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# Degenerate Systems of Capacitively-Coupled Josephson Junctions



Circuit graphs of maximally symmetric systems of N junctions for N = 3,4,5,6,7.

# Zech's question:

Consider a system of 3 Josephson junctions coupled by capacitors. How do the energy levels change if the junctions are connected in a symmetric way?

#### Zech's conclusion:

The first excited states become degenerate.



## My question:

How do we find the degeneracies of an arbitrary system of such junctions?

## My conclusion:

Degeneracies are given by the dimensions of the invariant subspaces of unitary representations of the symmetry group of the system Hamiltonian.





#### Systems with degenerate metastable states

Degeneracies of first-excited states for several other systems:



\* "Maybe" does not belong in a mathematical proof. Ask me about this one later.

# What is a Josephson Junction?

- In a superconductor, electrons can become correlated to form Cooper pairs.
- Cooper pairs are bosons, thus many can occupy the same state at low temperature.
- ♠ A Josephson junction is a weak link placed between two superconductors.

Some examples from [1] are shown below:



# Why study systems of Josephson junctions?

## Practical value:

- Systems of multiple junctions can be used as components in a quantum computer.
- Can be used to build S.Q.U.I.D.s and other high-precision sensors and amplifiers.

## Mathematical value:

- The mathematical techniques used to describe systems of junctions are also used to describe other composite quantum systems, e.g. molecules and crystals.
- Approximating the Schrödinger equation requires advanced numerical techniques.

## Theoretical value:

- Junction systems provide tests for theories of decoherence and teleportation.
- Josephson junctions are macroscopic examples of quantum entanglement.

If the superposition principle really works, is it possible to entangle a cat?







Josephson junction ~  $10^{-5}$  meter

Cat ~ 10<sup>0</sup> meter

#### Josephson's Equations à la Feynman: Two Buckets of Bosons

The image at right is from [2]. In this experiment, two containers of liquid <sup>3</sup>He are separated by a small aperture.

A Josephson junction consists of two superconductors separated by a thin dielectric barrier. Both are examples of *weakly coupled macroscopic systems.* 



Composite wavefunction in terms of individual wavefunctions:

$$\Psi(t) = \alpha \Psi_1(0) + \beta \Psi_2(0) \qquad ||\alpha||^2 = n_1 \qquad ||\beta||^2 = n_2$$
$$\Psi(t) = \sqrt{n_1} e^{i\phi_1} \Psi_1(0) + \sqrt{n_2} e^{i\phi_2} \Psi_2(0)$$

Schrödinger equation:

$$\partial_t \Psi = -\frac{\imath}{\hbar} \hat{H} \Psi \quad \Leftrightarrow \quad \begin{bmatrix} \dot{\alpha} \\ \dot{\beta} \end{bmatrix} = \frac{-\imath}{\hbar} \begin{bmatrix} E_1 & K \\ K & E_2 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

#### Josephson's Equations, part I

# Feynman:Schrödinger: $\Psi(t) = \alpha \Psi_1(0) + \beta \Psi_2(0)$ $\begin{bmatrix} \dot{\alpha} \\ \dot{\beta} \end{bmatrix} = \frac{-\imath}{\hbar} \begin{bmatrix} E_1 & K \\ K & E_2 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$ $\alpha = \sqrt{n_1} e^{\imath \phi_1}$ $\beta = \sqrt{n_2} e^{\imath \phi_2}$

The rate of change of particle density in each bucket is:  $\dot{n_1} = \alpha^*(\dot{\alpha}) + \alpha(\dot{\alpha})^*$   $\dot{n_2} = \beta^*(\dot{\beta}) + \beta(\dot{\beta})^*$ 

Electrical current in terms of particle density is:  $I_s = -q\dot{n}_1 = (2e)\dot{n}_1$ 

$$i\hbar \ \dot{n_1} = E_1 ||\alpha||^2 + K\alpha^*\beta - E_1 ||\alpha||^2 - K\alpha\beta^* = K(\alpha^*\beta - \alpha\beta^*)$$
$$\dot{n_1} = 2\frac{K}{\hbar}\sqrt{n_1 n_2} \sin(\phi_2 - \phi_1) \qquad \dot{n_1} = -i\frac{K}{\hbar}\sqrt{n_1 n_2}(e^{i(\phi_2 - \phi_1)} - e^{i(\phi_1 - \phi_2)})$$
$$I_s = -2e \ \dot{n_2} = 2e \ \dot{n_1} = 4e\frac{K}{\hbar}\sqrt{n_1 n_2} \ \sin(\phi_2 - \phi_1)$$

If the buckets contain enough particles that  $\sqrt{n_1 n_2} \approx$  constant, then we can write:

$$I_s = I_0 \sin(\gamma)$$
  $\gamma \equiv \phi_2 - \phi_1$   $I_0 \equiv 4e \frac{K}{\hbar} n_1 \cdot (\text{volume of subsystem 1})$ 

#### Josephson's Equations, part II

Feynman:Schrödinger: $\Psi(t) = \alpha \Psi_1(0) + \beta \Psi_2(0)$  $\begin{bmatrix} \dot{\alpha} \\ \dot{\beta} \end{bmatrix} = \frac{-\imath}{\hbar} \begin{bmatrix} E_1 & K \\ K & E_2 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$  $\alpha = \sqrt{n_1} e^{\imath \phi_1}$  $\beta = \sqrt{n_2} e^{\imath \phi_2}$ 

The rate of phase change of the particles in each bucket is:

$$\dot{\phi_1} = \frac{-\imath}{2||\alpha||^2} (\alpha^* \dot{\alpha} - \alpha(\dot{\alpha})^*) \qquad \dot{\phi_2} = \frac{-\imath}{2||\beta||^2} (\beta^* \dot{\beta} - \beta(\dot{\beta})^*)$$

The voltage across the junction is given by:  $qV = -2eV = E_2 - E_1$ 

 $\dot{\alpha} = \frac{-i}{\hbar} (E_1 \alpha + K\beta) \qquad \dot{\beta} = \frac{-i}{\hbar} (K\alpha + E_2 \beta) \qquad \dot{\phi}_1 = \frac{-i}{2\hbar ||\alpha||^2} (\alpha^* (-iE_1 \alpha - iK\beta) - \alpha (iE_1 \alpha^* + iK\beta^*))$   $\hbar \dot{\phi}_1 = -E_1 - \frac{1}{2||\alpha||^2} K(\alpha^* \beta + \alpha \beta^*) \qquad \hbar \dot{\phi}_1 = -E_1 - \frac{1}{2n_1} K\sqrt{n_1 n_2} (e^{i(\phi_2 - \phi_1)} + e^{i(\phi_1 - \phi_2)})$   $\hbar (\dot{\phi}_2 - \dot{\phi}_1) = (E_1 - E_2) + K(\frac{\sqrt{n_1 n_2}}{n_1} - \frac{\sqrt{n_1 n_2}}{n_2}) \cos(\phi_2 - \phi_1)$ 

Assuming an equal number of particles in each bucket and using  $~\gamma\equiv\phi_2-\phi_1~$  ,

$$V = \frac{\Phi_0}{2\pi} \dot{\gamma}$$
  $\Phi_0 \equiv \frac{h}{2e}$  where the constant  $\Phi_0$  is called the *flux quantum*.

#### **Resistor + Capacitor + Shunted Junction (RCSJ) model**

What happens if an external power supply drives current through a junction? The RCSJ model treats a single junction as three parallel channels:

**R channel**: Current conducts through the junction barrier as if the entire junction was a classical resistor.

C channel: Charge accumulates on either side of the barrier as if the junction was a classical capacitor.



X channel: Electron pairs tunnel through through the barrier via the Josephson effect. (There is no classical circuit element corresponding to this, hence the X.)

If the barrier is a strong insulator, current through the R channel becomes negligible.

Kirchhoff's circuit laws then impose constraints on the system:

$$I_{bias} = I_s + \frac{d}{dt}Q \qquad \qquad V_{bias} = V_s = \frac{Q}{C_J}$$

(The voltage across every channel is equal, so we refer to "the" junction voltage.)

### **RCSJ Equation of Motion**

Substituting Josephson's equations into Kirchhoff's laws, we find:



What should we choose for the conjugate momentum and Hamiltonian of this system? Consider a completely different system with an identical equation of motion:



360<sup>°</sup> pendulum with

applied torque  $\Gamma$ 

Equation of motion:

Conjugate momentum:

 $\Gamma = mgr\sin(\gamma) + mr^2(\ddot{\gamma})$ 

Lagrangian:

$$\mathfrak{L} = \frac{1}{2}mr^2(\dot{\gamma})^2 + mgr\cos(\gamma) + \Gamma\gamma$$

$$\mathfrak{p} = (\frac{\partial \mathfrak{L}}{\partial \dot{\gamma}}) = mr^2(\dot{\gamma})$$

Hamiltonian:

 $\mathcal{H} = \frac{1}{2}mr^2(\dot{\gamma})^2 - mgr\cos(\gamma) - \Gamma\gamma$ 

#### **RCSJ Hamiltonian and conjugate momentum**

These systems are equivalent under the following replacement of constants:

Each term in the Hamiltonian has a physical interpretation as a type of energy:

$$\mathcal{H} = \frac{1}{2}C_{J}V^{2} - I_{0}\left(\frac{\Phi_{0}}{2\pi}\right)\cos(\gamma) - \left(\frac{\Phi_{0}}{2\pi}\right)I_{b}\gamma$$

$$(apacitor energy) - (apacitor from power supply) - energy input from power supply - energy - energy input from power supply - energy - energ$$

#### Phase interference between coupled quantum systems

The energy term in the RCSJ Hamiltonian has a purely quantum-mechanical origin.

$$\mathcal{H} = \frac{1}{2}C_J V^2 - I_0 \left(\frac{\Phi_0}{2\pi}\right) \cos(\gamma) - \left(\frac{\Phi_0}{2\pi}\right) I_b \gamma$$
capacitor energy symphonic energy - energy input from power supply

What does the middle term represent? Look closely at the energies in this diagram [4] :



The composite wavefunction for two particles in adjacent wells is written as a sum of singleparticle states. For the ground states, the inphase combination has lower energy!

The out-of-phase state requires a node within the barrier. This node is energetically costly.

Feynman's junction model assumes that each subsystem is in its ground state, so we ignore the higher-energy substates. Those states may be useful for generalizing Feynman's model in a future project ... but not today.

#### The washboard potential

The RCSJ Hamiltonian resembles that of a particle in a washboard-shaped potential:



There are a few perplexing features about this Hamiltonian, however.

• If  $\gamma$  is a relative phase, why isn't the washboard potential  $2\pi$ -periodic?

• The coordinate  $\gamma$  and its conjugate momentum  $\mathfrak{p}$  are specified simultaneously! A coordinate and its conjugate momentum should not commute:  $[\gamma, \mathfrak{p}] = \imath \hbar \neq 0$ 

#### **Decompactification of the pendulum**

It may be helpful to consider the pendulum system again. Split the Hamiltonian into:

$$\mathcal{H} = E(t) - \Gamma \gamma$$
  $E(t) = \frac{\mathfrak{p}^2}{2mr^2} - mgr\cos(\gamma)$ 

The total Hamiltonian is constant in time, but the individual components need not be. E(t) can increase without bound for certain initial conditions and applied torques.

- If the initial energy E(0) is low and applied torque is weak, the pendulum oscillates.
- If E(0) or applied torque is slightly larger, the oscillations become nonlinear.
- If E(t) is ever greater than mgr, the pendulum becomes unbound!

Once the pendulum has gone "over the top," it is always unbound. With no friction to stop it, the angular momentum can increase forever (or until the pendulum breaks). In topology-speak, the pendulum's phase-space trajectory becomes *noncompact*.

#### **Decompactification of the washboard potential**

A quantum pendulum behaves even worse than a classical one - it can tunnel into a free-spinning state even if the applied torque is too weak to overcome gravity!

Spectroscopy experiments on Josephson junctions show a similar behavior. Junctions can switch from a zero-voltage state to a state with measurable voltage difference even when driven by currents less than the junction's critical current.

• The wavefunctions on either side of the barrier then have different energies. Their phase factors  $e^{-i\omega t}$  steadily drift apart, scrambling their earlier phase coherence.





driven quantum pendulums can tunnel over a finite energy barrier... driven Josephson junctions can also tunnel over a finite energy barrier. [5] please allow the presenter a few moments to set up

# NUMERICAL DEMONSTRATIONS

#### Quantum mechanics of the washboard potential

We now return to the problem of forming a quantum-mechanical Hamiltonian with the correct commutation relations for the RCSJ model. From before, we know:

Josephson:

Kirchhoff:

 $I_{s} = I_{0} \sin(\gamma) \qquad \qquad I_{b} = I_{s} + \frac{d}{dt}Q$  $V = \left(\frac{\Phi_{0}}{2\pi}\right)\dot{\gamma} \qquad \qquad Q = C_{J}V$ 



The phase coordinate and its conjugate momentum cannot both be known to arbitrary precision. Perhaps Josephson's equations are really *operator* equations.

Kirchhoff's laws and the ideal capacitor formulas are valid in *classical* physics.
 It seems reasonable to assume they apply to expectation values, not operators.

Ehrenfest's theorem (paraphrased): Put angle brackets around Heisenberg's equations to see if a Hamiltonian produces the correct classical behavior.

$$\frac{d}{dt}\langle\hat{Q}\rangle = \frac{\imath}{\hbar}\langle[\hat{H},\hat{Q}]\rangle = \frac{\imath}{\hbar}\left(\frac{\Phi_0}{2\pi}\right)^{-1}\langle[\hat{H},\hat{p}]\rangle$$

#### Does the washboard potential pass Ehrenfest's test?

Use the canonical commutation relation  $[\hat{\gamma}, \hat{p}] = \imath \hbar$  and do some algebra:

$$[\hat{W},\hat{p}]\Psi = \hat{W}\hat{p}\Psi - \hat{p}\hat{W}\Psi = -\left[\hat{W}(\hat{p}\Psi) \mp i\hbar\partial_{V}(\hat{W}_{2\pi}) + i\hbar\partial_{V}(\hat{W}_{$$

$$\hat{V} = \frac{1}{C_J} \left(\frac{\Phi_0}{2\pi}\right)^{-1} \hat{p} \qquad \Longrightarrow \qquad C_J \frac{d}{dt} \langle V \rangle + \langle I_s \rangle = \langle I_b \rangle$$

Yes! The Hamiltonian and conjugate momentum used earlier were wrong but useful. By replacing the coordinates with operators, we can describe a quantum system whose expectation values are consistent with classical circuit theory.

- Question: If voltage and supercurrent are operators, do they commute?
- Answer: No. In fact, these two operators obey an uncertainty principle:

$$[\hat{V}, \hat{I}_{s}] = (\underline{\Phi}_{0}) \mu^{-1} I_{0} [-\underline{M} ] [\underline{h}_{s} - \underline{h}_{s}] [\underline{h}_{s} -$$

CHALLENGE: Think of an experiment to (dis)prove this uncertainty relation.

#### Metastable states of the washboard potential

The generalized uncertainty principle allows us to define *metastable* states:

$$\Delta_E \Delta_t \ge \frac{1}{2}\hbar \qquad \Delta_t \equiv \Delta_A \left| \frac{d}{dt} \langle A \rangle \right|^{-1} \quad \Rightarrow \qquad \left| \frac{d}{dt} \langle A \rangle \right| \le \frac{2}{\hbar} (\Delta_E \Delta_A)$$

Here *A* is any operator whatsoever that does not explicitly depend on *t*. If the energy "width"  $\Delta_E$  of a state is small, then <*A*> evolves slowly.

A state in which the density operator  $\hat{\rho} = \Psi^* \Psi$  evolves slowly is *metastable*.



#### Metastable state energy levels

The energy gaps between the metastable states shown here are  $\sim 2.5 \ 10^{-24}$  joules. To prevent thermal interference, experiments must be cooled well below 0.1 K.

 $E_0 = -7.964 \ 10^{-24} \text{ joules} \qquad E_1 = -5.373 \ 10^{-24} = E_0 + 2.591 \ 10^{-24} \qquad E_2 = -2.941 \ 10^{-24} = E_1 + 2.432 \ 10^{-24}$  $kT = E_1 - E_0 \Rightarrow T \approx 0.18 \text{K} \qquad hf = E_1 - E_0 \Rightarrow f \approx 4 \text{GHz}$ 

• The energy levels are not evenly spaced:  $(E_2 - E_1) = 0.94 (E_1 - E_0)$ 

• Mean lifetimes for weakly-bound states at T ~ 10mK and  $I_b > 0.9(I_0)$  are in the range 100 µs  $\rightarrow$  1 ns.

Phase coherence for entangled states is shorter-lived than the states themselves: 1 ns - 100 ns is common for phase qubits.

 Resonant frequencies are near 5 GHz, which unfortunately coincides with 802.11a wireless internet! The 1-3GHz range is even more crowded.



#### **Multiple-junction systems: phase-coupled qubits**

Quantum computing requires the ability to transfer, store, and recall entanglement. One way to do this is by coupling systems of Josephson junctions with capacitors:



With three junctions, two different circuit diagrams are possible:



Serial 3-junction system



"Triangle" 3-junction system

#### **Dynamics of multiple-junction systems**

Solving (or approximating) the time-dependent behavior of systems of junctions is a difficult task. The first step is to write down all the terms in the Hamiltonian:

 $\hat{H} = \frac{1}{2}C_J\hat{V}_1^2 + \frac{1}{2}C_J\hat{V}_2^2 + \dots + \frac{1}{2}C_C(\hat{V}_2 - \hat{V}_1)^2 + \dots + \hat{W}_1 + \hat{W}_2 + \dots$ 



The capacitor terms can be written more conscisely using a capacitance matrix and row/column vectors of  $p_n$  operators. The Schrödinger equation then becomes:

$$i\hbar\partial_t \Psi = \frac{1}{2} \left(\frac{\Phi_0}{2\pi}\right)^2 \mathbf{p}^T [C]^{-1} \mathbf{p} + W_1(\gamma_1) + W_2(\gamma_2) + \cdots$$
$$\hat{p}_n = C_J \left(\frac{\Phi_0}{2\pi}\right) \hat{V}_n \qquad \mathbf{p}^T = [\hat{p}_1, \hat{p}_2, \cdots] \qquad \hat{W}_n = -\left(\frac{\Phi_0}{2\pi}\right) [I_0 \sin(\gamma_n) + I_n \gamma_n]$$

Unfortunately, the  $p_n$ 's here are **not** the operators conjugate to  $\gamma_n$  ! Finding the correct conjugate momenta takes a bit more work.

#### Graph theory short-cut to the multi-junction Hamiltonian

The conjugate momenta can be found using the same "pseudo-classical" Lagrangian method as before, but the results can get somewhat complicated.

• To simplify things, replace each circuit diagram with a simple undirected graph:



#### Finding the capacitance matrix

Each of these graphs can be represented by a unique Laplacian matrix  $\mathcal{L}$  :



The capacitance matrix can be found by writing  $C_{ij} = C_J \, \delta_{ij} + C_C \, \mathcal{L}_{ij}$ 

#### The Schrödinger equation for multiple junctions

Dividing the capacitance matrix by  $C_J$  produces a dimensionless matrix M:

$$M_{ij} = \delta_{ij} + \chi \mathcal{L}_{ij}$$
 where  $\chi \equiv \frac{C_C}{C_J}$ 

The *M* matrix can be used to write the conjugate momenta  $\hat{p}'_n$  in terms of  $\hat{p}_n$ :

 $\hat{p}_n = C_J \left(\frac{\Phi_0}{2\pi}\right) \hat{V}_n \quad \mathbf{p}^T = [\hat{p}_1, \hat{p}_2, \cdots] \quad \mathfrak{p}^T \equiv [\hat{p}'_1, \hat{p}'_2, \cdots] \quad \Rightarrow \quad \mathfrak{p}_i = M_{ij} \mathbf{p}_j$ 

The Hamiltonian can also be written in terms of the *M* matrix and **p** column vector:  $\hat{H} = \frac{1}{2\mu} \mathbf{p}^T [M] \mathbf{p} + \hat{W}_1 + \hat{W}_2 + \cdots$ 

Combining these expressions, we can (at last) write the Schrödinger equation:

$$i\hbar\partial_t = -\frac{\hbar^2}{2\mu}[\partial_{\gamma_1}, \partial_{\gamma_2}, \cdots] \begin{bmatrix} M^{-1} \end{bmatrix} \begin{bmatrix} \partial_{\gamma_1} \\ \partial_{\gamma_2} \\ \vdots \end{bmatrix} + W(\gamma_1) + W(\gamma_2) + \cdots$$

where we have written the canonical momentum operators as  $\hat{p}'_n = -\imath \hbar \partial_{\gamma_n}$ .

#### **Example: the serial 3-junction**

As an example, find the Schrödinger equation using the Laplacian-matrix method:

*M*<sup>-1</sup> can be cleaned up (some) by defining a coupling constant  $\kappa \equiv \frac{C_C}{C_J + C_J} = \frac{\chi}{1 + \chi}$ :

$$i\hbar\partial_t = -\frac{\hbar^2}{2\mu} \frac{1}{1+2\kappa} [\partial_{\gamma_1}, \partial_{\gamma_2}, \partial_{\gamma_3}] \begin{bmatrix} 1+\kappa-\kappa^2 & \kappa & \kappa^2 \\ \kappa & 1 & \kappa \\ \kappa^2 & \kappa & 1+\kappa-\kappa^2 \end{bmatrix} \begin{bmatrix} \partial_{\gamma_1} \\ \partial_{\gamma_2} \\ \partial_{\gamma_3} \end{bmatrix} + W(\gamma_1) + W(\gamma_2) + W(\gamma_3)$$

#### **Degeneracy and avoided crossings**

Metastable states can exist in multiple-junction systems, and they can be written as linear combinations of single-junction direct product states. For example:

$$2 - - \frac{1}{2\mu} i\hbar \partial_t = -\frac{\hbar^2}{2\mu} \frac{1}{\chi(\chi+2)} [\partial_{\gamma_1}, \partial_{\gamma_2}] \begin{bmatrix} 1+\chi & 1\\ 1 & 1+\chi \end{bmatrix} \begin{bmatrix} \partial_{\gamma_1}\\ \partial_{\gamma_2} \end{bmatrix} + W(\gamma_1) + W(\gamma_2)$$

If the labels 1,2 are switched, the Hamiltonian is unchanged. If we define an operator  $\hat{S}$  = "switch labels 1 and 2" then  $[\hat{H}, \hat{S}] = 0$ . Eigenstates of  $\hat{S}$  are :

$$\hat{S}_{\frac{1}{\sqrt{2}}}(|10\rangle + |01\rangle) = \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle) \qquad \hat{S}_{\frac{1}{\sqrt{2}}}(|10\rangle - |01\rangle) = \frac{1}{\sqrt{2}}(-|10\rangle + |01\rangle)$$

These states are the first-excited metastable states of the two-junction system.



spectroscopy data from [6]

- Resonances of the two-junction system are plotted at left as a function of bias current #2.
- The energy levels appear to repel each other; apparently this system forbids degenerate metastable states.

## Symmetries of multiple-junction systems

- Solving the Schrödinger equation for N junctions is a formidable task.
- If the solutions can be written as linear combinations of single-junction solutions, then the problem simplifies considerably.
- Symmetries of the Hamiltonian tell us how to write these linear combinations.
   These symmetries can also determine which combinations are degenerate.

Example: The triangle symmetry group is  $S_3$ , the permutation group of 3 objects.

♦ 3 rotations (including the identity rotation)





♦ 3 parity-reversed rotations

#### The triangle system continued

Every transformation in  $S_3$  leaves the Hamiltonian unchanged. Each of these transformations can be represented by a matrix acting on  $[\gamma_1, \gamma_2, \gamma_3]^T$ :

$$R_{123} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad R_{231} = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \qquad R_{312} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$
$$R_{213} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad R_{132} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \qquad R_{321} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

Energy eigenstates are found by looking for invariant subspaces of these matrices.

$$\frac{1}{\sqrt{3}} \Big( |100\rangle + |010\rangle + |001\rangle \Big)$$

is unchanged by any of these matrices.

 $\frac{\frac{1}{\sqrt{6}} \left( |100\rangle - 2|010\rangle + |001\rangle \right)}{\frac{1}{\sqrt{2}} \left( |100\rangle - |001\rangle \right)}$ 

Linear combinations of these states form an invariant subspace. Vectors in this space stay in the space when acted on by an  $S_3$  matrix.

The invariant subspace dimensions of  $S_3$  are  $\{1, 2\}$ .

#### Invariant subspaces and degeneracy

If a Hamiltonian has a symmetry group with an invariant subspace, all the states in that subspace must be degenerate. Here's a sketch of the proof:

- Every finite group can be represented by some set of unitary matrices.
- If the Hamiltonian has a group of symmetries, that group can be represented by unitary matrices that all commute with the Hamiltonian.

If V is an invariant subspace with dimension > 1, then two linearly independent states can be transformed into each other by a unitary matrix that commutes with the Hamiltonian. These states must have the same energy.

Therefore **states in an invariant subspace are degenerate.** Here are the systems from the first slide and their invariant subspace dimensions:



#### Invariant subspaces and degeneracy: a familiar example

$$\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$$

- This Hamiltonian depends only on *r*, so it is rotation-invariant.
- The symmetry group of 3D
   rotations is the Lie group SO(3).
- Invariant subspaces of SO(3) irreps have dimension  $2 \ell + 1$ .
- The degeneracies of this system are plotted to the right.



#### Invariant subspace dimensions for degree-N representations

Here are the earlier results lalong with each system's permutation symmetry group:



#### First steps towards time-dependent solutions

• For an *m*th-excited state, there are  $\frac{(N+m-1)!}{m!(N-1)!}$  different direct-product states. These states transform under larger-degree group representations.

The predicted degeneracies can be tested by spectroscopy experiments.
 Our real goal, however, is to know time-dependent behavior of these systems.

The group-theoretical methods here can be used to write system states in terms of direct-product states, but this is only a first step. Numerical methods and perturbation theory can be applied to find more general behavior.

Tetrahedron direct-product states:

$$\frac{\frac{1}{2} (|1000\rangle + |0100\rangle + |0010\rangle + |0001\rangle)}{\begin{cases} \frac{1}{\sqrt{2}} (|1000\rangle - |0100\rangle) \\ \frac{1}{\sqrt{2}} (|1000\rangle - |0010\rangle) \\ \frac{1}{\sqrt{2}} (|1000\rangle - |0001\rangle) \end{cases}$$



Hypercube system graph Symmetry group: *C*<sub>4</sub> Order of group: 384 Graph spectrum: {1,1,4,4,6} Degeneracy: ? Direct-product states: ?

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