Theory of STM Imaging of Fullerene Peapods

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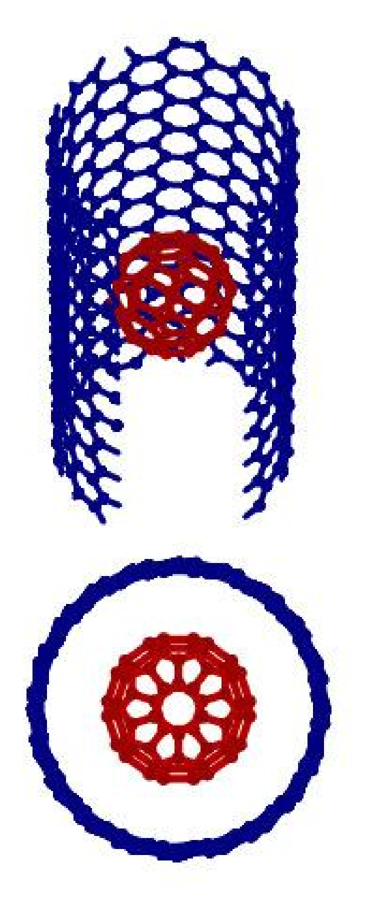
- **Tube states hybridize with C_{60} orbitals**
- **"Strongest" mixing in t_{1u} channel**
- **Coupling sensitive to tube chirality and ball setting**

LRSM the University of Pennsylvania's
Materials Research Science
and Engineering Center

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



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

crystal momentum: q_x

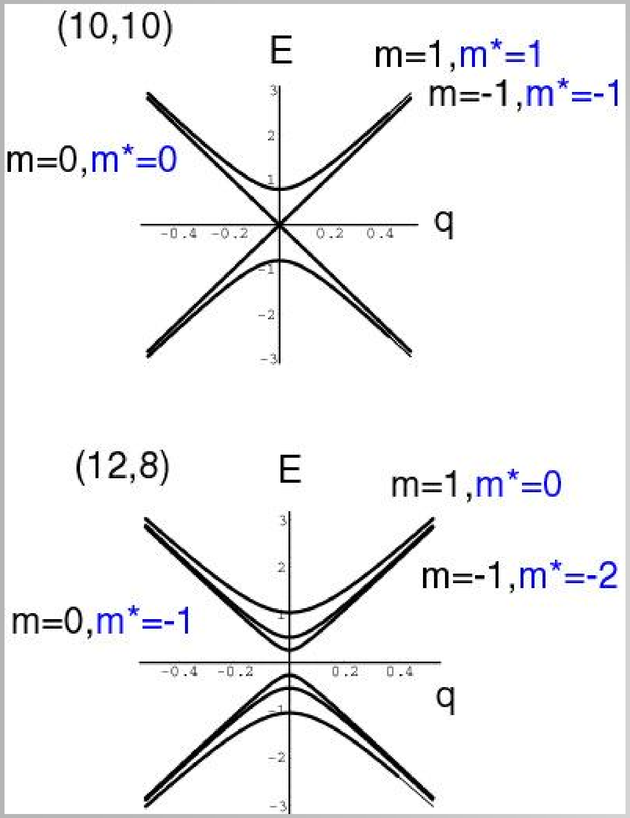
m* = m - int ((M-N)/3)

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

L=5 ⬇ $h_u + t_{1u} + \ldots$

L=6 ⬇ $t_{1g} + \ldots$

Tube states are indexed by m* = m - int[(M-N)/3]



$$\left[\begin{array}{ccccc}
M & N & & \Delta\ (m^*) & \\
10 & 10 & -1(-1) & 0(0) & 1(1) \\
10 & 11 & -4/3(-1) & -1/3(0) & 2/3(1) \\
10 & 12 & -2/3(0) & 1/3(1) & 4/3(2) \\
11 & 8 & -1(-2) & 0(-1) & 1(0) \\
11 & 9 & -4/3(-2) & -1/3(-1) & 2/3(0) \\
12 & 8 & -2/3(-2) & 1/3(-1) & 4/3(0) \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
17 & 0 & -4/3(-7) & -1/3(-6) & 2/3(-5)
\end{array}\right]$$

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

$$\left\{\begin{array}{ll} & -L \le m \le L \rightarrow \\ \alpha & \\ \downarrow & C_{\alpha m} = \left|\left\langle \Phi_\alpha \,|\, Lm \right\rangle\right|^2 \end{array}\right\}$$

$$h_u : \left\{\begin{array}{ccccccccccc} . & . & . & 0.46 & . & . & . & . & 0.54 & . & . \\ . & . & . & . & 0.65 & . & . & . & . & 0.35 & . \\ 0.5 & . & . & . & . & 0 & . & . & . & . & 0.5 \\ . & 0.35 & . & . & . & . & 0.65 & . & . & . & . \\ . & . & 0.54 & . & . & . & . & 0.46 & . & . & . \end{array}\right\}$$

L=5

“pseudotensor”

$$t_{1u} : \left\{\begin{array}{ccccccccccc} . & . & . & . & 0.25 & . & . & . & . & 0.75 & . \\ 0.11 & . & . & . & . & 0.78 & . & . & . & . & 0.11 \\ . & 0.75 & . & . & . & . & 0.25 & . & . & . & . \end{array}\right\}$$

L=5

“vector”

$$t_{1g} : \left\{\begin{array}{ccccccccccccc} 0.14 & . & . & . & . & 0.62 & . & . & . & . & 0.24 & . & . \\ . & 0.5 & . & . & . & . & 0 & . & . & . & . & 0.5 & . \\ . & . & 0.24 & . & . & . & . & 0.62 & . & . & . & . & 0.14 \end{array}\right\}$$

L=6

“pseudovector”

Electrons hop from the tube to the α-th ball orbital

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

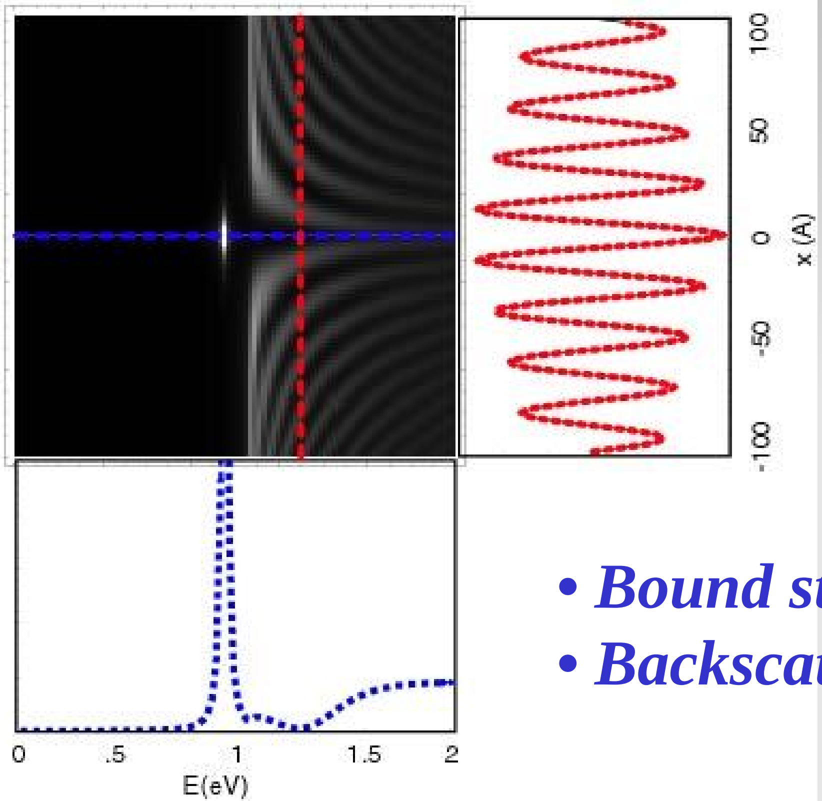
Eliminating the buckyball degrees of freedom using…

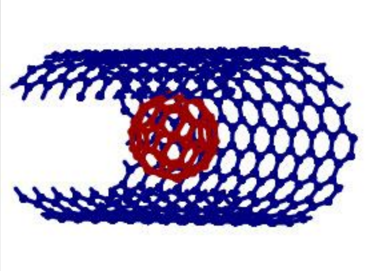
$$\hat{\Sigma}_{ij}(x,E)=\psi_i^{\dagger}(x)\frac{T_{i\alpha}T_{j\alpha}^{*}}{E-E_\alpha}\psi_j(x)a\delta\left(x-na\right)$$

..gives the effective Hamiltonian as seen from the tube

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

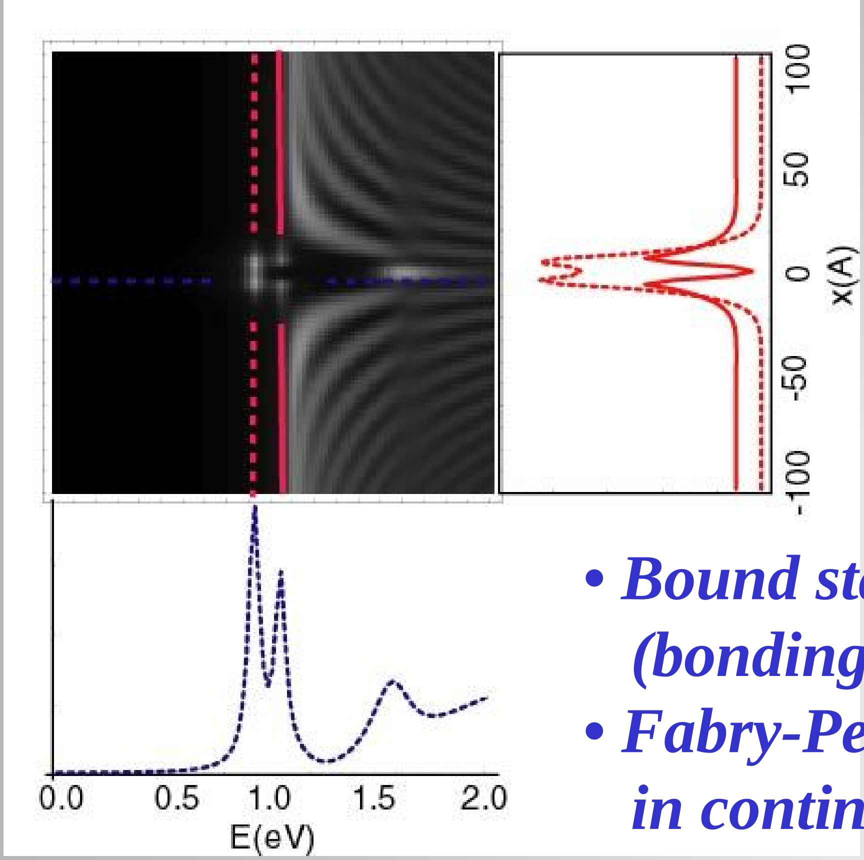
Spectrum for an Isolated Scatterer

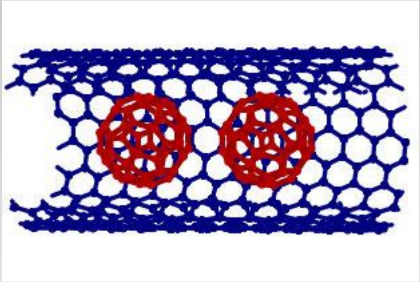




- *Bound state on tube wall*
- *Backscattering resonances*

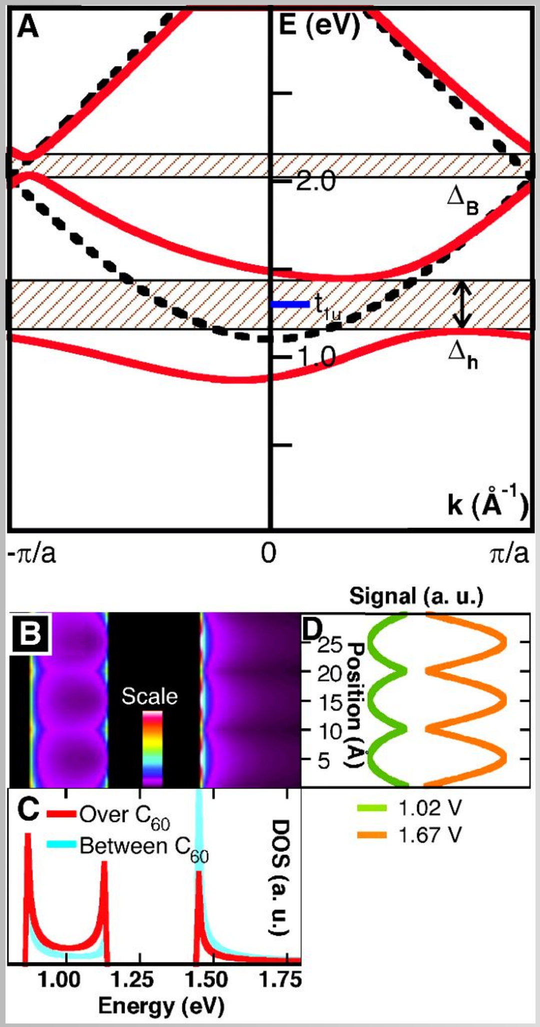
Spectrum for an Isolated Dimer





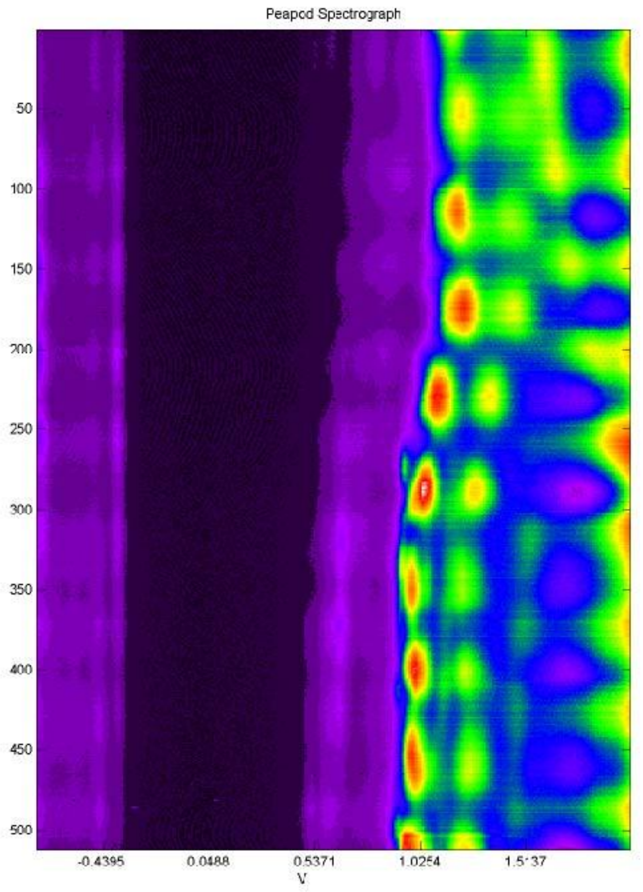
- ***Bound states split (bonding-antibonding)***
- ***Fabry-Perot resonances in continuum***

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 ⇒ impurity band*
- *phase reversal of density modulations ⇒ 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.