Tight-binding Scattering Solution for Electron Mediated Entanglement

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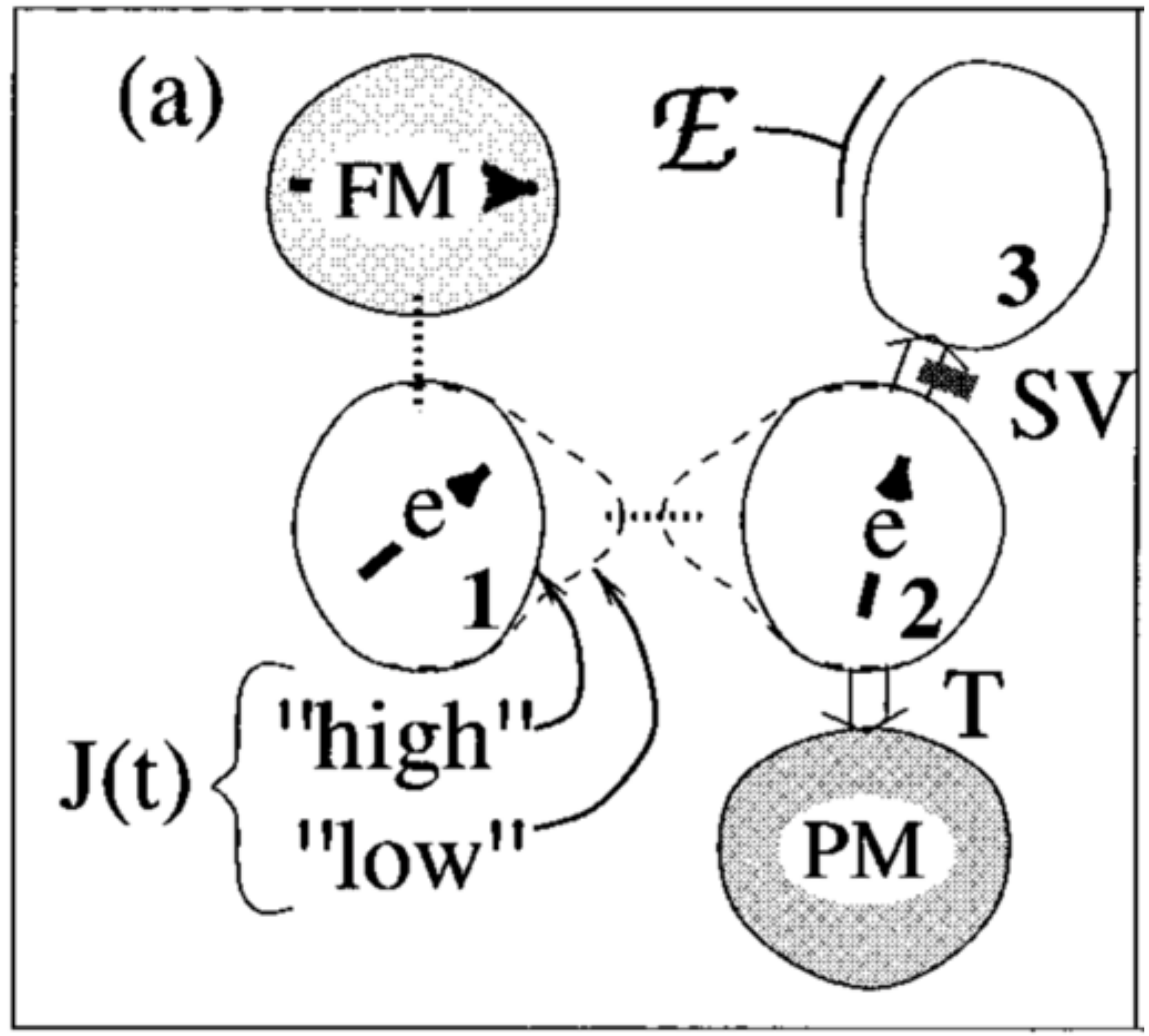
Motivation

- Controlled exchange $J(t)\mathbf{S}_1 \cdot \mathbf{S}_2$ is essential for molecular QIS (Gaita-Arino, Luis, Hill and Coronado, 2019)
- Work is ongoing to design linker complexes that enable controlled exchange (e.g. spin-crossover molecules)



Loss and DiVincenzo, 1997

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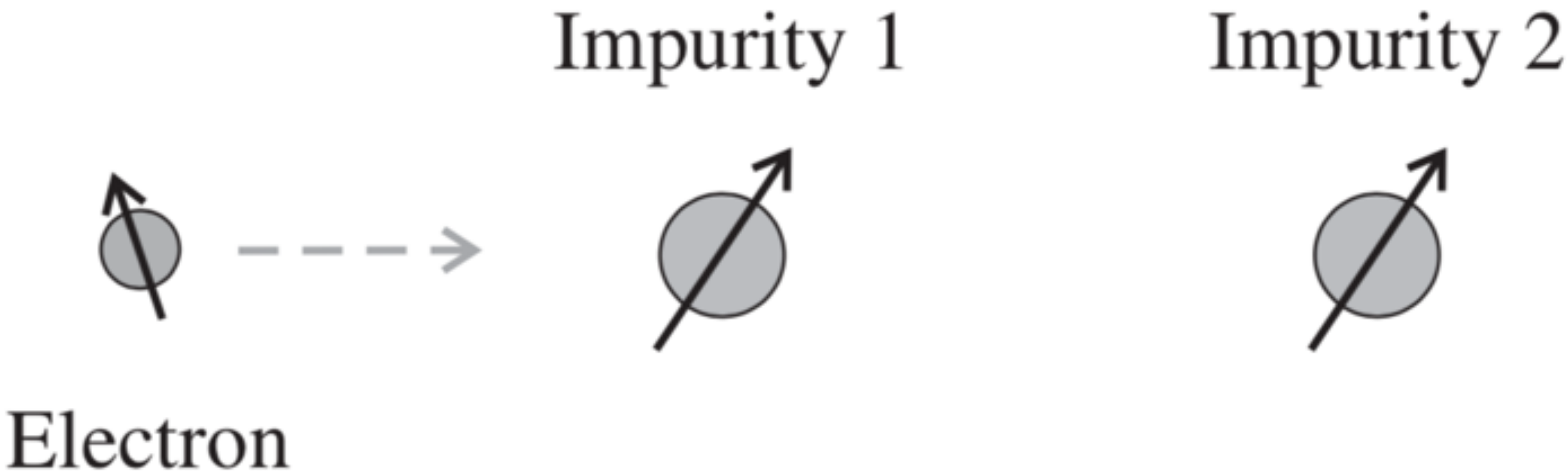
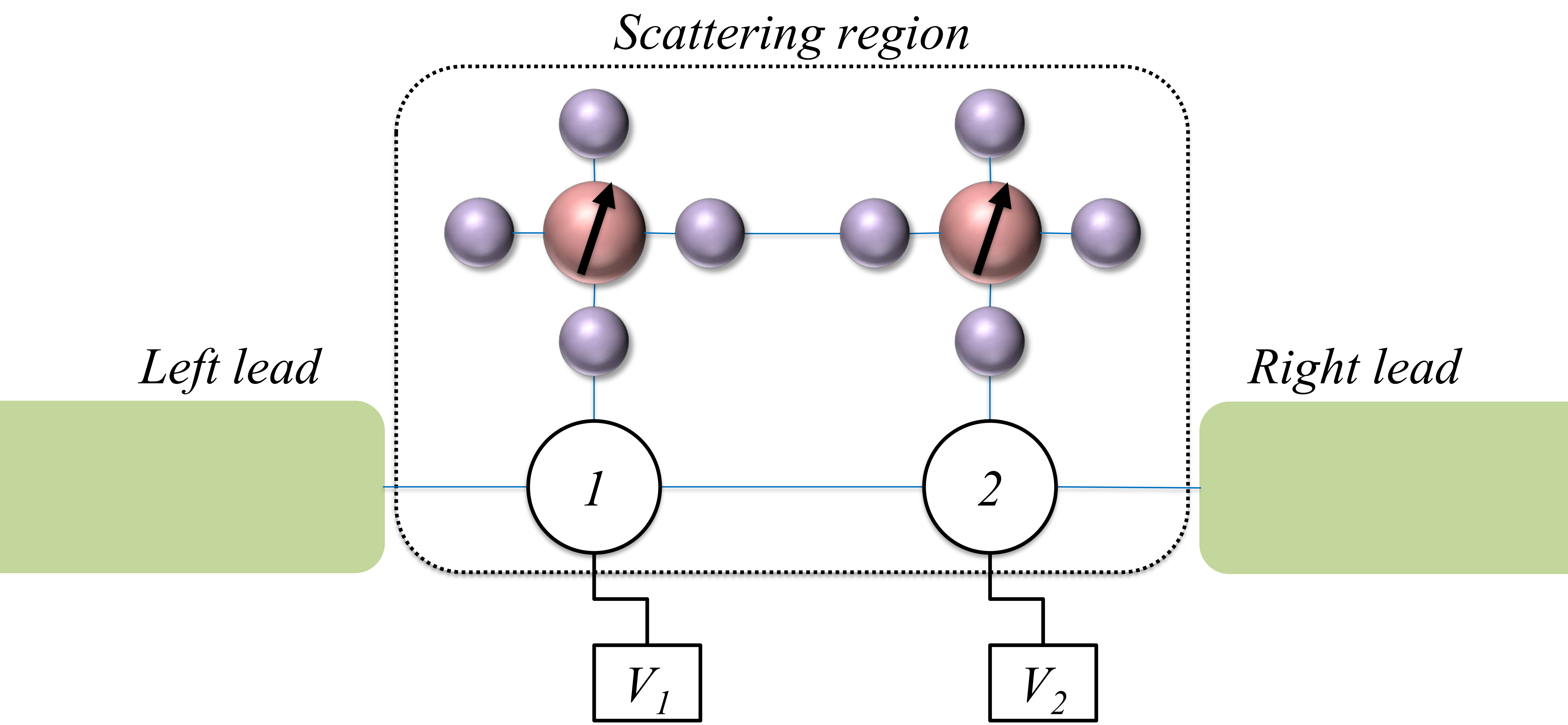
Motivation

- Solid state qubit implementations use a third particle, giving us a new knob of control

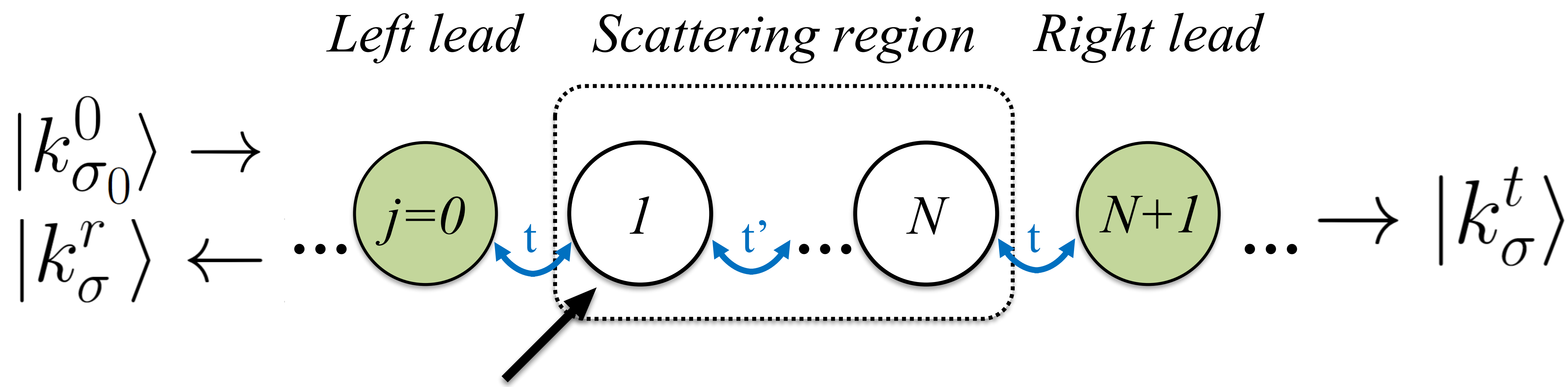


Costa et al., 2006

Setup (physical system)



Setup (model)



"Molecule"

= Spin + Magnetic Anisotropy + Exchange

$$\hat{H} = D_1(S_1^z)^2 + D_2(S_2^z)^2 + J_{12}^x S_1^x S_2^x + J_{12}^y S_1^y S_2^y + J_{12}^z S_1^z S_2^z + J\mathbf{S}_e \cdot \mathbf{S}_1 + J\mathbf{S}_e \cdot \mathbf{S}_2$$

$$\rightarrow T_\sigma = \frac{\hbar^2}{a^2} \left|G_{N+1,0,\sigma,\sigma_0}\right|^2 v_\sigma^t v_{\sigma_0}^0$$

Conserved Quantities

$$|\sigma_0\rangle \equiv |\downarrow\rangle_e |s\rangle_1 |s\rangle_2$$

- Total spin of the system in the z direction = 2s - 1/2
- Total spin magnitude of the molecules = 2s

$$|+\rangle \equiv |\uparrow\rangle_e \frac{1}{\sqrt{2}} \left(|s\rangle_1 |s-1\rangle_2 + |s-1\rangle_1 |s\rangle_2 \right)$$

- Total spin of the system in the z direction = 2s - 1/2
- Total spin magnitude of the molecules = 2s

Electron spin controls the entanglement!

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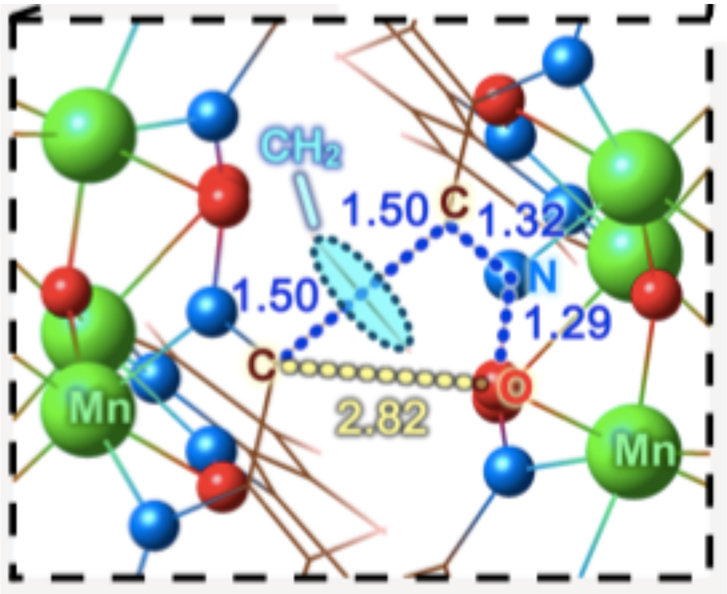
Tuning the Hamiltonian

$$\hat{H} = D_1(S_1^z)^2 + D_2(S_2^z)^2 + J_{12}^x S_1^x S_2^x + J_{12}^y S_1^y S_2^y + J_{12}^z S_1^z S_2^z + J\mathbf{S}_e \cdot \mathbf{S}_1 + J\mathbf{S}_e \cdot \mathbf{S}_2$$

- Heisenberg exchange coupling isotropic in the *xy*-plane
- Inversion symmetry ($D_1 = D_2$)



$D_1 = D_2 = -0.22\ \mathrm{cm}^{-1}$

$J_{12}^x = J_{12}^y = J_{12}^z = 0.025\ \mathrm{cm}^{-1}$

Yu, Christou and Cheng, 2020

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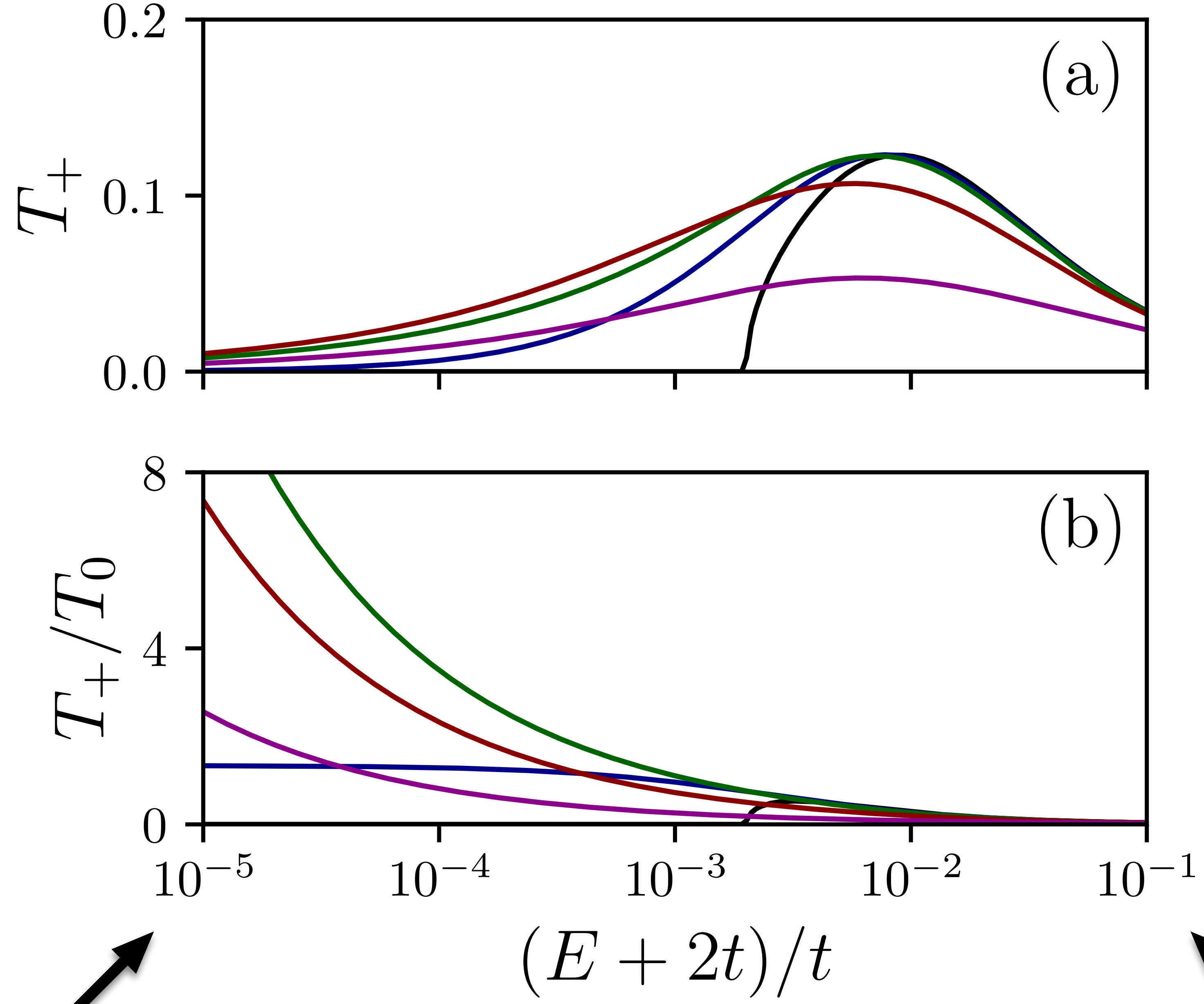
Results



v ~ 10^3 m/s

v ~ 10^5 m/s

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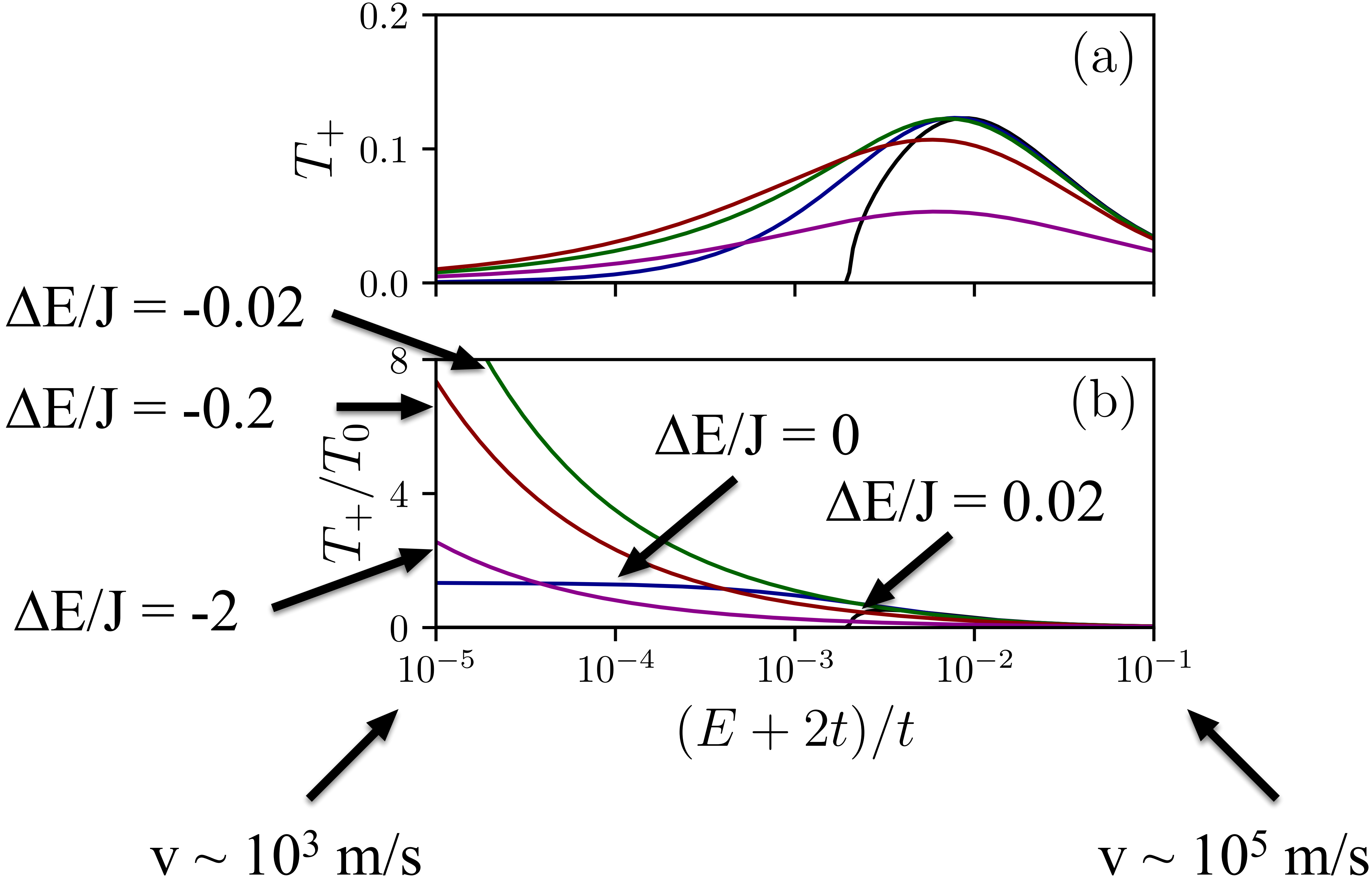
$$\Delta E = -(2s-1)(D_1+D_2)/2 - s(J_{12}^z - J_{12}^x)$$



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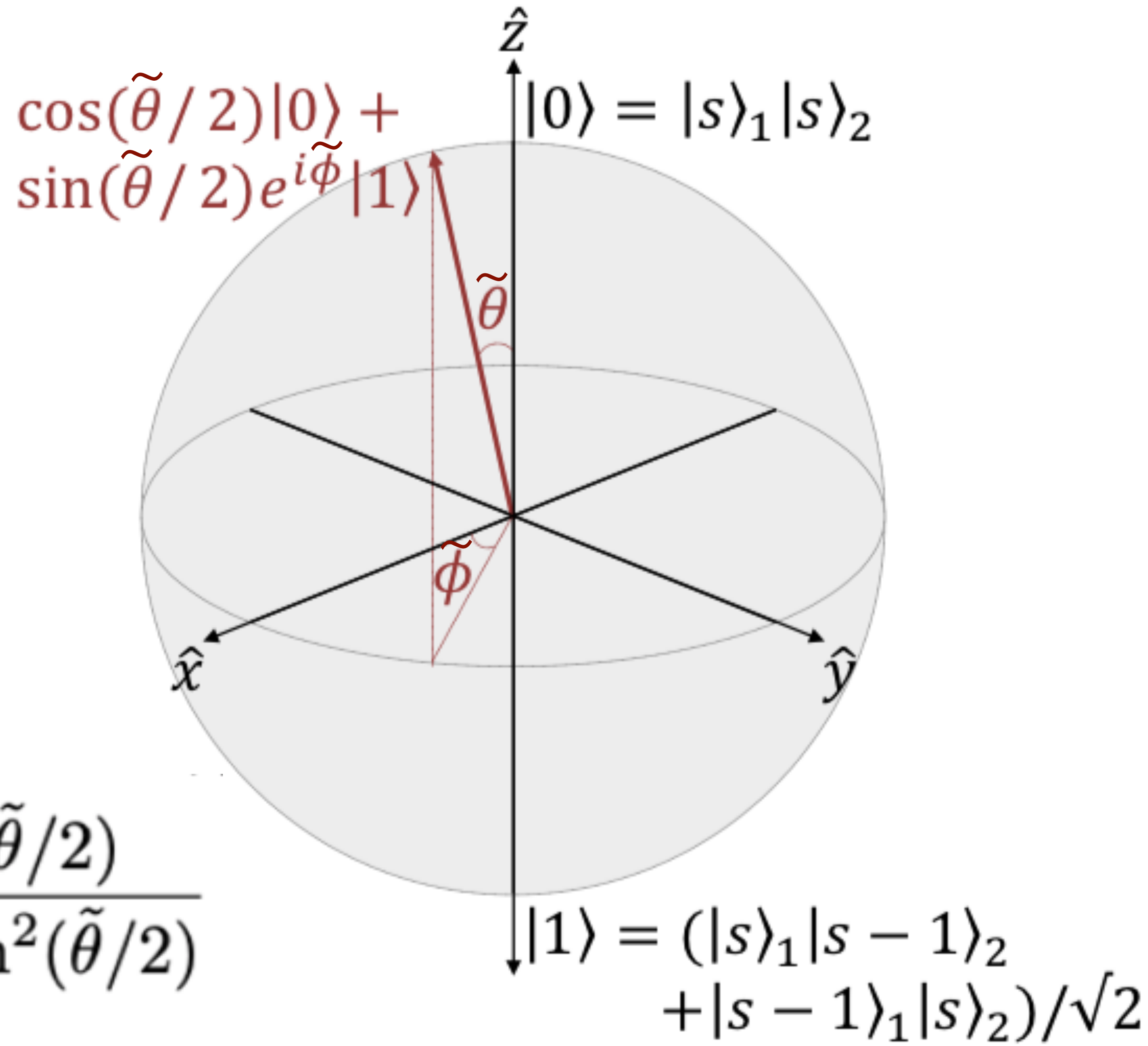
Results

Measure the electron spin observable $\mathbf{S}_e \cdot (\theta, \phi)$

$$\tan(\tilde{\theta}/2) \equiv \sqrt{\frac{T_+}{T_0}} \tan(\theta/2)\,,$$
$$\tilde{\phi} \equiv \phi + \phi_1 + \pi\,,$$



Probability of success

$$= \frac{T_+/T_0}{1 + T_+/T_0} \frac{1 + \tan^2(\tilde{\theta}/2)}{T_+/T_0 + \tan^2(\tilde{\theta}/2)}$$

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Conclusions

- Measurement of the mediating electron spin in the z direction can be used to probabilistically select a Bloch state
- Desirable molecular properties:
  - Inversion symmetry
  - Isotropic molecule-molecule exchange
  - Small negative energy splitting ΔE
- Unresolved:
  - Molecule-electron exchange

Thank You!

Funding provided by the Department of Energy,
Center for Molecular Magnetic Quantum Materials

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