DYNAMICAL SYMMETRIES for SCES

K. Kikoin

Harwell
1963-66
J. Hubbard

IFM-UrGU
1966
Yu.P. Irkhin

Moscow
1967-74
L.A. Maksimov

$$H\,|\Lambda\,\mu\rangle = E_\Lambda\,|\Lambda\,\mu\rangle$$

$$X^{\Lambda\mu,\Lambda'\mu'} = ||\Lambda\,\mu\rangle\langle\Lambda'\mu'|$$

Beer-Sheva-
Tel-Aviv
1997-2011
Y. Ne'eman

Hubbard atom:

$$\hat{H}_d = \epsilon_d \sum_{\sigma=\uparrow,\downarrow} d^\dagger_{i\sigma} d_{i\sigma} + U n_{id\uparrow} n_{id\downarrow}$$

N=0,1,2

Commutation relations for fifteen Hubbard operators:

$$[X^{\kappa\lambda}, X^{\mu\nu}]_{\mp} = X^{\kappa\nu}\delta_{\lambda\mu} \mp X^{\mu\lambda}\delta_{\kappa\nu}$$

Both Fermi-like and Hubbard-like operators form a superalgebra for *Spl(2,1)* group

Zaitsev (??), Wiegmann(88), Foerster & Karowski (92)…

so what ?

Neither of two generic models (Anderson model and Hubbard model, AM & HM) possess true supersymmetry, so one has to look for alternative closed algebra for these 15 operators. 15 is a good number from the point of view of the Lie algebras. There are at least two such group formed by 15 generators: ***SO(6)*** and ***SU(4)***. These groups may be reduced to ***SO(5)*** and ***SU(3)*** under special physical limitations. ***Zhang ('88)*** tried to apply the former group to *t-J* model in a context of the theory of HiTc (without great benefit).

Here I will try to convince you that ***SU(4)*** is the **generic** symmetry of the AM. What about benefits? Let's see.

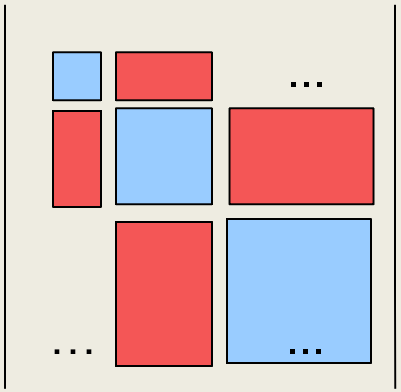
Symmetry of the Hamiltonian and dynamical symmetry of the energy spectrum

Any Hamiltonian H is characterized by some symmetry. Operations leaving H invariant generate corresponding symmetry group G .

Wigner theorem

> The wave functions belonging to a given eigen energy E transform along a representation of the group G of the Schroedinger equation

Secular matrix for Schroedinger equation .
Each diagonal block corresponds to some eigenstate E_Λ.



$$[X^{\Lambda\Lambda'}, \hat{H}] = (E_{\Lambda'} - E_\Lambda)\hat{H}$$

The right hand side of this relation turns into zero provided the states Λ and Λ' belong to the same irreducible representation of the group G_S.

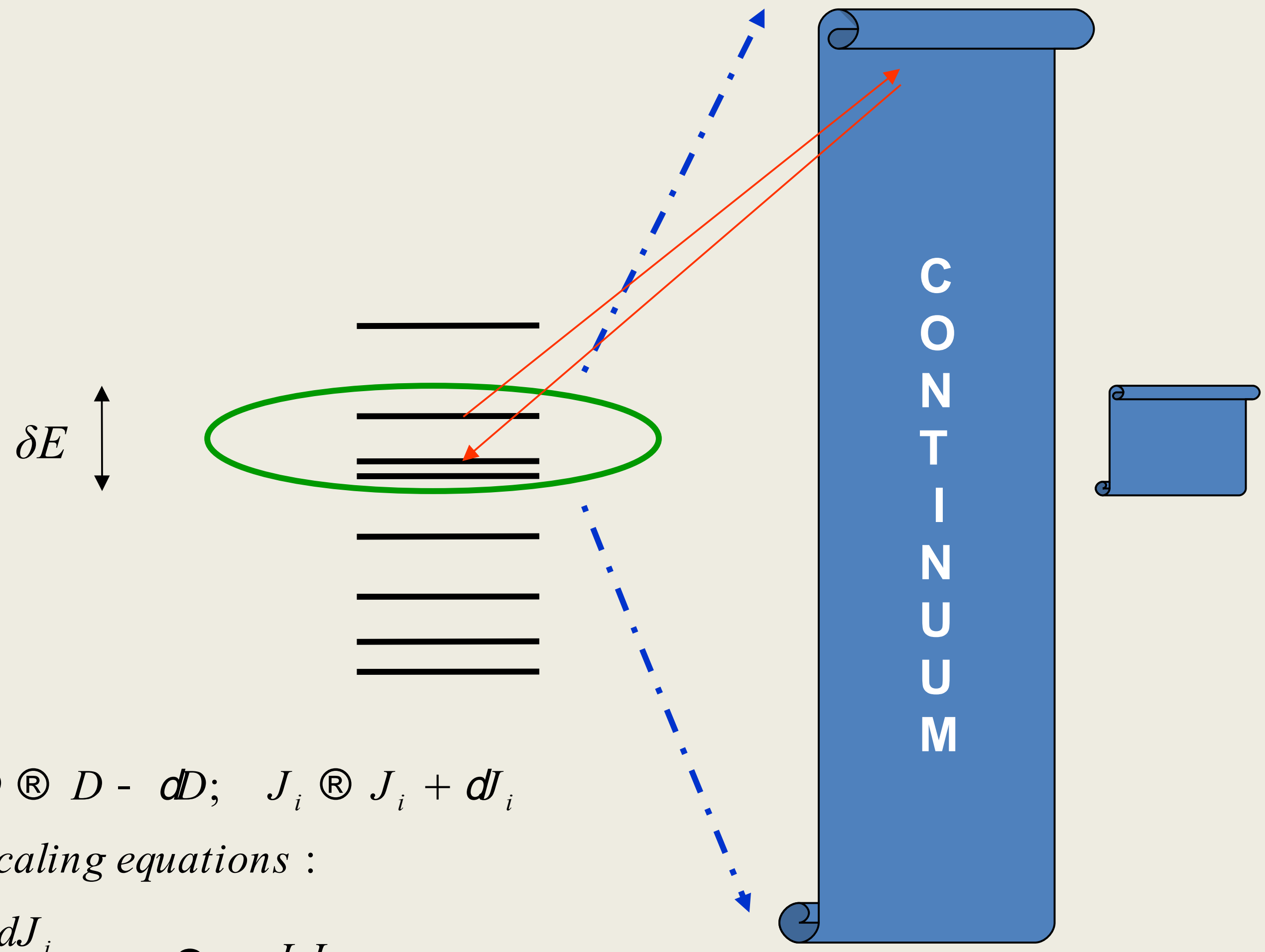
Off-diagonal operators $X^{\Lambda\Lambda'}$ belonging to different IRs complement algebra of generators of the symmetry group of Schroedinger equation to a set of generators of a **dynamical symmetry group** characterizing a "supermultiplet" of eigenstates, provided these operators form a closed algebra.

Off-diagonal operators $X^{\Lambda\Lambda'}$ generate the spectrum starting from any given state Λ.
Off-diagonal operators $X^{\Lambda\Lambda'}$ will be used below for construction of irreducible tensor operators describing observables (scalars, vectors, tensor

$$\mathcal{O}_\varrho^{(r)} = \sum_{\Lambda\Lambda'} \langle\Lambda|\mathcal{O}_\varrho^{(r)}|\Lambda'\rangle X^{\Lambda\Lambda'}.$$

Dynamical symmetry is not a universal characteristic: it depends on the number of off-diagonal blocks included into consideration and on the actual energy scale.
Examples: dipole transitions with $\Delta l = 1$, spin-flip transitions with ΔS=1, etc.

General view on emergence of dynamical symmetries in nanoobjects possessing RG invariance.



$$D \to D - \delta D; \quad J_i \to J_i + \delta J_i$$

Scaling equations :

$$\frac{dJ_i}{d \ln D} = - \sum_k a_{ik} J_i J_k$$

Flow RG?

Hubbard atom as a seed of SCES:

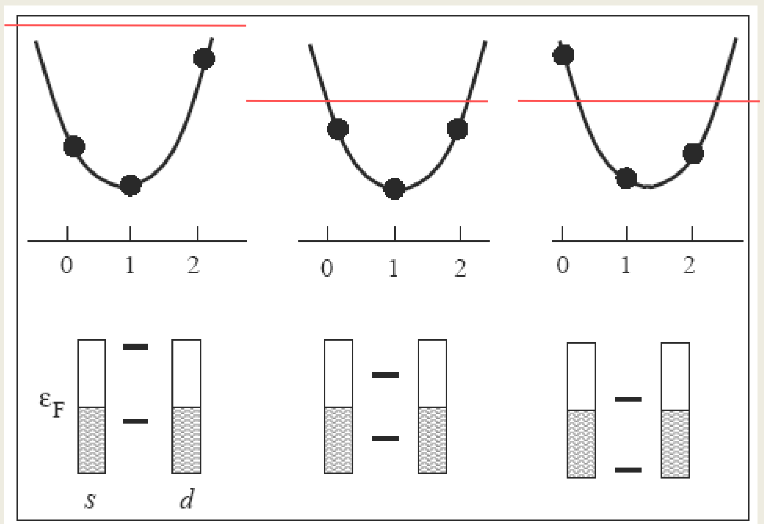
$$\hat{H}_d = \epsilon_d \sum_{\sigma=\uparrow,\downarrow} d^\dagger_{i\sigma} d_{i\sigma} + U n_{id\uparrow} n_{id\downarrow} = \sum_\Lambda E_\Lambda X^{\Lambda\Lambda}$$

where $\Lambda = 0, \sigma, 2$ and the energy levels E_Λ are

$$E_0 = 0, \quad E_\uparrow = E_\downarrow = E_1 \equiv \epsilon_d, \quad E_2 = 2\epsilon_d + U.$$

Hubbard parabolas for quantum dots:

E (N)



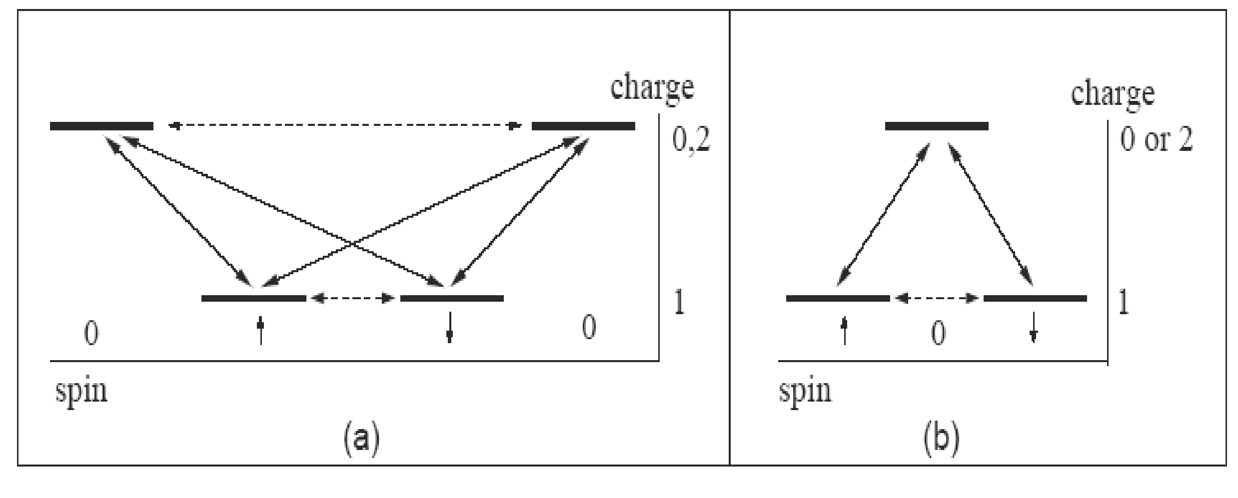
$$\bar{\Phi}_4 = (\uparrow \quad \downarrow \quad 0 \quad 2)$$

$$\bar{\Phi}_3 = (\uparrow \quad \downarrow \quad 0) \qquad (\uparrow \quad \downarrow \quad 2)$$

)

Useful tool for visualization of dynamical symmetries is the energy level diagrams arranged in accordance with relevant variables (***F. Onufrieva, 1981***).
In our case these variables are spin and charge (occupation number).

SU(4)



SU(3)

Florogrammes for Hubbard atom with variable charge and spin

Arrows connecting the levels E_Λ and $E_{\Lambda'}$ correspond to Hubbard operators $X^{\Lambda\Lambda'}$

The Bose-like transitions with even $\delta\mathcal{N} = 0, \pm 2$ are marked by the dashed arrows, the Fermi-like transitions with odd $\delta\mathcal{N} = \pm 1$ are marked by the solid arrows.

From the point of view of dynamical symmetry, one deals with a 4-level system in case of full Hubbard Hamiltonian, with a 3-level system in case when zero- or two-electron states are suppressed and with a 2-level system, when only spin degrees of freedom survive. The corresponding Fock spaces are Φ_4, Φ_3 and Φ_2, respectively.

Everybody knows that 2-level systems possess SU(2) symmetry with the basic matrices

$$\hat{\sigma}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

or the ladder operators

$$\hat{\sigma}^+ = \frac{1}{2}(\hat{\sigma}_x + i\hat{\sigma}_y) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}^- = \frac{1}{2}(\hat{\sigma}_x - i\hat{\sigma}_y) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

Pauli operators form closed *su(2)* algebra with commutation relations .

$$[\sigma_i, \sigma_k] = 2i\varepsilon_{ijk}\sigma_k \quad (i, j, k = x, y, z)$$

These operators generate *SU(2)* Lie group of infinitesimal rotations in a space Φ_2.

Our idea is to use the generators of SU(3) and SU(4) groups for representing the Hubbard and Anderson models. These generators are **the Gell-Mann matrices** of 3rd and 4th rank. These generators will be constructed from our beloved **Hubbard operators.**

Mathematical interlude: basic information about Gell-Mann matrices.

The number of group generators is n^2 -1 =15 or 8 (because of normalization condition).

SU(3):

$$\bar{\Phi}_3 = (\uparrow \quad \downarrow \quad 0) \quad \text{or} \quad (\uparrow \quad \downarrow \quad 2)$$

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.$$

SU(4) : $\bar{\Phi}_4 = (\uparrow \quad \downarrow \quad 0 \quad 2)$

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \lambda_9 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix},$$

$$\lambda_{10} = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}, \quad \lambda_{11} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \lambda_{12} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix},$$

$$\lambda_{13} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad \lambda_{14} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}, \quad \lambda_{15} = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix},$$

The traceless GM matrices describe ***all*** transitions between the levels 1,2,3,4 or 1,2,3. In other words, the Gell-Mann matrices generate the dynamical symmetry of 4-level or 3-level systems. Unit matrix λ_0 should be added in order to describe Hamiltonian and other physical operators.

The groups *SU(n)* with n>2 are semisimple, which means that their matrix representations are direct sums of simple *SU(2)* groups. It is convenient to use this fact explicitly, i.e. to introduce combinations of GM matrices (triads) with spin-like commutation relations. In case of *SU(3)* group these combinations are

$$\begin{aligned} \mathsf{T}^{\pm} &= \frac{1}{2}(\lambda_1 \pm i\lambda_2),\ \mathsf{T}_z = \lambda_3 \\ \mathsf{U}^{\pm} &= \frac{1}{2}(\lambda_6 \pm i\lambda_7),\ \mathsf{U}_z = \frac{1}{2}(-\lambda_3 + \sqrt{3}\lambda_8) \\ \mathsf{V}^{\pm} &= \frac{1}{2}(\lambda_4 \pm i\lambda_5),\ \mathsf{V}_z = \frac{1}{2}(\lambda_3 + \sqrt{3}\lambda_8), \end{aligned}$$

The operators belonging to the same triad commute like Pauli operators:

$$[\mathsf{O}_z, \mathsf{O}^{\pm}] = \pm 2\mathsf{O}^{\pm}, \quad [\mathsf{O}^{+}, \mathsf{O}^{-}] = \mathsf{O}_z.$$

The rest commutators are

$$[\mathsf{U}^{\pm}, \mathsf{V}^{\mp}] = \pm \mathsf{T}^{\mp},\ [\mathsf{U}^{\pm}, \mathsf{V}_{\mathsf{z}}] = \mp \mathsf{U}^{\pm},\ [\mathsf{U}_z, \mathsf{V}^{\pm}] = \pm V^{\pm},\ [\mathsf{U}_z, \mathsf{V}_z] = 0.$$

The matrix form of these operators is

$$\mathsf{T}^{+} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},\ \mathsf{T}^{-} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},\ \mathsf{T}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$\mathsf{U}^{+} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix},\ \mathsf{U}^{-} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},\ \mathsf{U}_z = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

$$\mathsf{V}^{+} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},\ \mathsf{V}^{-} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix},\ \mathsf{V}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Only eight of these operators are linearly independent.

The same trick for *SU(4)* groups results in appearance of 6 triades.
First three are the same matrices T, U, V, and the rest are W, Y, Z with the components:

$$\mathsf{W}^{\pm} = \frac{1}{2}\left(\lambda_9 \pm i\lambda_{10}\right), \; \mathsf{W}_z = \frac{1}{2}\left(\lambda_3 + \frac{1}{\sqrt{3}}\lambda_8 + \frac{4}{\sqrt{6}}\lambda_{15}\right)$$
$$\mathsf{Y}^{\pm} = \frac{1}{2}\left(\lambda_{11} \pm i\lambda_{12}\right), \; \mathsf{Y}_z = \frac{1}{2}\left(-\lambda_3 + \frac{1}{\sqrt{3}}\lambda_8 + \frac{4}{\sqrt{6}}\lambda_{15}\right)$$
$$\mathsf{Z}^{\pm} = \frac{1}{2}\left(\lambda_{13} \pm i\lambda_{14}\right), \; \mathsf{Z}_z = \frac{1}{\sqrt{3}}\left(-\lambda_8 + \sqrt{2}\lambda_{15}\right). \quad \text{(A3)}$$

Of course, only 15 operators of them are linearly independent. The choice of these 15 depend on the physics of the problem, you are interested in.

These triads ara matrices containing units and zeros as matrix elements.

In the Fock spaces Φ_n with n=3,4 each unit element may be represented by some Hubbard operator

$$\begin{aligned}
&\mathsf{T}^+ = X^{\uparrow\downarrow}, \quad \mathsf{T}^- = X^{\downarrow\uparrow}, \quad \mathsf{T}_z = X^{\uparrow\uparrow} - X^{\downarrow\downarrow} \\
&\mathsf{V}^+ = X^{\uparrow 0}, \quad \mathsf{V}^- = X^{0\uparrow}, \quad \mathsf{V}_z = X^{\uparrow\uparrow} - X^{00} \\
&\mathsf{U}^+ = X^{\downarrow 0}, \quad \mathsf{U}^- = X^{0\downarrow}, \quad \mathsf{U}_z = X^{\downarrow\downarrow} - X^{00} \\
&\mathsf{W}^+ = X^{\uparrow 2}, \quad \mathsf{W}^- = X^{2\uparrow}, \quad \mathsf{W}_z = X^{\uparrow\uparrow} - X^{22} \\
&\mathsf{Y}^+ = X^{\downarrow 2}, \quad \mathsf{Y}^- = X^{2\downarrow}, \quad \mathsf{Y}_z = X^{\downarrow\downarrow} - X^{22} \\
&\mathsf{Z}^+ = X^{02}, \quad \mathsf{Z}^- = X^{20}, \quad \mathsf{Z}_z = X^{00} - X^{22} \quad (
\end{aligned}$$

Non-zero commutation relations for the operators belonging to different triads: including those from *SU(4)* group:

$$[W^{\pm},Y^{\mp}]=\pm T^{\pm},\ [W^{\pm},Y_z]=\mp W^{\pm},\ [Y_z,W^{\pm}]=\pm W^{\pm},$$
$$[W^{\pm},Z^{\mp}]=\pm V^{\pm},\ [W^{\pm},Z_z]=\mp W^{\pm},\ [W_z,Z^{\pm}]=\pm Z^{\pm}$$
$$[Y^{\pm},Z^{\mp}]=\pm U^{\pm},\ [Y^{\pm},Z_z]=\mp Y^{\pm},\ [Y_z,Z^{\pm}]=\pm Z^{\pm}$$
$$[W^{\pm},T^{\mp}]=\mp Y^{\pm},\ [W^{\pm},T_z]=\mp W^{\pm},\ [W_z,T^{\pm}]=\pm T^{\pm},$$
$$[V^{\pm},W^{\mp}]=\mp Z^{\mp},\ [V^{\pm},W_z]=\mp V^{\pm},\ [V_z,W^{\pm}]=\pm W^{\pm},$$
$$[V^{\pm},Z^{\pm}]=\pm W^{\pm},\ [V^{\pm},Z_z]=\pm V^{\pm},\ [V_z,Z^{\pm}]=\mp Z^{\pm},$$
$$[U^{\pm},Z^{\pm}]=\pm Y^{\pm},\ [U^{\pm},Z_z]=\pm U^{\pm},\ [U_z,Z^{\pm}]=\mp Z^{\pm},$$
$$[Y^{\pm},T^{\pm}]=\pm W^{\pm},\ [Y^{\pm},T_z]=\pm Y^{\pm},\ [Y_z,T^{\pm}]=\mp T^{\pm},$$
$$[Y^{\pm},U^{\mp}]=\mp Z^{\pm},\ [Y^{\pm},U_z]=\mp Y^{\pm},\ [Y_z,U^{\pm}]=\pm U^{\pm}.$$

Thus instead of original superalgebra *Spl(2,1)* we get Pauli like algebras, which are more suitable for discussing the properties of SCES. There are some attempts to find supersymmetric SCES models involving Hubbard atom (e.g***., Essler, '95; Coleman et al, '01,'03***), but they are not too realistic and in fact Bose-Fermi duality merely reveals internal SU(n) dynamical symmetry of the Hubbard atom (***K.K., private communication***)

Now the last step: expressing the diagonal Hubbard operators entering the Hamiltonian of a Hubbard atom

$$\hat{H}_d = \sum_{\Lambda} E_\Lambda X^{\Lambda\Lambda} \qquad (*)$$

where $\Lambda = 0, \sigma, 2$ and the energy levels E_Λ are

$$E_0 = 0, \quad E_\uparrow = E_\downarrow = E_1 \equiv \epsilon_d, \quad E_2 = 2\epsilon_d + U$$

via the GM operators.

Following operators are involved in case of SU(4) symmetry (full Hubbard Hamiltonian)

$$\begin{aligned} \mathsf{Q}_z &= \mathsf{V}_z + \mathsf{U}_z = X^{11} - 2X^{00}, \\ \mathsf{P}_z &= \mathsf{W}_z + \mathsf{Y}_z = X^{11} - 2X^{22}, \\ 2\mathsf{Z}_z &= \mathsf{Q}_z - \mathsf{P}_z = 2(X^{22} - X^{00}) \end{aligned}$$

$$X^{00} + X^{11} + X^{22} = 1, \quad X^{11} = \sum_\sigma X^{\sigma\sigma}$$

Hubbard operators via GM operators

$$\begin{aligned} X^{00} &= \frac{1}{4} - \frac{1}{8}(3\mathsf{Q}_z - \mathsf{P}_z) \\ X^{22} &= \frac{1}{4} + \frac{1}{8}(\mathsf{Q}_z - 3\mathsf{P}_z) \\ X^{11} &= \frac{1}{2} + \frac{1}{4}(\mathsf{P}_z + \mathsf{Q}_z). \end{aligned}$$

Fermi operators via GM operators

$$d^\dagger_\uparrow = \mathsf{V}^+ + \mathsf{Y}^-, \quad d^\dagger_\downarrow = \mathsf{U}^+ - \mathsf{W}^-,$$

$$n_d = X^{\uparrow\uparrow} + X^{\downarrow\downarrow} + 2X^{22} = 1 + \frac{1}{2}(\mathsf{Q}_z - \mathsf{P}_z) = 1 + \mathsf{Z}_z.$$

Then

$$\hat{H}^{SU(4)} = \frac{2E_1+E_0+E_2}{4}\cdot \mathsf{G}_0 + \frac{h}{2}\cdot \mathsf{T}_z + \frac{E_{10}}{4}\cdot \mathsf{Q}_z + \frac{E_{12}}{4}\cdot \mathsf{P}_z + \frac{E_{20}}{4}\cdot \mathsf{Z}_z$$

Thus the operators $\mathsf{P}_z/4$, $\mathsf{Q}_z/4$, $\mathsf{Z}_z/4$ and $\mathsf{T}_z/2$
describe both Fermi-like and Bose-like excitations shown at "Florogrammes" .

Since the set of triads is overcomplete, only three of these diagonal operators correspond to some observables. Below some examples will be presented.

GM operators enter also the perturbation terms in SCES models. E.g. in Anderson model this perturbation describes hybridization/tunneling coupling with Fermi sea of conduction electrons:

$$H_{db} = \sum_{k\sigma} (t_k d_\sigma^\dagger c_{k\sigma} + \mathrm{H.c.})$$

In terms of GM operators it reads

$$\hat{H}_{db}^{SU(4)} = \sum_k t_k (\mathsf{V}^\dagger + \mathsf{Y}^\dagger) c_{k\uparrow} + (\mathsf{U}^\dagger - \mathsf{W}^-) c_{k\downarrow} + \mathrm{H.c.}$$

Unlike standard representation (*), the GM representation contains <u>excitation energies</u>, and thus can be directly used for construction of Green functions and concomitant diagrammatic techniques.

In case of reduced SU(3) model the same procedure gives

$$\hat{H}_d^{SU(3)} = \frac{2E_1 + E_0}{3} \cdot \mathsf{G}_0 + \frac{E_{10}}{3} \cdot (\mathsf{U}_z + \mathsf{V}_z) + \frac{h}{2} \cdot \mathsf{T}_z$$

$$\hat{H}_{db}^{SU(3)} = \sum_k t_k \left[(\mathsf{V}^+ c_{k\uparrow} + \mathsf{U}^+ c_{k\downarrow}) + \text{H.c.} \right].$$

Thus we rewrote the Anderson Hamiltonian in really invariant form. The eigenstates of operators U_z and V_z correspond to excitations of charge states with ΔN=1,-1 in the same sense as the eigenstates of spin operator $S_z = T_z/2$ with ΔS=1,-1. Below we will find corresponding quantum numbers.

Due to the commutation rule $[\mathsf{U}^\pm, \mathsf{V}^\mp] = \pm \mathsf{T}^\mp$ the spin sector is also involved in effective interaction (cf. Schrieffer –Wolff transformation which describe effective exchange between two subsystems. Thus the interaction with the bath (i) activates *dynamical SU(3)* symmetry.

Green functions:

There are Bose-like Green functions and Fermi-like Green functions for charge excitations. The question: how do these functions look in terms of GM operators?

There is nothing new about propagators for spin excitations: S = T/2,

$$G_s = \langle\langle \mathsf{S}^-(t) \cdot \mathsf{S}^+(0)\rangle\rangle,$$

"Atomic" spin propagator is

$$G_s = \frac{i}{2\pi}\frac{\langle \mathsf{S}_z\rangle}{\omega - h}.$$

Charge propagators are

$$G_v = \langle\langle \mathsf{V}^-(t)\mathsf{V}^+(0)\rangle\rangle, \quad G_u = \langle\langle \mathsf{U}^-(t)\mathsf{U}^+(0)\rangle\rangle$$

To calculate them one needs anticommutation relations for operators V,U.

$$\{\mathsf{U}^+, \mathsf{U}^-\} = \frac{2 + \mathsf{V}_z - 2\mathsf{U}_z}{3} \qquad \{\mathsf{V}^+, \mathsf{V}^-\} = \frac{2 + \mathsf{U}_z - 2\mathsf{V}_z}{3}$$

Using these anticommutators, one gets the bare atomic propagators:

$$G_v(\omega) = \frac{i}{2\pi}\frac{(2 + \langle \mathsf{V}_z\rangle - 2\langle \mathsf{U}_z\rangle)/3}{\omega - \epsilon_d},$$

$$G_u(\omega) = \frac{i}{2\pi}\frac{(2 + \langle \mathsf{U}_z\rangle - 2\langle \mathsf{V}_z\rangle)/3}{\omega - \epsilon_d}.$$

But the averages in the numerators are nothing but

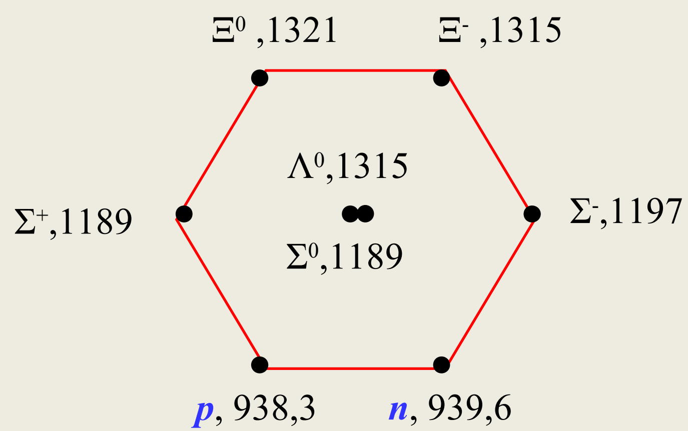
$$\langle X^{00}\rangle + \langle X^{\uparrow\uparrow}\rangle \text{ and } \langle X^{00}\rangle + \langle X^{\downarrow\downarrow}\rangle,$$

so everybody recognizes familiar Hubbard atomic propagators!

Historical Interlude

<u>Eight-fold way</u> offered in 1964 by Gell-Mann - Ne'eman and Zweig

Baryonic octet in QCD



This octet includes *neutral* and *charged* particles with *integer* and *half-integer* spin. Quark model offered in order to explain the origin of this multiplet as well as other baryonic and mesonic multiplet is nothing but realization of dynamical SU(3) symmetry .
Baryonic octet realizes the irreducible representation $D^{(11)}$ of the group *SU(3)* .
Other multiplets transform along other $D^{(nn')}$ representations.

The baryonic octet consists of two doublets, one singlet and one triplet. It is described in terms of so called strong interaction. The levels are split because of brocken symmetry due to electro-weak interaction, so the “elementary” particles are unstable. Particle transformation is in fact an inter-level transition within the multiplet.

Dynamical symmetry of baryon octet: “interlevel” transitions

mass, MeV

Ξ^0 ,1321
Ξ^- ,1315

Σ^-,1197
Σ^0,1192
Σ^+,1189

Λ^0,1315

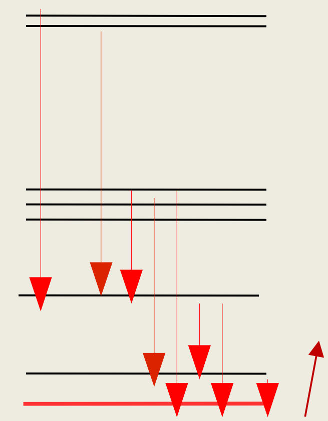
n, 939,6
p, 938,3

$$\Xi^0 \longrightarrow \Lambda + \pi^0$$
$$\Xi^- \longrightarrow \Lambda + \pi^-$$

$$\Sigma^- \longrightarrow n + \pi^-$$
$$\Sigma^0 \longrightarrow \Lambda + \gamma$$
$$\Sigma^+ \longrightarrow p + \pi^0, \quad \Sigma^+ \longrightarrow n + \pi^+$$

$$\Lambda \longrightarrow p + \pi^-, \quad \Lambda \longrightarrow n + \pi^0$$

$$n \longrightarrow p + e^- + \nu$$



“Elementary” particles / energy levels

reactions / interlevel transitions

True elementary particles behind this symmetry are “colored” quarks u,d,s possessing SU(3) symmetry

Hadron states are described by spin, charge, isospin and hypercharge

Unlike the case of SU(2) group, not one but two matrices representing generators of SU(3) group may be diagonalized simultaneously. It is natural to choose for diagonalization the matrices T_z and Q

$$\mathsf{T}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathsf{Q} = \frac{1}{3}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

Their eigenvalues are

$$M_T = 1, -1,\ 0; \quad M_Q = 1/3,\ 1/3, -2/3$$

for the states $|\uparrow\rangle, |\downarrow\rangle, |0\rangle$, respectively.

Thus the set of eigenstates is defined by two sets of quantum numbers. Conventional representation uses two sets of integer numbers

$$M_T = \lambda + \mu, \quad M_Q = \frac{1}{3}(\lambda - \mu).$$

Then the eigenvalues of infinite U Hubbard atom are represented as

λ	μ	M_T	M_Q	Λ
1	0	1	1/3	u
0	-1	-1	1/3	d
-1	1	0	-2/3	h

Quantum numbers for Hadron supermultiplet

	spin s	charge e	isospin T	M_T	hypercharge Q	
Ξ^0	**½**	**0**	**½**	**½**	**-1**	D
Ξ^-	½	-1	**½**	-½	-1	
Σ^-	½	-1	**1**	-1	0	T
Σ^0	½	0	**1**	0	0	S
Σ^+	½	1	**1**	1	0	
Λ^0	½	0	**0**	0	0	D
n	½	0	**½**	-½	1	
p	½	1	**½**	½ Q	1	

What does the hexagon ordering mean?

Octet of light hadrons contains elementary particles with spin ½, charge -1,0,1 plus isospin and hypercharge. The two last variables are described by quantum numbers M_T and M_Q ., which are the eigenstates of operators T_z and Q introduced above:

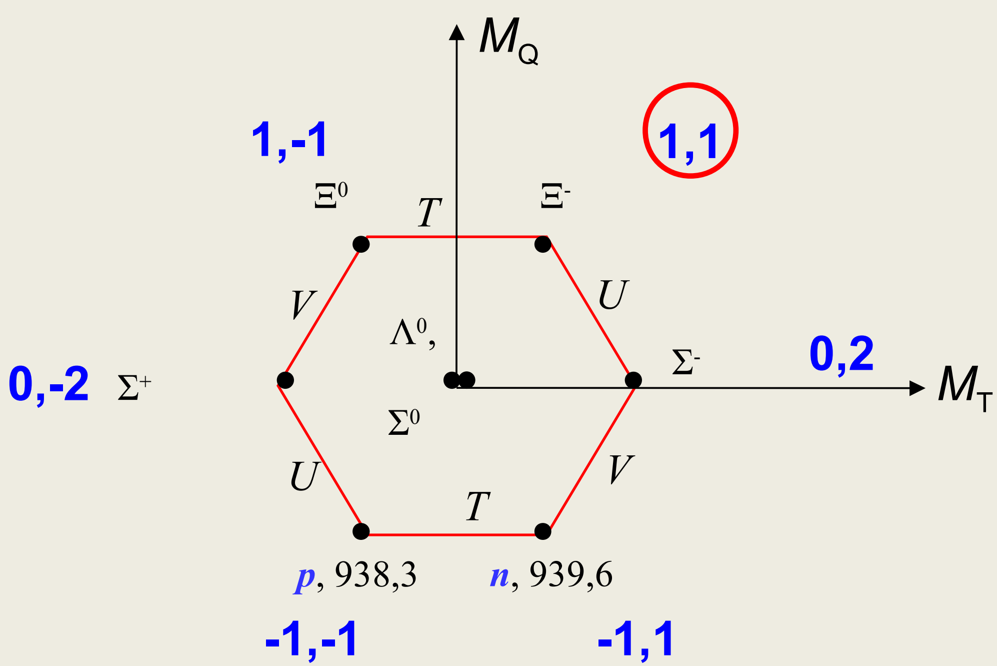
$$\mathsf{T}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathsf{Q} = \frac{1}{3}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

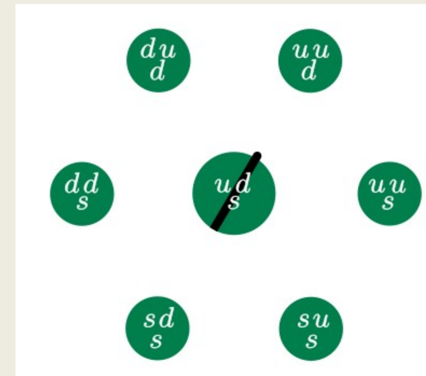
Thus the set of eigenstates is defined by two sets of quantum numbers.
Conventional representation uses two sets of integers

$$M_T = \lambda + \mu, \quad M_Q = \frac{1}{3}(\lambda - \mu).$$

Then the members of the hadron family can be arranged as the points on a triangular lattice in the plane (M_T , M_Q).

The set of basic vectors classifies the irreducible representations of *SU(3)* group.
In λμ classification the corresponding irreducible representation for baryon multiplet is $D^{(11)}$.





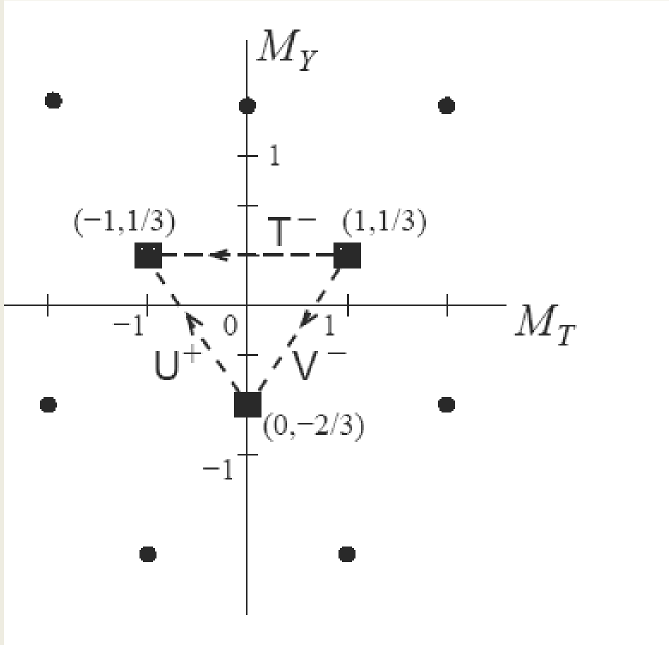
λ	μ	M_T	M_Q	Λ
1	0	1	1/3	u
0	-1	-1	1/3	d
-1	1	0	-2/3	h

h → s

Looking at mass values, we see that the SU(3) symmetry of strong interaction is conserved only approximately due to contribution of electroweak interactions. Real elementary particles are quarks and real symmetries are SU(3n) with SU(3) subgroups of quark triplets (*u,d,s*) with charge -1/3, 2/3.

Let us return to our Hubbard atom treated as a 3-level system.
The Gell-Mann procedure gives in this case the lowest irreducible representation $D^{(10)}$.

Horizontal arrows correspond to Bose like excitations (spin-flips with spin 1), Slanting arrows stand for Fermi-like excitations (adding/removing electron with spin ½).



: Irreducible representation $D^{(10)}$ for the set $\bar{\Phi}_3$

λ	μ	M_T	M_Q	Λ
1	0	1	1/3	u
0	-1	-1	1/3	d
-1	1	0	-2/3	h

The generic algebra is neither Bose, nor Fermi, it is Pauli-like!

In our case the number 1/3 is nothing but the normalization factor, because we deal only with charge and spin and there is no analogs of hypercharge and isospin in non-degenerate Hubbard model

The above procedure can be generalized for the full Hubbard model treated as a 4-level system:

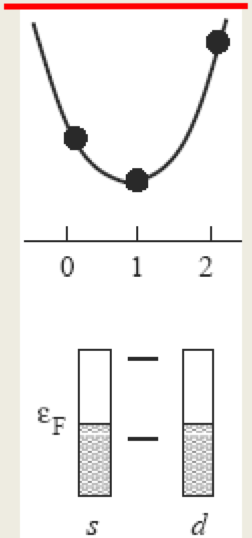
Generalization of this description for the $SU(4)$ group is straightforward. In this case the phase space for the irreducible representations is defined by the eigenvalues of the operators P_z, Q_z, T_z, and the lowest irreducible representation of this group $D^{(100)}$ is represented by a triangular pyramid in this 3D space. Three indices of the representation $D^{(\lambda\mu\nu)}$ determine the eigenvalues M_T, M_Q, M_P of the operators $\mathsf{T}_z/2$, $\mathsf{Q}_z/4$, $\mathsf{P}_z/4$:

$$M_T = \frac{\lambda+\mu-\nu}{2}, \quad M_Q = \frac{\lambda-\mu+\nu}{4}, \quad M_P = \frac{\lambda-\mu-\nu}{4}.$$

λ	μ	ν	M_T	M_Q	M_P	M_Z	Λ
1	0	0	1/2	1/4	1/4	0	$\uparrow$
0	-1	0	-1/2	1/4	1/4	0	$\downarrow$
-1	0	-1	0	-1/2	0	-1/4	h
0	1	1	0	0	-1/2	1/4	d

The quartet of Hubbard states form a triangle in the 3D space constituted by *z*-projections of group generators. In the conventional Hubbard atom with $U > 0$ the relevant operators are P,Q,T. In the model with negative U another triad is relevant, namely P,Q,Z (see below).

Physical applications: multistage Kondo screening in metals with magnetic impurities and quantum dots.



In the process of RG transformation, the symmetry reduces as

$$SU(4) \to SU(3) \to SU(2)$$

following the reduction of the energy scale from 4-level system to 2-level system at low energy. At the first two stages the excitation energy states are renormalized logarithmically (***Haldane '78***).

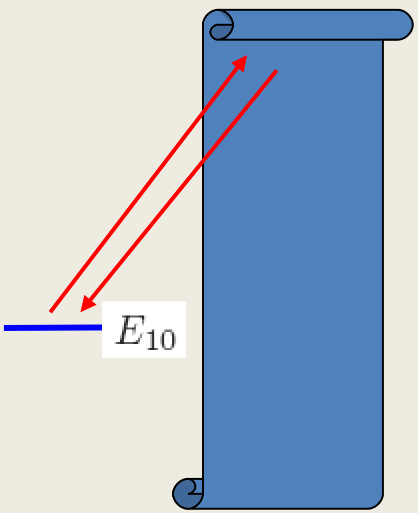
Scaling equation

$$\epsilon_d = E_{10} + \frac{\Gamma}{\pi}\int_0^D \frac{d\varepsilon}{E_{10}-\varepsilon} \quad \to \quad \frac{d\epsilon_d}{dD} = \frac{\Gamma}{\pi D}$$

the scaling invariant

$$\epsilon_d^* = \epsilon_d + \frac{\Gamma}{\pi}\ln\left(\frac{\pi D}{\Gamma}\right).$$

$$H_{\mathrm{SW}} = J\vec{S}\cdot\vec{s}$$



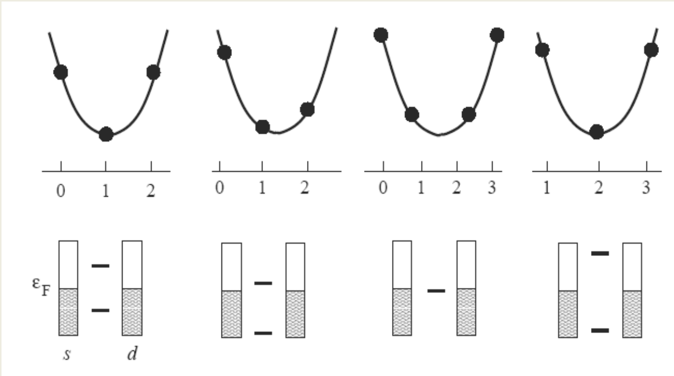
$$D \to D - \delta D; \quad J_i \to J_i + \delta J_i$$

Scaling equations :

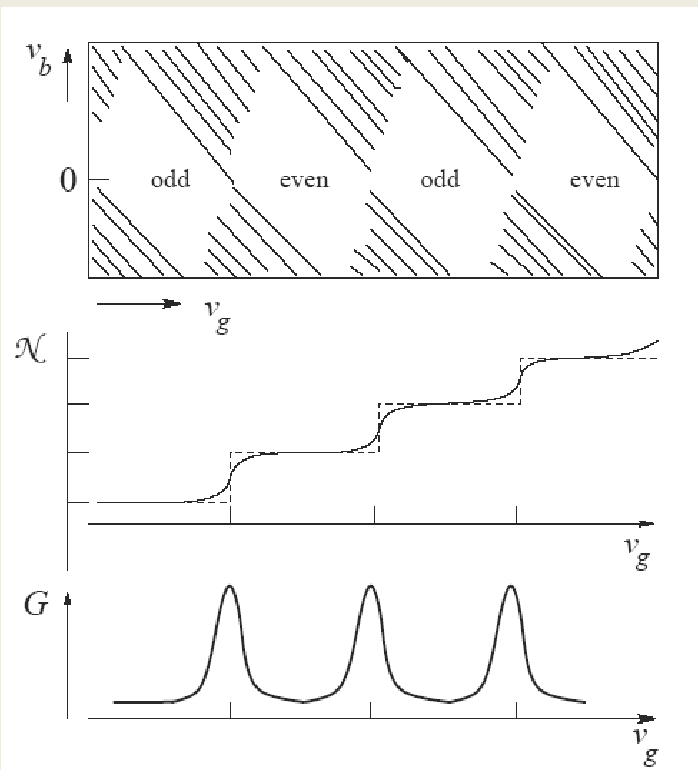
$$\frac{dJ_i}{d\ln D} = -\sum_k a_{ik} J_i J_k \quad \to \quad J(E,T) = \frac{\bar{J}}{1-2\rho_0\bar{J}\ln(\bar{D}/\max\{E,T\})}.$$

$$T_K = \sqrt{\Gamma D}\, e^{-\pi|\varepsilon_d|/2\Gamma}$$

Experimental realizations of Hubbard parabolas in quantum dots

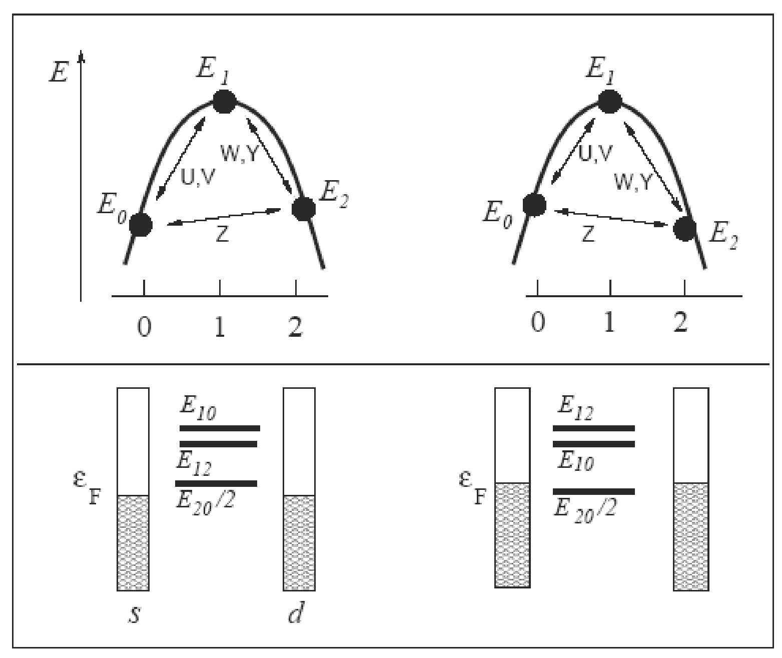


SU(4) → SU(3) → MV → SO(4)



The case N=2 in QD needs another approach involving *spin singlet - spin triplet excitations* within the same charge sector, but this is a separate story about *SO(n)* dynamical symmetries with $n > 3$.
(***K.K., Y. Avishai, M. Kiselev '98 – '08***)

Anderson model with negative U. Two-electron tunneling



Phonon-mediated attractive interaction change the sign of Hubbard parameter

$$U' = U - 2\lambda^2\Omega_0 \ .$$

Due to this "disproportionation" bipolaronic effect the lowest excitation energy is the energy of two-electron transition E_{20} and the spin flip processes are frozen out. In this physical reality the SU(4) group is formed by the vectors

$$\vec{Z}\,\vec{U}, \vec{V}, \vec{W}, \vec{Y}$$

This model is **dual** to *SU(4)* model with positive U!

The same 3-stage RG procedure results in the following strongly anisotropic SW Hamiltonian

$$\hat{H}_{\text{cotun}} = N\frac{J_\perp}{2}\left(\mathsf{Z}^+\mathsf{B}^- + \mathsf{Z}^-\mathsf{B}^+\right) + NJ_\parallel \mathsf{Z}_z\mathsf{B}_z \ ,$$

The components of the vector $\vec{\mathsf{B}}$ defined in the space of two-particle itinerant excitations are

$$\mathsf{B}^+ = N^{-1}\sum_{kk'} c^\dagger_{k\uparrow}c^\dagger_{k'\downarrow}, \quad \mathsf{B}^- = N^{-1}\sum_{kk'} c_{k\downarrow}c_{k'\uparrow},$$

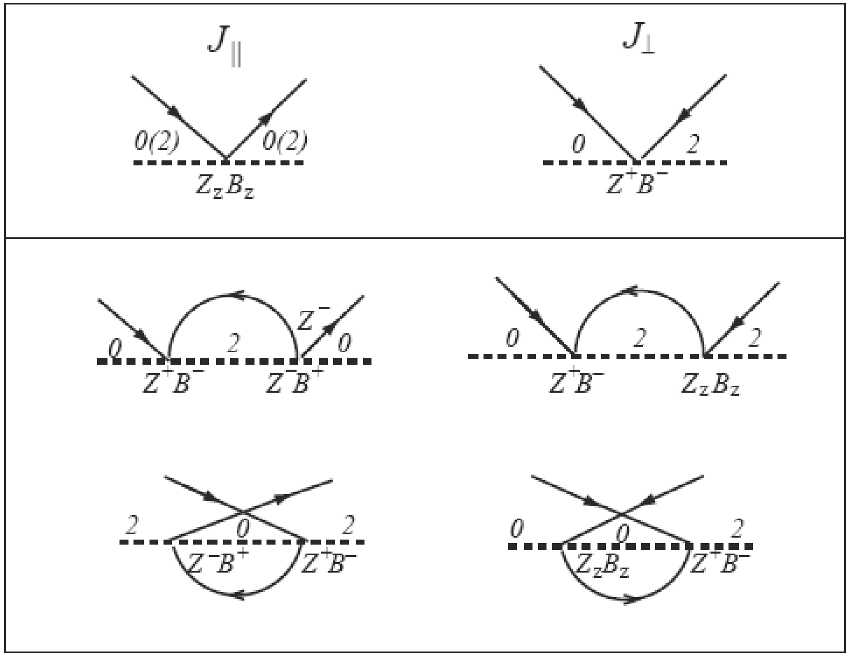
$$\mathsf{B}_z = N^{-1}\sum_{kk'}\left(c^\dagger_{k\uparrow}c_{k'\uparrow} - c_{k'\downarrow}c^\dagger_{k\downarrow}\right)$$

$$\frac{J_\perp}{J_\parallel} = \langle 2|0\rangle \sim e^{-2(\lambda/\Omega_0)^2}.$$

$$(\lambda/\Omega_0)^2 = S \gg 1$$

Instead of spin SU(2) space we arrive at holon-doublon SU(2) space $\bar{\Phi}_2 = (0, 2)$.
and the anisotropic Kondo problem is mapped on the two-electron tunneling model

$\vec{S} \to \vec{Z},\ \vec{s} \to \vec{B}.$



Scaling equations:

$$\frac{dj_{\|}}{d\eta} = -j_{\perp}^2, \quad \frac{dj_{\perp}}{d\eta} = -j_{\perp} j_{\|}$$

$$T_K \sim \left(\frac{j_{\perp}}{j_{\|}}\right)^{1/j_{\|}} \sim \bar{D} \exp\left[-\frac{\pi\Omega_0}{2\Gamma}\left(\frac{\lambda}{\Omega_0}\right)^4\right].$$

(*Aleksandrov, Bratkovskii ’03;*
Cornaglia et al ‘05)

This mapping is a bright manifestation of intrinsic SU(4) symmetry of Anderson model.

One more realization of SU(3) symmetry in nanoobjects: (***M.Kiselev and K.K., 2009***)

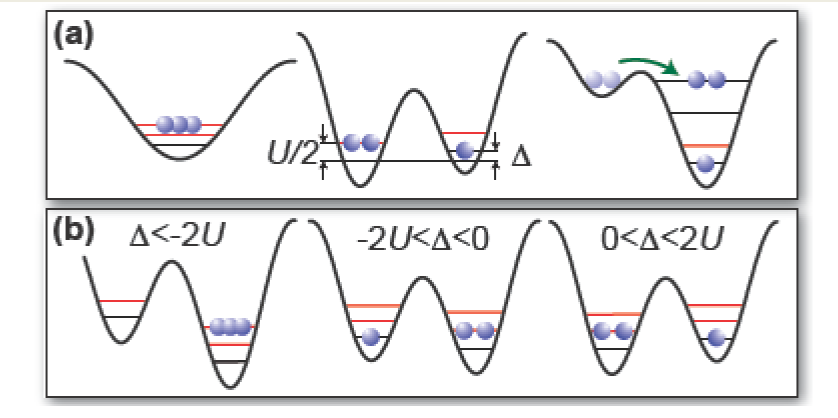
Double well traps in optical lattices

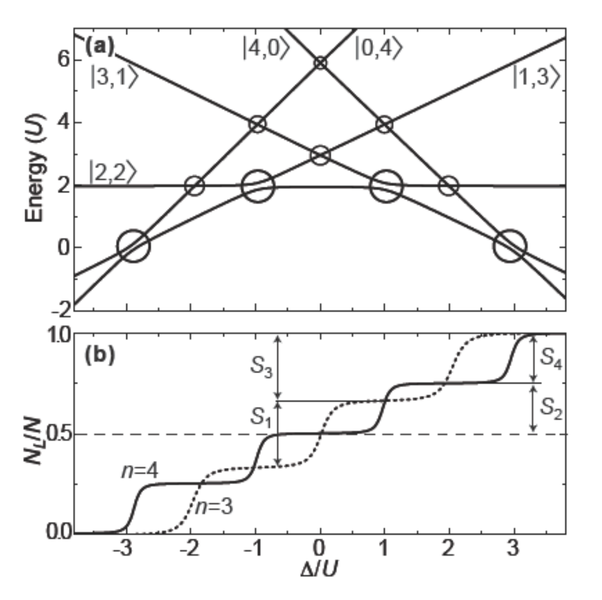
Experiment: (***P. Cheinet et al, PRL, 2008***)

87 Rb cold atoms in a bichromatic tetragonal optical lattice with a beam splitter

$$V(x) = V_s \cos^2(4\pi x/\lambda_l - \phi) + V_l \cos^2(2\pi x/\lambda_l),$$

where ϕ is the relative phase between the short and long period lattices. $V_{s,l,t}$ denote the lattice depths of the short, long and transverse lattices.

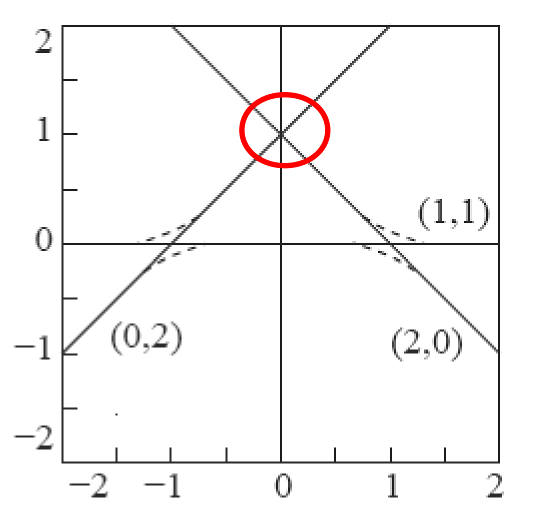




Model: double-well trap with tunneling between two wells with total occupation $N = 2$.

$$H_{\rm DW} = \sum_j (\varepsilon_j n_j + U n_j^2) - \Delta_0 (c_l^\dagger c_r + \text{H.c.}).$$

To describe a doubly occupied DW trap in pseudospin representation we introduce notation $|1\rangle, |0\rangle, |\bar{1}\rangle$ for eigenstates $E_1 = 2\varepsilon_0 - \delta_0 + U, E_0 = 2\varepsilon_0, E_{\bar{1}} = 2\varepsilon_0 + \delta_0 + U$ of the Hamiltonian (1) with $N = 2$ and $\Delta_0 = 0$ in configurations (2,0), (1,1), (0,2), respectively. Evolution of these levels as a function of the ratio δ_0/U is shown in Fig. 1



The effective pseudospin Hamiltonian for this 3-level system in this basis is

$$H_{\rm DW}^{(2)} = U S_z^2 - \delta_0 S_z + \Delta_1 (S^+ + S^-) - \mu_0 (N - 2).$$

$$S_z = |1\rangle\langle 1| - |\bar{1}\rangle\langle \bar{1}|, \quad S^+ = \sqrt{2}(|1\rangle\langle 0| + |0\rangle\langle \bar{1}|)$$

This is spin 1 Hamiltonian with single-site anisotropy, which allows transitions with $\Delta S_z = 2$.

As a result we have a three-level system with a dynamical symmetry SU(3).

In the first example of Hubbard atom we combined 8 Gell-Mann matrices
in two vectors **V, U** and two scalars T_z, Q . In this case another representation is used, namely irreducible vector T and and irreducible tensor $Q^{(2)}$ of the second rank with components

$$\hat{Q}_{(+1)} = \frac{1}{2}(T^+ - U^+) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{Q}_{(-1)} = \frac{1}{2}(U^- - T^-) = \begin{pmatrix} 0 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

$$\hat{Q}_{(+2)} = V^+, \quad Q_{(-2)} = V^-, \quad \hat{Q}_{(0)} = \frac{1}{3}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \frac{2}{3}(T_z - U_z). \qquad (592)$$

or in terms of Hubbard operators

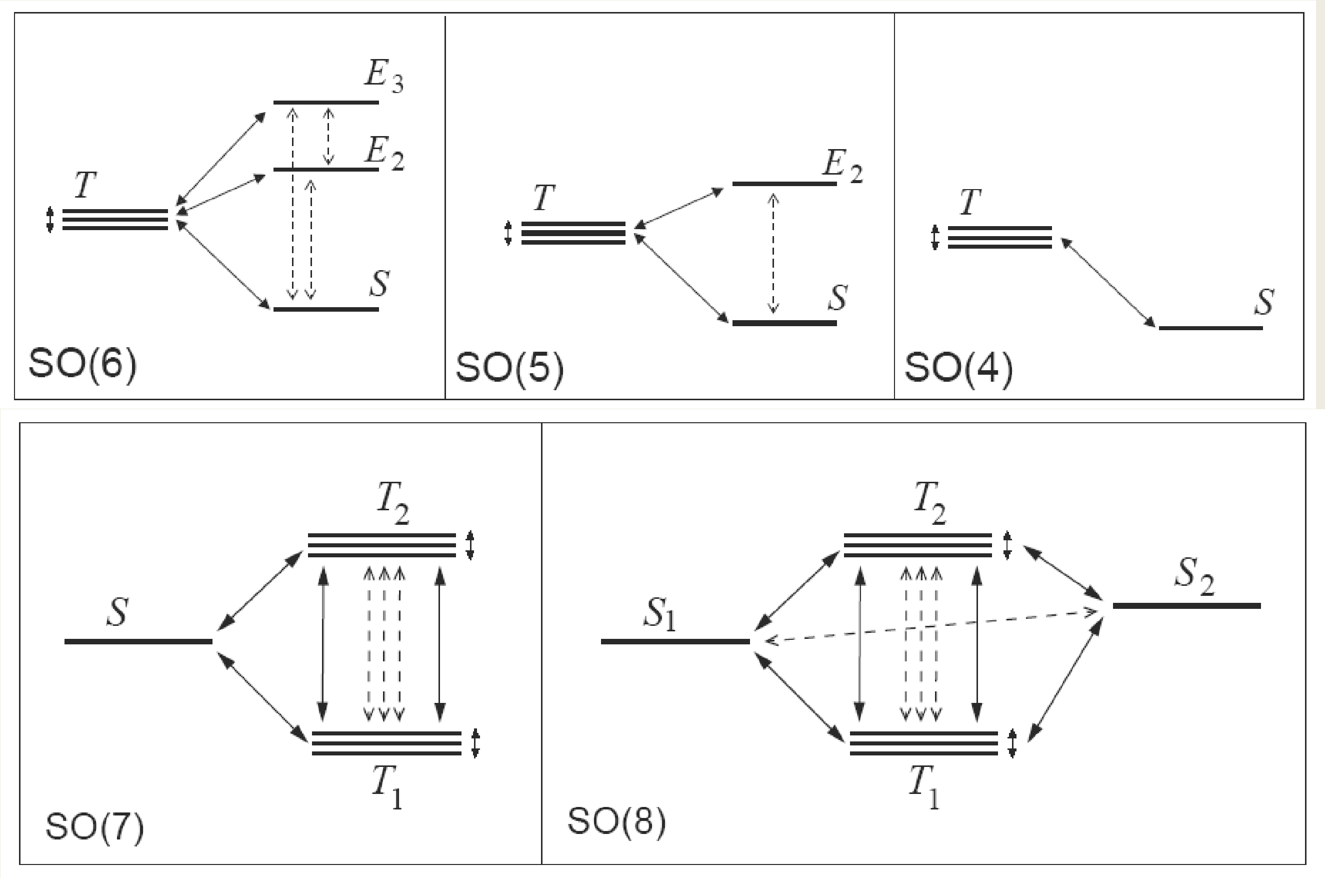
$$\begin{aligned} &\hat{Q}^{(2)}_{+2} = X^{1\bar{1}} \sim (S^+)^2, \quad \hat{Q}^{(2)}_{-2} = X^{\bar{1}1} \sim (S^-)^2, \\ &\hat{Q}^{(2)}_{0} = (X^{11} + X^{\bar{1}\bar{1}}) - 2/3 \sim S_z^2 - 2/3, \\ &\hat{Q}^{(2)}_{+1} = X^{10} - X^{0\bar{1}} \sim (S_z S^+ + S^+ S_z), \\ &\hat{Q}^{(2)}_{-1} = X^{\bar{1}0} - X^{01} \sim (S_z S^- + S^- S_z). \end{aligned}$$

(***Onufrieva ’81***)

This representation allows one to avoid square operators in the Hamiltonian and describe repopulation dynamics in generic variables of SU(3) group.

Florogrammes for double quantum dots with even number of electrons

In this case the relevant dynamical symmetry groups are semisimple SO(n) Lie groups



To summarize the survey of possible $SO(n)$ symmetries in spin systems described in the following chapters we present a table of representations of semisimple groups $SO(n)$ with n from 4 to 8 via scalar and vector irreducible operators (2.8):

n	rank	V	A	
4	6	2	0	S,T
5	10	3	1	2S,T
6	15	4	3	3S,T
7	21	6	3	S,2T
8	28	8	4	2S,2T

In the third and fourth columns the number of vector (V) and scalar (A) operators is shown, the last column explains the structure of energy spectrum, namely the number of spin singlets (S) and spin triplets (T) entering the corresponding super-multiplet.

CONCLUSIONS

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Dynamical Symmetries for Nanostructures

September 2, 2011

Springer

ПОКОЛЕНИЯ ВОЛХВОВ

Волхвы забудут адрес твой
И. Бродский

Когда зажжется над Москвой
Вечерняя звезда,
Волхвы припомнят адрес твой,
И явятся сюда.
Они придут из дальних стран,
Из ближних палестин:
Волхв Михаил, волхв Александр,
И третий – Константин.
Они отложат на потом
Текущие дела,
Чтобы собраться за столом
Там, где звезда взошла.
Они вернутся в теплый хлев,
Где научили их,
Что черств порой научный хлеб
И путь научный лих.
Они не вышли из игры
Своих учителей,
Они несут свои дары
На скромный юбилей.
А тот, который их учил,
Где ж…а где перёд,
Отнюдь на лаврах не почил,
Совсем наоборот –
Все так же молод, хоть и сед,
И мудр зело на вид,
В свои осьмнадцать с чем-то лет
Максимов Леонид.