Quantum Computing with Polar Molecules

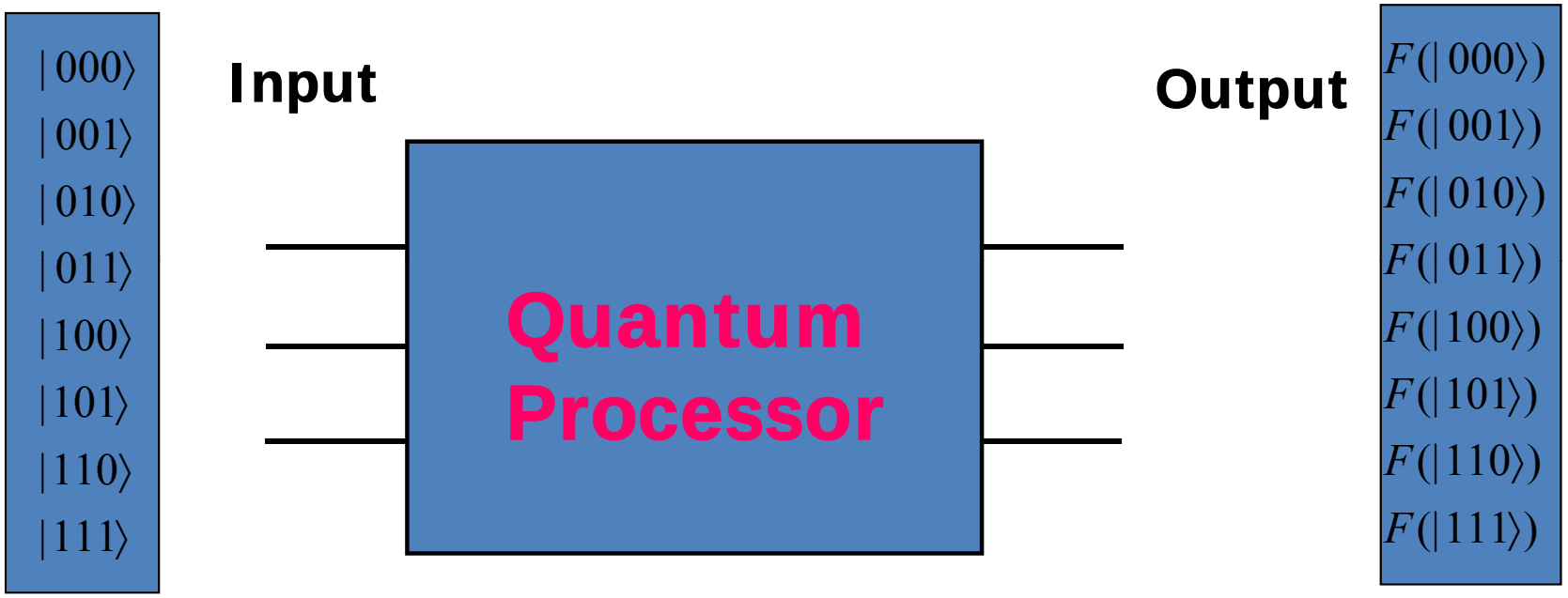
Sabre Kais

Department of Chemistry and Physics
Purdue University and QEERI, Qatar

Talk overview

- Introduction
- Polar molecules in optical lattice
- Entanglement in optical traps
- Alignment-mediated entanglement
- Dynamics of entanglement
- Quantum gates
- Applications

Quantum Computation



Preparing state

$$|\Psi_{in}\rangle$$

Processing state

$$|\Psi_{out}\rangle = U|\Psi_{in}\rangle$$

Detecting state

$$|\Psi_{out}\rangle$$

DeVincenzo Criteria (2001)

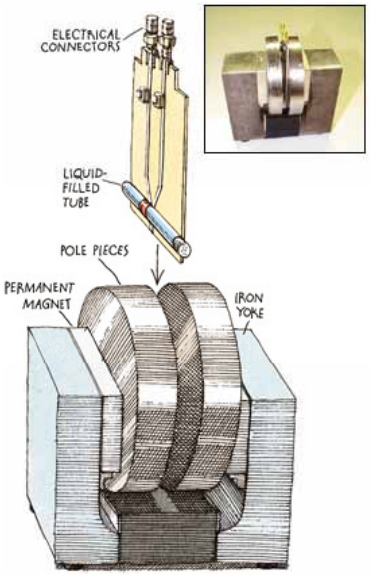
- A scalable physical system with well characterized qubits
- The ability to initialize the state of the qubits
- Long decoherence time relative to the gate operation time
- Universal set of quantum gates
- Qubit-specific measurement capability

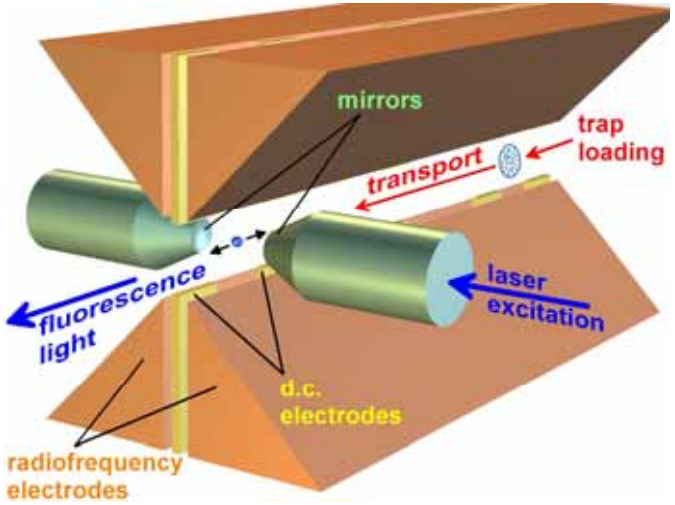
Prospects for Quantum Computing
David P. DiVincenzo
IBM TJ Watson Research Center, USA

Possible Systems

Quantum two-level systems:

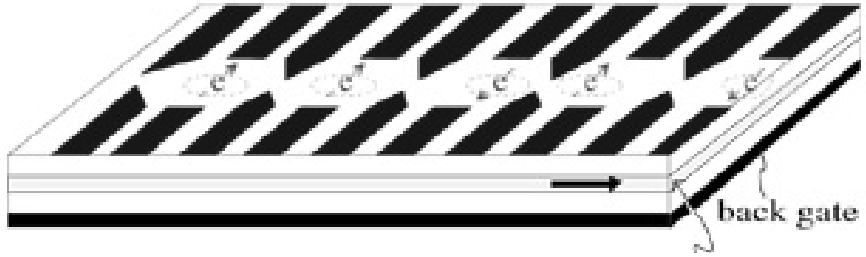
- **Electron Spin $|\uparrow\rangle, |\downarrow\rangle$**
- **Nuclear Spin $|+\rangle, |-\rangle$**
- **Polarized Photon $|L\rangle, |R\rangle$**
- **Trapped Ion $|L_0\rangle$, $|L_1\rangle$**
- **Quantum Dot $|g\rangle, |e\rangle$**





Quantum–dot array proposal:

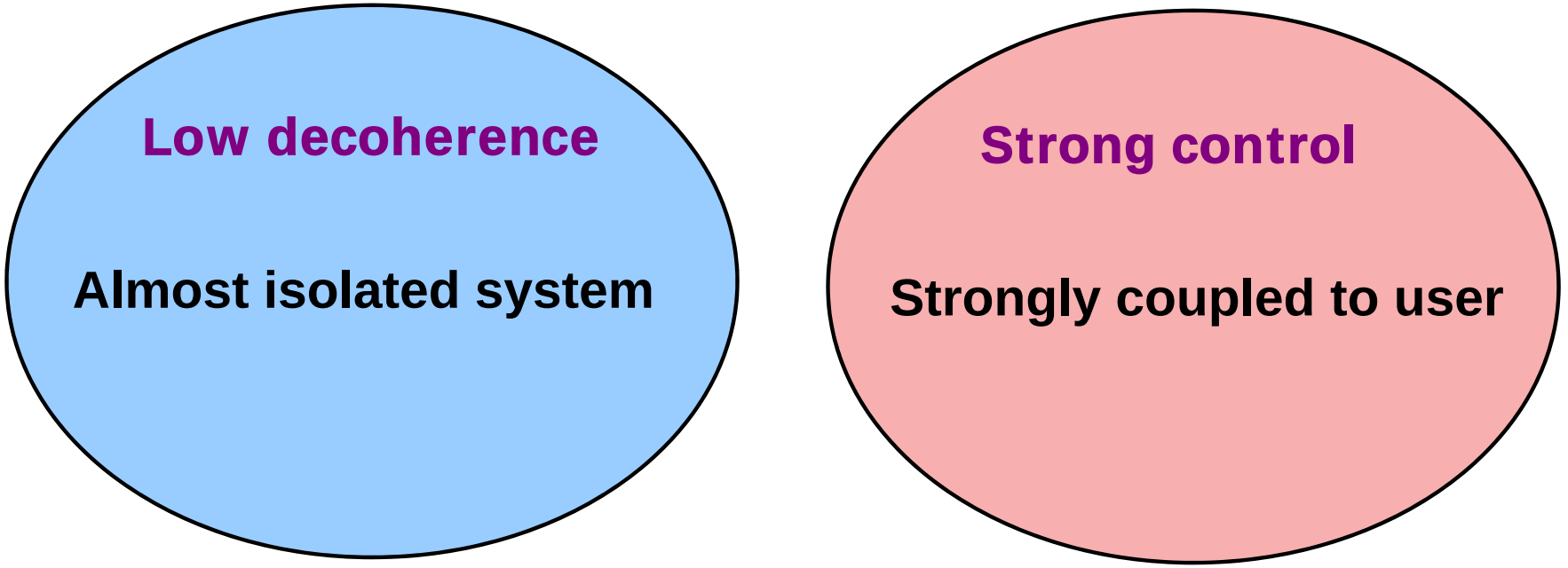
Loss & DiVincenzo, Phys. Rev. A 57, 120 (1998).



System	τ_Q	τ_{op}	$n_{op}=\lambda^{-1}$
Nuclear Spin	$10^2 - 10^8$	$10^{-3} - 10^{-6}$	$10^5 - 10^{14}$
Electron spin	10^{-3}	10^{-7}	10^4
Ion Trap (In^+)	10^{-1}	10^{-14}	10^{13}
Electron – Au	10^{-8}	10^{-14}	10^6
Electron – GaAs	10^{-10}	10^{-13}	10^3
Quantum dot	10^{-6}	10^{-9}	10^3
Optical cavity	10^{-5}	10^{-14}	10^9
Microwave cavity	10^0	10^{-4}	10^4

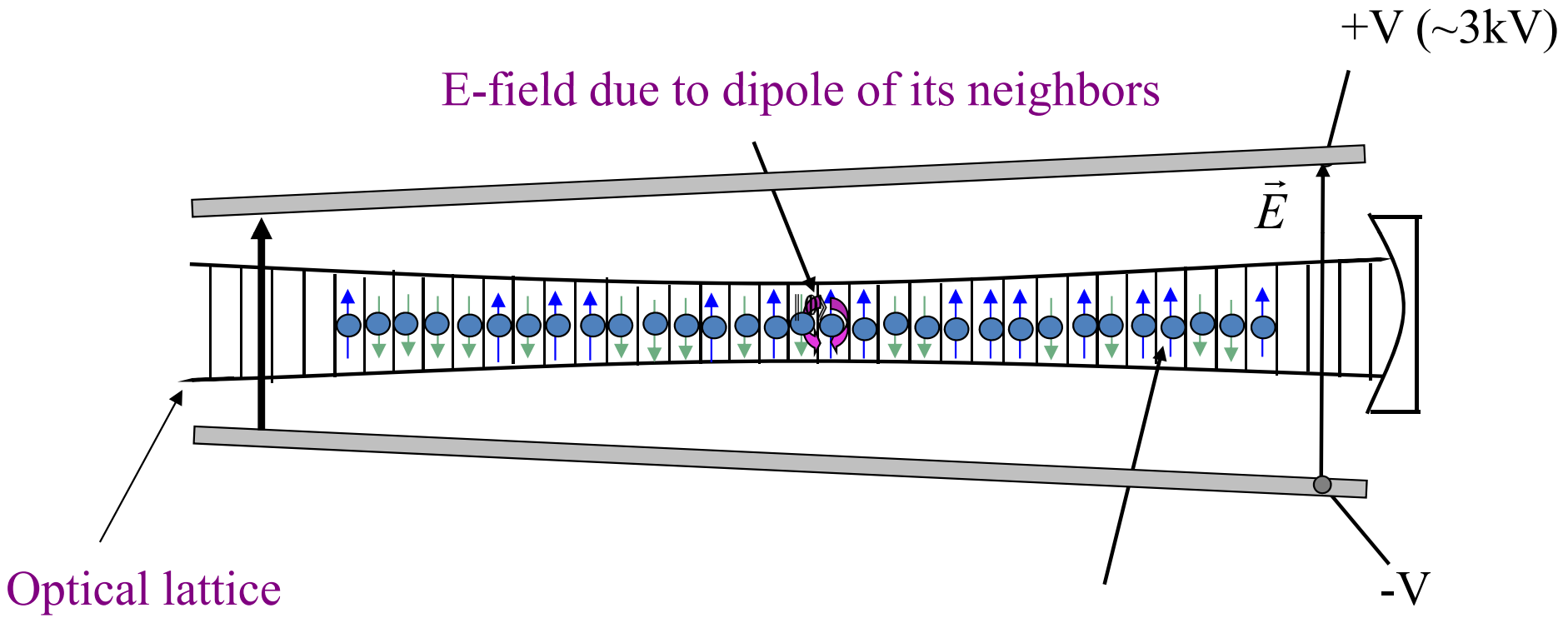
Crude estimates for decoherence times τ_Q (seconds), operation times τ_{op} (seconds), and maximum number of operations $n_{op}= \lambda^{-1}=\tau_Q/\tau_{op}$ for various candidate physical realizations of interacting systems of quantum bits.

What we need for Quantum Computation



Challange: to gain strong, precise control over quantum systems that maintain their quantum nature.

Quantum Computation with Cold Polar Molecules in an Optical Lattice



D. DeMille, PRL 88, 067901 (2002))

Features of the Proposed Approach

- Long decoherence time ~ 1 s or longer.
- Easy to scale up the number of quantum gates.
- Easy to address individual qubit due to introduced E-field gradient.
- Involved challenging technologies but achievable

http://qist.lanl.gov **the quantum computation roadmap**

Entanglement

Trapped Molecules Proposal for QC

Arrays of trapped ultracold polar molecules. Spin-less (S=0) polar molecules in their electronic-vibrational ground-state, with zero-projection (M=0) of the total angular momentum on the internuclear axis.

Qubits correspond to dipole moments up or down relative to the applied E-field.

A strong external field with appreciable gradient is imposed in order to prevent quenching of the dipole moments by rotation and to distinguish among the qubit sites.

Molecular dipoles undergo pendular oscillations, which markedly affect the qubit states and the dipole– dipole interaction.

Objectives

- Evaluate entanglement of the pendular qubit states for two linear dipoles, characterized by pairwise concurrence, as a function of:

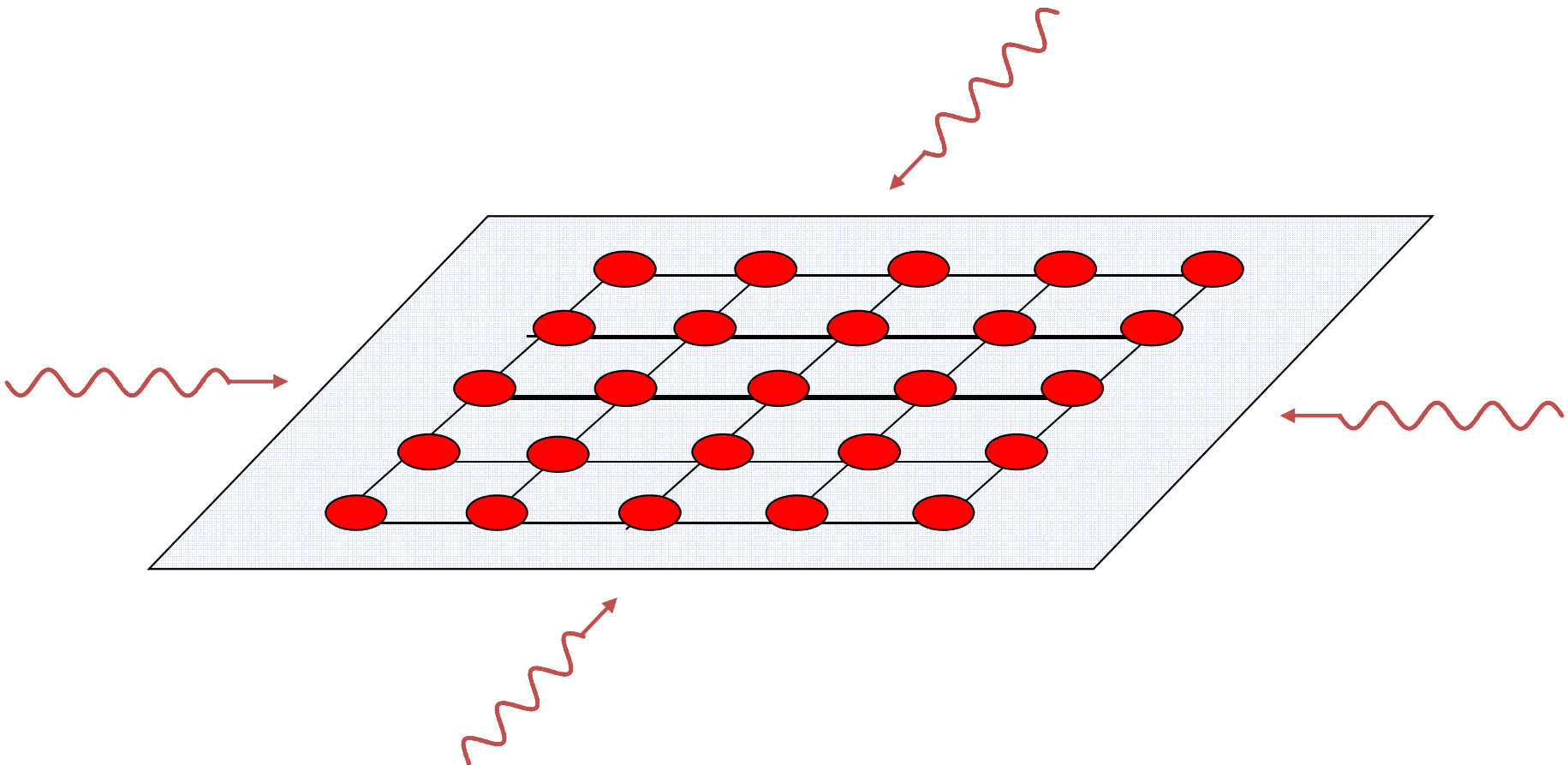
  (A) Molecular dipole moment rotational constant
  (B) Strengths of the external field
  (C) Dipole–dipole coupling
  (D) Temperature

  Extend the calculations to N-dipoles

- Evaluate the parameters needed for quantum gates
- Examine dynamics and decoherence of qubits

Optical Lattice

An **optical lattice** is formed by the interference of counter-propagating laser beams, creating a spatially periodic polarization pattern.

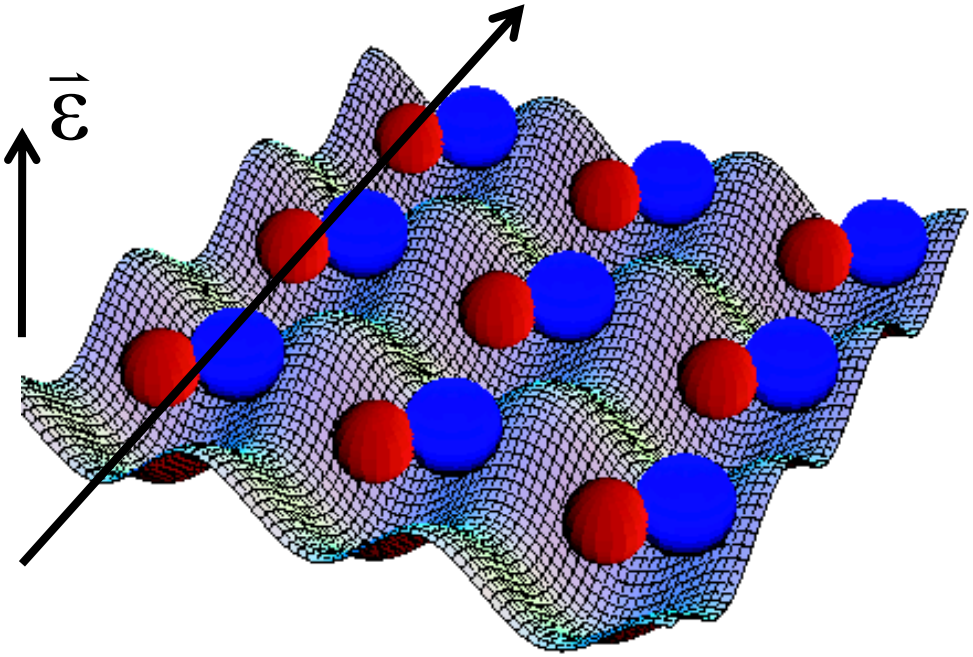


Hamiltonian for a Single Molecule

$$\hat{H} = \frac{P^2}{2m} + V_{trap}(\vec{r}) + BJ^2 - \vec{\mu}\cdot\vec{\mathcal{E}}$$

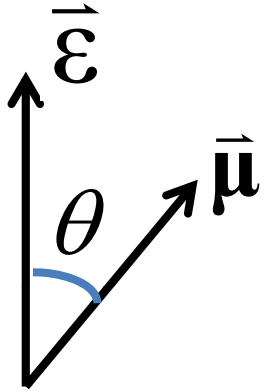
Kinetic energy | Trapping potential | Rotational energy | Electric field

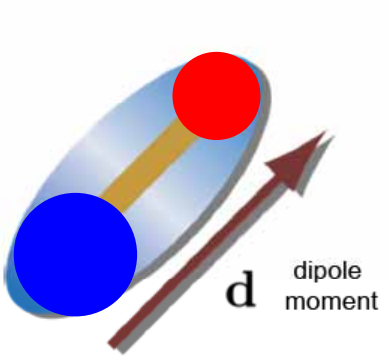
Assume | Rotational state H_S



$$\hat{H}_S = B\mathbf{J}^2 - \boldsymbol{\mu}\boldsymbol{\mathcal{E}}\cos\theta$$

Eigenfunctions : Pendular states





A Brief History of Pendular States

Directed States of Molecules:

Stationary quantum mechanical states for diatomic molecules whose geometrical axis is preferentially aligned in space, the molecular axis is directed (Generalized coherent states, minimal uncertainty states)

S. Kais and R.D. Levine, J. Phys. Chem. 91, 5461 (1987)

Pendular States of Molecules:

Directional hybrids , comprised of linear combinations of the field-free rotor states **|J,M>** with a range of **J** values but the same fixed value of the **M** quantum number

"Spatial orientation of molecules in strong electric fields and evidence for pendular states"

B. Friedrich and D.R. Herschbach, ***Letters to Nature*** *353,412 (1991)*

Experimental demonstration for the diatomic molecule **iodine monochloride , ICl**

Taken by S. Rais, 1991

Pendular States Qubits

$$|0\rangle = \sum_j a_j Y_{j,0}(\theta,\varphi), \qquad |1\rangle = \sum_j a'_j Y_{j,0}(\theta,\varphi)$$

For the simplest case of a diatomic molecule, the qubit eigenstates resulting from the Stark effect are linear combinations of Spherical Harmonics, with coefficients that depend markedly on the field strength.

There are three dimensionless variables:

$\mu\varepsilon/B$ The ratio of the Stark energy (magnitude of permanent dipole moment times electric field strength) to the rotational constant (proportional to inverse of molecular moment of inertia).

Ω/B with $\Omega=\mu^2/r^3$ The square of the permanent dipole moment divided by the cube of the separation distance.

k_BT/B The ratio of thermal energy (Boltzmann constant times Kelvin temperature) to the rotational constant

THE JOURNAL OF CHEMICAL PHYSICS **134**, 124107 (2011)

Entanglement of polar molecules in pendular states

Qi Wei,[1,2] Sabre Kais,[2] Bretislav Friedrich,[3] and Dudley Herschbach[1,a)]

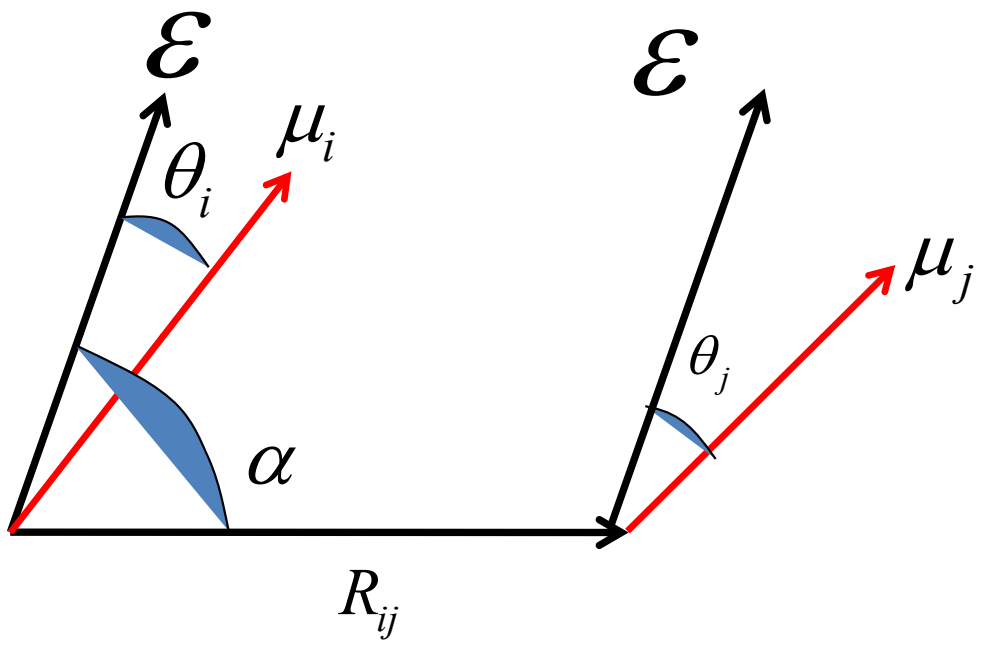
[1]*Department of Physics, Texas A & M University, College Station, Texas 77843, USA*

[2]*Department of Chemistry, Purdue University, West Lafayette, Indiana 47907, USA*

[3]*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany*

(Received 21 January 2011; accepted 28 February 2011; published online 24 March 2011)

Dipole-Dipole Interaction



$$V_{d-d}^{i,j} = \frac{\mu_i \mu_j}{R_{ij}^3}(1-3\cos^2\alpha)\cos\theta_i \cos\theta_j$$

Multi-dipole Hamiltonian

$$\hat{H} = \hat{H}_S + \hat{H}_{dd} = \sum_{i=1}^{N} H_S^i + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} V_{d-d}^{i,j}$$

For N = 2, we expand the $\hat{H}$ in the basis of $|00\rangle, |01\rangle, |10\rangle$ and $|11\rangle$

$$\hat{H}_S = \begin{pmatrix} W_0 + W_0' & 0 & 0 & 0 \\ 0 & W_0 + W_1' & 0 & 0 \\ 0 & 0 & W_1 + W_0' & 0 \\ 0 & 0 & 0 & W_1 + W_1' \end{pmatrix}$$

$$\hat{H}_{d-d} = \Omega(1 - 3\cos^2\alpha) \begin{pmatrix} C_0 C_0' & C_0 C_X' & C_X C_0' & C_X C_X' \\ C_0 C_X' & C_0 C_1' & C_X C_X' & C_X C_1' \\ C_X C_0' & C_X C_X' & C_1 C_0' & C_1 C_X' \\ C_X C_X' & C_X C_1' & C_1 C_X' & C_1 C_1' \end{pmatrix}, \qquad \Omega = \frac{\mu^2}{R^3}$$

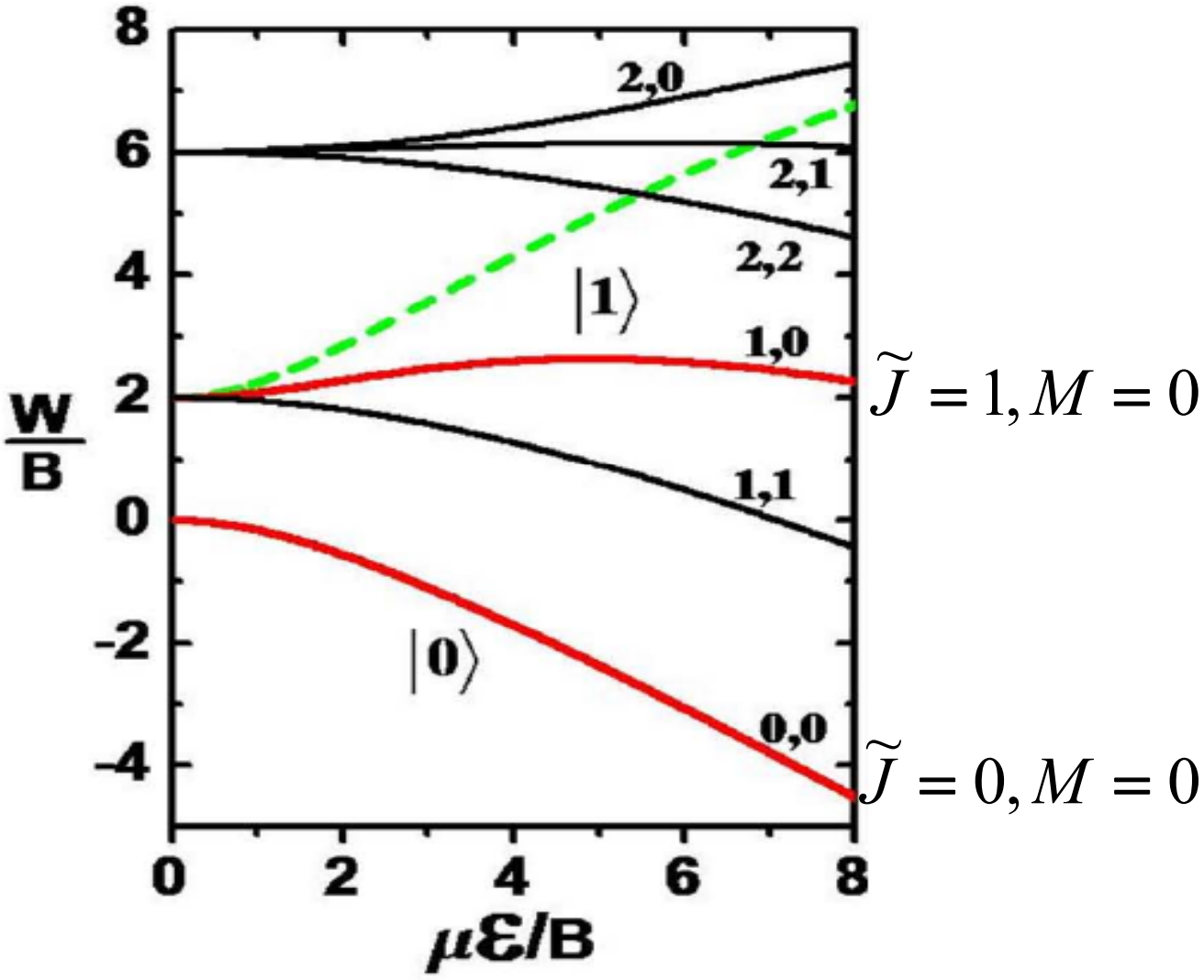
Where $C_0 = \langle 0|\cos\theta|0\rangle \quad C_X = \langle 0|\cos\theta|1\rangle \quad C_1 = \langle 1|\cos\theta|1\rangle$

Pendular Eigenenergies

Energy levels, **W**, for a polar diatomic molecule in an electric field. States are labeled by quantum numbers **J, M**

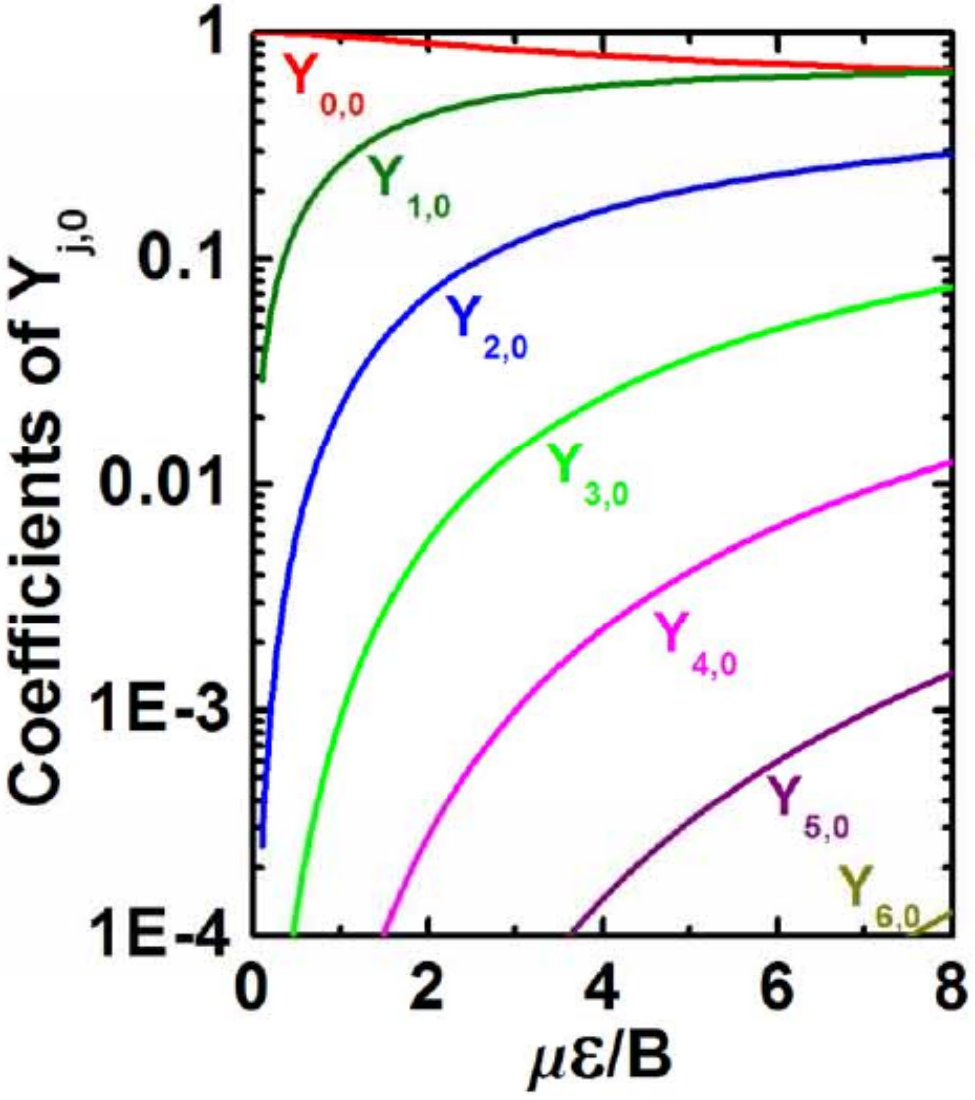
J denotes total angular momentum **M** projection on direction of electric field Qubit states **|0> and |1> are in red.**

Green is the transition energy.

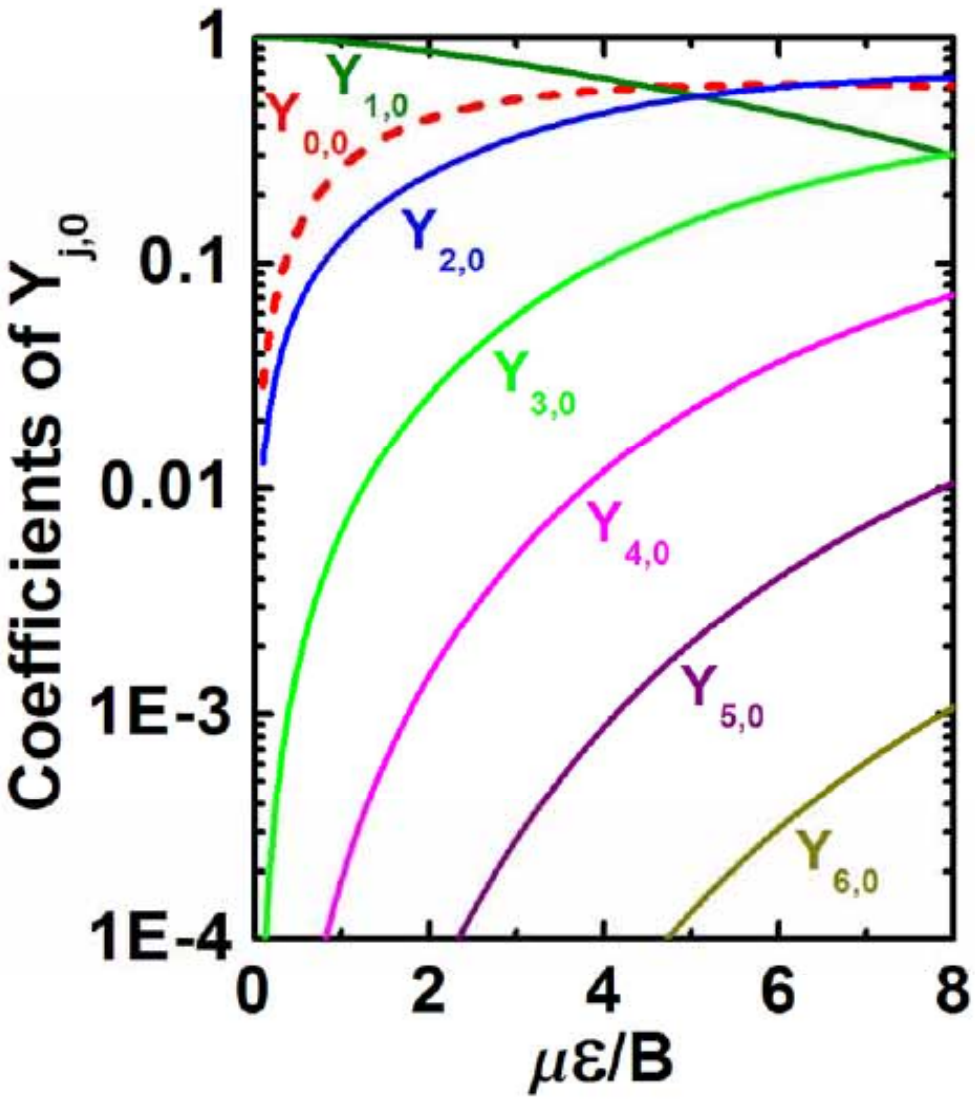


$$|0\rangle = \sum_j a_j Y_{j,0}(\theta,\varphi), \qquad |1\rangle = \sum_j a'_j Y_{j,0}(\theta,\varphi)$$

$$|0\rangle = \sum_j a_j Y_{j,0}(\theta,\varphi), \qquad |1\rangle = \sum_j a'_j Y_{j,0}(\theta,\varphi)$$

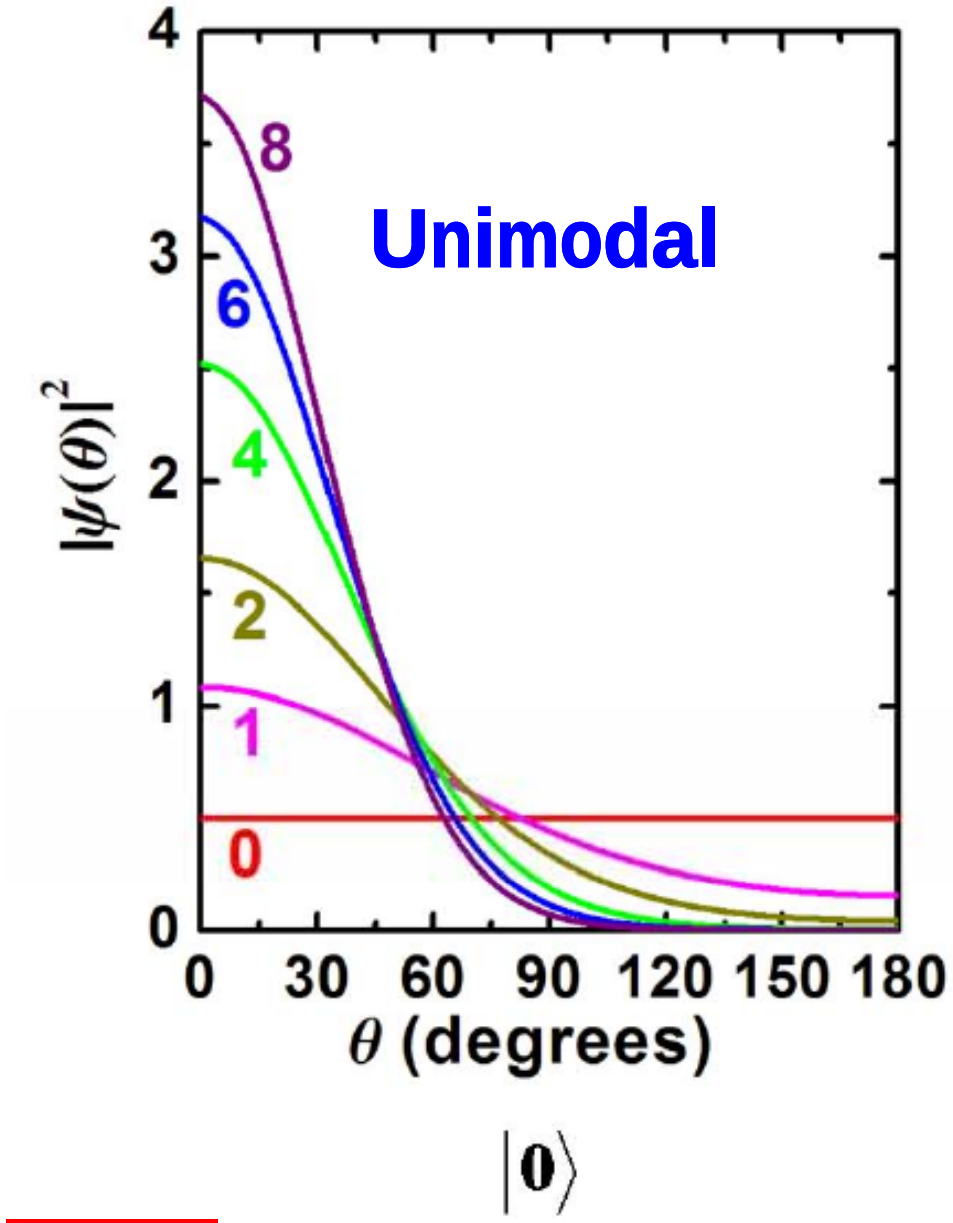


$|0\rangle$

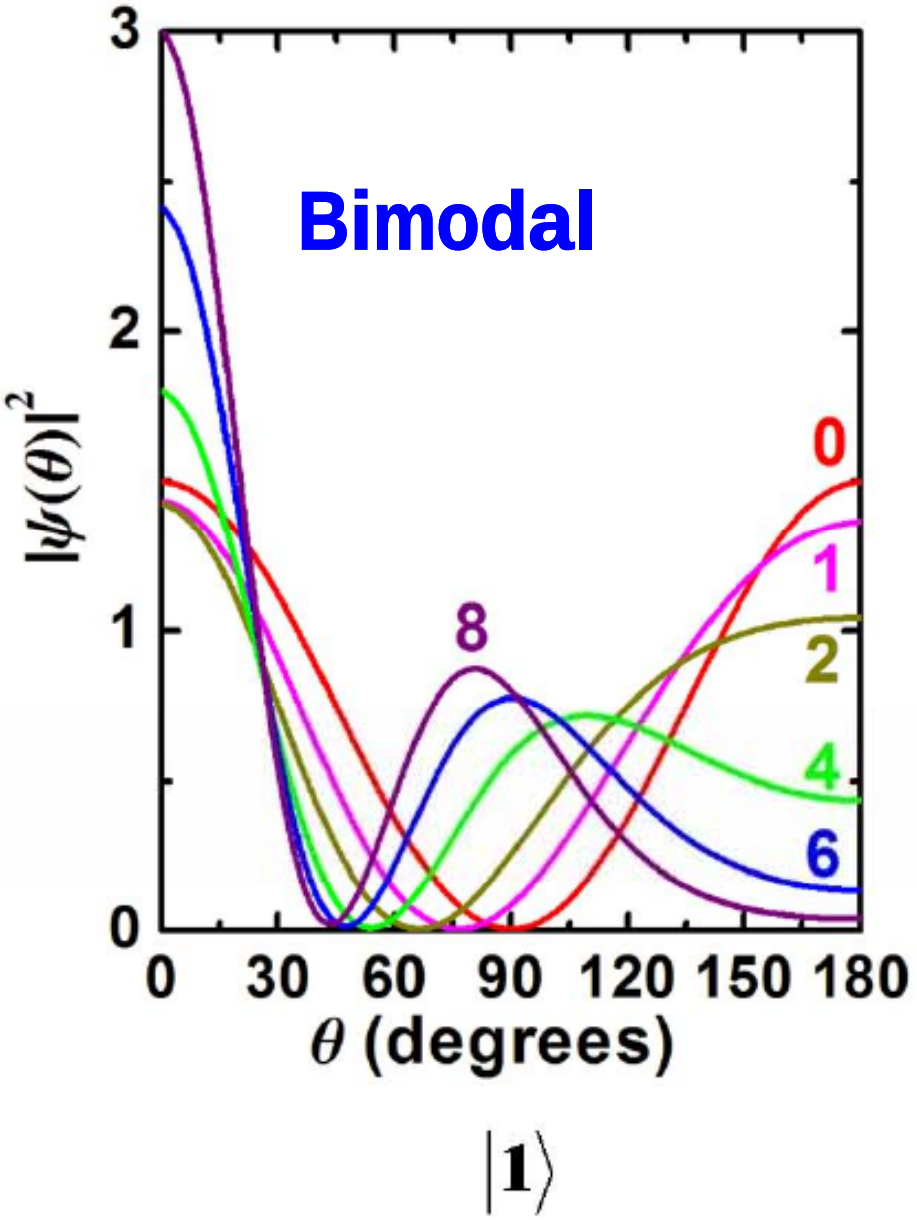


$|1\rangle$

Angular distributions of the pendular qubits

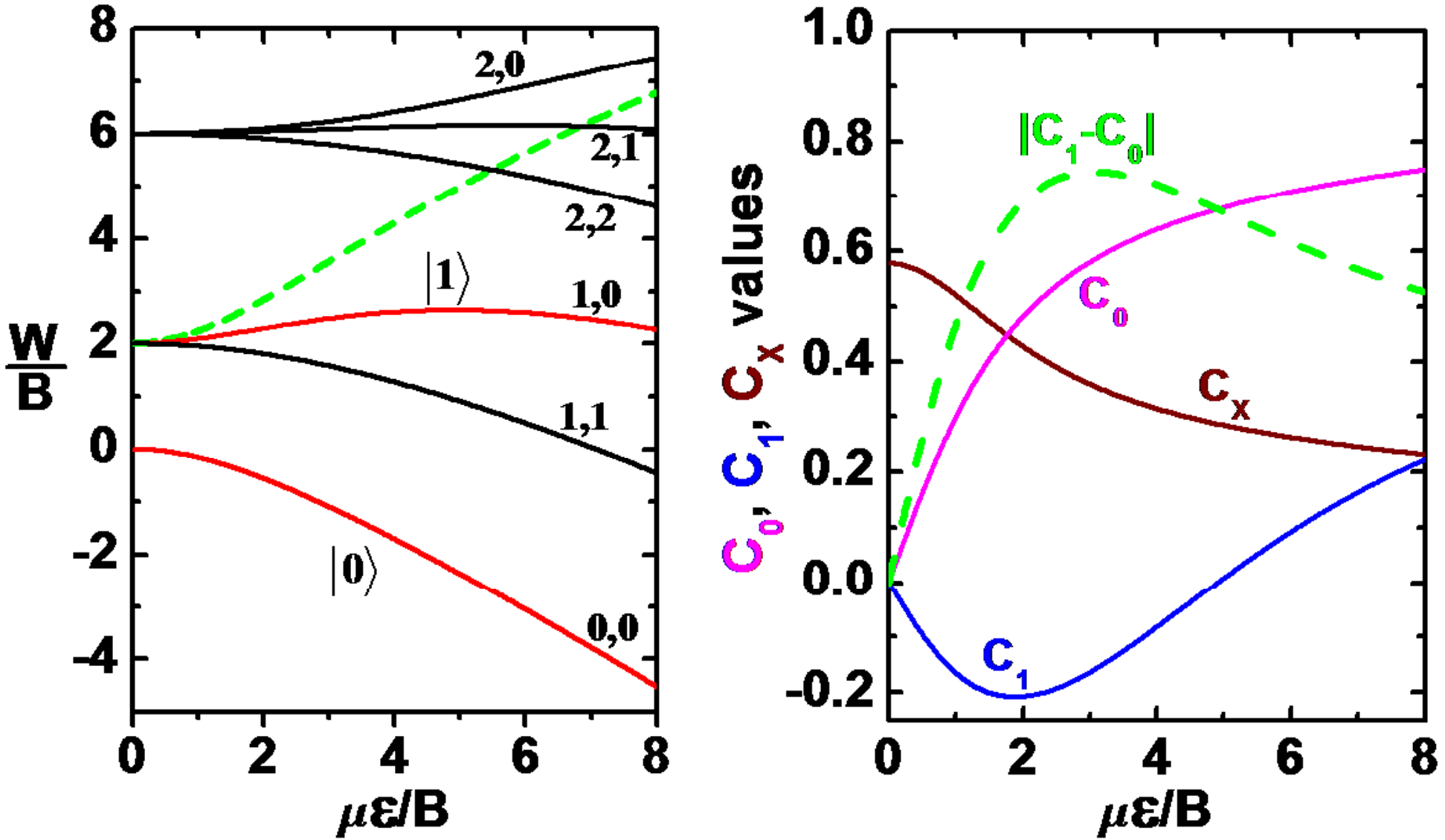


$|\mathbf{0}\rangle$



$|\mathbf{1}\rangle$

Angular distributions of the $|0\rangle$ and $|1\rangle$ pendular states for values of $\mu\varepsilon/B$ between 0 and 8.


W/B
με/B
2,0
2,1
2,2
|1⟩
1,0
1,1
|0⟩
0,0
C0, C1, Cx values
|C1-C0|
C0
Cx
C1
(a)
(b)

Quantify Entanglement

Entanglement of Formation

We calculate the entanglement of formation, $E(\rho) = \mathcal{E}(C(\rho))$

which characterizes the amount of entanglement needed in order to prepare a state described by a density matrix

$$\rho_A = Tr_B(\rho), \qquad \rho = |\phi><\phi|$$

Concurrence is the simply expression of Entanglement

$$\mathcal{E} = h\left(\frac{1+\sqrt{1-C^2}}{2}\right) \qquad h(x) = -x log_2 x - (1-x) log_2 (1-x)$$

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y) \qquad R \equiv \sqrt{\sqrt{\rho}\,\tilde{\rho}\,\sqrt{\rho}}$$

$$C(\rho) = max\{0,\ \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\ \}$$

W. K. Wootters, Phys. Rev. Lett. 80, 2245 (1998)

Recipe for Concurrence

A Measure of Pairwise Entanglement
C = 0 means no entanglement
C = 1 means maximum entanglement

1. Construct **density matrix**, ρ

2. Construct **flipped density matrix**, $\tilde{\rho}$

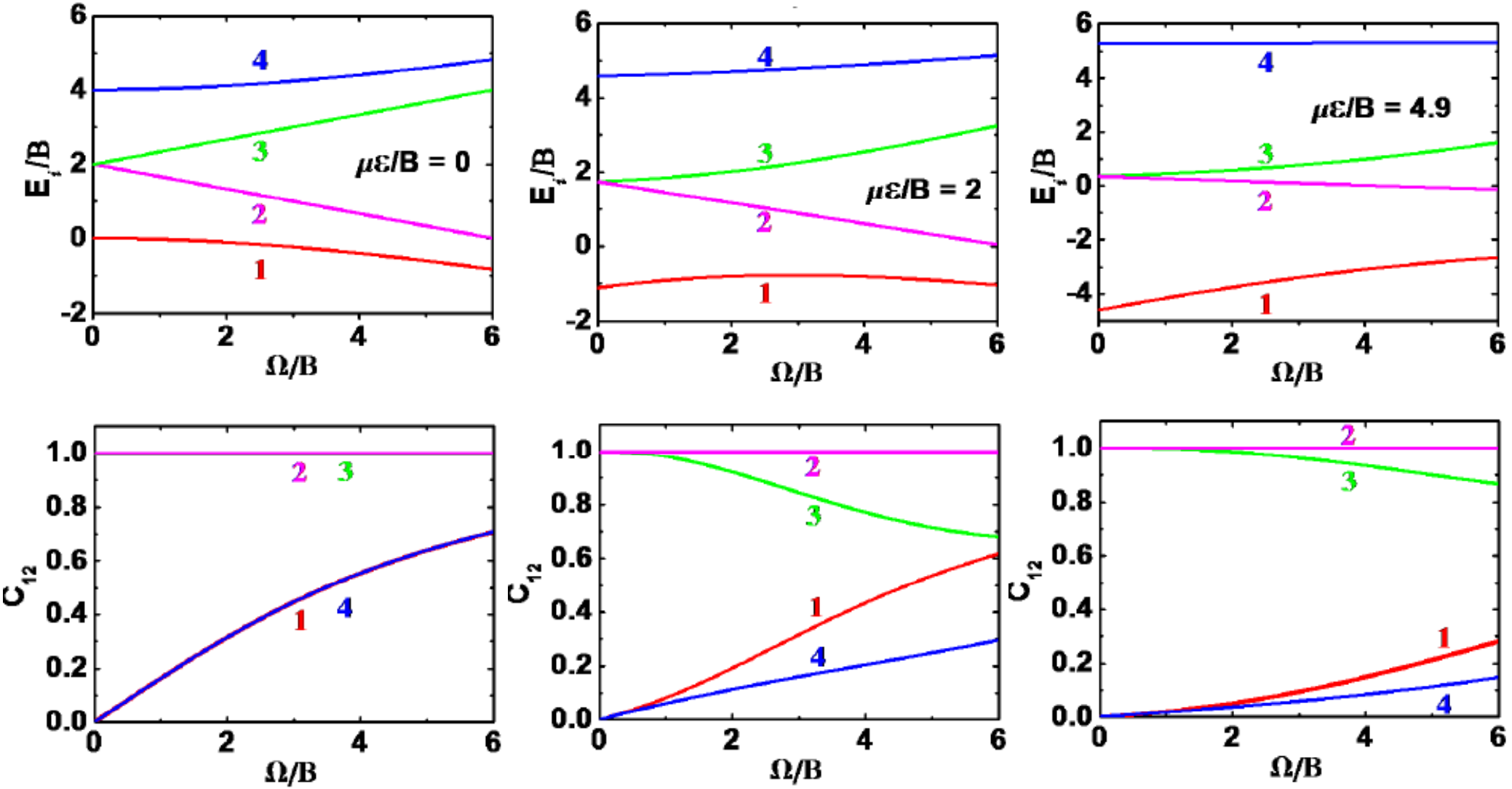
3. Construct **product matrix**, $\rho\tilde{\rho}$

4. Find **eigenvalues** $\lambda_1, \lambda_2, \ldots$ of $\rho\tilde{\rho}$

5. Calculate **Concurrence** from square roots of eigenvalues via

$$\mathbf{C} = \max[0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \cdots]$$

Pairwise Concurrences

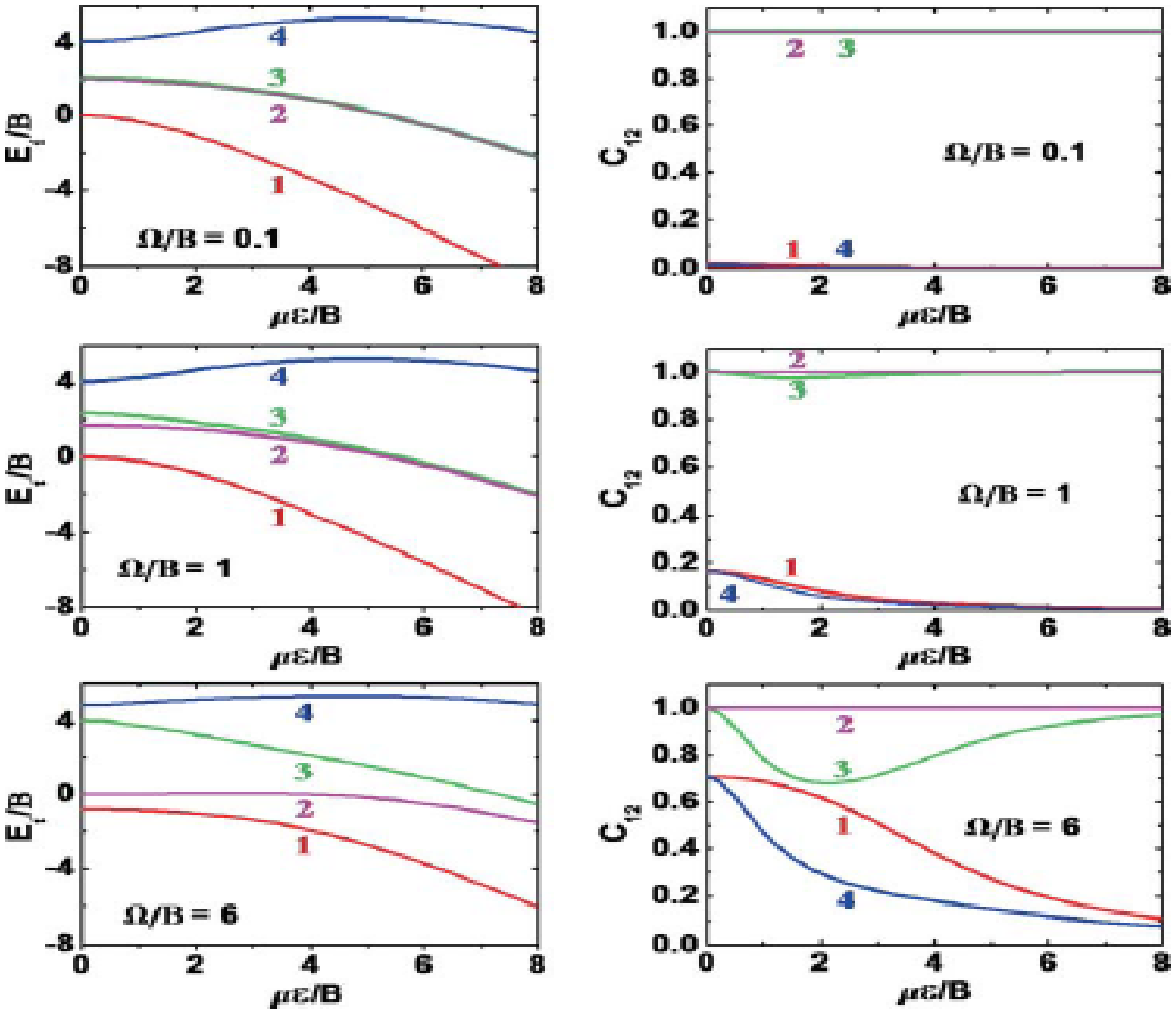


Using a basis of Bell states:

$$\frac{|11\rangle + |00\rangle}{\sqrt{2}}, \quad \frac{|11\rangle - |00\rangle}{\sqrt{2}}, \quad \frac{|10\rangle + |01\rangle}{\sqrt{2}}, \quad \frac{|10\rangle - |01\rangle}{\sqrt{2}}$$

$$H_{S1} + H_{S2} = \left(\begin{array}{cc:cc} W_+ & W_- & 0 & 0 \\ W_- & W_+ & 0 & 0 \\ \hdashline 0 & 0 & W_+ & 0 \\ 0 & 0 & 0 & W_+ \end{array}\right), \qquad V_{d-d} = \Omega(1 - 3\cos^2\alpha) \left(\begin{array}{ccc:c} \hat{A}_+ & \hat{B} & \hat{C}_+ & 0 \\ \hat{B} & \hat{A}_- & \hat{C}_- & 0 \\ \hat{C}_+ & \hat{C}_- & \hat{D}_+ & 0 \\ \hdashline 0 & 0 & 0 & \hat{D}_- \end{array}\right),$$

where $W_\pm = W_1 \pm W_0$, $\hat{A}_\pm = \frac{1}{2}(C_1^2 + C_0^2) \pm C_\chi^2$, $\hat{B} = \frac{1}{2}(C_1^2 - C_0^2)$, $\hat{C}_\pm = C_\chi(C_1 \pm C_0)$, and $\hat{D}_\pm = C_1 C_0 \pm C_\chi^2$.



. Eigenenergies and concurrences for the four eigenstates for two dipoles as a function of reduced variables, $\mu\varepsilon/B$ for electric field and Ω/B for dipole–dipole coupling.

Superposition Basis Set

- The new basis set is defined as

$$\uparrow = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle);\ \downarrow = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

- The new basis set arrangement

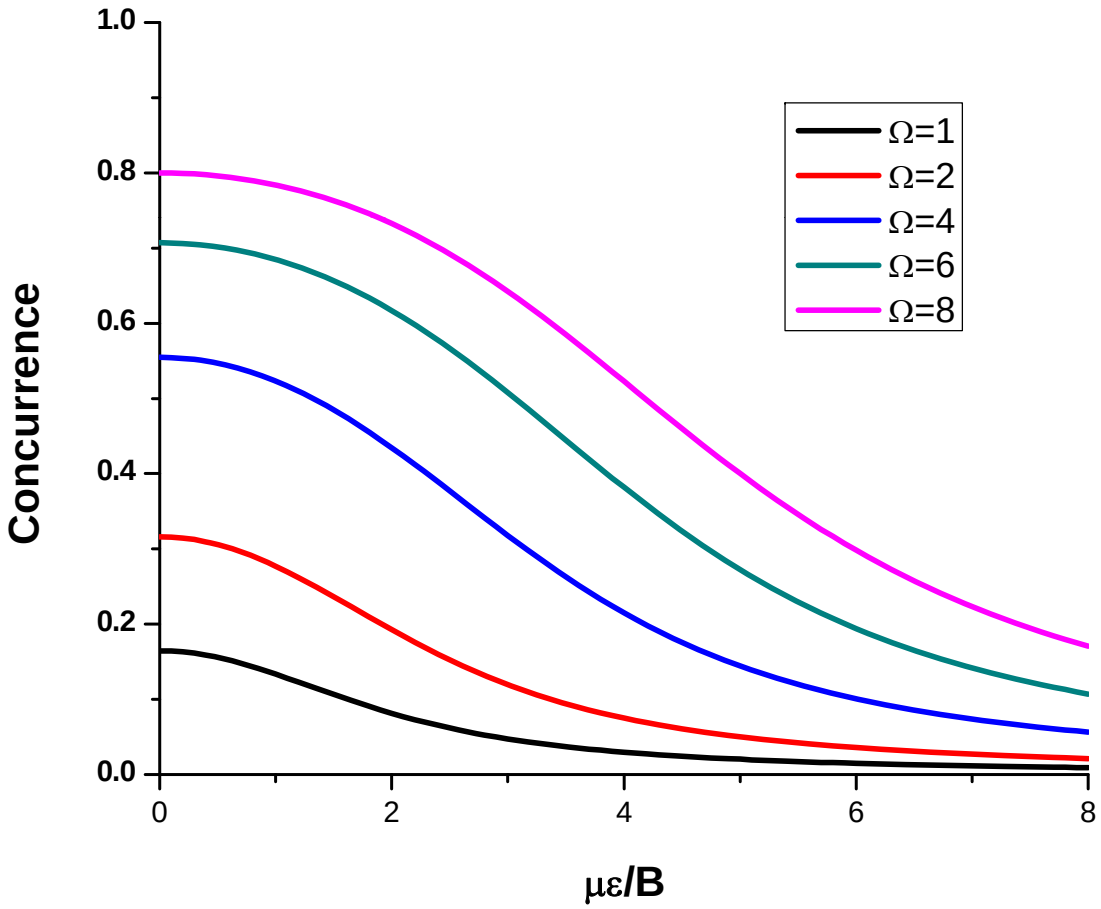
$$(\uparrow\uparrow \quad \uparrow\downarrow \quad \downarrow\uparrow \quad \downarrow\downarrow)$$

Dan Elliott and Yong Chen (EE and Physics, Purdue)

Investigate superpostion of ultracold

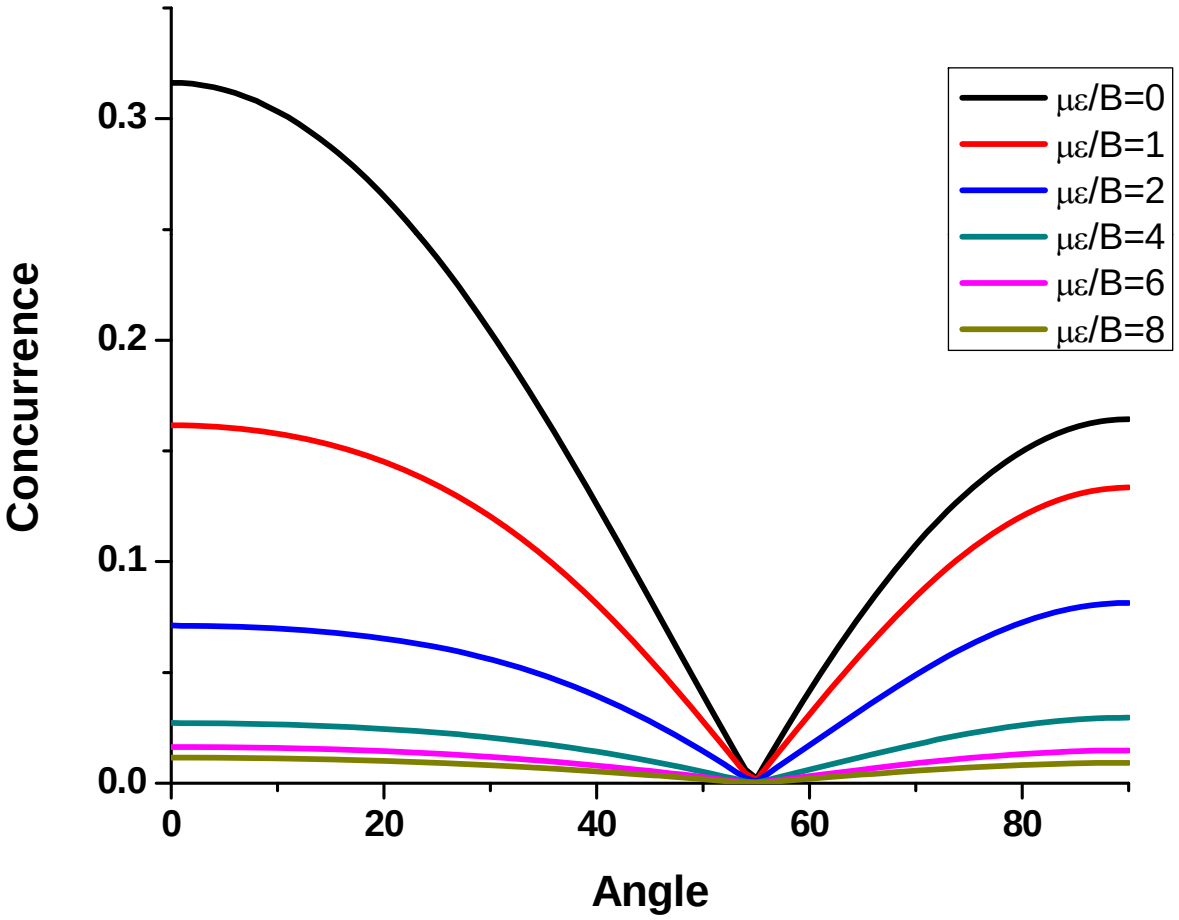
LiRb molecules

Concurrence v.s. με/B & Ω



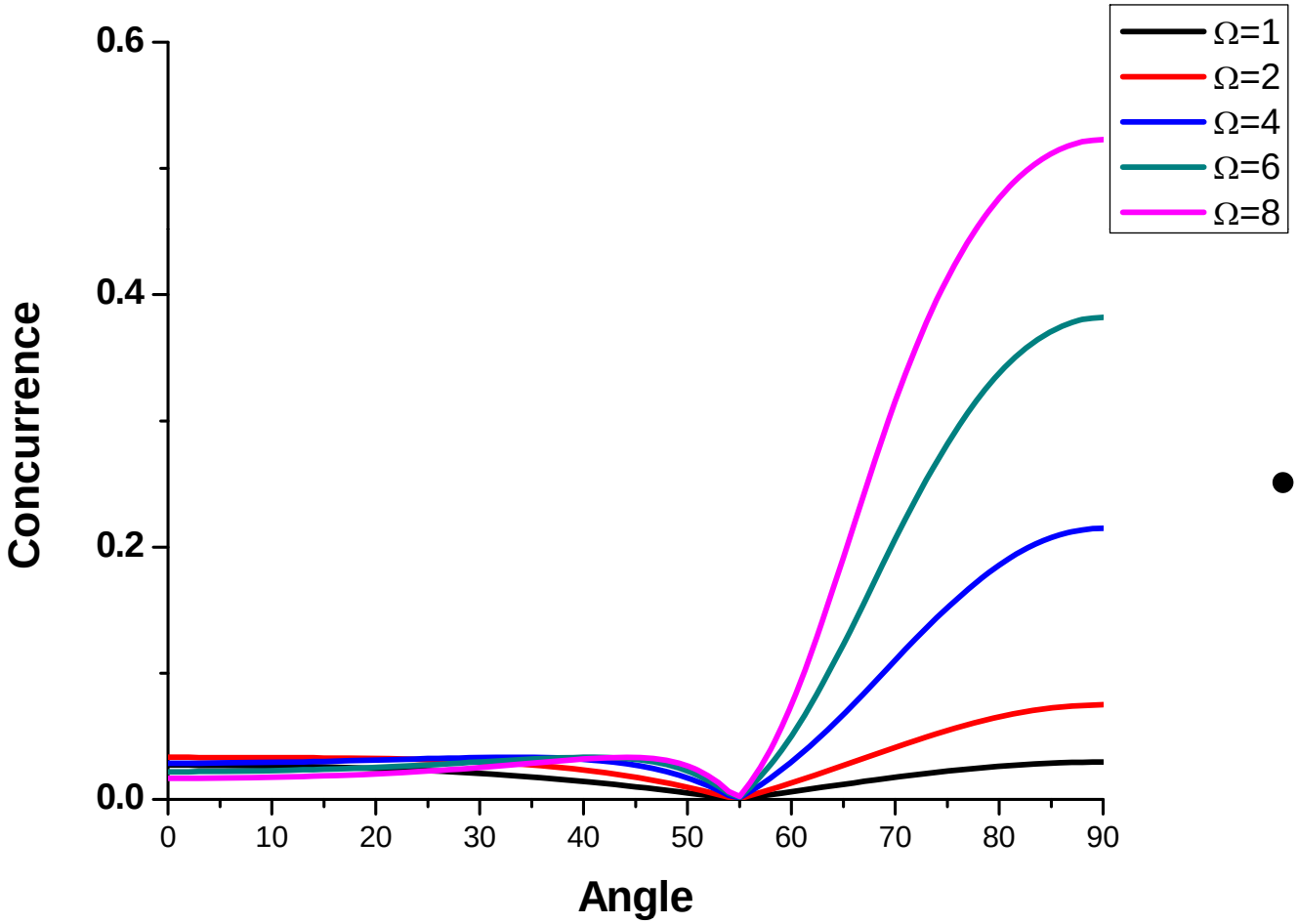
- The ground state entanglement decreases when με/B increases.
- The ground state entanglement increased as the coupling constant Ω increases ($\alpha=90^{O}$)

Concurrence v.s. α & με/B



- There is a magic angle (54.74 degrees) where no entanglement exists.
- Before the magic angle, the entanglement decreases. Beyond that, the entanglement increases.
- Similar to the previous one, the entanglement decreases when the external electric fields increases (Ω=1)

Concurrence v.s. α & Ω



- The entanglement stays at almost zero before the magic angle. While that increases fast beyond the magic angle.
- When Ω becomes large, the increase of the entanglement becomes faster. ($\mu\varepsilon/B=4$)

Thermal Entanglement

In order to evaluate thermal entanglement, we need a temperature dependent density matrix, $\rho = \exp(-\beta H)/Z(T)$, with $\beta = 1/k_B T$ and $Z(T)$ the partition function

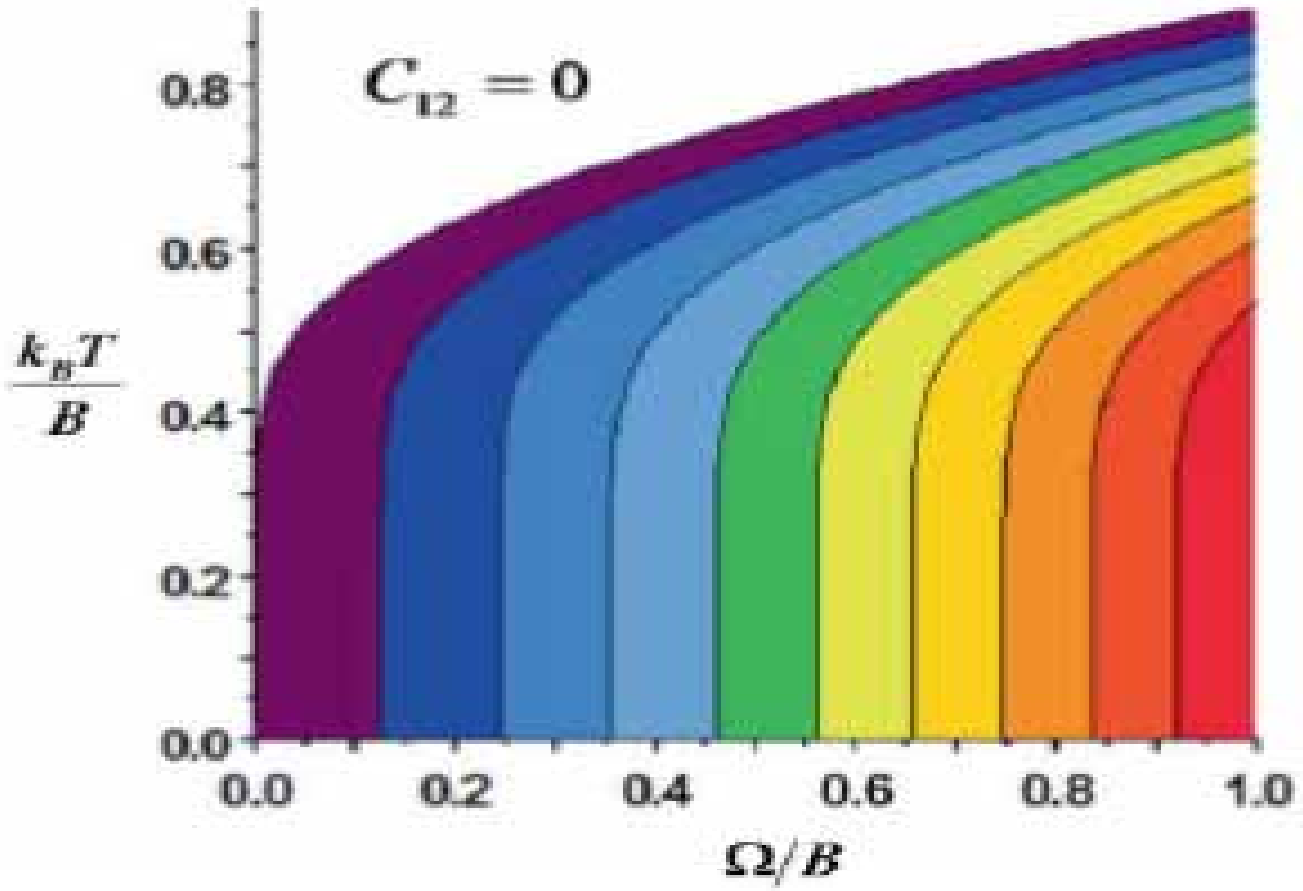
$$Z(T) = tr[\exp(-\beta H)] = \sum_i g_i e^{-\beta E_i},$$

with E_i the ith eigenvalue and g_i its degeneracy. Hence the density matrix can be written as

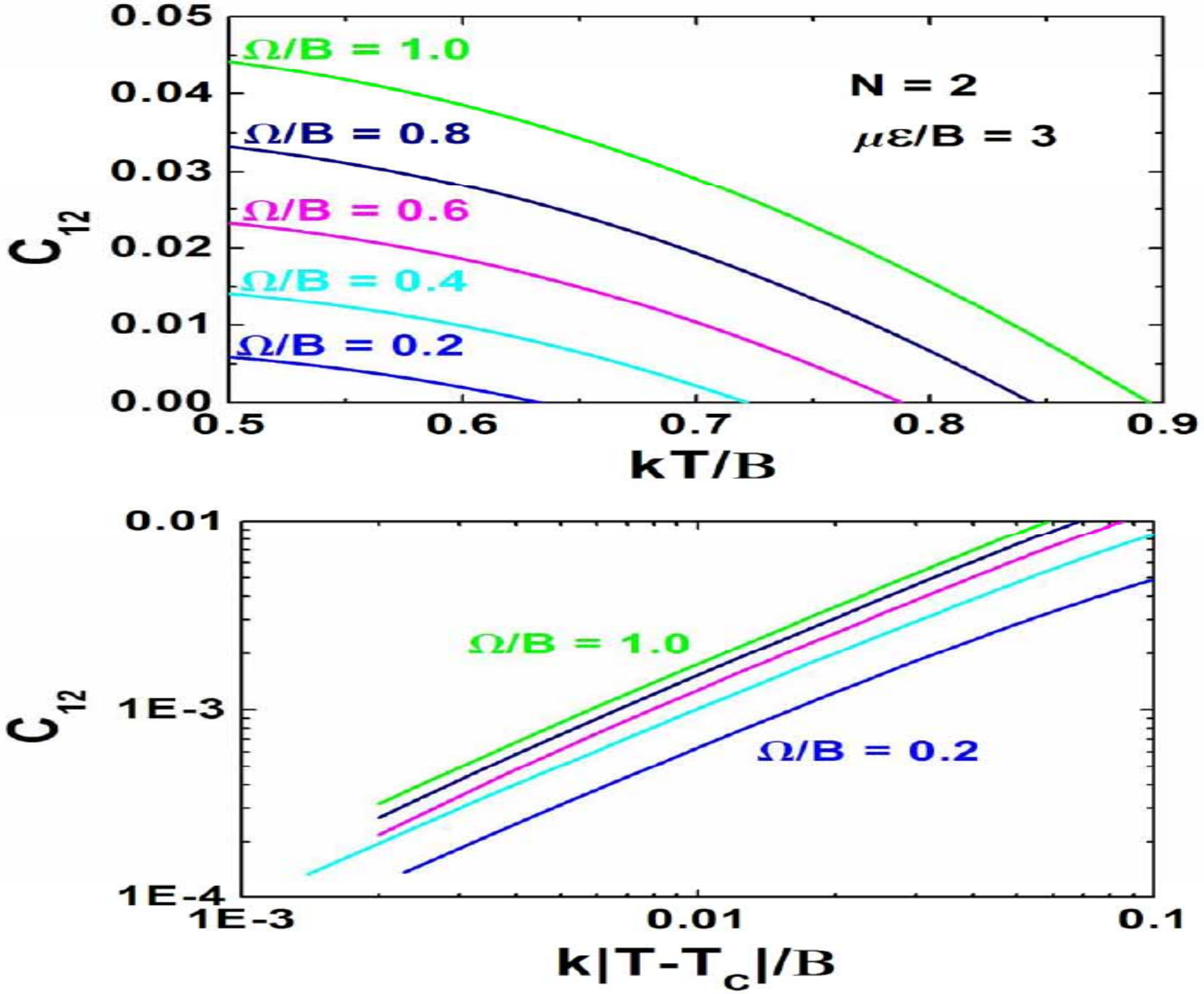
$$\rho(T) = \frac{1}{Z} \sum_i^N e^{-\beta E_i} |\Psi_i\rangle\langle\Psi_i|,$$

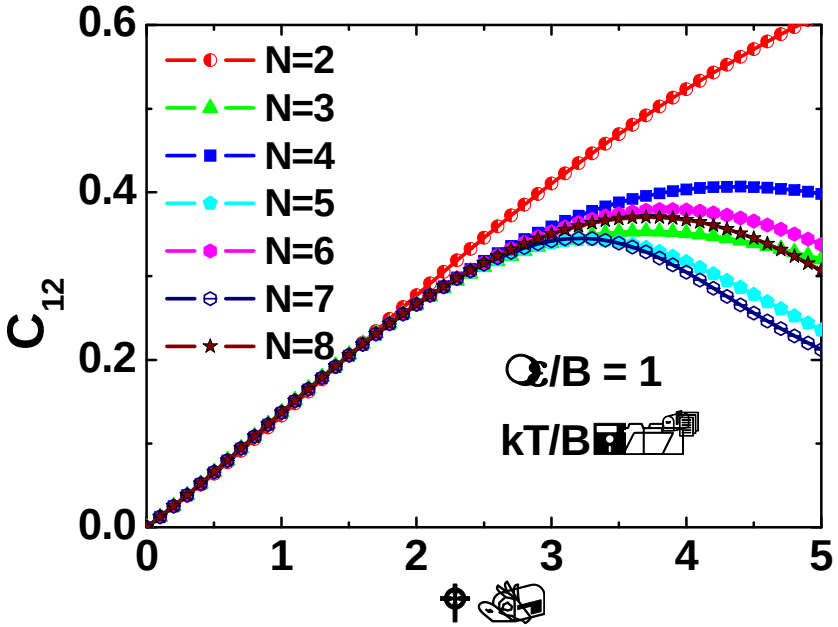
where $|\Psi_i\rangle$ is the ith eigenfunction. From the density matrix $\rho(T)$, we can obtain the reduced density matrix for any pair of dipoles and thence evaluate the concurrence at any temperature.

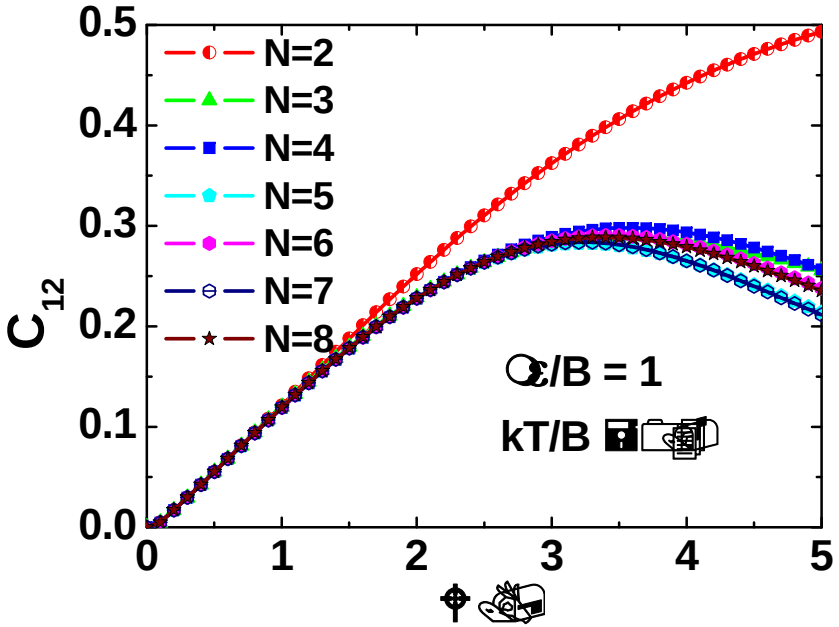
Thermal Pairwise Concurrence

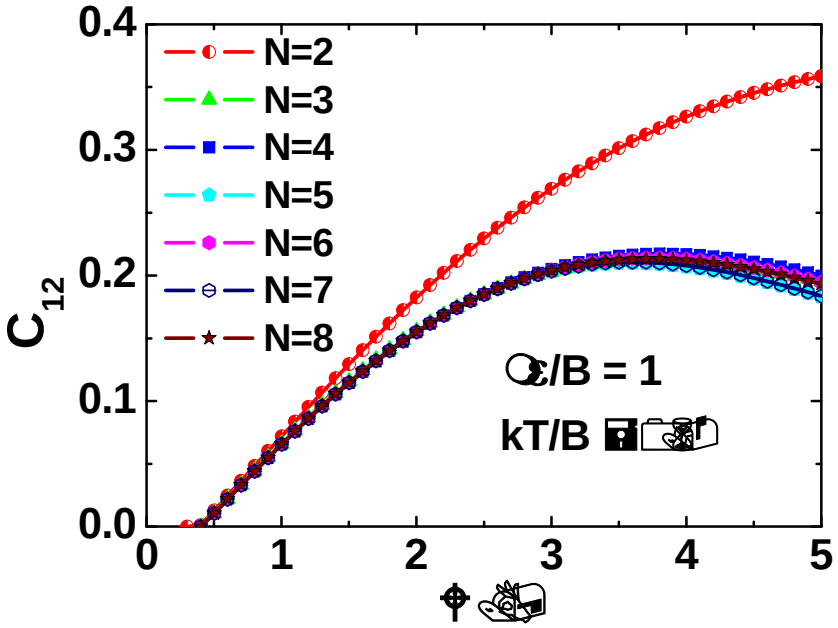


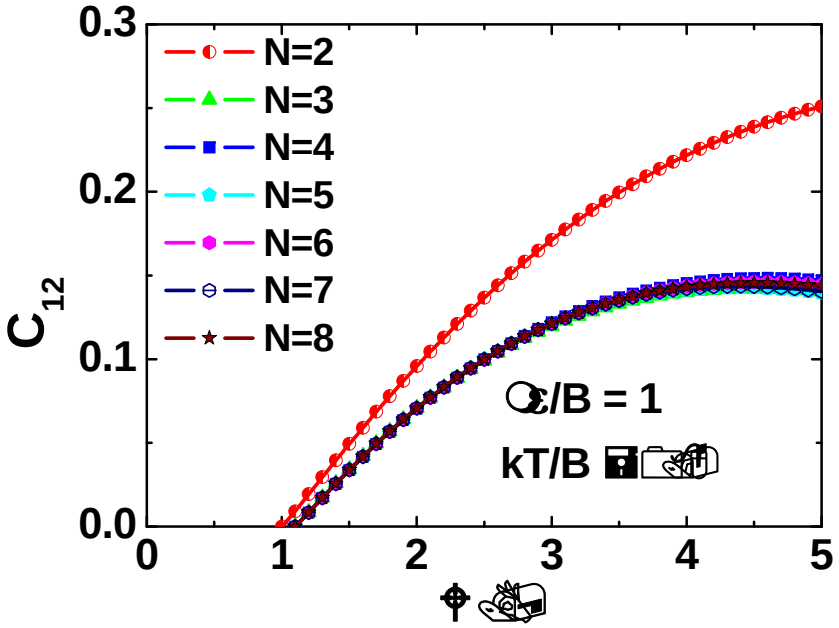
Contour plot of thermal pairwise concurrence for two dipoles, for $\mu\varepsilon/B = 3$. For $0 < \Omega/B < 1$, the maximum concurrence $C_{12}(\text{max}) = 0.0473$, occurs at $T = 0$, $\Omega/B = 1$. The plot displays normalized contours. Within each colored band, the variation of $C_{12}/C_{12}(\text{max})$ is 0.1; thus, the normalized concurrence in the right most band (red) ranges from 0.9 to 1, and in the next band (orange red), from 0.8 to 0.9, etc. A striking feature is the large region (uncolored) where $C_{12} = 0$. There, entanglement does not occur unless the dipole–dipole coupling exceeds a critical value dependent on the temperature.

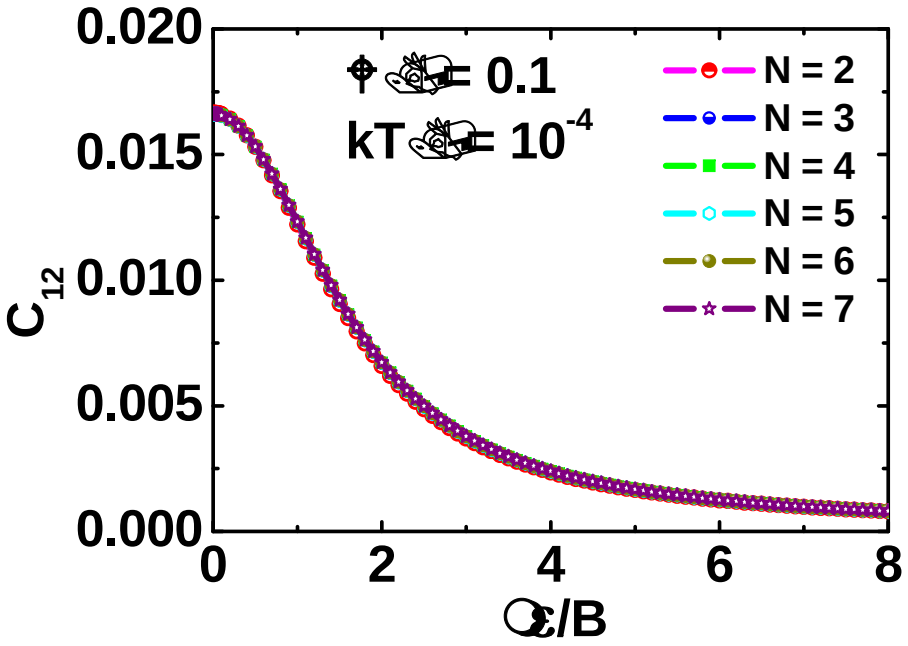

0.05
0.04
0.03
0.02
0.01
0.00
C_{12}
Ω/B = 1.0
Ω/B = 0.8
Ω/B = 0.6
Ω/B = 0.4
Ω/B = 0.2
N = 2
με/B = 3
0.5
0.6
0.7
0.8
0.9
kT/B
0.01
1E-3
1E-4
C_{12}
Ω/B = 1.0
Ω/B = 0.2
1E-3
0.01
0.1
$k|T-T_c|/B$

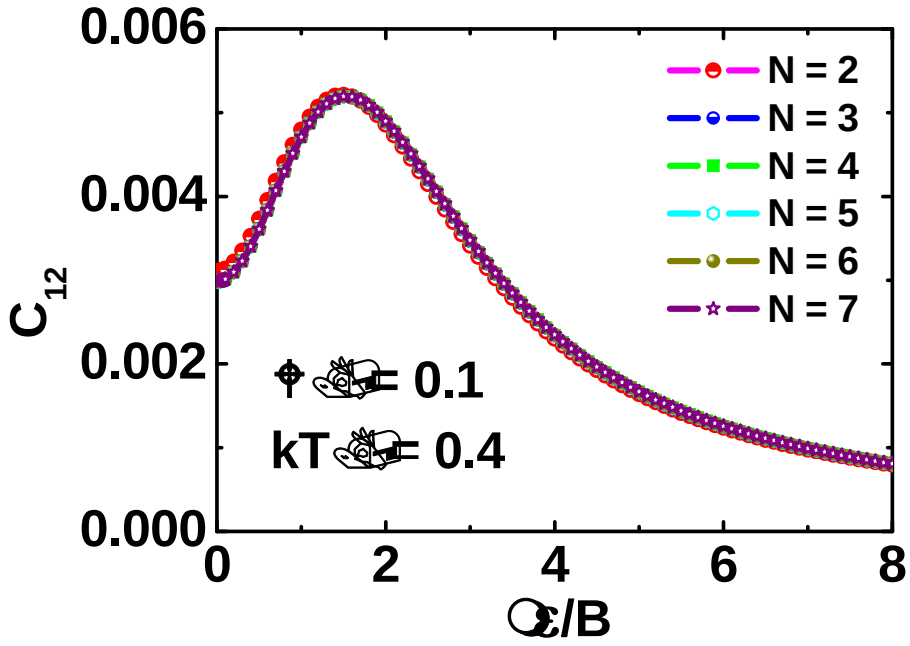

N=2
N=3
N=4
N=5
N=6
N=7
N=8
ε/B = 1
kT/B
C12
0.0
0.2
0.4
0.6
0
1
2
3
4
5

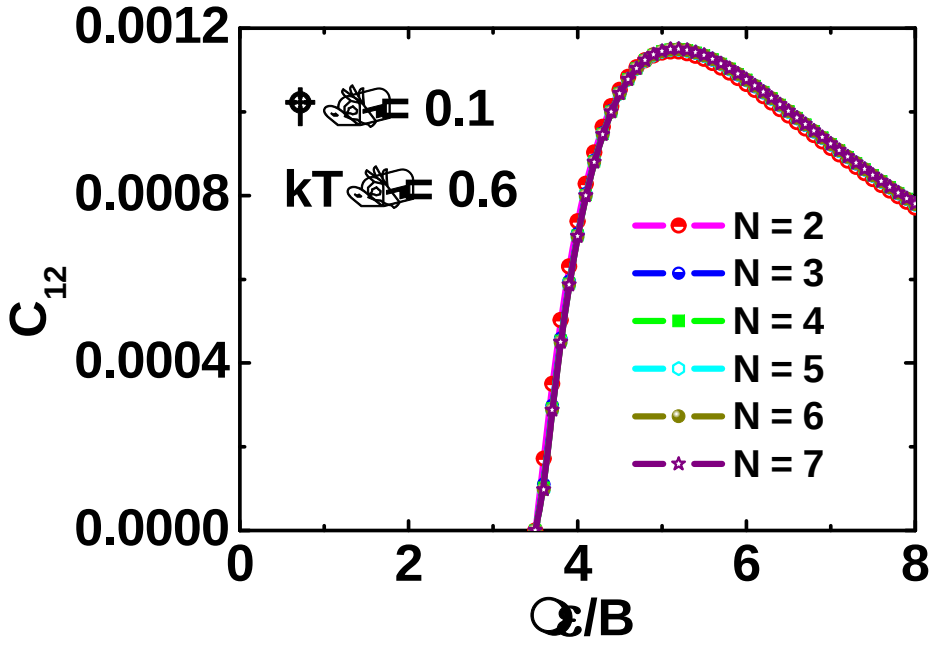

N=2
N=3
N=4
N=5
N=6
N=7
N=8
ε/B = 1
kT/B
C12
0.0
0.1
0.2
0.3
0.4
0.5
0
1
2
3
4
5


N=2
N=3
N=4
N=5
N=6
N=7
N=8
ε/B = 1
kT/B
C12
0.0
0.1
0.2
0.3
0.4
0
1
2
3
4
5


N=2
N=3
N=4
N=5
N=6
N=7
N=8
ε/B = 1
kT/B
C12
0.0
0.1
0.2
0.3
0
1
2
3
4
5


0.020
0.015
0.010
0.005
0.000
C_{12}
0
2
4
6
8
ε/B
= 0.1
kT = 10^{-4}
N = 2
N = 3
N = 4
N = 5
N = 6
N = 7


0.006
0.004
0.002
0.000
C_{12}
0
2
4
6
8
ε/B
= 0.1
kT = 0.4
N = 2
N = 3
N = 4
N = 5
N = 6
N = 7


0.0012
0.0008
0.0004
0.0000
C_{12}
0
2
4
6
8
ε/B
= 0.1
kT = 0.6
N = 2
N = 3
N = 4
N = 5
N = 6
N = 7

Dynamics of Entanglement of Polar Molecules in Pendular States

- Quantum Liouville equation

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho]$$

$$\hbar = 1$$

ρ ~ density matrix of the system

Objective

Investigate the dynamics of entanglement of the dipoles system under different initial conditions: external electric field, dipole-dipole coupling constant and the angle between external field and the dipole chain.

Experimental parameters

External field : $\varepsilon \sim$ **a few** kV/cm

Trap temperatures $\leq \mu K \Rightarrow k_B T/B \sim 10^{-5} - 10^{-6} \Rightarrow$ **Ground**

Space of optical lattice $r = \lambda/2$ **and** $\lambda \sim 0.3 - 1\ \mu m \Rightarrow \Omega/B \leq 10^{-4}$

SrO : $\mu = 8.9\ D,\ B = 0.33\ cm^{-1},\ \lambda = 1\ \mu m \Rightarrow \Omega/B \sim 10^{-5}$

When $\Omega/B \leq 10^{-4}$, $C_{12} \sim 10^{-5}$

Potential candidate molecules: **KCs, CsI, SrO, …**

The key aspect is that although entanglement needs to be large for some quantum computing algorithms, it need not be appreciable or even present in the ground eigenstate of the system; it can be induced dynamically during operation of the computer

The Simulation Procedure

- Five different initial conditions:

$$|00\rangle\,,\ |11\rangle\,,\ |10\rangle\,,\ |11\rangle\,,\ \frac{1}{\sqrt{2}}\left(|00\rangle+|11\rangle\right)\ \text{and}\ \frac{1}{\sqrt{2}}\left(|01\rangle+|10\rangle\right)$$

- Relationship between concurrence & external electric fields ($\mu\varepsilon/B$)
  - we set $\Omega=5$ & $\alpha=90^{O}$
- Concurrence verses coupling constant (Ω)
  - The other coefficients are $\mu\varepsilon/B=3$ & $\alpha=90^{O}$
- Concurrence verses Angle (α)
  - The other coefficients are $\mu\varepsilon/B=3$ & $\Omega=3$

Units

- H is the Hamiltonian with the unitless parameters με/B and Ω/B. The rotational constant B is dealt as the basic unit in the Hamiltonian.

$$\mu\varepsilon/B = 0.0168\ \mu(\text{Debye})\varepsilon(\text{kV/cm})/B(\text{cm}^{-1}),$$

$$\Omega/B = 5.04 \times 10^{-9}\mu^2(\text{Debye})/r^3(\mu)/B(\text{cm}^{-1}),$$

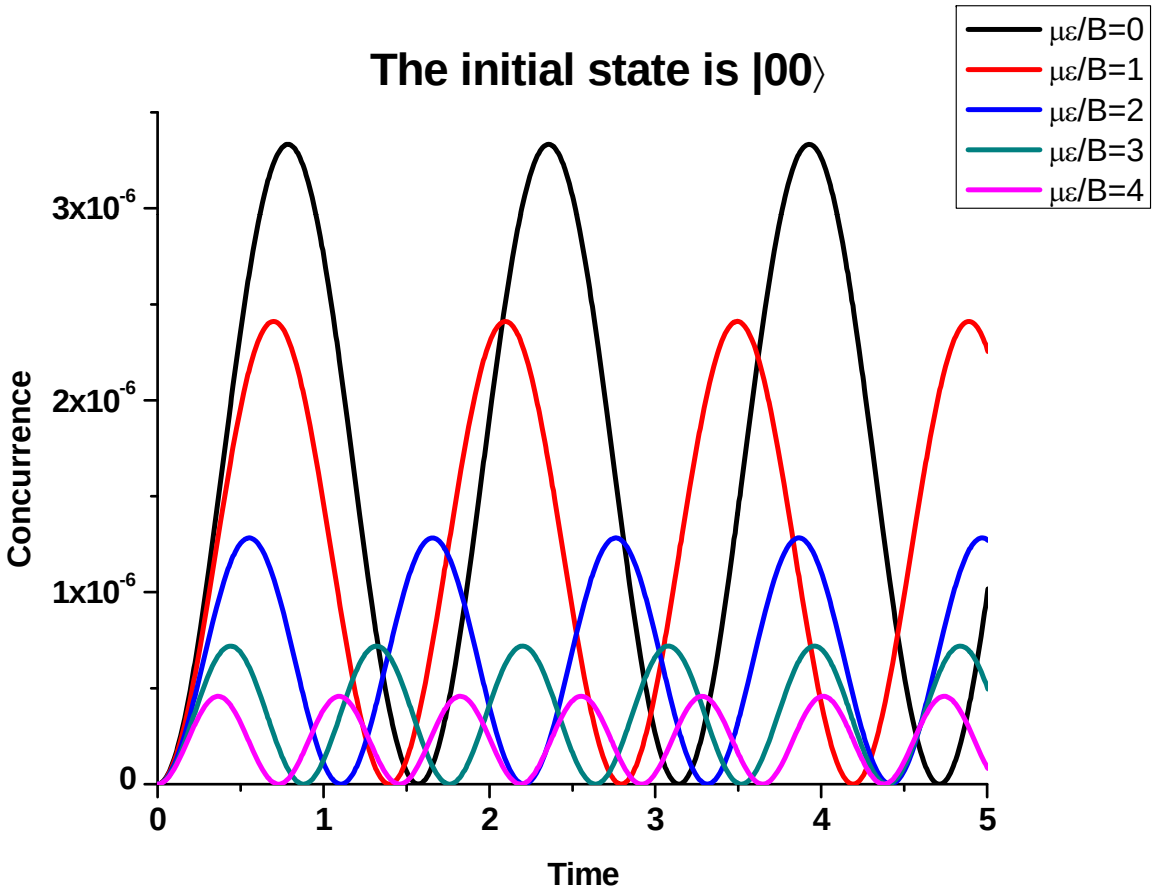
$$k_\text{B}T/B = 0.695\ T(K)/B(\text{cm}^{-1}).$$

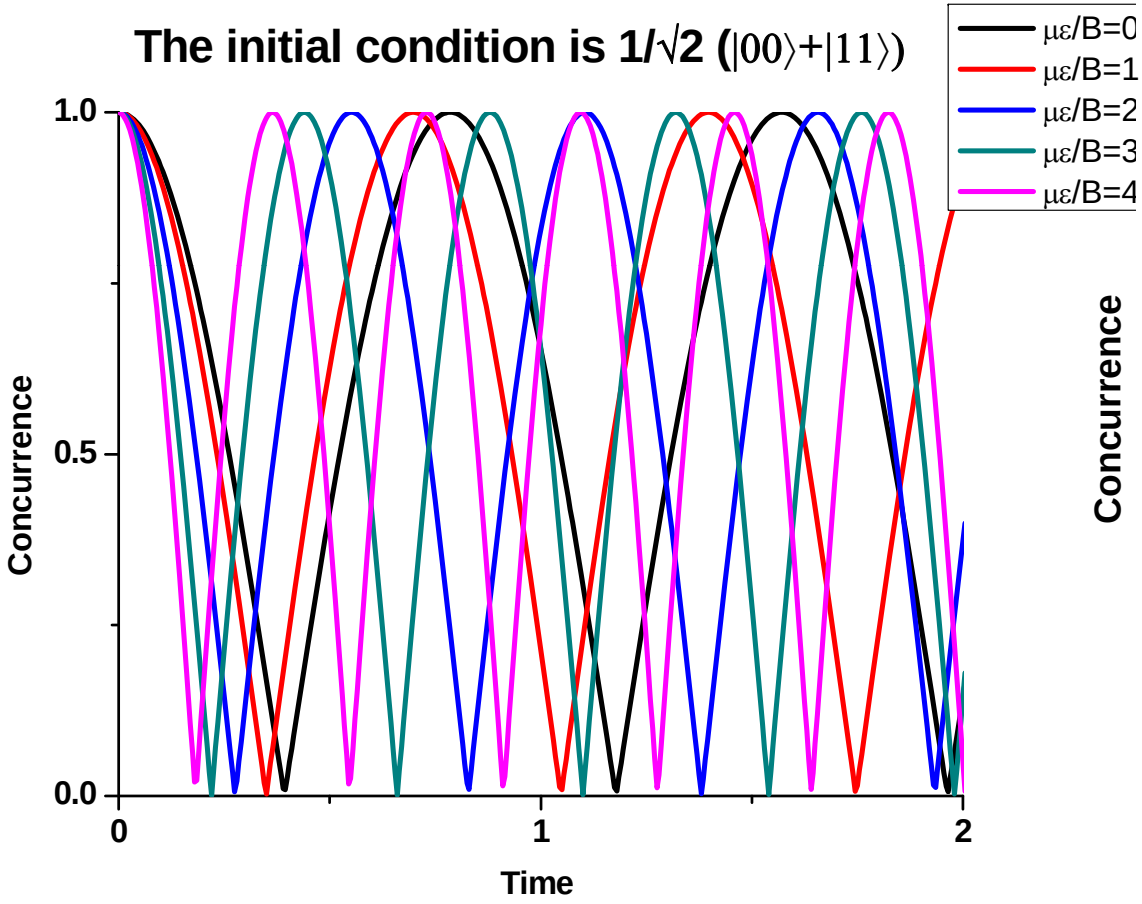
The time scale for the Liouville equation is

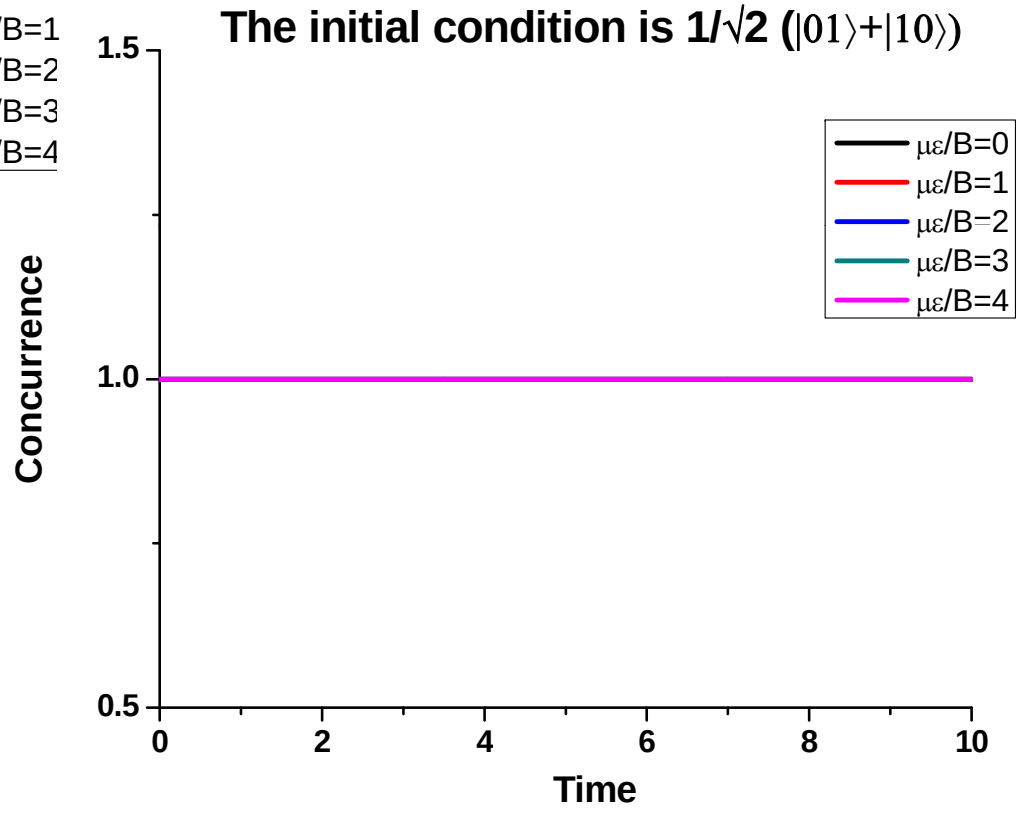
$$\frac{\hbar}{B} = \frac{5.3088\ cm^{-1}ps}{0.33\ cm^{-1}} = 16.1\ ps$$

- Each time step is equal to **t=1 --> 16ps**

Relationship between Concurrence & με/B; Ω=1E-5 & α=90°




The initial condition is 1/√2 (|00⟩+|11⟩)
Concurrence
Time
1.0
0.5
0.0
0
1
2
με/B=0
με/B=1
με/B=2
με/B=3
με/B=4


The initial condition is 1/√2 (|01⟩+|10⟩)
Concurrence
Time
1.5
1.0
0.5
0
2
4
6
8
10
με/B=0
με/B=1
με/B=2
με/B=3
με/B=4

CNOT Gate

Gates:

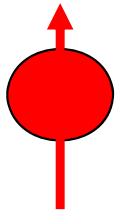
Classical

Information is encoded in a series of **bits**, and these bits are manipulated via Boolean logic gates arranged in succession to produce an end result.

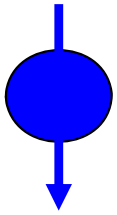
Quantum

Manipulates **qubits** by executing a series of quantum gates, each a unitary transformation acting on a single qubit or pair of qubits. The qubits can then be measured, with this measurement serving as the final computational result.

Matrix representation of simple quantum logic gates



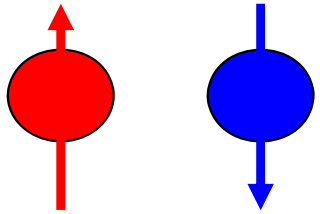
$|\uparrow\rangle = |1\rangle$: $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$



$|\downarrow\rangle = |0\rangle$: $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$

A general unitary transformation is a 2x2 matrix:

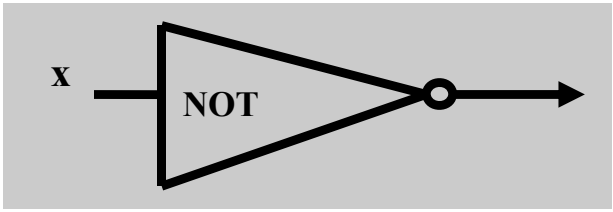
$$U_\theta = \begin{pmatrix} \cos(\theta/2) & \sin(\theta/2) \\ -\sin(\theta/2) & \cos(\theta/2) \end{pmatrix}$$



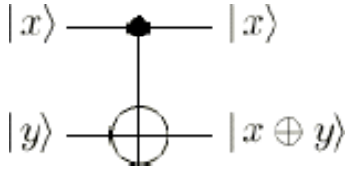
$U_\pi |1\rangle = |0\rangle$

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

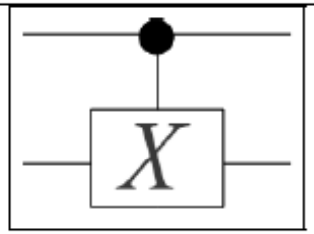
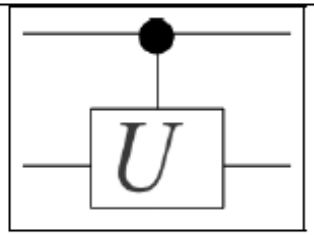
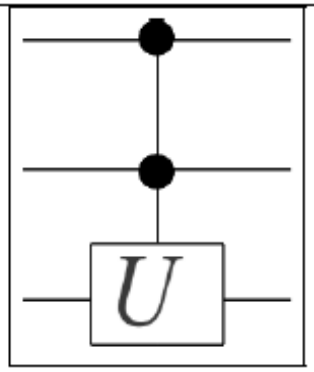
"NOT" gate



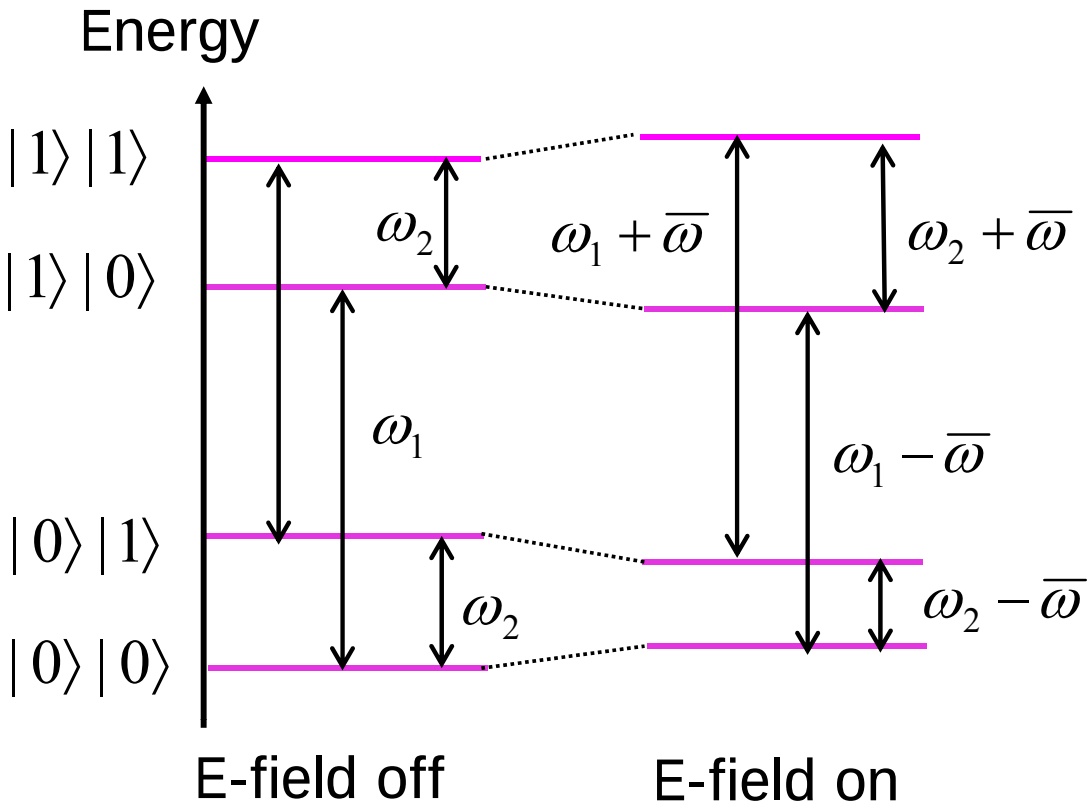
$$\text{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

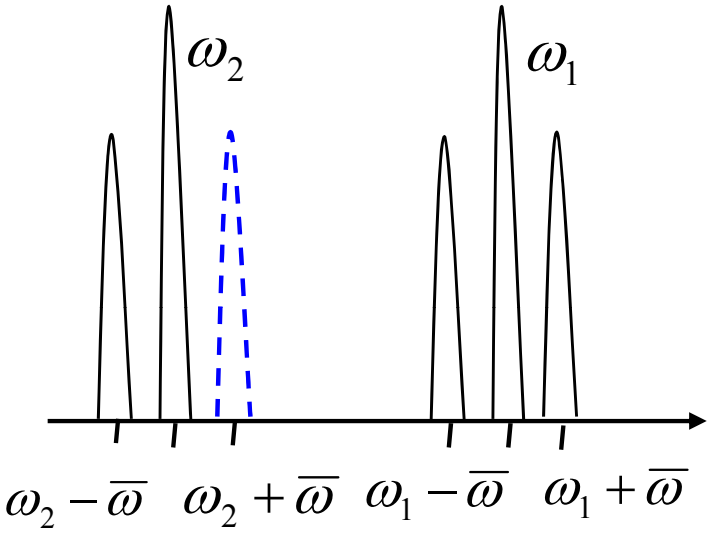


Quantum Gates

The name of the gate	The schematic view of the gate	The unitary matrix for the gate
CNOT (Control X)		$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
General control gate		$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & u_{00} & u_{01} \\ 0 & 0 & u_{10} & u_{11} \end{pmatrix}$
Multi control gate		$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & u_{00} & u_{01} \\ 0 & 0 & 0 & 0 & 0 & 0 & u_{10} & u_{11} \end{pmatrix}$

Controlled-NOT Gate

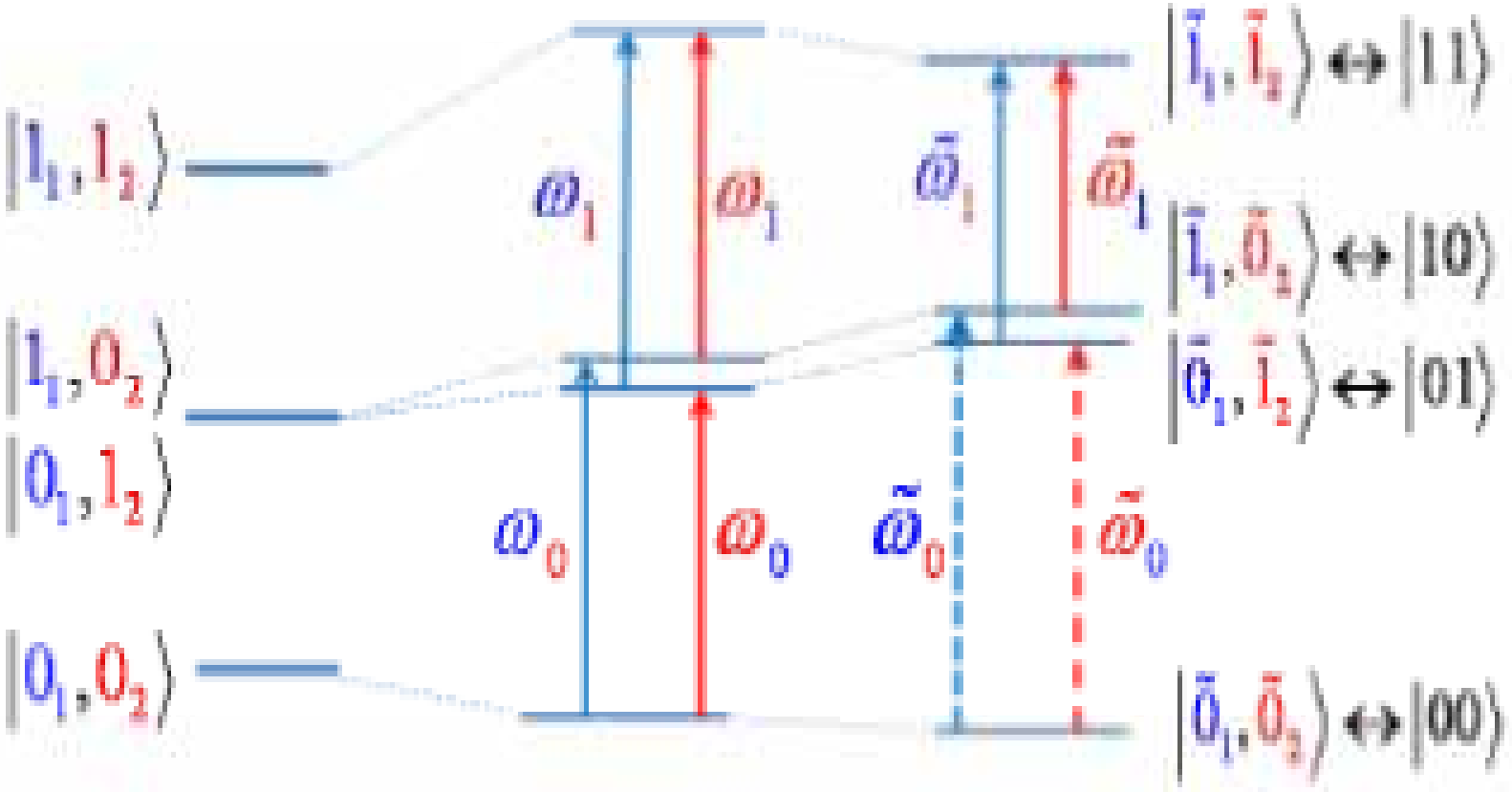




π-pulse at $\omega_2+\overline{\omega}$

$$|0\rangle\otimes|0\rangle\rightarrow|0\rangle\otimes|0\rangle$$
$$|0\rangle\otimes|1\rangle\rightarrow|0\rangle\otimes|1\rangle$$
$$|1\rangle\otimes|0\rangle\rightarrow|1\rangle\otimes|1\rangle$$
$$|1\rangle\otimes|1\rangle\rightarrow|1\rangle\otimes|0\rangle$$

CNOT Gate for Pendular States



Estimation of Characteristic Values

$$\vec{E}_{ext}(x) = [E_0 + x(\partial E/\partial x)]\hat{z}, \vec{E}_a = \vec{E}_{ext}(x_a) + \vec{E}_{\text{int}}(x_a)$$

$$\vec{E}_{\text{int}} = \sum_{b \neq a} -\vec{d}_b \Big/ |x_a - x_b|^3$$

Resonant frequency $\nu_a = \nu_0 + d_{eff} E_a / h \sim$ 3.5-6.0 GHz for E_{ext}=2-5 kV/cm

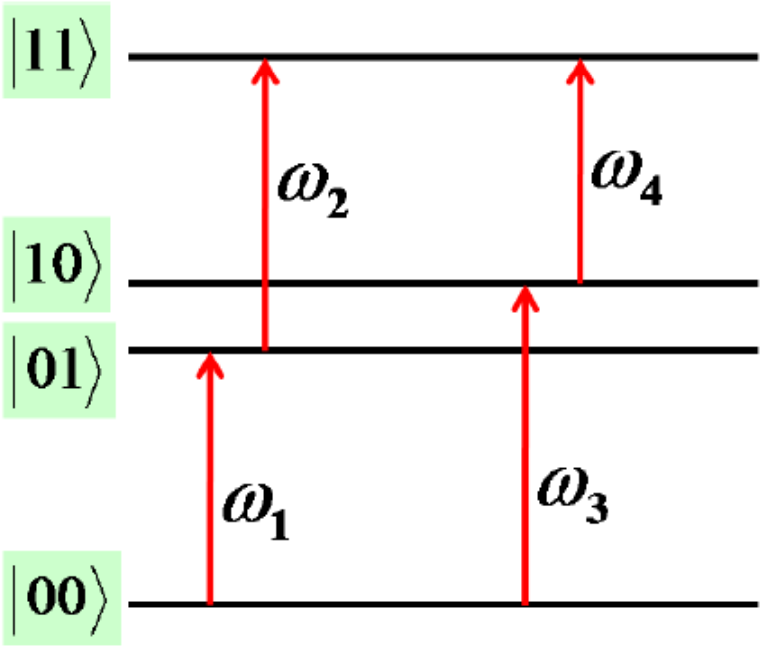
Resonant frequency difference per lattice site ~250kHz

$$\delta\nu = d^2{}_{eff} / 4\pi\varepsilon_0 (\lambda/2)^3 \sim 3kHz$$

CNOT Gate time $\tau \sim (2\pi\delta\upsilon)^{-1} \approx 50\mu s$

For a microwave π pulse, required field strength ~ 10 mV/cm

Generate Bell state



$$\omega_1 = W_1' - W_0' + \Omega_\alpha C_0 (C_1' - C_0')$$

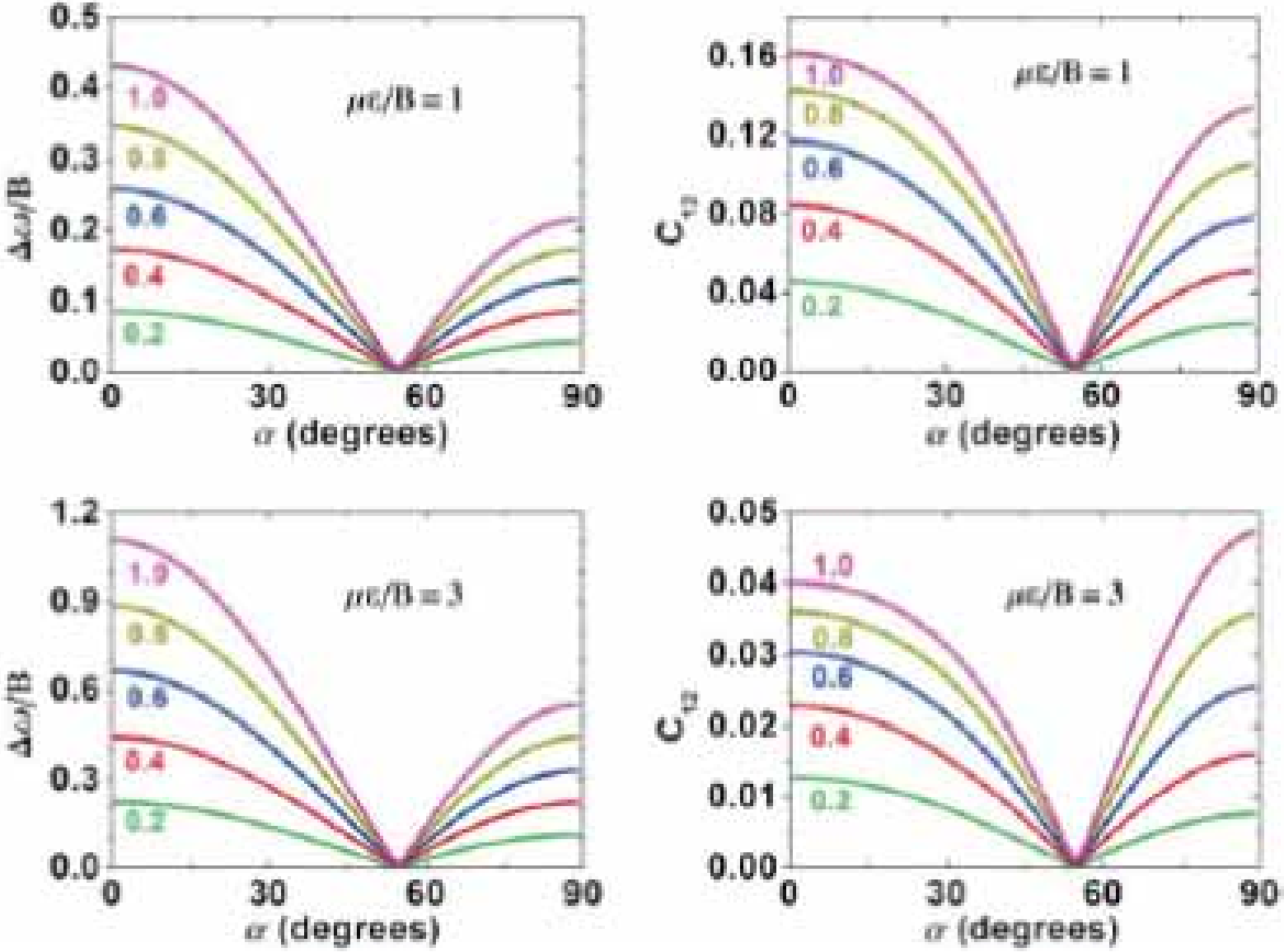
$$\omega_2 = W_1 - W_0 + \Omega_\alpha C_1' (C_1 - C_0)$$

$$\omega_3 = W_1 - W_0 + \Omega_\alpha C_0' (C_1 - C_0)$$

$$\omega_4 = W_1' - W_0' + \Omega_\alpha C_1 (C_1' - C_0')$$

$$|00\rangle \xrightarrow{\omega_1, \pi/2} \frac{|00\rangle + |01\rangle}{\sqrt{2}} \xrightarrow{\omega_2, \pi} \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

$$|00\rangle \xrightarrow{\omega_3, \pi/2} \frac{|00\rangle + |10\rangle}{\sqrt{2}} \xrightarrow{\omega_4, \pi} \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$



Frequency shift $\Delta\omega/B$ (left panels) and ground-state concurrence C_{12} (right panels) as functions of α, the orientation angle of the electric field. Curves are shown for $\Omega/B = 0.2$ to 1.0 with $\mu\varepsilon/B = 1$ or 3.

Frequency Shift

SrO : $\mu = 8.9\ D,\ B = 0.33\ cm^{-1},\ \lambda = 1\ \mu m \ \Rightarrow\ \Omega_\alpha / B \sim 10^{-5}$

$\mu\varepsilon/B$	$\mu\varepsilon'/B$	$\Delta\omega/B$	C_{12}
1.00	1.01	2.19×10^{-6}	1.20×10^{-6}
1.00	1.10	2.33×10^{-6}	1.17×10^{-6}
3.00	3.03	5.52×10^{-6}	3.57×10^{-7}
3.00	3.30	5.51×10^{-6}	3.34×10^{-7}

$$\Delta\omega = \omega_3 - \omega_2 = \omega_4 - \omega_1 = \Omega_\alpha (C_1 - C_0)(C_1' - C_0').$$

$$\Delta\omega \sim 20 - 60 \ \mathbf{kHz}$$

Experimental Resolution

$\Delta\omega \sim 20 - 60$ **kHz**

Line widths for rotational transition:

- Ultracold molecules trapped in optical lattice

No data have been reported on line widths for rotational transitions of ultracold molecules trapped in an optical lattice and subject to an external electric field

- Ordinary gas phase conditions: ~ a few 100 kHz

Conclusions

For quantum computing, a crucial issue is whether ω is large enough to enable the ω_2 transition to be reliably distinguished from ω_3 (and, equivalently, ω_1 from ω_4). For typical candidate polar molecules, this requires resolving transitions separated by only tens of kHz. That would not be feasible in conventional molecular spectroscopy. Under ordinary gas phase conditions, transitions between molecular rotational or pendular states have line widths of the order of a few 100 kHz.

At present, no data have been reported on line widths for rotational transitions of ultracold molecules trapped in an optical lattice and subject to an external electric field

THE JOURNAL OF CHEMICAL PHYSICS **138**, 024104 (2013)

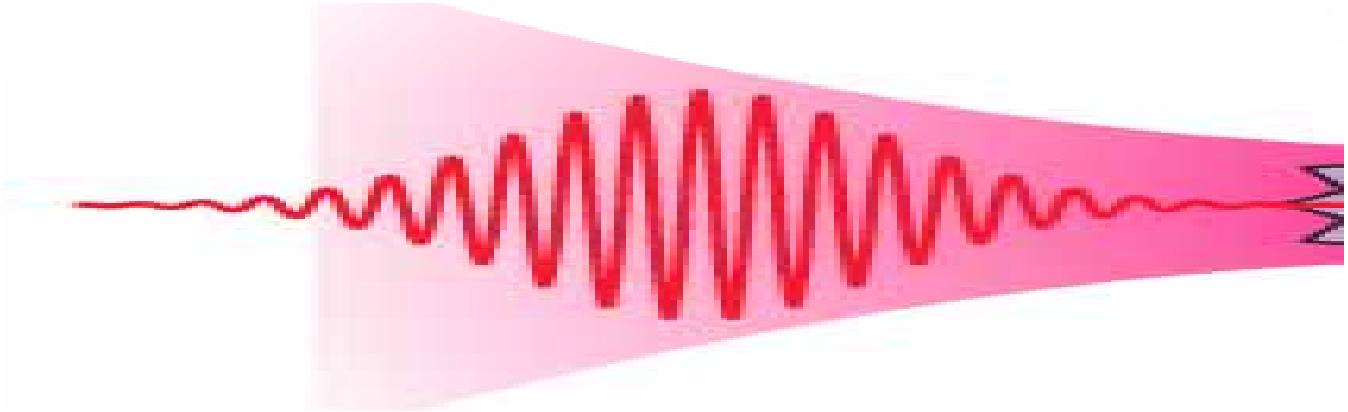
Implementation of quantum logic gates using polar molecules in pendular states

Jing Zhu,[1] Sabre Kais,[1,a)] Qi Wei,[2] Dudley Herschbach,[2] and Bretislav Friedrich[3]
[1]*Department of Chemistry, Physics and Birck Nanotechnology Center, Purdue University, West Lafayette, Indiana 47907, USA*
[2]*Department of Physics, Texas A&M University, College Station, Texas 77843, USA*
[3]*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany*

(Received 12 October 2012; accepted 18 December 2012; published online 10 January 2013)

Introduction of MTOCT

- Multi-target optimal control theory
  - The tool for calculating laser pulse guiding the quantum system to the selected objective state
  - Transfer an arbitrary number of *k* initial states into *k* target state simultaneously by just one laser field



Korff, B. M. R.; Troppmann, U.; Kompa, K. L. & de Vivie-Riedle, R., Journal of Chemical Physics, 2005, 123, 244509
Tesch, C. M. and de Vivie-Riedle,R. , Physical Review Letters, 2002,89, 157901

Research Objective

Implement laser pulses to realize different quantum logic gates

(such as NOT, Hadamard and CNOT)

on system of linear trapped polar molecules

System

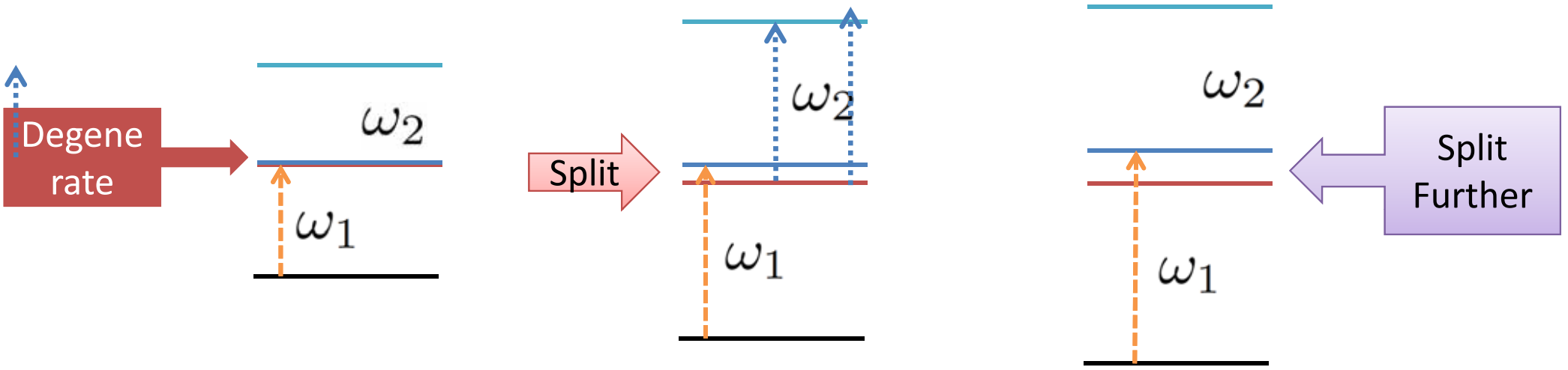
- Two polar molecules trapped in the electric field at low temperature (μK)
- The polar molecule candidate in the simulation is SrO
  - Permanent dipole moment of 8.9 Debye
  - Rotational constant B=0.33 cm^{-1}
  - The optical lattice wavelength of SrO λ=1μm and the space between them is λ/2.

Strategies to increase Δω

- Place two dipoles into different external electric fields
  - 1st dipole: $\mu\epsilon/_B = 2$ 2nd dipole: $\mu\epsilon/_B = 3$
  - External electric field strength: ~120-180 kV/cm
- Short the distance between two dipoles
  - The distance in the simulation is 0.05 μm , which is 10% of their length at optical lattice.

Wei, Q.; Kais, S.; Chen, Y. P.Journal of Chemical Physics, 2010, 132, 121104.
Murphy, B.; Hau, L. V.Physical Review Letters, 2009, 102, 033003.

Relations between dipole-dipole interaction; external electric field and frequency shift



Original State

Introduce dipole-dipole coupling

Further introduce external electric field

$$\Delta\omega = \omega_2 - \omega_1$$

$|00\rangle$ $|01\rangle$ $|10\rangle$ $|11\rangle$

System Hamiltonian

$$\mathcal{H}_{tot} = \mathcal{H}_{S1} + \mathcal{H}_{S2} + V_{dd}$$

$$\mathcal{H}_{S1} = \begin{pmatrix} W_0 & \\ & W_1 \end{pmatrix} \otimes \mathbf{I}_2 \qquad \mathcal{H}_{S2} = \mathbf{I}_2 \otimes \begin{pmatrix} W_0' & \\ & W_1' \end{pmatrix}$$

$$V_{dd} = \Omega \left(1 - \cos^2 \alpha\right) \left[\begin{pmatrix} C_0 & C_x \\ C_x & C_1 \end{pmatrix} \otimes \begin{pmatrix} C_0' & C_x' \\ C_x' & C_1' \end{pmatrix} \right]$$

$$C_0 = \langle 0 \left| \cos\theta \right| 0 \rangle ; \quad C_1 = \langle 1 \left| \cos\theta \right| 1 \rangle ; \quad C_x = \langle 0 \left| \cos\theta \right| 1 \rangle$$

MTOCT

- The target function:

$$J\left[\psi_{ik}\left(t\right),\,\psi_{fk}\left(t\right),\,\epsilon\left(t\right)\right]=\sum_{k=1}^{z}\left\{\left|\left\langle\psi_{ik}\left(T\right)\left|\phi_{fk}\right\rangle\right|^{2}-\alpha_{0}\int_{0}^{T}\frac{\left|\vec{E}\left(t\right)\right|^{2}}{S\left(t\right)}dt-2Re\left\{\left\langle\psi_{ik}\left(T\right)\left|\phi_{fk}\right\rangle\right.\right.\right.$$
$$\left.\left.\left.\times\int_{0}^{T}\left\langle\psi_{fk}\left(t\right)\left|\frac{i}{\hbar}\left[H-\vec{\mu}\cdot\vec{E}\left(t\right)\right]+\frac{\partial}{\partial t}\right|\psi_{ik}\left(t\right)\right\rangle dt\right\}\right\}$$

  - 1st term of RHS: Overlap of the initial wave functions ψ_{ik} driven by laser field, with the target ϕ_{fk} .
  - 2nd term: Controls the intensity of the laser
  - 3rd term: Ensures Time-dependent Schrödinger Equation is fulfilled for all time steps.

The Laser Pulse

$$E(t) = -\frac{z \cdot S(t)}{\hbar \cdot \alpha_0} \cdot \sum_{k=1}^{z} \mathrm{Im}\left\{\left\langle \psi_{ik}(t) \left| \psi_{fk}(t) \right\rangle \right.\right.$$
$$\left.\left. \left\langle \psi_{fk}(t) \left| \mu_1 \cdot cos\theta_1 + \mu_2 \cdot cos\theta_2 \right| \psi_{ik}(t) \right\rangle \right\}$$

$$\left\langle \psi_{fk}(t) \left| \mu_1 \cdot cos\theta_1 + \mu_2 \cdot cos\theta_2 \right| \psi_{ik}(t) \right\rangle = \mu \cdot \left\langle \psi_{fk}(t) \left| cos\theta_1 + cos\theta_2 \right| \psi_{ik}(t) \right\rangle$$

Numerical Approach to Obtain the Optimized Laser Pulse

- Rapid convergent iteration approach developed by the Rabitz in 1998

Step 1:

$$i\frac{\partial}{\partial t}\psi_i^{(0)}(t)=(H_0+V)\psi_i^{(0)}(t)-\mu\overline{\epsilon(t)}\psi_i^{(0)}(t),$$

$$i\frac{\partial}{\partial t}\psi_f^{(1)}(t)=(H_0+V)\psi_f^{(1)}(t)+\frac{\mu}{\alpha_0}\psi_f^{(1)}(t)$$
$$\times\mathrm{Im}(\langle\psi_i^{(0)}(t)|\psi_f^{(1)}(t)\rangle\langle\psi_f^{(1)}(t)|\mu|\psi_i^{(0)}(t)\rangle$$

Step 2:

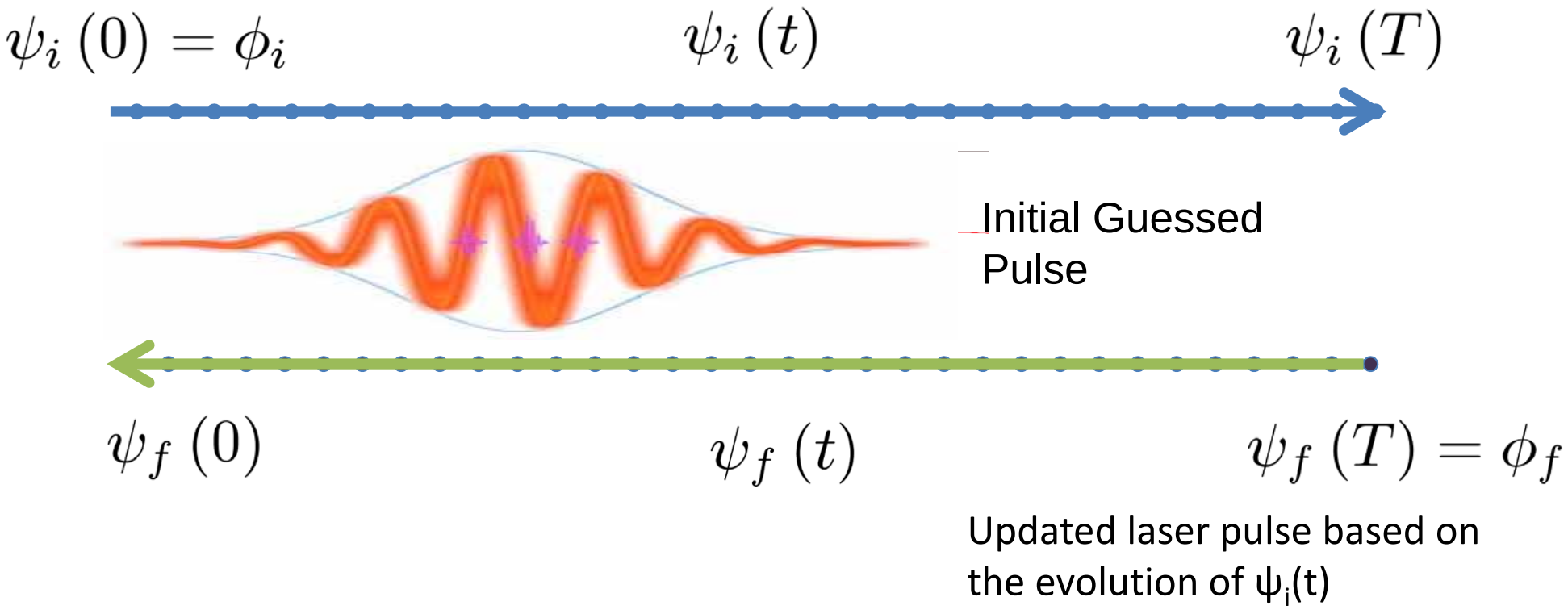
$$i\frac{\partial}{\partial t}\psi_i^{(1)}(t)=(H_0+V)\psi_i^{(1)}(t)+\frac{\mu}{\alpha_0}\psi_i^{(1)}(t)$$
$$\times\mathrm{Im}(\langle\psi_i^{(1)}(t)|\psi_f^{(1)}(t)\rangle\langle\psi_f^{(1)}(t)|\mu|\psi_i^{(1)}(t)\rangle)$$

$$i\frac{\partial}{\partial t}\psi_f^{(2)}(t)=(H_0+V)\psi_f^{(2)}(t)+\frac{\mu}{\alpha_0}\psi_f^{(2)}(t)$$
$$\times\mathrm{Im}(\langle\psi_i^{(1)}(t)|\psi_f^{(2)}(t)\rangle\langle\psi_f^{(2)}(t)|\mu|\psi_i^{(1)}(t)\rangle$$

Zhu, W. S.; Botina, J.; Rabitz, H.Journal of Chemical Physics 1998, 108, 1953-1963.

Numerical Approach Continued

- Illusion of the iteration approach:



Coefficients to check convergence

- The average transition probability

$$\bar{P} = \frac{1}{z} \cdot \sum_{k=1}^{z} \left| \langle \psi_{ik}(T) | \Phi_{fk} \rangle \right|^2$$

- The fidelity

$$F = \frac{1}{z^2} \cdot \left| \sum_{k=1}^{z} \langle \psi_{ik}(T) | \Phi_{fk} \rangle \right|^2$$

- The coupling constant $\Omega/B=0.01$
- The frequency shift $\Delta\omega=1.69\times10^{-3}$ cm^{-1}
- The time duration of the laser pulse should be $10\,\hbar/\Delta\omega$, which is 32 ns for this case.
- The self evolution of the SrO system is about 29 ps per circle.
- In the simulation, the basic time step at 0.25ps and the total length of the pulse is 32 ns. The max iterations are set at 300.

Bomble, L.; Pellegrini, P.; Ghesquiere, P.; Desouter-Lecomte, M.Physical Review A2010, 82,062323

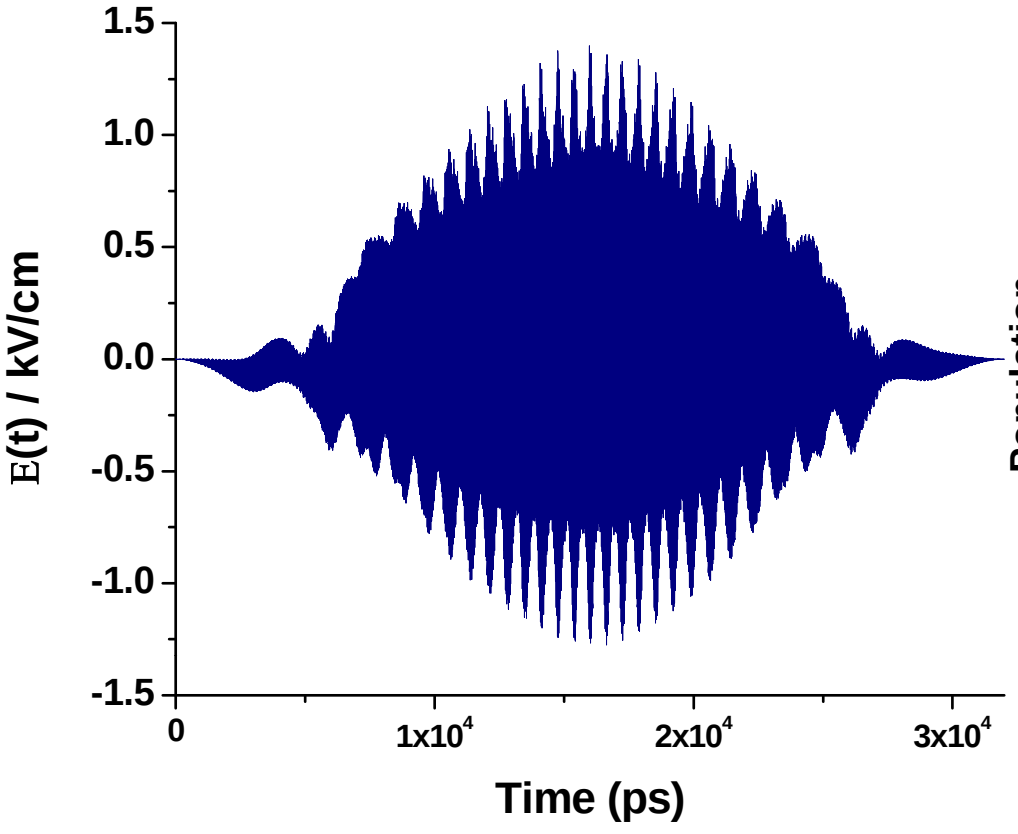
Simulation Result

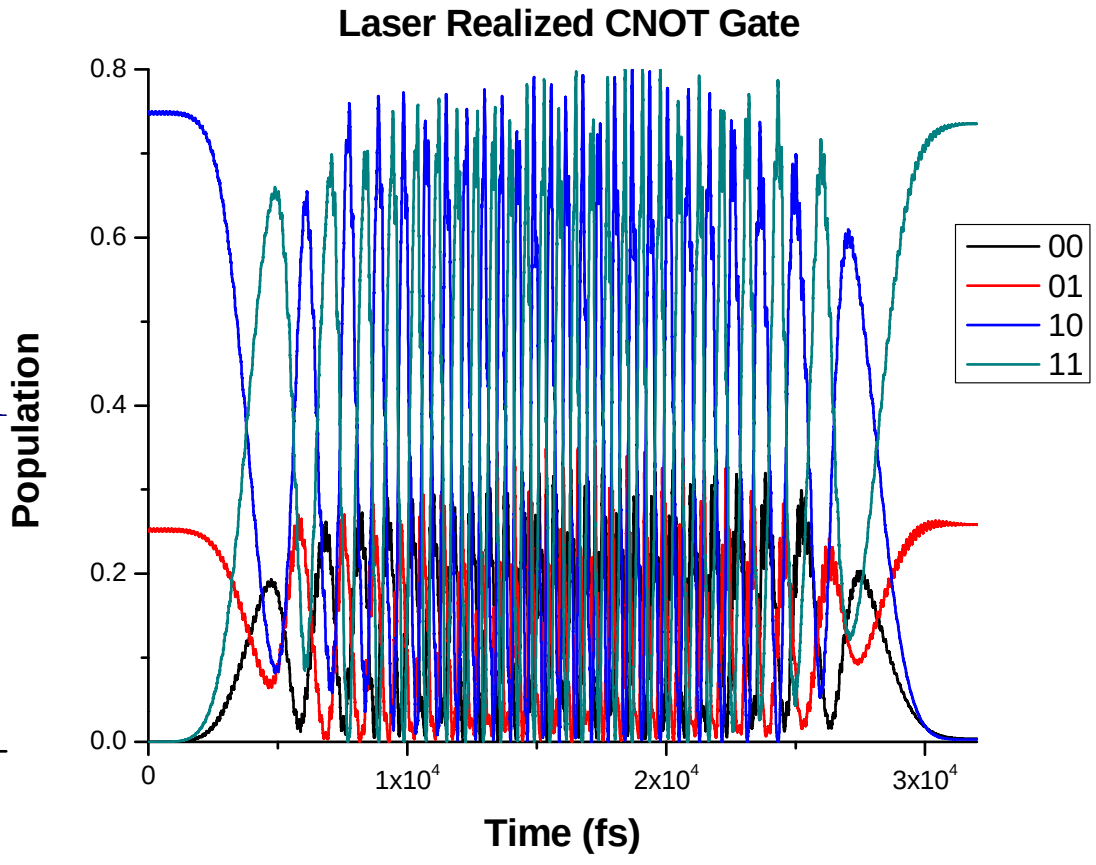
Table I: The initial and traget state of CNOT gate

i	Initial State	Target State
1	$\|00\rangle$	$\|00\rangle$
2	$\|01\rangle$	$\|01\rangle$
3	$\|10\rangle$	$\|11\rangle$
4	$\|11\rangle$	$\|10\rangle$
5	$\frac{1}{2}\left(\|00\rangle + \|01\rangle + \|10\rangle + \|11\rangle\right)$	$\frac{1}{2}e^{i\phi} \cdot \left(\|00\rangle + \|01\rangle + \|11\rangle + \|10\rangle\right)$

The Pulse for Realizing CNOT Gate

- CNOT Gate
  - $00 \rightarrow 00;\ 01 \rightarrow 01;\ 10 \rightarrow 11;\ 11 \rightarrow 10$
  - $\begin{pmatrix} 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 & \frac{1}{2} & 0 & \frac{\sqrt{3}}{2} \end{pmatrix}$



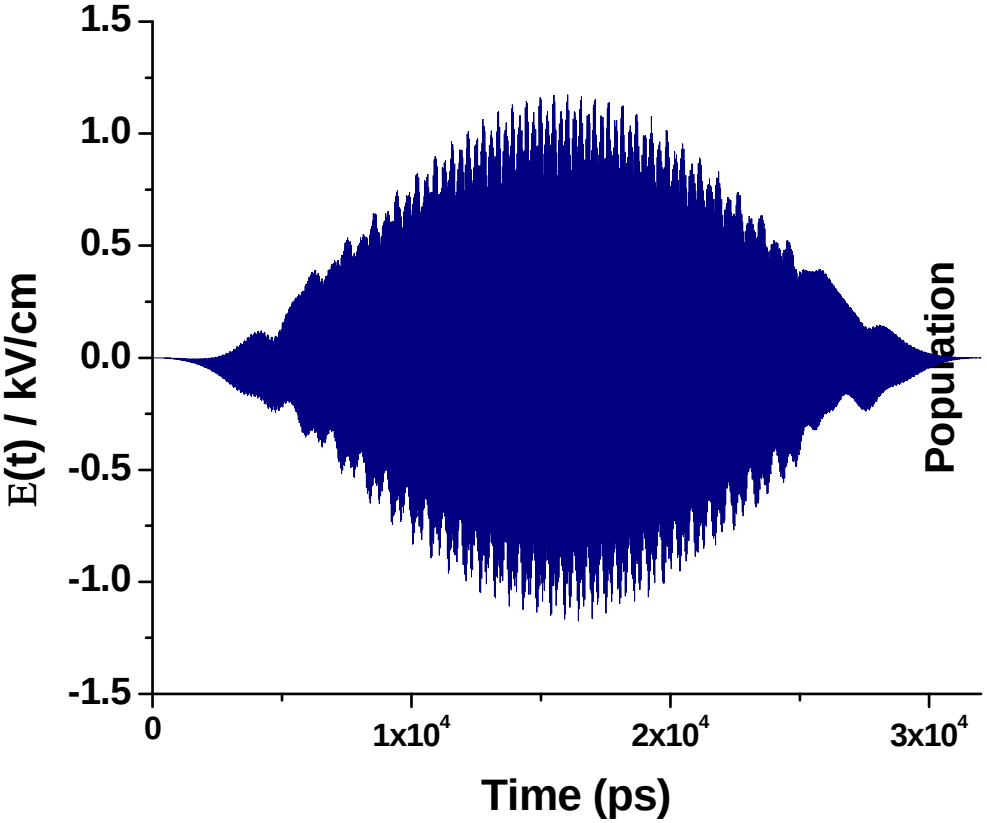


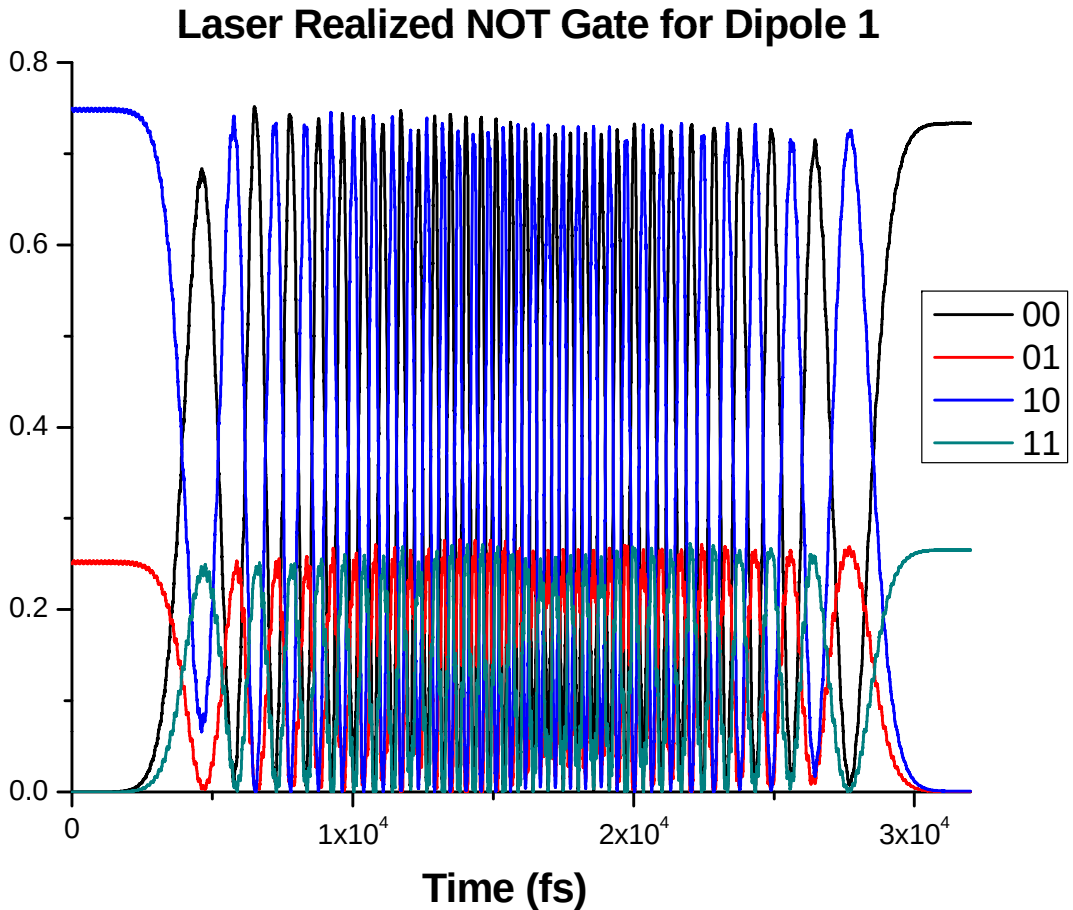
NOT gates for Molecule 1 and 2

i	Initial State	Target State	
		NOT gate for Molecule 1	NOT gate for Molecule 2
1	$\|00\rangle$	$\|10\rangle$	$\|01\rangle$
2	$\|01\rangle$	$\|11\rangle$	$\|00\rangle$
3	$\|10\rangle$	$\|00\rangle$	$\|11\rangle$
4	$\|11\rangle$	$\|01\rangle$	$\|10\rangle$
5	$\frac{1}{2}(\|00\rangle + \|01\rangle + \|10\rangle + \|11\rangle)$	$\frac{1}{2}e^{i\phi} \cdot (\|10\rangle + \|11\rangle + \|00\rangle + \|01\rangle)$	$\frac{1}{2}e^{i\phi} \cdot (\|01\rangle + \|00\rangle + \|11\rangle + \|10\rangle)$

The Pulse for NOT Gate for Dipole 1

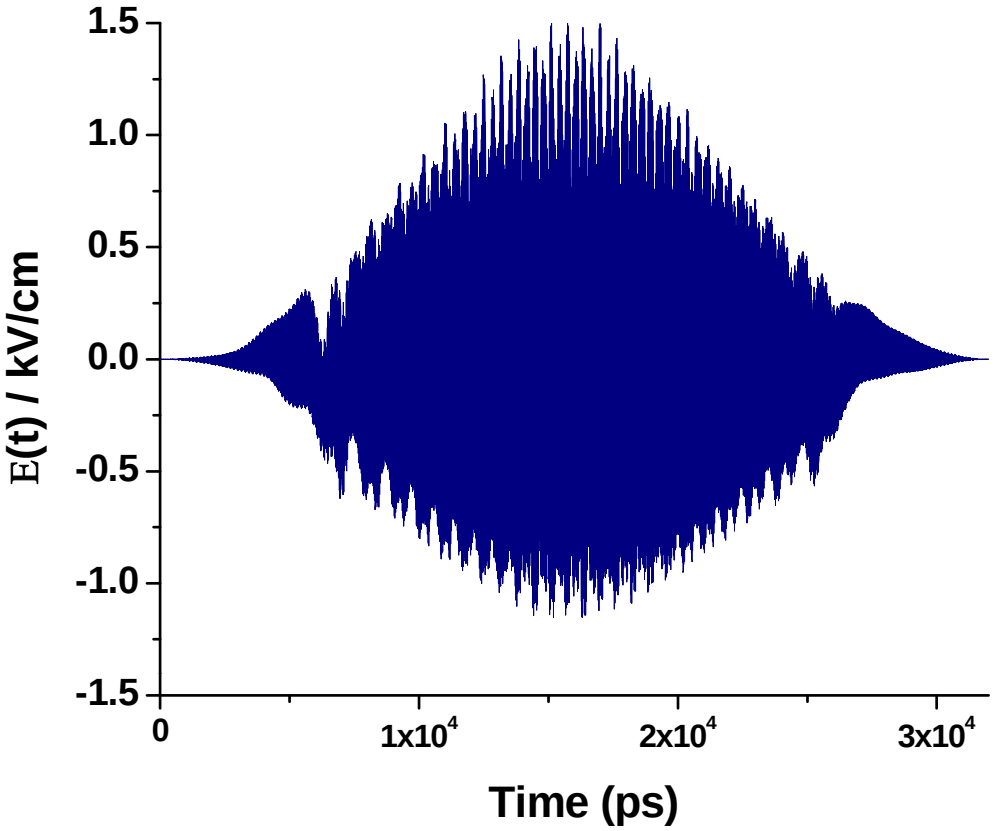
- NOT Gate for Dipole 1
  - $00 \rightarrow 10;\ 01 \rightarrow 11;\ 10 \rightarrow 00;\ 11 \rightarrow 01$
  - $\begin{pmatrix} 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \end{pmatrix} \rightarrow \begin{pmatrix} \frac{\sqrt{3}}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix}$

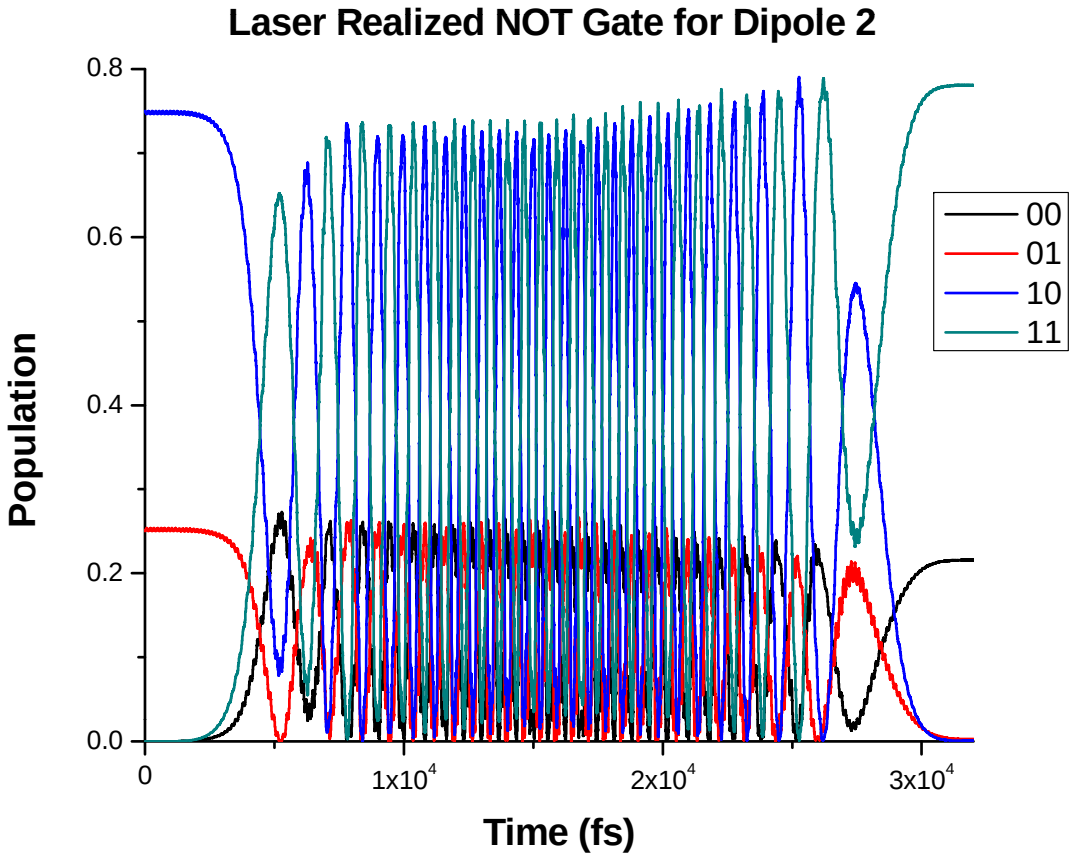




The Pulse for NOT Gate for Dipole 2

- NOT Gate for Diple 2
  - $00 \rightarrow 01;\ 01 \rightarrow 00;\ 10 \rightarrow 11;\ 11 \rightarrow 10$
  - $\begin{pmatrix} 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \end{pmatrix} \rightarrow \begin{pmatrix} \frac{1}{2} & 0 & 0 & \frac{\sqrt{3}}{2} \end{pmatrix}$



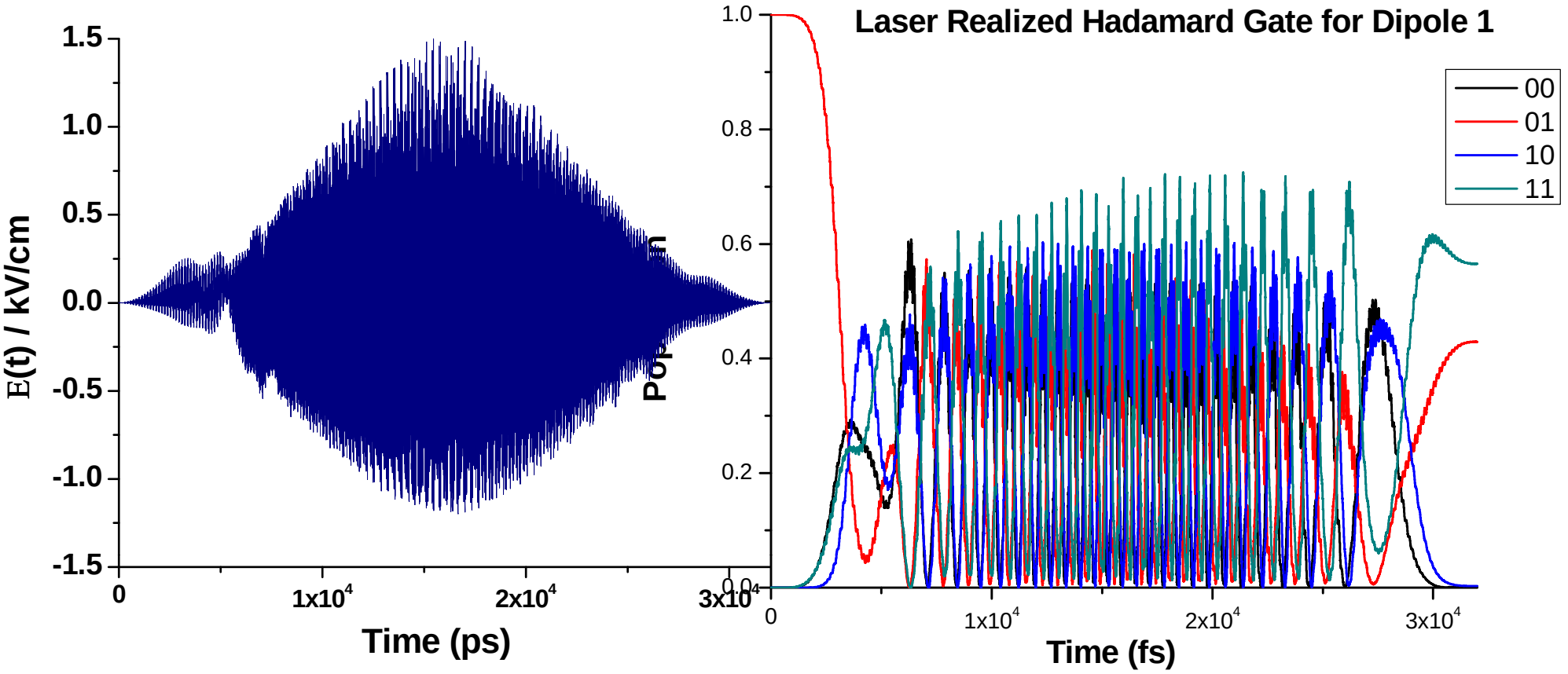


Hadamard gate for both molecules

i	Initial State	Target State	
		Hadamard gate for Molecule 1	Hadamardgate for Molecule 2
1	$\|00\rangle$	$\frac{1}{\sqrt{2}}(\|00\rangle + \|10\rangle)$	$\frac{1}{\sqrt{2}}(\|00\rangle + \|01\rangle)$
2	$\|01\rangle$	$\frac{1}{\sqrt{2}}(\|01\rangle + \|11\rangle)$	$\frac{1}{\sqrt{2}}(\|00\rangle - \|01\rangle)$
3	$\|10\rangle$	$\frac{1}{\sqrt{2}}(\|00\rangle - \|10\rangle)$	$\frac{1}{\sqrt{2}}(\|10\rangle + \|11\rangle)$
4	$\|11\rangle$	$\frac{1}{\sqrt{2}}(\|01\rangle - \|11\rangle)$	$\frac{1}{\sqrt{2}}(\|10\rangle - \|11\rangle)$
5	$\frac{1}{2}(\|00\rangle + \|01\rangle + \|10\rangle + \|11\rangle)$	$\frac{1}{\sqrt{2}}e^{i\phi} \cdot (\|00\rangle + \|01\rangle)$	$\frac{1}{\sqrt{2}}e^{i\phi} \cdot (\|00\rangle + \|10\rangle)$

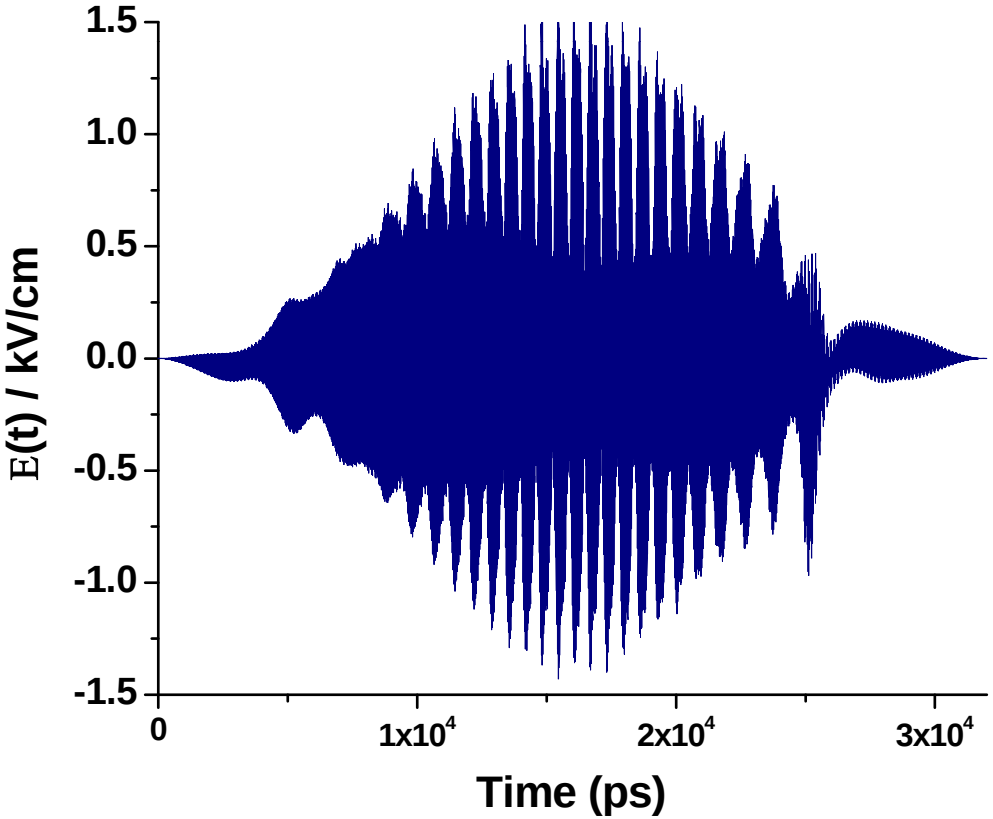
The Pulse for Hadamard Gate for Dipole 1

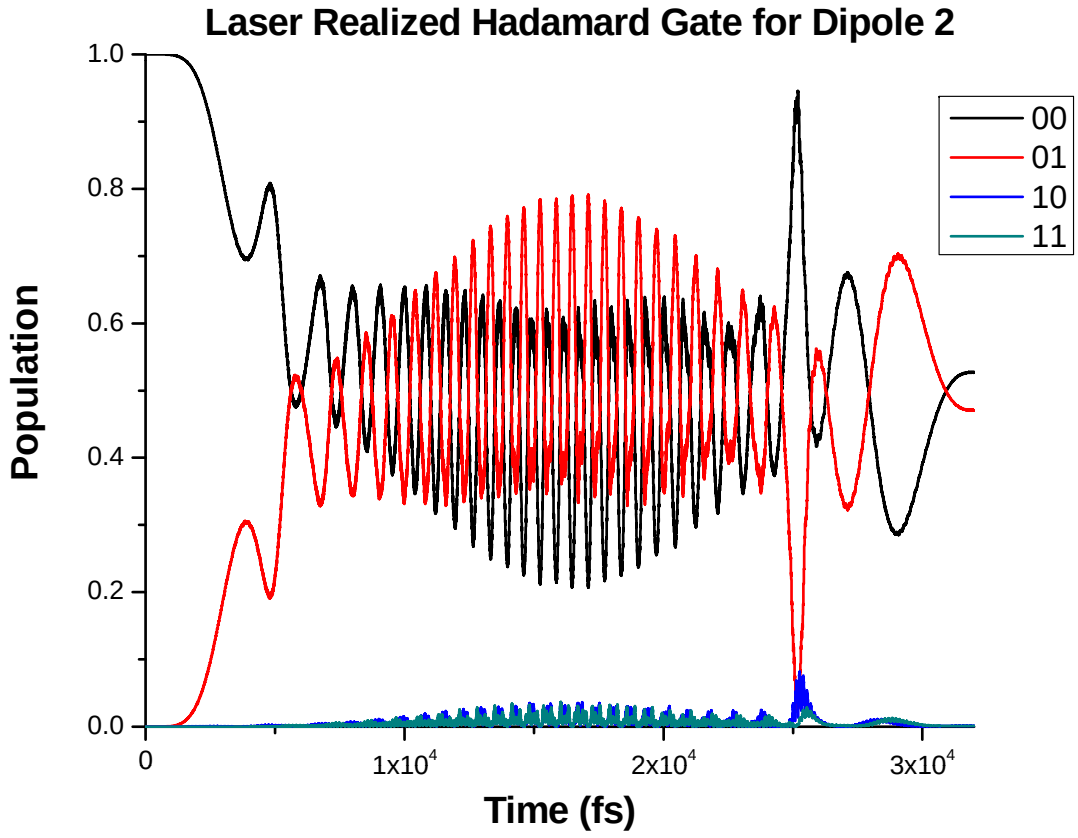
- Hadamard Gate for Dipole 1
  - $00 \rightarrow \frac{1}{\sqrt{2}}(0+1) \otimes 0;\ 01 \rightarrow \frac{1}{\sqrt{2}}(0+1) \otimes 1;\ 10 \rightarrow \frac{1}{\sqrt{2}}(0-1) \otimes 0$
    $11 \rightarrow \frac{1}{\sqrt{2}}(0-1) \otimes 1$



The Pulse for Hadamard Gate for Dipole 2

- Hadamard Gate for Dipole 2
  - $00 \rightarrow 0 \otimes \frac{1}{\sqrt{2}}(0+1)\,;\; 01 \rightarrow 0 \otimes \frac{1}{\sqrt{2}}(0-1)\,;\; 10 \rightarrow 1 \otimes \frac{1}{\sqrt{2}}(0+1)$
    $11 \rightarrow 1 \otimes \frac{1}{\sqrt{2}}(0-1)$





Conclusion

- Applied the MTOCT theory to obtain the optimized laser pulse to quantum logic gates, such as CNOT, NOT and Hadamdard gates, with high fidelity
- After reducing the distance to 10% of that in the optical lattice, the energy shift becomes 51MHz and can be resolved by the laser with the duration time of 32μs

New Directions

THE JOURNAL OF CHEMICAL PHYSICS **135**, 154102 (2011)

Entanglement of polar symmetric top molecules as candidate qubits

Qi Wei,[1] Sabre Kais,[2] Bretislav Friedrich,[3] and Dudley Herschbach[1,a)]

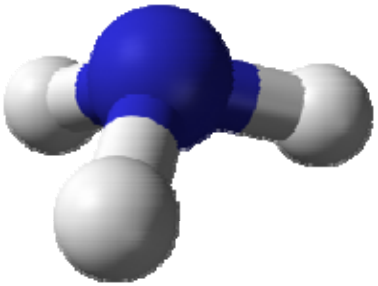
[1]*Department of Physics, Texas A & M University, College Station, Texas 77843, USA*

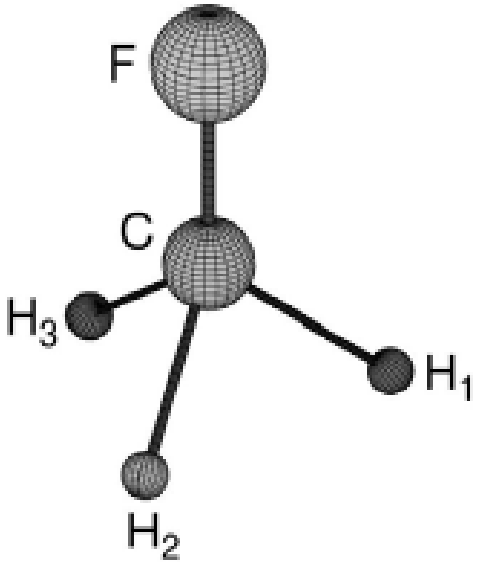
[2]*Department of Chemistry, Purdue University, West Lafayette, Indiana 47907, USA*

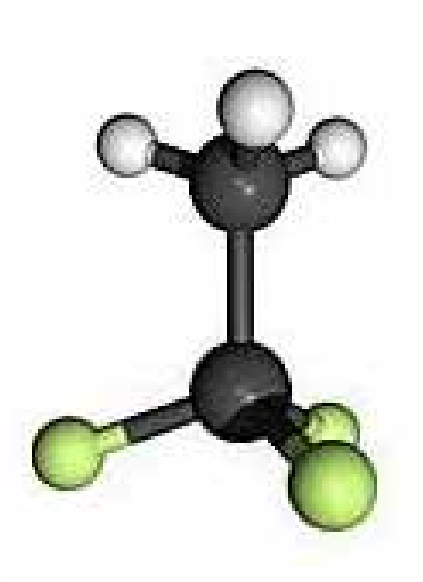
[3]*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany*

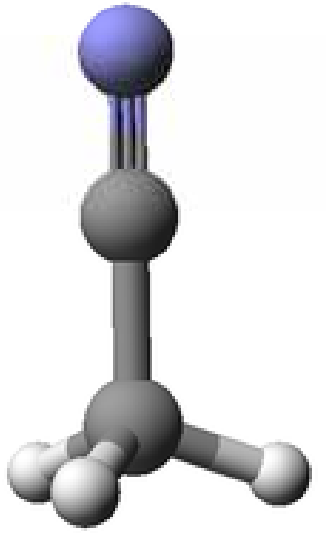
(Received 1 August 2011; accepted 21 September 2011; published online 17 October 2011)

Symmetric Top Molecules



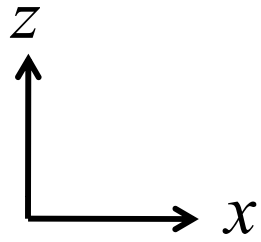






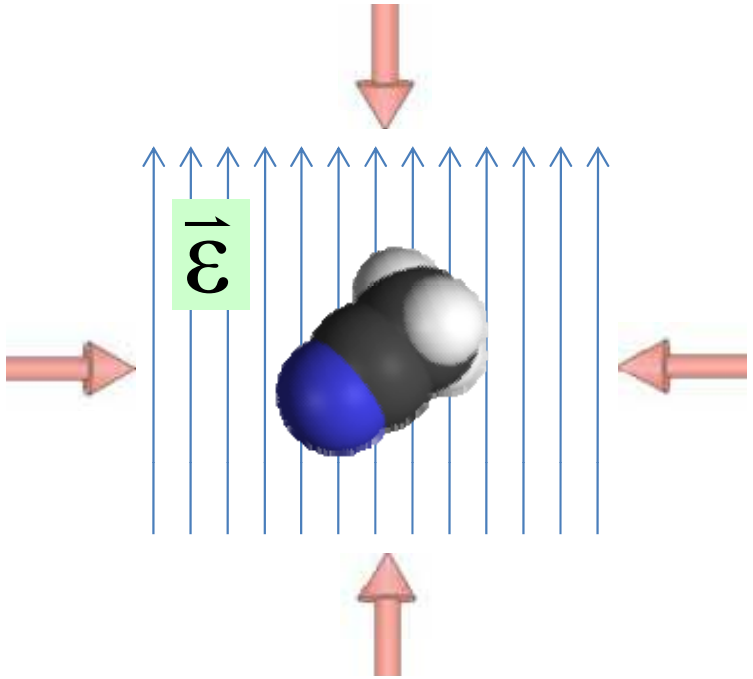
NH_3 CH_3F CH_3CF_3 CH_3CN

Property : $I_x = I_y \neq I_z$



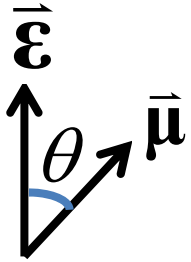
Hamiltonian of Single Molecule

$$\hat{H} = \hat{H}_R + \hat{H}_S + \hat{H}_T$$



$$\hat{H}_R = B\hat{\mathrm{J}}^2 + (A-B)\hat{\mathrm{J}}_z^2 \Leftarrow \text{Rotational}$$

$$\hat{H}_S = \vec{\mu}\cdot\vec{\varepsilon} = \mu\varepsilon\cos\theta \Leftarrow \text{Stark}$$



$$\hat{H}_T = \frac{p^2}{2m} + V_{trap} \Leftarrow \text{Trapping (assume constant)}$$

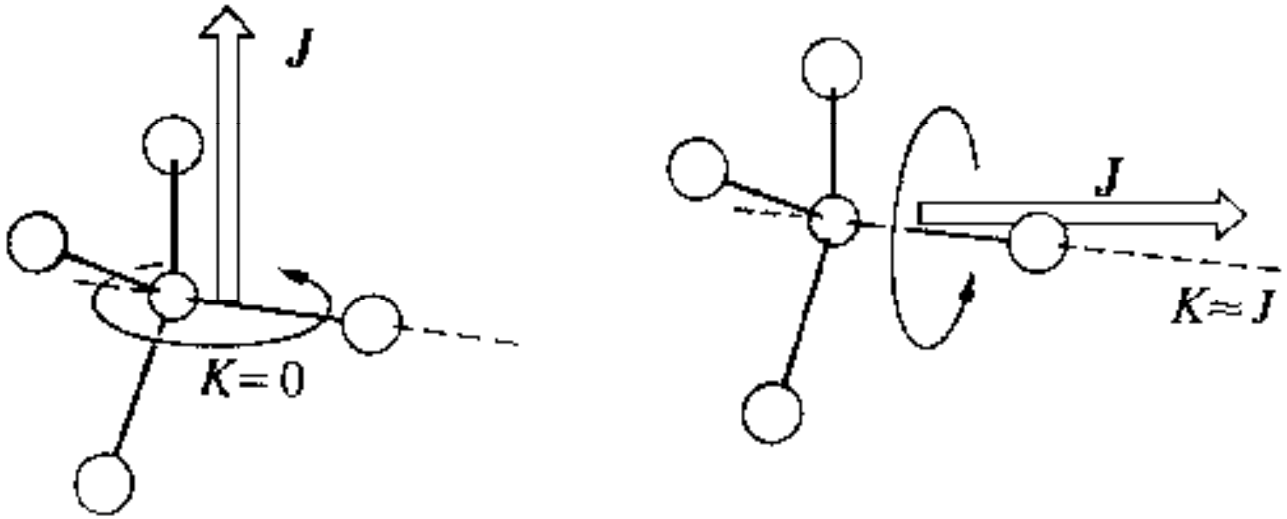
Rotational & Stark

Rotational energy : $\mathrm{E_R}(J,K) = BJ(J+1) + (A-B)K^2$

Total rotational angular momentum : $J = 0, 1, 2, 3, 4, ...$

Projection of J along molecular axis : $K = 0, \pm 1, \pm 2, ...,\pm J$

CH_3F



Stark energy : $\mathrm{E_S}(J,K,M_J) = -\mu\mathcal{E}M_J K/J(J+1)$

Projection of J along external field : $M_J = 0, \pm 1, \pm 2, ...,\pm J$

Effective dipole moment : $\mu_{\mathrm{eff}} = -\partial E_S/\partial\mathcal{E} = -\mu M_J K/J(J+1)$

Symmetric Top Molecules

Qubits:

$|0\rangle = |J,K,M\rangle = |1,1,+1\rangle$

$|1\rangle = |J,K,M\rangle = |1,1,-1\rangle$

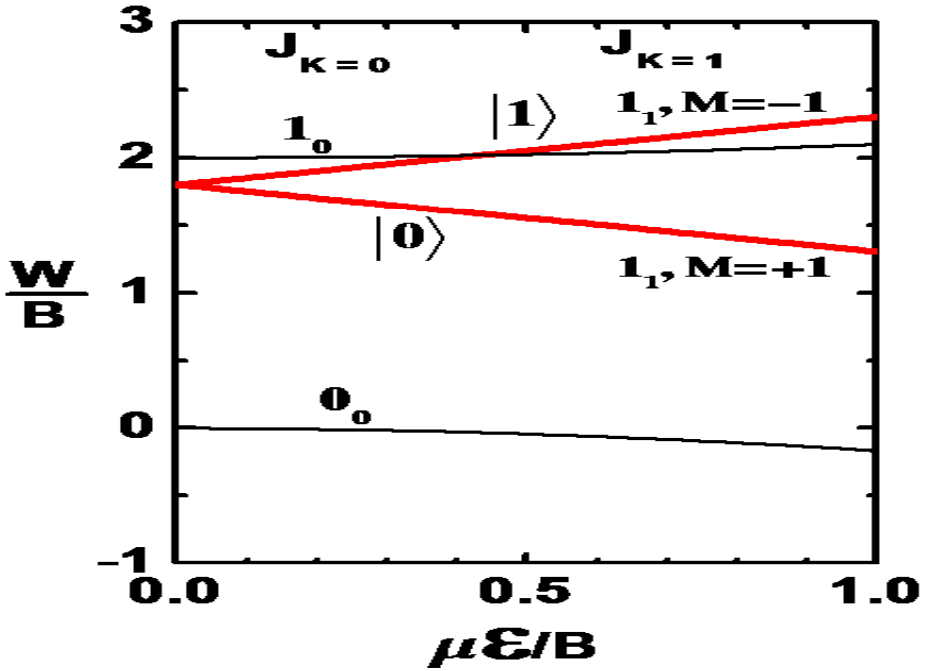
$J=0,1,2,\ldots \quad K=0,\pm1,\pm2,\ldots$

$\Delta J=0,\pm1 \qquad \Delta K=0 \qquad$ for $K\neq0$

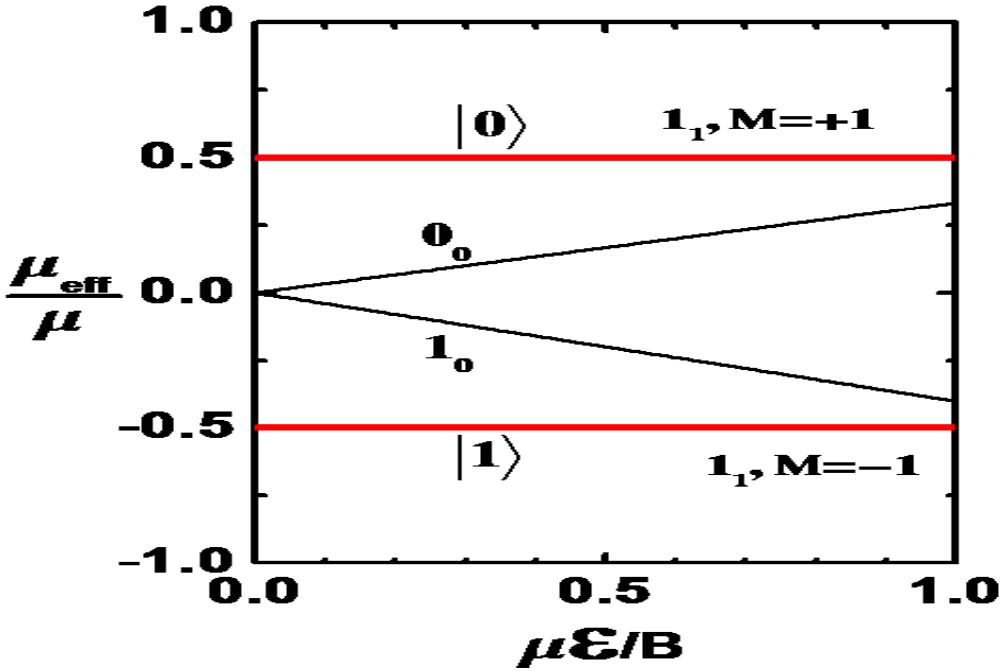
$\Delta J=\pm1 \qquad \Delta K=0 \qquad$ for $K=0$

Energy levels W and effective dipole moments μ_{eff} for a symmetric top molecule in an electric field

K = quantum number denoting projection of J on the symmetry axis of the molecule



(a)



(b)

Note that, in contrast to the diatomic case, here the qubit states split apart linearly as field increases; allows use low field strength to increase Ω/ω greatly, giving access to region where entanglement is large

Symmetric Top

- **Initial Hamiltonian**

$$\mathcal{H}^{st} = \mathcal{H}_R^{st} + \mathcal{H}_S^{st} + \mathcal{H}_T^{st} + \mathcal{H}_{s.q.}^{st}$$
$$\mathcal{H}_R^{st} = B \cdot \boldsymbol{J}^2 + (A - B) \cdot \boldsymbol{J}_z^2$$
$$\mathcal{H}_S^{st} = -\vec{\mu} \cdot \vec{\epsilon} = -\mu\epsilon \cos\theta$$

$$\left|0^{st}\right\rangle = \left|J = 1,\ K = 1,\ M_J = +1\right\rangle$$
$$\left|1^{st}\right\rangle = \left|J = 1,\ K = 1,\ M_J = -1\right\rangle$$

$$W_0^{st} = A + B - \frac{\mu\epsilon}{2};\ W_1^{st} = A + B + \frac{\mu\epsilon}{2}$$

$$C_0^{st} = \langle 0 \left|\cos\theta\right| 0\rangle = \frac{1}{2};\ \ C_1^{st} = \langle 1 \left|\cos\theta\right| 1\rangle = -\frac{1}{2};\ \ C_x^{st} = \langle 0 \left|\cos\theta\right| 1\rangle = 0$$

- **Simplified Hamiltonian**

$$\mathcal{H}_{total}^{st} = 2(A + B) \cdot \mathbf{I}_4 + \frac{\mu}{2}\left(\epsilon \cdot \sigma_z \otimes \mathbf{I}_2 + \epsilon' \cdot \mathbf{I}_2 \otimes \sigma_z\right) + \frac{\Omega\left(1 - \cos^2\alpha^{st}\right)}{4} \cdot \sigma_z \otimes \sigma_z$$

- **NMR Hamiltonian**: $\mathcal{H} = v_1 \hat{\mathbb{I}}_{1z} + v_2 \hat{\mathbb{I}}_{2z} + J_{12} \hat{\mathbb{I}}_{1z} \hat{\mathbb{I}}_{2z}$

Conclusions

Symmetric top molecules, with first-order Stark effect, offer a means to obtain $\Omega/\omega \sim 1$ and hence large concurrence.

In the region $\Omega/\omega <$ or ~ 1 the max concurrence occurs for temperatures so low that only ground state concurrence matters much.

ENTANGLEMENT CREATION IN COLD MOLECULAR GASES USING STRONG LASER PULSES

Felipe Herrera, Purdue - Harvard
Birgitta Whaley and Berkeley
Sabre Kais Purdue

New Journal of Physics (submitted, 2013)

Entanglement of cold molecules with off-resonant laser pulses

Rotational structure in off-resonant optical fields

$$\hat{H} = \hat{H}_{\mathrm{R}} + \hat{H}_{\mathrm{AC}}$$

Rigid Rotor

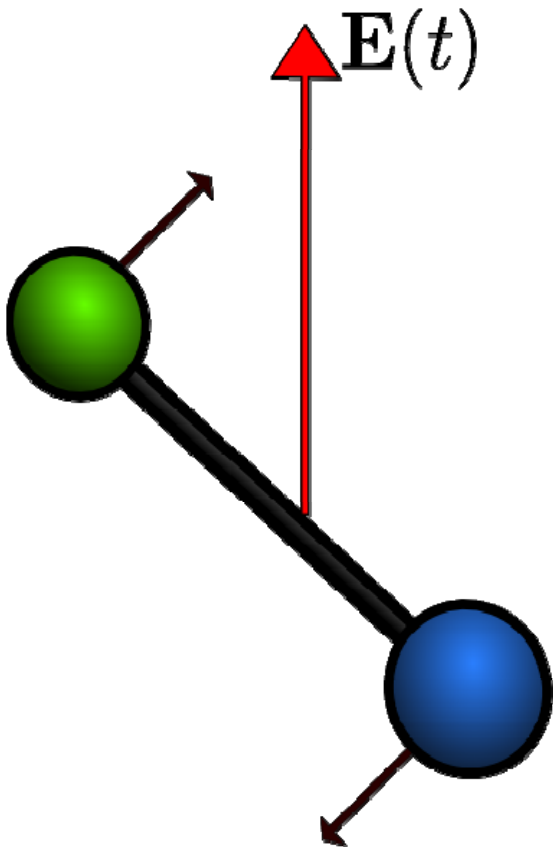
$$\hat{H}_{\mathrm{R}} = B_e \hat{N}^2$$

Light-induced potential

$$\hat{H}_{\mathrm{AC}} = -\frac{|E_0|^2}{4}\left\{\frac{1}{3}(\alpha_{\parallel} + 2\alpha_{\perp}) + \frac{2}{3}(\alpha_{\parallel} - \alpha_{\perp})C_{2,0}(\theta)\right\}$$

Molecules in far-detuned laser fields

- Semiclassical picture



Strong off-resonant laser field

$$\mathbf{E}(t) = E_0 \mathbf{e}_Z \cos(\omega t)$$

Instantaneous dipole moment

$$\mathbf{d}(t) = \alpha \mathbf{E}(t)$$

Light-matter interaction

$$U = -\langle \mathbf{d}(t) \cdot \mathbf{E}(t) \rangle$$

Molecules in far-detuned laser fields

- Rotational structure

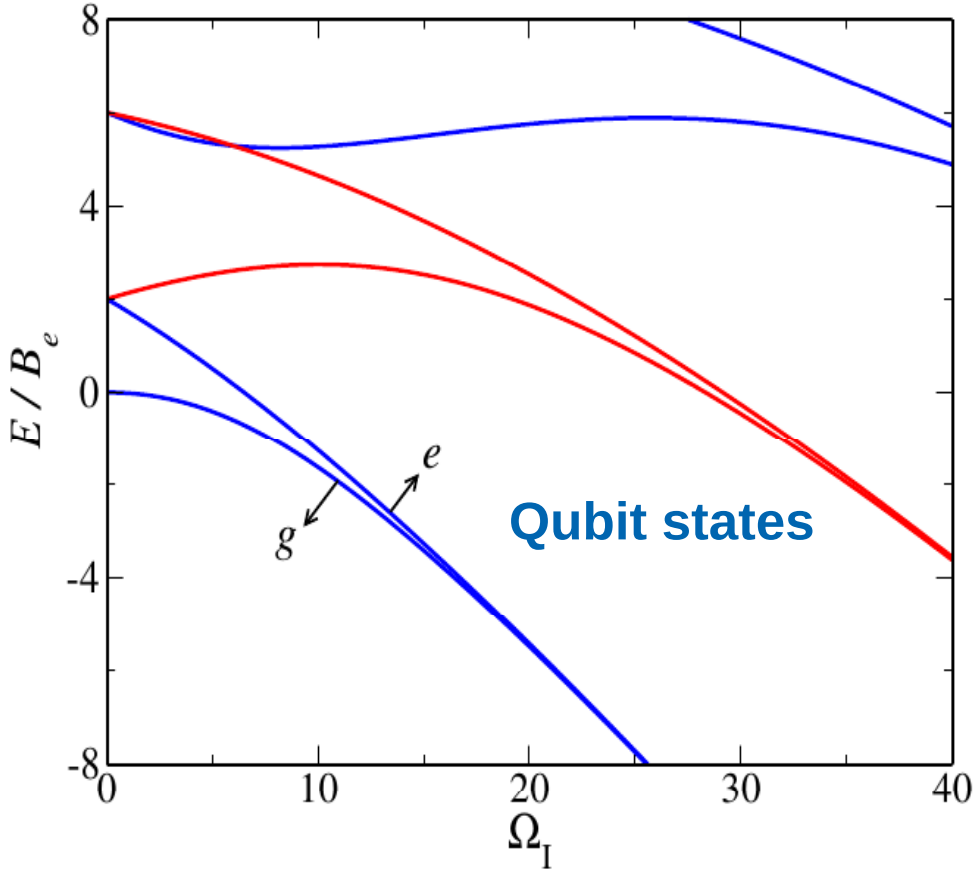
Light-matter Hamiltonian

$$\hat{H} = \hat{N}^2 - \Omega_I \cos^2\theta$$

Laser intensity parameter

$$\Omega_I = \frac{(\alpha_\parallel - \alpha_\perp)|E_0|^2}{4B_e}$$

Field-dressed rotational spectrum



Eigenstates have definite parity

Qubit transition energy decreases exponentially with inter

Alignment-mediated entanglement

- Two-molecule evolution in a strong pulse

$$|\Psi(t)\rangle = a(t)|g_1 g_2\rangle + b(t)|e_1 e_2\rangle$$

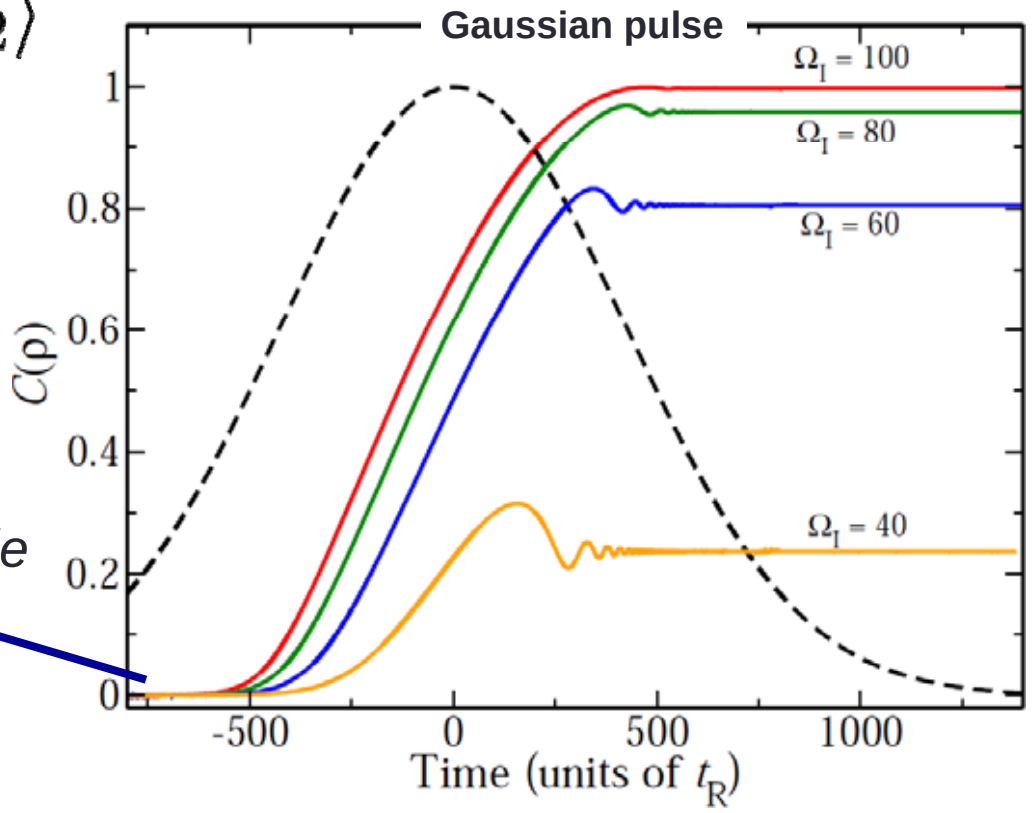
Bipartite concurrence

$$C(\rho) = 2|ab|$$

Interaction time

$$t_{\mathrm{dd}} = \hbar / U_{\mathrm{dd}}$$

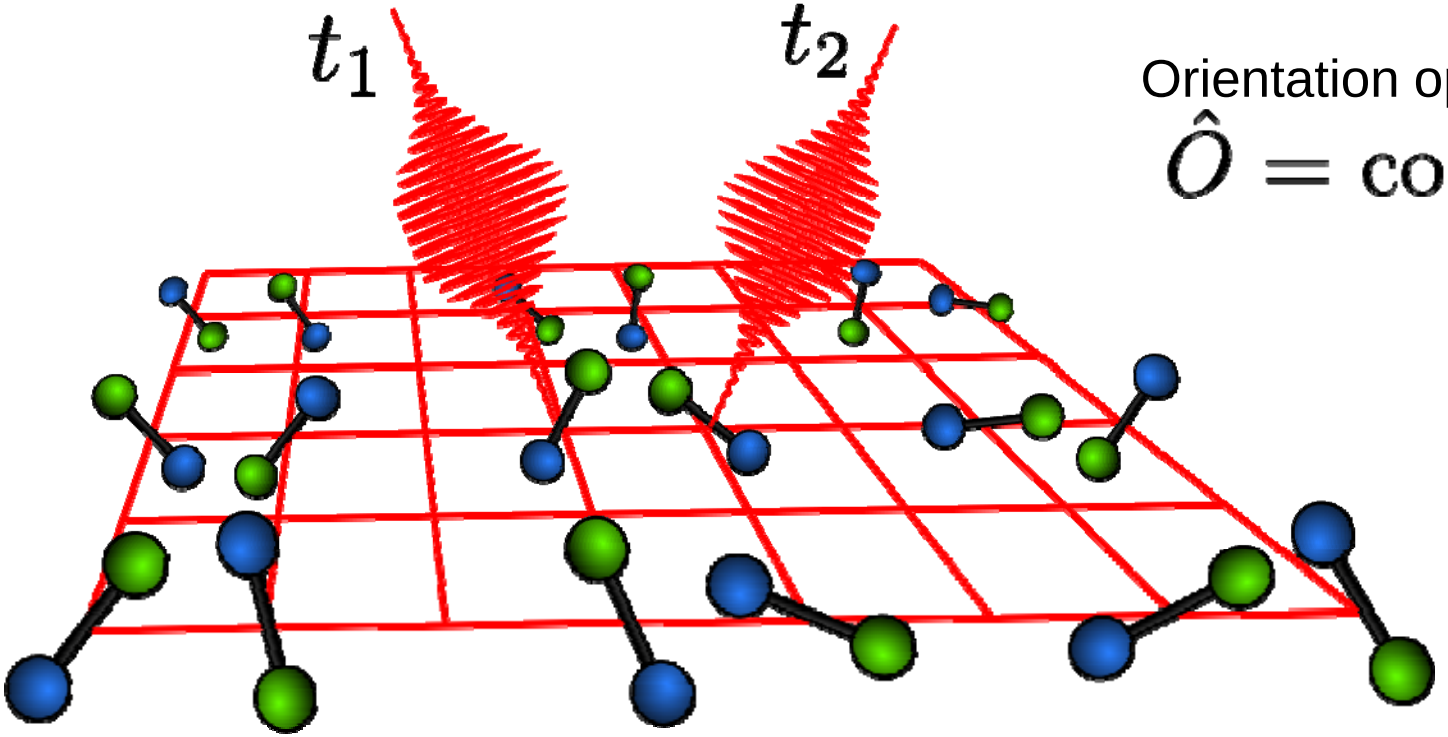
Initially separable states



Molecules remain entangled after the pulse is

Entanglement in optical traps

- Binary correlations in double well lattices



Orientation operator

$$\hat{O} = \cos\theta$$

Orientation correlation measurements

$$E(t_1, t_2) = \langle \hat{O}(t_1)\hat{O}(t_2) \rangle$$

Violation of Bell's inequalities with polar molecules in optical lattices

$$|\Psi\rangle = a|g_1 g_2\rangle + b|e_1 e_2\rangle$$

$$E(t_a, t_b) = \frac{1}{3}\left(2|ab|\right)\cos\left(\omega_{10} t_a + \omega_{10} t_b + \theta_{ba}\right)$$

$$S_1(t) = E(0,0) + E(0,t) + E(t,0) - E(t,t)$$

$$a^* b = |ab| \mathrm{e}^{i\theta_{ba}} \qquad t_a = t_b = 0$$

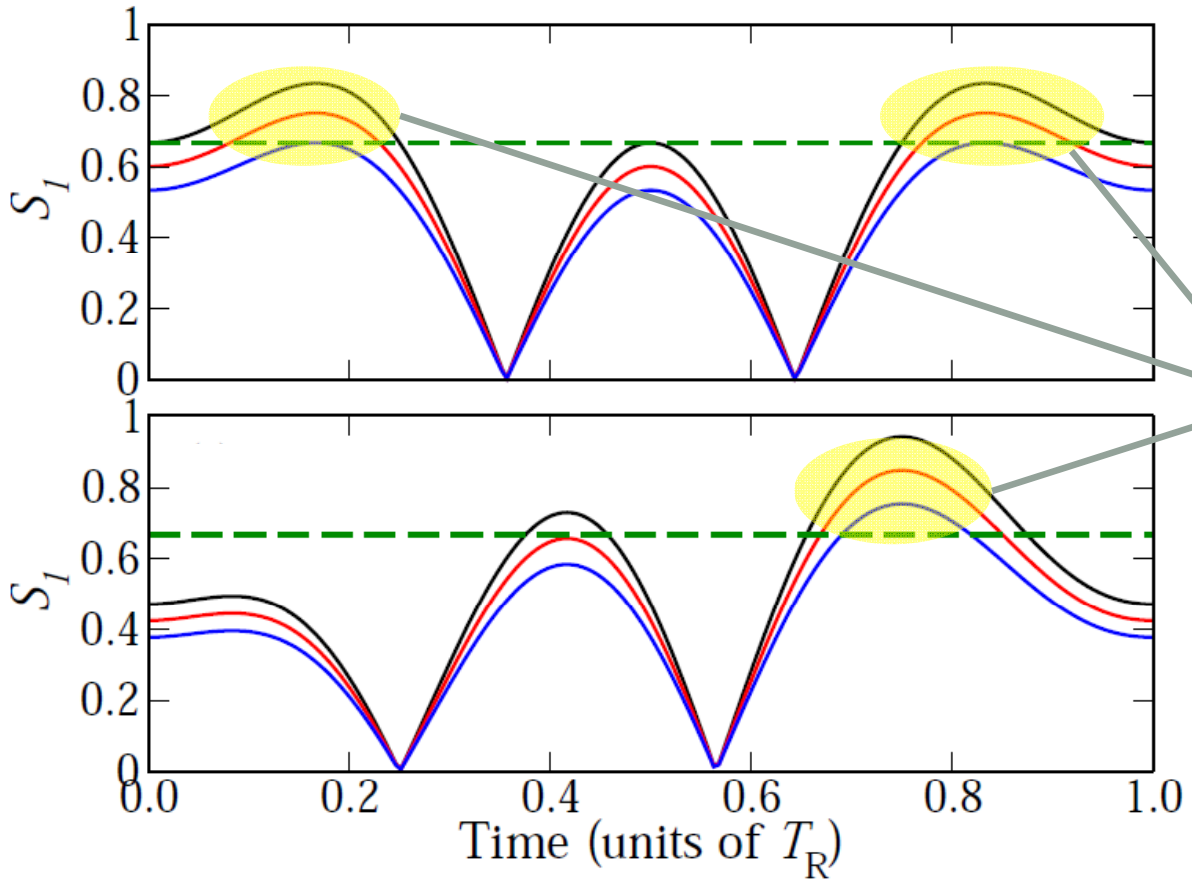
$$\omega_{10} = 2B_e/\hbar \qquad t'_a = t'_b = t$$

$$|E(\vec{a},\vec{b}) + E(\vec{a},\vec{b}') + E(\vec{a}',\vec{b}) - E(\vec{a}',\vec{b}')| \leq 2\lambda^2_{\max}$$

Entanglement in optical traps

- Bell inequality for orientation correlations

$$E(t_a, t_b) + E(t_a, t_b') + E(t_a', t_b) - E(t_a', t_b') \leq 2/3$$



Inequality violations on the picosecond timescale

Phonon-induced decoherence

- Local qubit decoherence
  - External field fluctuations (classical noise)
  - Spontaneous emission (quantum noise)
- Nonlocal decoherence
  - Phonon-modulated intermolecular coupling

Phonon-induced decoherence

- Phonon-modulated excitation hopping
  - Motion in trap modulates dipole-dipole energy
  - Optical trapping laser has intensity and frequency noise
  - Optical lattice phonons can influence system dynamics

Spin-boson model

$$\mathcal{H} = \sum_i \epsilon_{eg} \hat{c}_i^\dagger \hat{c}_i + \sum_{i,j} J_{ij} \hat{c}_i^\dagger \hat{c}_j + \sum_k \hbar\omega_k \hat{a}_k^\dagger \hat{a}_k + \sum_{i,j\neq i} \sum_k \lambda_{ij}^k \hat{c}_i^\dagger \hat{c}_j \left(\hat{a}_k + \hat{a}_k^\dagger\right)$$

system environment interaction

Summary

1) Strong laser pulses can mediate long range entanglement in dipolar molecular gases

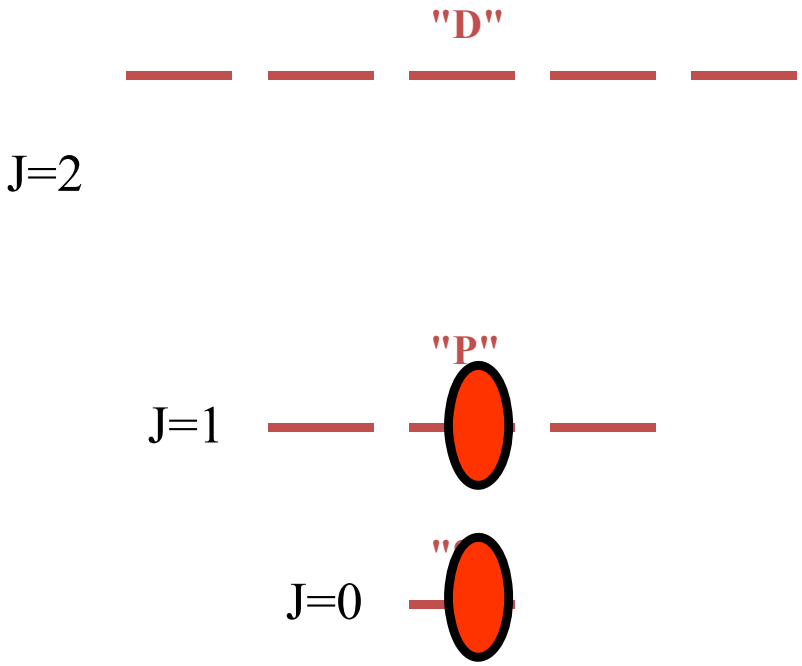
2) Arbitrary degree of entanglement can be prepared by tuning laser pulse parameters

3) Entangled states are robust against motional decoherence in optical lattices

Identifying Qubits

- rigid rotor

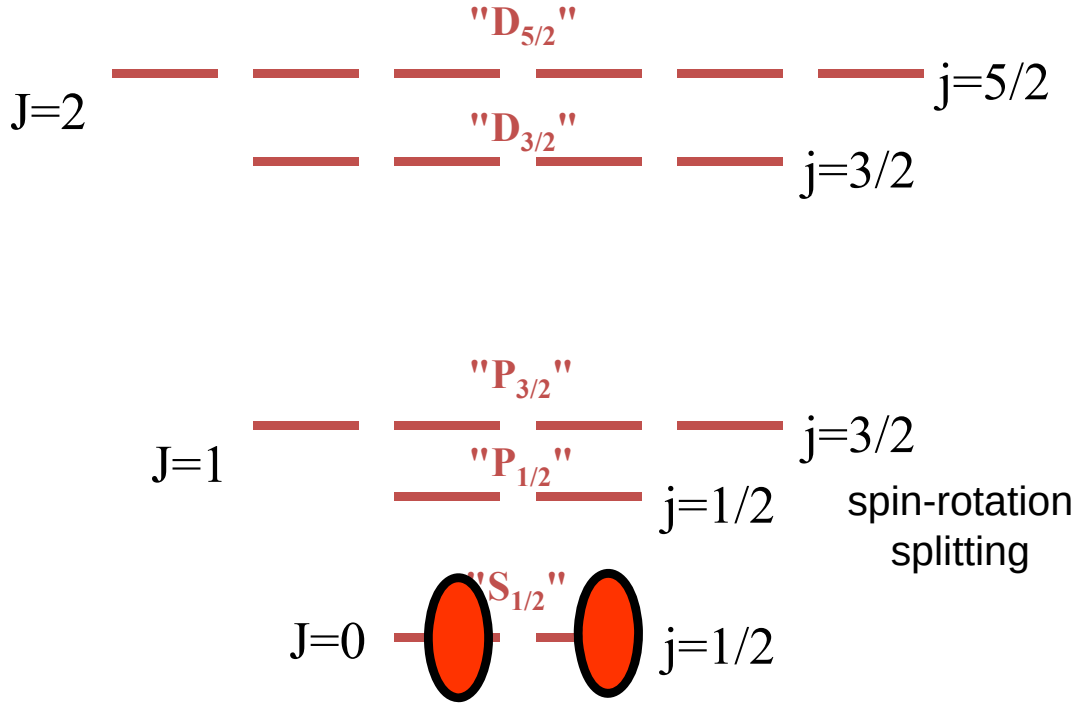
$$H = B\,\mathbf{J}^2$$



charge qubit

- adding spin-rotation coupling (S=1/2)

$$H = B\,\mathbf{J}^2 + \gamma\,\mathbf{J}\cdot\mathbf{S}$$



spin qubit

Supersymmetry in Molecules

We consider a $^1\Sigma$ molecule with a rotational constant B, a permanent dipole moment μ along the internuclear axis, and polarizability components $\alpha_{\parallel}$ and $\alpha_{\perp}$ parallel and perpendicular to the internuclear axis. The molecule is subjected to an electrostatic field ε combined with a nonresonant laser field of intensity I, whose linear polarization is collinear with ε. With energy expressed in terms of B, the Hamiltonian takes the dimensionless form [2]

$$H = \mathrm{J}^2 + V_{\mu,\alpha}(\theta),$$

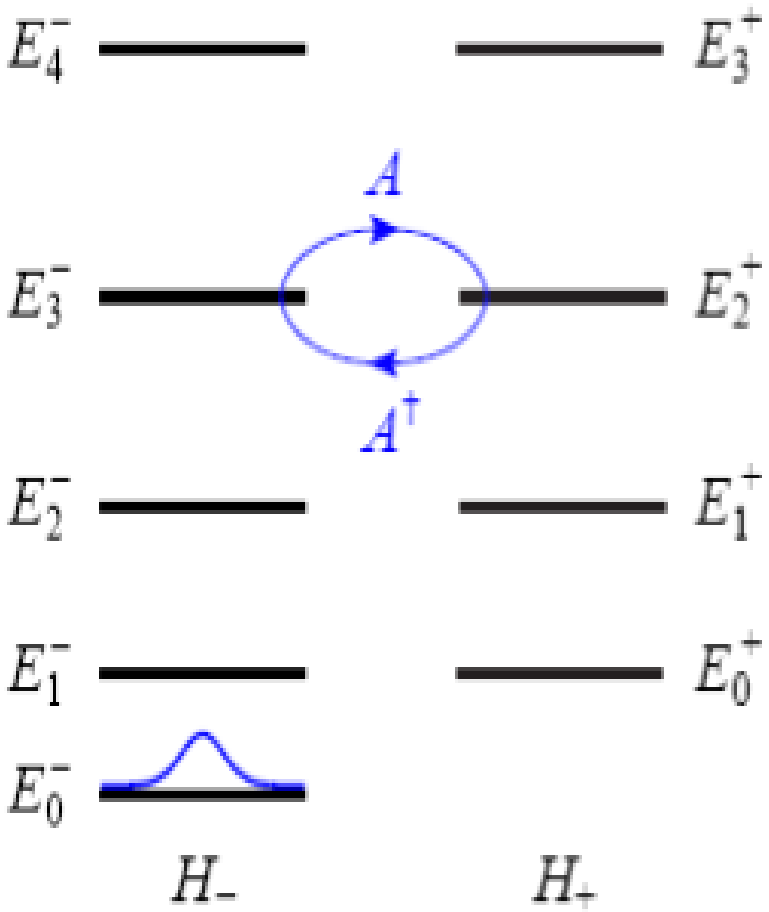
with the angular momentum operator

$$\mathrm{J}^2 = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

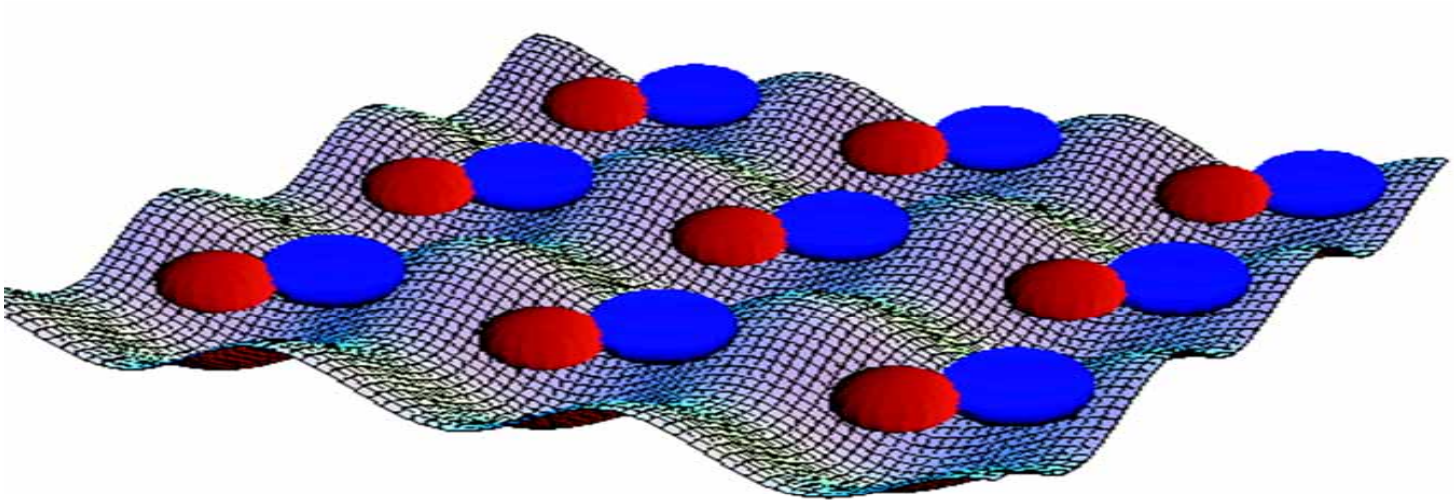
and the interaction potential

$$V_{\mu,\alpha}(\theta) = -\omega\cos\theta - \left(\Delta\omega\cos^2\theta + \omega_{\perp}\right)$$

The dimensionless interaction parameters are given as $\omega \equiv \mu\varepsilon/B$ and $\Delta\omega \equiv \omega_{||} - \omega_{\perp}$, with $\omega_{||,\perp} \equiv 2\pi\alpha_{||,\perp}I/(Bc)$.


E_4^-
E_3^+
A
E_3^-
E_2^+
$A^\dagger$
E_2^-
E_1^+
E_1^-
E_0^+
E_0^-
H_-
H_+

Advances in the field of ultracold atomic and molecular gases give us the capability to engineer a wide range of quantum systems



The possibilities are almost limitless, with real-time control over features such as lattice structure, density, temperature, level of impurities and disorder, quantum statistics, spin, dimensionality, and interactions by changing the symmetry, strength, and range.

References

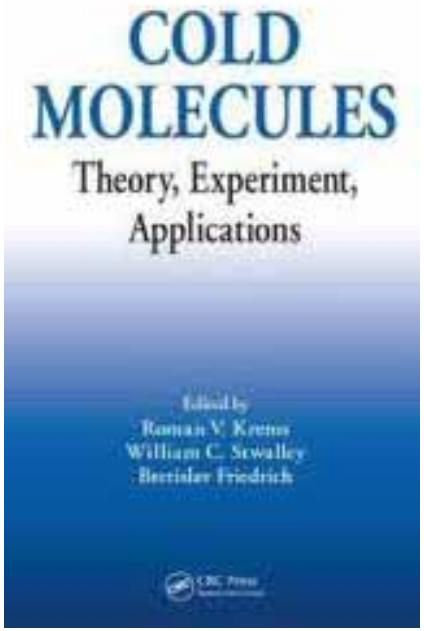
- *Molecular alignment and orientation*
  - Friedrich & Hershbach, PRL 74, 4623 (1995)
  - Seideman & Hamilton, Adv. At. Mol. Phys. 52, 289 (2005)

- *Dipole-dipole interaction in external fields*
  - Herrera & Krems, PRA 84, 051401(R) (2011)
  - Lemeshko & Friedrich, Mol. Phys. 110, 1873 (2012)
  - Carr, DeMille, Krems, Ye, New J. Phys. 11, 055049 (2009)

- *Entanglement creation and detection*
- *S. Kais, Adv. Chem. Phys. 134, 493 (2007).*
  - Amico, Fazio, Osterloh, Vedral, Rev. Mod. Phys 80, 517 (2008)

Cold molecules

- Applications include:
  - Cold chemistry and controlled collisions
  - Dipolar effects in quantum gases
  - Quantum simulation of condensed matter
  - Precision measurements
  - Quantum information processing



New Journal of Physics
The open-access journal for physics

Cold and ultracold molecules: science, technology and applications

Lincoln D Carr[1], David DeMille[2], Roman V Krems[3] and Jun Ye[4]

Finite Size Scaling and Quantum Criticality

Ross Hoehn (CHEM)
Edwin Antillon (PHYS)
Xu Qing (PHYS)

Quantum Computing and Quantum Information Theory

Jing Zhu (PHYS)
Shuhao-Yeh (CHEM)
Yting Zhang (PHYS)
Anmer Daskin (CS)
Shuxian Jiang (CS)
Yudong Cao (ME)
Rishabh Chandra (ME)
Cyrus Vandrevala (PHYS)
Felipe Herrera (CHEM)

QIQC

PURDUE
RESEARCH FOUNDATION

QIQC

QUANTUM INFORMATION FOR QUANTUM CHEMISTRY

- Alan Aspuru-Guzik (Harvard)
- Kenneth R. Brown (Georgia Tech)
- Daniel A. Lidar (USC)
- Peter J. Love (Haverford)
- Sabre Kais (Purdue, PI)

http://web.ics.purdue.edu/~kais/qc/

QIQC

CCI Director

Internal Advisory Committee: Phase I Team

External Advisory Committee

NSF CCI Program Officer(s)

CCI Innovation Partners

Alan Aspuru-Guzik

Peter Love

Ken Brown

Daniel Lidar

Bill Bayley

Seth Lloyd

Joseph Traub

Brigitta Whaley

David Mazziotti

Greg Engel

Garnet Chan

Graduate/Undergraduate Students and Postdoctoral Fellows

(25+?)

Thank you!