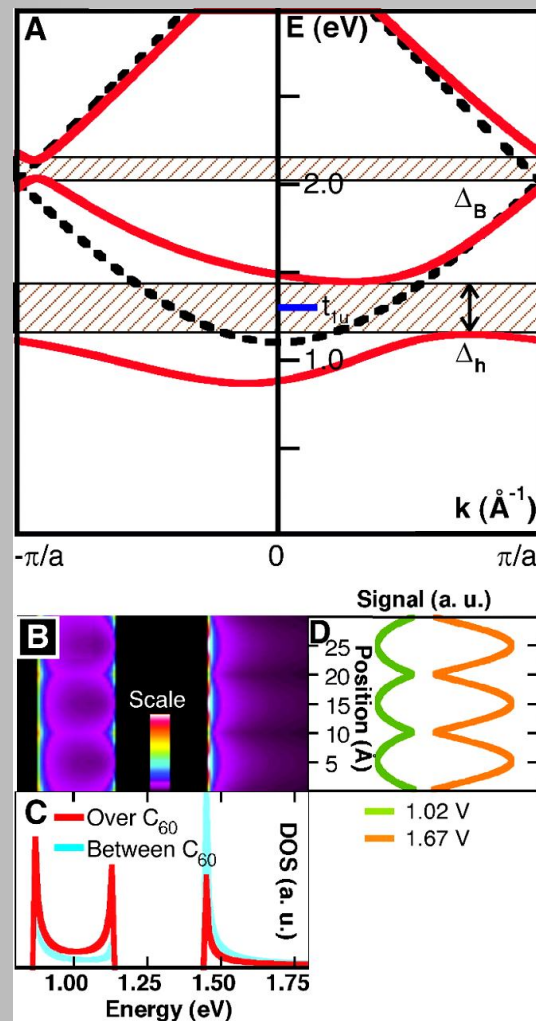
- *Bound state on tube wall*
- *Backscattering resonances*

# Spectrum for an Isolated Dimer



- *Bound states split (bonding-antibonding)*
- *Fabry-Perot resonances in continuum*

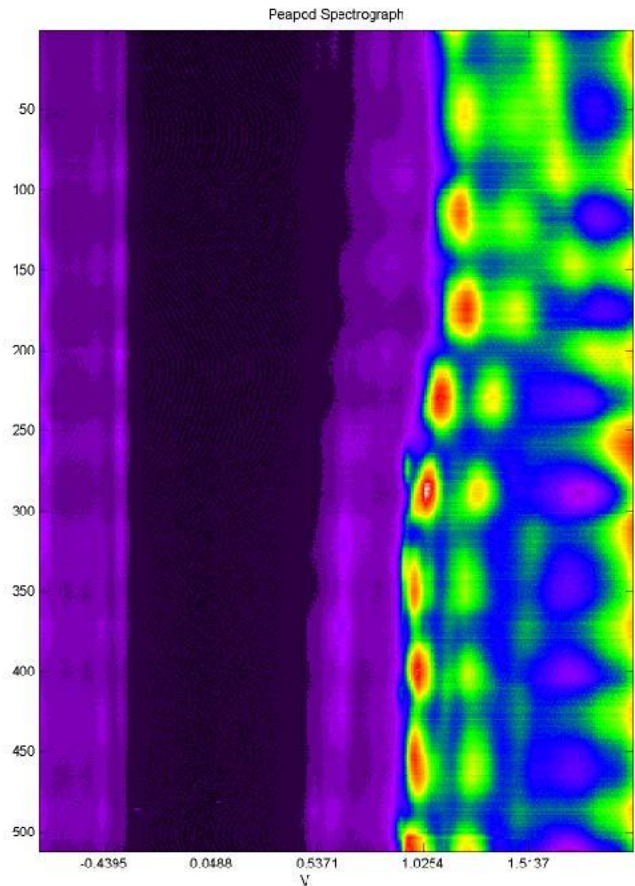
# Hybridized Bands of a Peapod Lattice



- *Tube states hybridize with  $C_{60}$  orbitals*
- *Hybridization gap*
- *Bragg gap*



# Spatially Resolved Differential Conductance



- *peapod-induced features at positive bias*
- *coupling of  $t_{1u}$  in “third subband”*
- *doublet features  $\Downarrow$  impurity band*
- *phase reversal of density modulations  $\Downarrow$  hybridization gap*



## More Questions

Why are only the  $t_{1u}$  levels active? (Coupling through  $h_u$  and  $t_{1g}$  is allowed for other nanotubes.)

What is the role of orientational disorder? (Different azimuthal settings with five fold axes along tube)

Charging effects in measured conductance spectra.