What is the mean field theory of a weak or strong dynamical symmetry group?

George Rosensteel
Tulane University
george.rosensteel@tulane.edu

Irreducible representations (Irreps)

- U(n), n=dim s.p. space, Irrep=shell model space.
- O(2n), Irrep = shell model + pair creation and annihilation < Fock space.
- G = Lie group, Irrep = Hilbert space of a strong dynamical symmetry.

Algebraic mean field theory (AMFT)

G = Lie group,

$\pi(g)$ = group representation on some Hilbert space, not necessarily irreducible.

Mean field states = Orbit space $\subset$ Hilbert space:

$$\mathcal{O}_\Psi = \{\pi(g)\Psi, g \in G\}.$$

The orbit space $\mathcal{O}_\Psi$ consists of *coherent* states (Perelomov).

U(n) Hartree-Fock (HF) (1980 Rowe, Gilmore, and GR)

O(2n) HFB (1981 GR)

Why use AMFT?

- Easy. AMFT manifold is an enormous simplification compared to irreps.
- Flexible. L = Lie algebra of group G includes most significant degrees of freedom.

Density matrix

$$
\begin{aligned}
L^* &= \text{dual space to Lie algebra } L \\
&= \text{space of real-valued linear functions on } L \\
&= \text{space of “densities.”}
\end{aligned}
$$

When L is a semisimple matrix Lie algebra, $L^* \cong L$ and

$$\langle \rho, X \rangle = \mathrm{Tr}(\rho X) \quad \text{for } X \in L \text{ and } \rho \in L^*.$$

Example: Hartree-Fock

$$
\begin{aligned}
X &\in u(n) \\
\hat{X} &= \sum X_{ij}\, a_i^\dagger a_j \\
\rho_{ij} &= M(\Psi) = \langle \Psi \,|\, a_j^\dagger a_i \Psi \rangle \\
\langle \Psi \,|\, \hat{X} \Psi \rangle &= \mathrm{Tr}(\rho X) = \langle \rho, X \rangle.
\end{aligned}
$$

Moment map M

$$\begin{aligned} M : \text{representation space} &\longrightarrow L^* \\ \Psi &\longmapsto \rho = M(\Psi) \end{aligned}$$

where

$$\langle \rho, X \rangle = \frac{\langle \Psi \,|\, \dot{\pi}(X)\Psi \rangle}{\langle \Psi \,|\, \Psi \rangle}$$

$X \in L$, $\hat{X} = \dot{\pi}(X)$ is the operator representation of the matrix X.

Advantages to density

1. For HF, $\langle \Psi \,|\, \Psi^{\text{exact}} \rangle \approx 0$, yet $\rho \approx \rho^{\text{exact}}$. AMFT aims to derive accurate densities ρ, and doesn't try to find Ψ

2. Group transformation simplifies. $\Psi \mapsto \pi(g)\Psi$ is hard to compute. But the density corresponding to the coherent state $\pi(g)\Psi$ is $\mathrm{Ad}^*_g \rho = g\,\rho\,g^{-1}$, the product of three matrices. Ad^*_g is called the coadjoint transformation.

Coadjoint orbit

$$\mathcal{O}_\rho = \{\mathrm{Ad}^*_g \rho = g\,\rho\,g^{-1}, g \in G\}.$$

The moment map, restricted to the set of coherent states,

$$M : \mathcal{O}_\Psi \longrightarrow \mathcal{O}_\rho,$$

is, in general, many-to-one.

1-1 exceptions: (a) Ψ is a highest weight vector and (b) Slater determinants $\leftrightarrow$ Idempotent densities.

Strong versus weak dynamical symmetry

- Strong: States are vectors in one *irreducible representation* space.
- Weak: Densities are points in one *coadjoint orbit*.

Casimirs

$$\mathcal{C}_p(\rho) = \mathrm{Tr}(\rho^p), p = 1, 2, \ldots.$$

The Casimirs are constant functions on each coadjoint orbit:

$$\mathcal{C}_p(\mathrm{Ad}^*_g\rho) = \mathrm{Tr}\left((g\rho g^{-1})^p\right) = \mathrm{Tr}\left(g\rho^p g^{-1}\right) = \mathcal{C}_p(\rho).$$

Conversely, for a compact Lie group, every coadjoint orbit is a level surface of the Casimir functions.

Weak dynamical symmetry example

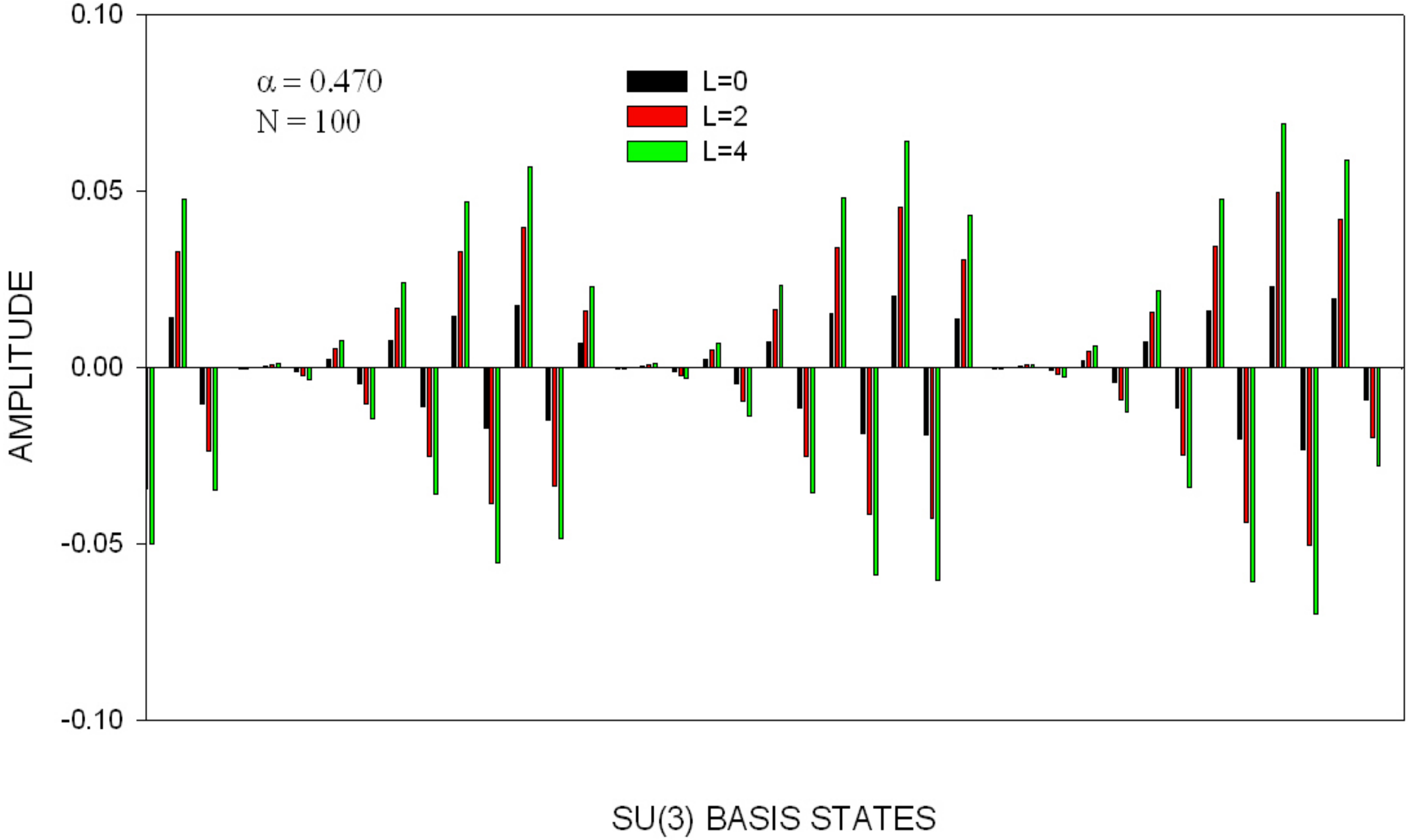
U(6) interacting boson model. Fix irrep [N].

$$H(\alpha) = (1-\alpha)H_1 + \alpha H_2, \ 0 \le \alpha \le 1,$$

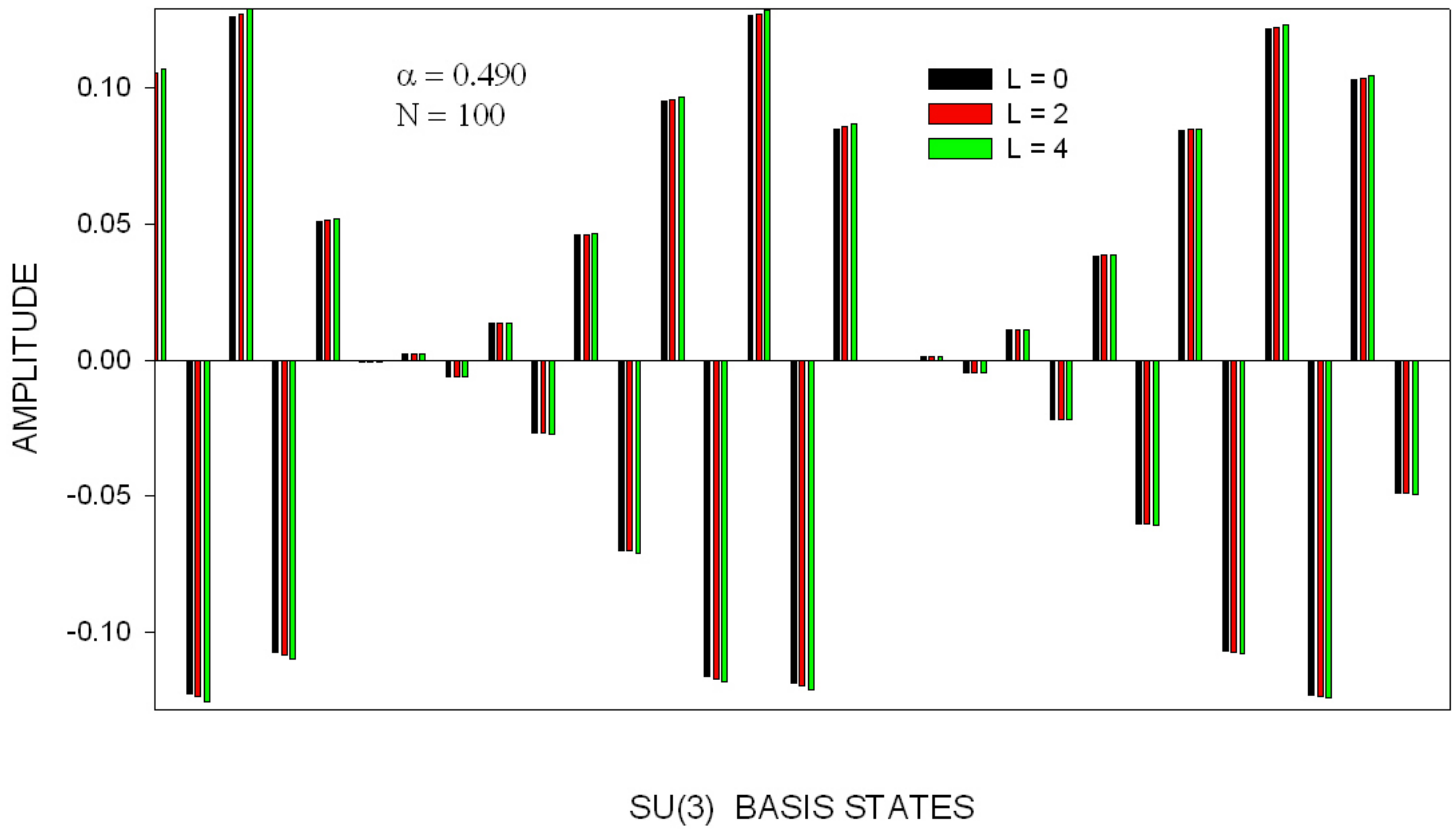
where $H_1 = \hat{n}_d$, the u(5) d-boson number operator, and $H_2 = -\hat{Q}\cdot\hat{Q}$, the su(3) quadrupole-quadrupole interaction.

For large N, this Hamiltonian has a quantum phase transition.

- $\alpha < \alpha_c \Rightarrow$ u(5) vibrational phase
- $\alpha > \alpha_c \Rightarrow$ su(3) rotational phase



$\alpha = 0.470$
$N = 100$
L=0
L=2
L=4
0.10
0.05
0.00
-0.05
-0.10
AMPLITUDE
SU(3) BASIS STATES



α = 0.490
N = 100
L = 0
L = 2
L = 4
0.10
0.05
0.00
-0.05
-0.10
AMPLITUDE
SU(3) BASIS STATES

$$|I\rangle, I = 0, 2, 4, \ldots$$

Strong su(3) dynamical symmetry when all states of band belong to one irrep of su(3).

Weak su(3) dynamical symmetry when the band's densities lie on a level surface of the su(3) Casimirs. For $\alpha > \alpha_c$ in the IBM quantum phase transition example,

$$|I\rangle = \sum_{(\lambda,\mu)} A_{(\lambda,\mu)} \, |(\lambda, \mu)I\rangle,$$

where the coefficients $A_{(\lambda,\mu)}$ in the expansion are independent of I. The expectation of any su(3) Casimir is

$$\langle I \,|\hat{C}\,|\, I\rangle = \sum_{(\lambda,\mu)} |A_{(\lambda,\mu)}|^2 \, C((\lambda, \mu)),$$

where $C((\lambda, \mu))$ is the value of the Casimir operator $\hat{C}$ in the irrep (λ, μ).

Representations of Lie groups

- Highest weight
- Duality, Permutation group and U(n)
- Induced
- Geometric quantization

Starting point: coadjoint orbit

(Kirillov, Kostant, Souriau,Vogan)

Kirillov metatheorem

- Every property of a Lie group irrep may be determined from an analysis of the corresponding coadjoint orbit.
- Branching rules, group characters, etc.
- Kirillov “The orbit method in representation theory” (AMS)

Symplectic structure

- Every coadjoint orbit is a symplectic manifold or phase space
- $\Omega(X,Y) = < \rho, [X, Y] >$ is nondegenerate
- $E(\rho)$ = energy functional on coadjoint orbit
- $h[\rho]$ = mean field Hamiltonian, where

$$dE\,(X) = \Omega(X,h[\rho])\ .$$

Dynamics on a coadjoint orbit

Dynamics is determined for semisimple Lie groups by a Lax equation:

$$\frac{d}{dt}\rho = [\rho, h[\rho]].$$

Casimir functions are constants of the motion because

$$\frac{d}{dt}\mathrm{Tr}(\rho^p) = 0.$$

Nonabelian density functional theory

Suppose $E : L^* \to \mathbf{R}$ is an energy functional.

$E_X(\rho) = E(\rho) - \langle \rho, X \rangle$ for $X \in L$.

Hohenberg-Kohn (GR and Dankova JPA 31 (1998) 8933).

$$E(\rho) = \inf_{M(\Psi)=\rho} \frac{\langle \Psi \mid \hat{H} \mid \Psi \rangle}{\langle \Psi \mid \Psi \rangle}$$

Conventional DFT:

L = set of one-body multiplication operators, $V = \Sigma_i v(r_i)$,

$L^* = \mathcal{L}^{(1)}(\mathbf{R}^3)$,

$$\langle \rho, V \rangle = \int \rho(\vec{r}) v(\vec{r}) d^3 r.$$

SU(3) densities

$\rho = q - \frac{1}{2} i l \in \mathrm{su}(3)^* \cong \mathrm{su}(3)$, where

$$
\begin{aligned}
q_{ij} &= \langle \Psi \,|\, \hat{Q}_{ij}\, \Psi \rangle \\
l_{ij} &= \langle \Psi \,|\, \hat{L}_{ij}\, \Psi \rangle .
\end{aligned}
$$

$Z = Y + iX \in \mathrm{su}(3)$, $\dot{\pi}(Z) = \Sigma_{ij}\, Y_{ij} \hat{Q}_{ij} - \frac{1}{2} \Sigma_{ij}\, X_{ij} \hat{L}_{ij}$,

$$\langle \rho, Z \rangle = \mathrm{Tr}(\rho\, Z) = \langle \Psi \,|\, \dot{\pi}(Z) \Psi \rangle$$

SU(3) Coadjoint orbit

Density matrix of highest weight is diagonal:

$$\rho = \frac{1}{3}\,\mathrm{diag}(-\lambda + \mu, -\lambda - 2\mu, 2\lambda + \mu).$$

Casimir functions:

$$\begin{aligned}
\mathcal{C}_2(\rho) &= \mathrm{Tr}(\rho^2) = \frac{2}{3}(\lambda^2 + \lambda\mu + \mu^2) \\
\mathcal{C}_3(\rho) &= \mathrm{Tr}(\rho^3) = \frac{1}{9}(2\lambda^3 + 3\lambda^2\mu - 3\lambda\mu^2 - 2\mu^3).
\end{aligned}$$

Intrinsic frame densities

An intrinsic frame density is a density with a diagonal quadrupole matrix,

$$\tilde{q} = RqR^T = \mathrm{diag}(q_1, q_2, q_3).$$

AMFT system of equations for intrinsic $\tilde{\rho} = \tilde{q} - \frac{1}{2}iI$:

$$\begin{aligned} q_1 + q_2 + q_3 &= 0 \\ I_1^2 + I_2^2 + I_3^2 &= I^2 \\ \sum_k q_k^2 + \frac{1}{2}I^2 &= \mathcal{C}_2(\lambda, \mu) \\ \sum_k q_k^3 - \frac{3}{4}\sum_k q_k I_k^2 &= \mathcal{C}_3(\lambda, \mu) \end{aligned}$$

Principal axis rotation

$I_2 = I_3 = 0$:

$$q_1 = -\frac{\lambda + 2\mu}{3}, q_{2,3} = \frac{\lambda + 2\mu}{6} \pm \frac{1}{2}\sqrt{\lambda^2 - I^2},$$

for $0 \leq I \leq \lambda$.

$$q_1 = \frac{2\lambda + \mu}{3}, q_{2,3} = -\frac{2\lambda + \mu}{6} \pm \frac{1}{2}\sqrt{\mu^2 - I^2},$$

for $0 \leq I \leq \mu$.

Routhian

Lax equation in intrinsic frame:

$$i\frac{d}{dt}\tilde{\rho} = [h_\Omega[\tilde{\rho}], \tilde{\rho}],$$

where the Routhian is $h_\Omega[\tilde{\rho}] = h[\tilde{\rho}] + i\Omega$, $\Omega = \dot{R}R^T$ is the angular velocity of the rotating frame relative to the lab frame.

A rotating equilibrium density $\tilde{\rho}$ satisfies $[h_\Omega[\tilde{\rho}], \tilde{\rho}] = 0$.

Normal modes

Suppose $E(\rho) = A_1 I_1^2 + A_2 I_2^2 + A_3 I_3^2$. Normal mode analysis via linearization of Lax equations near an equilibrium density determines wobbling frequency about short principal axis:

$$\omega = \frac{2I\sqrt{(A_1 - A_2)(A_3 - A_2)}}{1 + \left(\frac{I^2}{4\mu(\lambda+\mu)}\right)}$$

for $0 \le I \le \lambda$. The denominator contains the su(3) correction in parentheses.

The End Part

- GCM(3) Riemann ellipsoidal or Bohr-Mottelson model
- Sp(3,R) symplectic collective model
- O(6) = SU(4) interacting boson model
- SO(5) = USp(4) ibm

Internally consistent

- Correct group representation properties are built into each coadjoint orbit. Branching rules for $H<G$ derived from geometric analysis of H-orbits in coadjoint G-orbit space.
- DFT Hohenberg-Kohn assures the existence of an energy functional for which the exact ground state density is a minimum.

Simple to use

- AMFT calculations use n x n matrices, e.g., SU(3) works with 3 x 3 matrices. The (possibly infinite) dimension of the representation under investigation is irrelevant.
- Method applies to nonintegral orbits which is necessary for weak dynamical symmetry.

Questions

- Is weak dynamical symmetry ubiquitous?
- What's the best way to find the universal energy functional for a given algebra L?