

Chapter 2

HIDDEN AND DYNAMICAL SYMMETRIES OF ATOMS AND MOLECULES

We concentrate in this book on the symmetry properties of nanoobjects (quantum dots, rings and short chains of quantum dots, molecular complexes) in a weak tunneling and/or capacitive contact with reservoirs (metallic electrodes attached to quantum dots, metallic substrates or edges of nanowires for molecular complexes deposited on these surfaces and points, etc). Before turning to these artificially engineered devices, we will review in brief the origin of dynamical symmetry in "natural" quantum objects, i.e. in some integrable quantum systems with well defined energy spectrum and quantum numbers. Conventionally the symmetry of such systems is considered in terms of the symmetry group $G_{\mathcal{S}}$ of Schrödinger equation. This description is based on the fundamental Wigner theorem [428] which states that the eigenfunctions which belong to a given energy level E are transformed along the same irreducible representation of the group $G_{\mathcal{S}}$.

Sometimes two or more energy levels coincide not because of symmetry demands but due to *accidental degeneracy*. Such a degeneracy will play important part in the following chapters of this book. Here we concentrate on two other aspects of the symmetry of quantum systems, namely on the *dynamical* and *hidden* symmetries inherent in some integrable quantum objects.

Following the definition used in Ref. [274], we define the dynamical symmetry group $D_{\mathcal{S}}$ as a Lie group characterized by the irreducible representations which act in the whole Hilbert space of eigenstates $|\lambda\rangle$ of a Schrödinger equation

$$\hat{H}|\lambda\rangle = E_l|\lambda\rangle \quad (2.1)$$

describing quantum system $\mathcal{S}$. Here l is the index of irreducible representation and λ enumerates the lines of this representation. Projection operators for an irreducible

representation l

$$X_{(l)}^{\lambda\mu} = |l\lambda\rangle\langle l\mu| \quad (2.2)$$

play central part in the procedure of construction of irreducible representations of a group of Schrödinger equation $G_{\mathcal{S}}$. The basic property of these operators is given by the equation

$$X_{(l)}^{\lambda\mu} |l'\nu\rangle = \delta_{ll'} \delta_{\mu\nu} |l\lambda\rangle. \quad (2.3)$$

These operators are useful for construction of basis functions for irreducible representations of $G_{\mathcal{S}}$. Group generators obeying algebra $\mathfrak{g}_{\mathcal{S}}$ may be represented via operators (2.2) (see Chapter 9).

To construct an algebra which generates a dynamical group, one should add to the set (2.2) the operators

$$X_{(l'l'')}^{\lambda\mu} = |l\lambda\rangle\langle l'\mu| \quad (2.4)$$

which project the states belonging to different irreducible representations ($l \neq l'$) of the group G_S one onto another. Unifying the notations $|l\lambda\rangle = |\Lambda\rangle$, one may write the commutation relation

$$[X^{\Lambda\Lambda'}, \hat{H}] = (E_{\Lambda'} - E_{\Lambda}) \hat{H} \quad (2.5)$$

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 $G_{\mathcal{S}}$.

If one succeeds in constructing a closed algebra $\mathfrak{d}_{\mathcal{S}}$ from the set of operators (2.2),(2.4) then it is possible to say that the system described by the Hamiltonian (2.1) possesses the dynamical symmetry $D_{\mathcal{S}}$. This algebra is conditioned by the norm

$$\sum_{\lambda} X^{\lambda\lambda} = 1 \quad (2.6)$$

and the commutation relations for the operators $X^{\kappa\lambda}$. In general case these relations may be presented in the following form [170]

$$[X^{\kappa\lambda}, X^{\mu\nu}]_{\mp} = X^{\kappa\nu} \delta_{\lambda\mu} \mp X^{\mu\lambda} \delta_{\kappa\nu} \quad (2.7)$$

“General case” means that the Fock space includes states which may belong to different charge sectors, where changing the state λ for the state κ implies changing the number of fermions $N_{\lambda} \rightarrow N_{\kappa}$ in a many-particle system. If both $N_{\lambda} - N_{\kappa}$ and $N_{\nu} - N_{\mu}$ are odd numbers (Fermi-type operators), the plus sign should be chosen

in Eq. (2.7). If at least one of these difference is zero or even number (Bose-type operators), one should take the minus sign.

The operators $X^{\kappa\lambda}$ were exploited by J. Hubbard as a convenient tool for description of elementary excitations in strongly correlated electron systems (SCES). His seminal model of interacting electron motion in a narrow band, known now as a Hubbard model [169, 170, 171] was the first microscopic model of SCES for which the conventional perturbative approach based on Landau Fermi liquid hypothesis turned out to fail (see detailed discussion in Ref. [157]. Now the realm of SCES is really vast, and the most of artificial nanostructures belong to this realm. In particular, complex quantum dots under strong Coulomb blockade are typical examples of short Hubbard chains or rings (see Chapter 4).

The Hubbard operators (2.4) obeying the commutation relation (2.5) is a convenient tool for construction of the algebras generating the dynamical symmetry groups of the resolvent operator $\hat{R} = (\hat{H} - E)^{-1}$ or Schrödinger operator $\hat{R}^{-1}$. We will use these operators in a systematic way to construct the irreducible tensor operators $\mathcal{O}^{(r)}$ (scalars, $r = 0$, vectors, $r = 1$, and tensors $r = 2$) which transform along the representation of the dynamical group which characterizes the symmetry properties of the supermultiplet of the eigenstates of the Schrödinger equation:

$$\mathcal{O}_\rho^{(r)} = \sum_{\Lambda\Lambda'} \langle \Lambda | \mathcal{O}_\rho^{(r)} | \Lambda' \rangle X^{\Lambda\Lambda'}. \quad (2.8)$$

Here the index ρ stands for components of irreducible tensor operator of the rank r . On the one hand, it is clear that the operators $X^{\Lambda\Lambda'}$ are able to generate all the eigenstates of the Hamiltonian $\hat{H}$ from any given initial state Λ' . On the other hand, the components of the operators $\mathcal{O}^{(r)}$ form a closed algebra, which characterizes the dynamical symmetry group provided the Hamiltonian $\hat{H}$ possesses such symmetry. Having in mind future applications to geometrically confined nanoobjects, we restrict ourself mainly by discrete eigenstates.

In the two following sections we discuss the symmetry properties of two integrable quantum mechanical systems (rigid rotator and hydrogen atom) and show how the dynamical symmetries $D_{\mathcal{J}}$ emerge from the apparent symmetry $SO(3)$ of the Schrödinger equation.

2.1 Rigid Rotator

A simplified quantum-mechanical description of molecular motion in a framework of rigid rotator model implies quenching of vibrational excitations, whereas the rotational degrees of freedom are described as rotation of a "solid body" around some axis $\mathbf{n} = n_\xi, n_\eta, n_\zeta$ which in turn precesses around a fixed z axis in a 3D space. The Hamiltonian of symmetric rotator is

$$\hat{H} = \frac{\hbar^2}{2I_\perp} (L_\xi^2 + L_\eta^2) + \frac{\hbar^2}{2I_\parallel} L_\zeta^2 = \frac{\hbar^2}{2I_\perp} \mathbf{L}^2 + \frac{\hbar^2}{2} \left(\frac{1}{I_\parallel} - \frac{1}{I_\perp} \right) L_\zeta^2 \quad (2.9)$$

Here the coordinates (ξ, η, ζ) are bound to the rotation axis, $(I_\perp, I_\parallel)$ are two component of the moment of inertia. Both types of rotations are quantized but the energy levels depend only on the quantum number l and the eigenvalues κ of the operator L_ζ which change in the interval $\kappa = -l, \dots, l$

$$E_{j\kappa} = \frac{\hbar^2}{2I_\perp} l(l+1) + \frac{\hbar^2}{2} \left(\frac{1}{I_\parallel} - \frac{1}{I_\perp} \right) \kappa^2. \quad (2.10)$$

In case of fully symmetric rotator with $I_\perp = I_\parallel$ the levels lose dependence on κ and acquire $2l + 1$ -fold degeneracy. Additional degeneracy in projection of the angular momentum on the z -axis of fixed reference frame results in total $(2l + 1)^2$ -fold degeneracy of the level E_j of spherically symmetric rotator. This additional symmetry is inessential for the level classification, but it is meaningful from the point of view of the dynamical symmetry of rigid rotator [95, 275, 289]. Indeed, any rotation

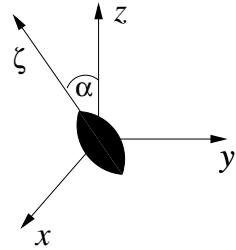


Fig. 2.1 Rigid rotator precessing around the axis z .

of the coordinates is characterized by three Euler angles in the precessing system (ξ, η, ζ) and one more angle α between the axes ζ and z (Fig. (2.1)). Corresponding spherical coordinates are $(r, \varphi, \vartheta, \alpha)$. The basis functions for description of such a motion are the hyperspherical harmonics $Y_{nlm}(\alpha, \vartheta, \varphi)$. On the other hand, these

harmonics form the basis for the irreducible representations of the group $SO(4)$ of rotations on a 4D sphere (see Section 9.2.1). The six generators $\mathbf{L}, \mathbf{K}$ of this group obey $o(4)$ algebra defined in Eq. (9.14). One may then turn to linear combinations $\mathbf{J}_{(1,2)} = (\mathbf{L} \pm \mathbf{K})/2$ (9.16). These two vectors describe the two types of rotations mentioned above. Due to the kinematic constraint (9.19) these operators have the same eigenvalues $j_1(j_1 + 1) = j_2(j_2 + 1) = l(l + 1)$ and their projections $J_{1\zeta}$ and $J_{2\zeta}$ have $2l + 1$ values. Thus, the total degeneracy of an eigenstate with given l is $(2l + 1)^2$.

The operators $L^\pm, L_\zeta$ performing rotations around the axes n_ξ, n_η, n_ζ generate the $o(3)$ algebra for the subgroup $SO(3)$ (invariance group), whereas the operators $K^\pm, K_\zeta$, which depend on all rotation angles $(\varphi, \vartheta, \alpha)$ (9.21) generate the dynamical algebra $o(4)$, and thus define the dynamical symmetry group $SO(4)$ of a rigid rotator which unites all the energy levels of rigid rotator in an infinite “supermultiplet” [289].

To show this, let us consider the vector $\mathbf{K}$ as an irreducible tensor of the 1-st rank and express its components K_τ^1 via projection operators (2.4) following the pattern (2.8). Here $\tau = 0, \pm 1$ stands for $K_\zeta, K_\pm$, respectively. In this case, one should use the operators $X_{mm'}^{(ll')}$ describing transitions between states with given momentum l and its projection m and the states with other values $l'm'$ of these quantum numbers,

$$K_\tau^{(1)} = \sum_{lm, l'm'} \langle lm | K_\tau^{(1)} | l'm' \rangle X_{mm'}^{ll'} \quad (2.11)$$

Then, using the Wigner-Eckart theorem, we represent the coefficients in this expansion as

$$\langle lm | K_\tau^{(1)} | l'm' \rangle = (-1)^{l-m} \begin{pmatrix} l & 1 & l' \\ -m & \tau & m' \end{pmatrix} \langle l || K^{(1)} || l' \rangle \quad (2.12)$$

(cf. Eq. 2.8) The factors in the r.h.s. of this equation are the Wigner $3j$ -symbol and the reduced matrix element of the vector K . Explicit form of these matrix elements may be found in [275, 289, 291].

It follows from the triangle rule for $3j$ -coefficients in Eq. (2.12) that the transversal components $K^\pm = K_x \pm iK_y$ of the operator $\mathbf{K}$, work as ladder operators which connect the states with $\Delta l = \pm 1$ and thus unite all the energy levels of rigid rotator into an infinite multiplet of the semisimple group $SO(4)$ with generators $\mathbf{L}, \mathbf{K}$ and two Casimir operators (9.18) or (9.19).

One may perceive from the above procedure that the choice of dynamical symmetry is not a unique procedure. For example, one may change the signature in the metrics from $\{+, +, +, +\}$ to $\{+, +, +, -\}$ and introduce generators $\tilde{K}_j$ (9.27) in-

stead of K_j . These operators represent dynamical symmetry $SO(3, 1)$. Usually the choice of enveloping group is determined by physical reasons (e.g., by the type of perturbation which actuates the dynamical symmetry). In particular, in case when this perturbation implies the selection rules $\Delta l = 0, \pm 1, \pm 2$ for transitions between different states, then one has to use the irreducible tensor $K_\tau^{(2)}$ of the 2nd rank in the expansion (2.8). Five components of this tensor together with the operators L_j of the invariance group $SO(3)$ form the set of generators of the dynamical group $SU(3)$ (see Sections 2.3 and 9.2.4).

2.2 Hydrogen atom and Runge-Lenz vector

The quantum mechanical problem of electronic spectrum of hydrogen atom inherited its peculiar properties from its classical analog, i.e. from the mechanical problem of rotation of one celestial body in the gravitational field $\sim 1/r$ of another body (Kepler problem). It was realized three centuries ago that the orbital rotation of celestial body in such a field is characterized by a specific constant of motion which is known now as a Laplace-Runge-Lenz vector (although two latter physicists only used this vector in their own tutorial and scientific texts). This vector arose anew in the analysis of the Schrödinger equation for an electron wavefunction $\psi(\mathbf{r})$ in the potential field created by a proton. This equation in atomic units ($e = 1, \hbar = 1, m = 1$) has the form:

$$\left(-\frac{\Delta}{2} - \frac{1}{r}\right) \psi(\mathbf{r}) = E \psi(\mathbf{r}). \quad (2.13)$$

Here Δ is the 3D Laplacian.

This equation obviously has the spherical symmetry $SO(3)$ generated by operators of infinitesimal 3D rotations, but the eigenlevels corresponding to discrete states with $E < 0$ depend only on the principal quantum number,

$$E_n = -\frac{1}{2n^2} \quad (2.14)$$

and not on the orbital momentum $l = n - 1, n - 2, \dots, 1, 0$, thus possessing the n^2 -fold degeneracy. All peculiarities of the behavior of an electron in a potential $\sim 1/r$ stem from the fact that the rotation group $SO(3)$ is only a subgroup of the true symmetry group of Eq. (2.14). To reveal this symmetry let us follow the approach used in Refs. [36, 111] and turn to the momentum representation of the Schrödinger equation (2.13)

$$\frac{p^2}{2}\psi(\mathbf{p}) + \frac{1}{2\pi} \int \frac{\psi(\mathbf{q})d\mathbf{q}}{(\mathbf{p}-\mathbf{q})^2} = -\frac{p_0^2}{2}\psi(\mathbf{p}) \quad (2.15)$$

where

$$\psi(\mathbf{p}) = \frac{1}{(2\pi)^{3/2}} \int \psi(\mathbf{r})e^{-i(\mathbf{p}\cdot\mathbf{r})}d\mathbf{r}, \quad -\frac{p_0^2}{2} = E \quad (2.16)$$

Then we make a conformal mapping of each point $(\mathbf{p}, p_0)$ onto a point on the surface of the 4D sphere of unit radius with the coordinates $(\xi_1, \xi_2, \xi_3, \xi_4)$

$$\xi_i = \frac{2p_0}{p_0^2 + p^2} p_i \quad (i = 1, 2, 3); \quad \xi_4 = \frac{p_0^2 - p^2}{p_0^2 + p^2}; \quad \sum_{i=1-4} \xi_i^2 = 1 \quad (2.17)$$

Then by means of substitution

$$\Psi(\xi_1, \xi_2, \xi_3, \xi_4) = \frac{\pi}{\sqrt{8}} (p_0)^{5/2} (p_0^2 + p^2)^2 \psi(\mathbf{p}) \equiv \Phi(\mathbf{p})$$

Eq. (2.15) is transformed into

$$\Psi(\xi_1, \xi_2, \xi_3, \xi_4) = \frac{1}{2\pi^2 p_0} \int_{R_4} \frac{\Psi(\xi'_1, \xi'_2, \xi'_3, \xi'_4) d^4 \xi'}{|\xi_1 - \xi'_1|^2 + |\xi_2 - \xi'_2|^2 + |\xi_3 - \xi'_3|^2 + |\xi_4 - \xi'_4|^2} \quad (2.18)$$

The latter equation is invariant relative to rotations in a 4D space. Thus, we see that the real symmetry of an electron in a Coulomb field is $SO(4)$. One may construct the infinitesimal rotation operators in the space $\{\xi_1, \xi_2, \xi_3, \xi_4\}$. There are six such operators describing rotations in six 2D planes $(\xi_i \xi_j)$. Details of this construction may be found in the book [327]. Returning back from ξ -space to original variables $\{\mathbf{p}, p_0\}$ and changing p_0 for the operator $\sqrt{-\hat{H}}$, where $\hat{H}$ is the Hamiltonian operator in Eq. (2.13), one eventually finds equations for these generators:

$$\mathbf{L} = \frac{\mathbf{r} \times \mathbf{p} - \mathbf{p} \times \mathbf{r}}{2} \quad (2.19)$$

$$\mathbf{F} = \left(\frac{\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p}}{2} - \frac{\mathbf{r}}{r} \right) \sqrt{\frac{1}{-2\hat{H}}}$$

The vector of orbital momentum $\mathbf{L}$ contains three generators of the group $SO(3)$, which in this case is only a subgroup of the true symmetry group $SO(4)$ [111, 324]. Three more generators of the latter group are given by the components of the vector $\mathbf{F}$. The Runge – Lenz vector mentioned above is in fact

$$\mathbf{A} = \mathbf{F} \sqrt{-2\hat{H}}. \quad (2.20)$$

It commutes with the Hamiltonian $\hat{H}$. After replacing the operator $\hat{H}$ by its eigenvalue E in Eq. (2.19) for $\mathbf{F}$, the commutation relations for the generators $\mathbf{L}, \mathbf{F}$ acquire the form

$$\begin{aligned} [L_i, L_j] &= i\epsilon_{ijk}L_k, \\ [F_i, F_j] &= i\epsilon_{ijk}L_k, \\ [F_i, L_j] &= i\epsilon_{ijk}F_k. \end{aligned} \quad (2.21)$$

which is exactly the algebra $o(4)$ of the $SO(4)$ group generators (see Section 9.2.1). Besides, these operators are subject to kinematic restrictions

$$\mathcal{C}_1 = \mathbf{L}^2 + \mathbf{F}^2 = -1 - \frac{1}{-2\hat{H}}, \quad \mathcal{C}_2 = \mathbf{L} \cdot \mathbf{F} = 0, \quad (2.22)$$

which are in fact two Casimir operators for the group $SO(4)$ [cf. Eq. (9.18)]. Using (2.22), one may express the Coulomb Hamiltonian via Casimir invariants:

$$\hat{H} = -\frac{1}{2} \frac{1}{\mathcal{C}_1 + \mathcal{C}_2 + 1} = -\frac{1}{2} \frac{1}{(\mathbf{L} + \mathbf{F})^2 + 1} \quad (2.23)$$

Next, we make the rotation

$$\mathbf{J} = \frac{1}{2}(\mathbf{L} + \mathbf{F}), \quad \mathbf{K} = \frac{1}{2}(\mathbf{L} - \mathbf{F}), \quad (2.24)$$

and transform the first Casimir operator into

$$\mathbf{J}^2 = \mathbf{K}^2 = -\frac{1}{4} \left(1 + \frac{1}{2\hat{H}} \right) \quad (2.25)$$

The commutation relations for the last set of generator are

$$\begin{aligned} [J_i, J_j] &= i\epsilon_{ijk}J_k, \\ [K_i, K_j] &= i\epsilon_{ijk}K_k, \\ [K_i, J_j] &= 0. \end{aligned} \quad (2.26)$$

[cf. Eq. (9.19)]. As is discussed in Section 9.2.1, these relations points at the local isomorphism $SO(4) = SO(3) \times SO(3)$. Inserting the eigenvalues $j(j+1) = k(k+1)$ of the operators $\mathbf{J}^2 = \mathbf{K}^2$ and the eigenvalues E of the Hamiltonian $\hat{H}$ into Eq. (2.25) one obtains $E = -1/2(2j+1)^2$. Since j is integer, one may take $2j+1 = n = 1, 2, \dots$ and just come to the well known result (2.14). Thus, we see that the additional degeneracy of discrete spectrum of hydrogen atom is a direct consequence of an

additional "hidden" dimension which results in appearance of additional Casimir operator.

To reveal the dynamical symmetry of an electron in the Coulomb field, one should notice that the solutions of Eq. (2.18) may be represented by means of harmonic polynomials $\varphi(\{\xi_j\})$ of the vector ξ on the 4D sphere, which satisfy the equation

$$\Delta_4 \varphi = 0, \quad (2.27)$$

where

$$\Delta_4 = \sum_{j=1}^4 \frac{\partial^2}{\partial \xi_j^2}$$

is the 4D Laplacian. One may construct operators of infinitesimal transformations, which commute with Δ_4 [274]. These are

$$\begin{aligned} L_j &= i \sum_{k,l} \varepsilon_{jkl} \left(\xi_k \frac{\partial}{\partial \xi_l} \right), \\ R_j &= \sum_k \left(\xi_k^2 \frac{\partial}{\partial \xi_j} - 2 \xi_j \xi_k \frac{\partial}{\partial \xi_k} - 2 \xi_j \right) \\ P_j &= -i \frac{\partial}{\partial \xi_j} \\ I &= 1 + \sum_k \xi_k \frac{\partial}{\partial \xi_k} \end{aligned} \quad (2.28)$$

or, in alternative notations M_{kl} :

$$L_j \equiv \varepsilon_{jkl} M_{kl} \quad (2.29)$$

[see Eq. (9.12) in the Mathematical Annex (Chapter 9)].

These operators may be combined in antisymmetric linear combinations $L_{\mu\nu}$ ($\mu, \nu = 0, 1, 2 \dots 5$),

$$\begin{aligned} L_{\mu\nu} &= M_{\mu\nu} \quad (\mu, \nu = 1 \dots 4), \\ L_{\mu 5} &= (R_\mu + iP_\mu)/2 \quad (\mu = 1 \dots 4), \\ L_{\mu 0} &= (R_\mu - iP_\mu)/2 \quad (\mu = 1 \dots 4), \\ L_{50} &= -I. \end{aligned} \quad (2.30)$$

which form the algebra of the conformal group $SO(4,2)$ (see Section 9.2.2) and obey the commutation relations (9.32).

The operators $L_{\mu\nu}$ in the first line of Eq. (2.30) form the algebra $\mathfrak{o}(4)$ for the subgroup $SO(4)$ of dynamical group $SO(4, 2)$. The representations of this subgroup are characterized by the principle quantum number n of discrete hydrogen levels E_n (2.14), whereas the radial quantum numbers, namely j, k and their projections related to the hidden symmetry determine the degeneracy of discrete electron states in a Coulomb potential. Like in the case of rigid rotator, the operators $L_{\mu 5}$ and $L_{\mu 0}$ involving two additional dimensions in the Fock space work as ladder operators in the basis $|j, j_z; k, k_z\rangle$ just connecting the states with different quantum numbers n and thereby realizing the dynamical symmetry $SO(4, 2)$ [41, 274]. This dynamical symmetry is realized in electric dipole transition between neighboring energy states ($n \rightarrow n \pm 1, j \rightarrow j \pm 1$) [41]. It is worth noting that the dipole transitions realize the dilatation operation (9.30) of this conformal group.

Although the above considerations are confined to three-dimensional rigid rotator and Coulomb atom, the results can be generalized to any dimension n . In the general case the invariance group $SO(n)$ generates the enveloping dynamical group $SO(n+1)$ or $SO(n, 1)$ as a compact or non-compact dynamical group for n -dimensional rigid rotator [289].

Similar studies of the Coulomb problem [11, 212, 274, 289, 387] show that the invariance group of n -dimensional hydrogen atom is $SO(n+1)$ due to existence of additional invariant, i.e. Runge – Lenz vector. Its form is a natural extension of Eq. (2.20). Using the notation M_{jk} for the definition of the infinitesimal rotation in the plane (x_j, x_k) dissecting the n -dimensional sphere [see Eq. (9.12), the component A_j of this vector reads

$$A_j = M_{jk} \frac{\partial}{\partial x_k} + \frac{\partial}{\partial x_k} M_{jk} - \frac{x_j}{r}. \quad (2.31)$$

With the help of this equation one constructs the component j of the n -dimensional vector $\mathbf{F}$

$$F_j = \frac{1}{\sqrt{-2\hat{H}}} A_j \quad (2.32)$$

and repeat the above analysis in order to reveal the dynamical symmetry $SO(n, 2)$ [274].

Another important aspect of hidden symmetry of the hydrogen atom is its supersymmetry intimately related to the projection of the Runge-Lenz vector on the electron spin direction [394]. We postpone discussion of this problem till Section 2.6.1, where this property will be considered together with other examples of supersymmetries.

2.3 Dynamical symmetries for spin systems

In Sections 2.1 and 2.2 we dealt with integrable systems where the dynamical symmetry emerges due to rotations R_n in real space and the invariance group is a group $SO(n)$ of rotations on an n -dimensional sphere. Now we turn to the problems where the spinor structure of wave function predetermines both the symmetry group of Schrödinger equation and the dynamical symmetry group of supermultiplet. The source of spinor structure may be the spin variable alone, or some other discrete index (color), i.e. number of wells in a trap with several minima, or combination of both mechanisms. In any case the invariance group is the group $SU(2)$ of unimodular matrices of 2nd rank (see Section 9.1 for mathematical definitions).

To introduce the $SU(2)$ symmetry group and its generalization $SU(n)$, we first consider a handbook problem of one or several particles in shallow enough quantum trap with two minima and assume that each of two wells contains a single discrete s -level with zero orbital momentum. This elementary quantum object known under the name of two-level system (TLS) is used as a constituent of various physical applications some of which will be discussed in subsequent chapters of this book. Since the TLS model may be solved exactly for any occupation of double quantum well, we use it as a toy model with an energy spectrum consisting of few levels which allows one to demonstrate how dynamical symmetry of the spectrum emerges from the symmetry of the Hamiltonian. We will consider here the cases of two-well trap with occupation $\mathcal{N} = 1, 2$. The extension of this approach for multiwell traps and larger occupation numbers $\mathcal{N}$ is straightforward.

Let us start with a Hamiltonian for a single particle in a double-well potential $V_{\text{TLS}}(\mathbf{r})$,

$$\hat{H} = H_1 + H_2 + H_t. \quad (2.33)$$

Two wells are labeled with indices 1 and 2. A particle in an individual well j is described by the Schrödinger equation

$$\left(-\frac{\Delta_r}{2} + V_j(r) \right) \psi_j(\mathbf{r}) = \varepsilon_j \psi_j(\mathbf{r}). \quad (2.34)$$

Then the last term in Eq. (2.33) which describes the tunneling barrier between two wells is defined as

$$V_t(\mathbf{r}) = V_{\text{TLS}}(\mathbf{r}) - V_1(\mathbf{r}) - V_2(\mathbf{r}) \quad (2.35)$$

For the sake of simplicity it is assumed that the direct overlap between the wavefunctions of the particles in two wells is negligibly small and the width of the tunneling barrier is parametrized as $W = \langle \psi_1 | V_t | \psi_2 \rangle$.

Like in previous cases [see Eqs. (2.9) and (2.23)], our aim is to write the Hamiltonian of TLS in terms of invariant operators. For this case we reformulate the Schrödinger equation via spinor wave function $\hat{\psi} = \{ \psi_1 \chi, \psi_2 \chi \}$, where χ is a two-component spinor

$$\chi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (2.36)$$

In this representation the effective Hamiltonian $\hat{H}_{\text{eff}} = \langle \hat{\psi} | \hat{H} | \hat{\psi} \rangle$ acquires the matrix form

$$\hat{H}_{\text{eff}} = \varepsilon_0 \hat{t}_0 + \delta\varepsilon \hat{t}_z + W \hat{t}_x \quad (2.37)$$

where

$$\varepsilon_0 = \frac{\varepsilon_1 + \varepsilon_2}{2}, \quad \delta\varepsilon = \frac{\varepsilon_1 - \varepsilon_2}{2}$$

and the Pauli matrices $\hat{t}_i$ are defined in Eq. (9.3). Diagonalization of this Hamiltonian is an easy task. It gives the two-level spectrum

$$E_{(b,a)} = \varepsilon_0 \mp \sqrt{\delta\varepsilon^2 + W^2} \quad (2.38)$$

The subindices b, a correspond to the bonding and antibonding combination of eigenfunctions $\psi_{(b,a)}$.

$$\begin{pmatrix} \psi_b \\ \psi_a \end{pmatrix} = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}. \quad (2.39)$$

The mixing angle is defined as

$$\tan \theta = \frac{2W}{|\varepsilon_1 - \varepsilon_2|}. \quad (2.40)$$

One should note that the above results are valid both for Bose particles and spinless Fermi particles. When one deals with electron or other fermion with spin 1/2 and the wave function $\psi_{(b,a),\sigma}$, the energy levels are degenerate in spin index σ unless the tunneling is spin-sensitive. Then the energy spectrum of TLS consists of two spin doublets. Transitions within the spin doublet are determined by usual spin 1/2 matrices $\sigma = \tau/2$. The set of spin 1/2 operators may be constructed by means of Hubbard operators $X^{\sigma\sigma'}$

$$\sigma_z = \frac{1}{2}(X^{\uparrow\uparrow} - X^{\downarrow\downarrow}), \quad \sigma^+ = X^{\uparrow\downarrow}, \quad \sigma^- = X^{\downarrow\uparrow}. \quad (2.41)$$

In order to construct the algebra of operators describing transitions between the levels which belong to the supermultiplet (2.38) consisting of two spin doublets, one may use the same Pauli matrices as in the Hamiltonian (2.37), whereas transitions between the bonding and antibonding states are given by the Hubbard operators $X^{ab} = |a\rangle\langle b|$ and the like. One may construct the Pauli matrices acting in subspace $\{\psi_b, \psi_a\}$ in the following way:

$$\tau_0 = (X^{bb} + X^{aa}), \quad \tau_3 = (X^{bb} - X^{aa}), \quad \tau^+ = X^{ba}, \quad \tau^- = X^{ab}. \quad (2.42)$$

It is clear that all possible transitions between the energy levels (2.38) are described by composite Hubbard operators of the type $X^{\sigma\sigma'}X^{ab}$ which can be represented as components of a direct product $\sigma \otimes \tau$ of spin and pseudospin operators. These components provide 15 generators of $su(4)$ algebra [99]:

$$(\sigma_0, \sigma^+, \sigma^-, \sigma_3,) \otimes (\tau_0, \tau^+, \tau^-, \tau_3) - \sigma_0 \otimes \tau_0. \quad (2.43)$$

Thus, the dynamical symmetry of full TLS supermultiplet is $SU(4)$.

If one is interested only in spin conserving transitions between bonding and antibonding states, then two subspaces remain orthogonal and the matrix (2.43) reduces to

$$\begin{pmatrix} \sigma_0 \tau & 0 \\ 0 & \sigma \tau_0 \end{pmatrix} \quad (2.44)$$

where the first block corresponds to tunneling transitions without spin flips, and the second block is created by the spin-flip processes within each spin doublet E . Then the dynamical symmetry reduces from $SU(4)$ to $SU(2) \times SU(2)$.

Next we turn to a double quantum well occupied by two electrons, $\mathcal{N} = 2$. In the general case two more parameters enter the game, namely, the Coulomb and exchange energy of a two-electron system. In our case both electrons are in orbital s -states, and the Coulomb repulsion parameter U between the two electrons within the same well is enough to describe both Coulomb and exchange components of the interaction. The latter may appear in the problem, e.g. as an indirect exchange $J \sim W^2/U$ induced by virtual interdot tunneling (see below). From the point of view of quantum-mechanical description, a doubly occupied two-well trap is a caricature of a hydrogen molecule, where all vibrational and rotational degrees of freedom are frozen and the Coulomb attraction of two protons is modeled by a trap with

two potential minima. However, unlike the “natural” hydrogen molecule, which is strictly symmetric relative to permutation of two hydrogen atoms and should be classified in terms of even and odd combinations of wavefunctions ψ_j , the double quantum well is asymmetric in the general case. The measure of this asymmetry is the parameter $\delta\epsilon$. It controls the energy spectrum of doubly occupied trap together with parameters U and W .

It is known that one may use two types of basis functions in a description of two-electron states depending on the ratio between the tunneling amplitude W and the Coulomb repulsion U . If the tunneling is dominant, $W \gg U$, the appropriate basis is a set $\psi_{\pm}$ of bonding/antibonding states (the Hund-Mulliken method). In the opposite limit of strong interaction, $U \gg W$ the natural basis is the Slater determinant of antisymmetrized products $\psi_i(\mathbf{r})\psi_j(\mathbf{r}')$ with $i, j = 1, 2$ (the Heitler-London method). In the latter case the weight of “polar” states with two electrons in the same well is suppressed by strong repulsive interaction.

Of course, the spectrum contains the same number of energy levels (namely, six) in both limits. In any case the ground state is singlet, the first excited state is triplet, and the two other states are charge transfer excitons [206]. In the forthcoming chapters various examples of this six-level spectrum will be considered in more detail. Here we confine ourselves with general discussion of dynamical symmetry for a supermultiplet consisting of one spin triplet and three spin singlets. Let us present the Hamiltonian of a two-well trap in the diagonal form

$$\hat{H} = \sum_{\Lambda} E_{\Lambda} |\Lambda\rangle\langle\Lambda| \equiv \sum_{\Lambda} E_{\Lambda} X^{\Lambda\Lambda} \quad (2.45)$$

[cf. Eq. (2.4)]. Here $\Lambda = S, T\mu, E_2, E_3$ stands for the ground state singlet, triplet with spin projection $\mu = 1, 0, \bar{1}$ and two excitons, respectively.

All possible transitions between these levels are presented in Fig. 2.2(a). It is immediately seen from this level scheme, that one may organize all interlevel transitions in the supermultiplet by means of three irreducible scalars A_{α} and four irreducible vectors, $\mathbf{S}, \mathbf{R}_{\alpha}$ ($\alpha = 1, 2, 3$), namely

$$\begin{aligned} A_1 &= i(X^{E_2E_3} - X^{E_3E_2}), \quad A_2 = i(X^{E_3S} - X^{SE_3}), \quad A_3 = i(X^{SE_2} - X^{E_2S}), \\ S_z &= (X^{11} - X^{\bar{1}\bar{1}}), \quad S^+ = \sqrt{2}(X^{10} + X^{0\bar{1}}), \quad S^- = \sqrt{2}(X^{01} + X^{\bar{1}0}), \\ R_{1z} &= -(X^{0S} + X^{S0}) \quad R_1^+ = \sqrt{2}(X^{1S} - X^{S\bar{1}}) \quad R_1^- = \sqrt{2}(X^{S1} - X^{\bar{1}S}) \\ R_{2z} &= -(X^{0E_2} + X^{E_20}) \quad R_2^+ = \sqrt{2}(X^{1E_2} - X^{E_2\bar{1}}) \quad R_2^- = \sqrt{2}(X^{E_21} - X^{\bar{1}E_2}) \\ R_{3z} &= -(X^{0E_3} + X^{E_30}) \quad R_3^+ = \sqrt{2}(X^{1E_3} - X^{E_3\bar{1}}) \quad R_3^- = \sqrt{2}(X^{E_31} - X^{\bar{1}E_3}) \end{aligned} \quad (2.46)$$

Here $\mathbf{S}$ is the usual spin one operator, and the appearance of three more vectors $\mathbf{R}_j$ reflects the extension of effective dimension of spin multiplet from 3D Fock space with the rotation group $SO(3)$ to 6D space with the symmetry group $SO(6)$. Each set of singlet/triplet transitions adds one more dimension to the effective spin space and the appearance of three scalars reflects permutation symmetry of the supermultiplet shown in Fig. 2.2(a).

The operator algebra $o(6)$ is given by the commutation relations (in Cartesian coordinates)

$$\begin{aligned} [S_j, S_k] &= i\epsilon_{jkl}S_l, \quad [R_{\alpha j}, R_{\alpha k}] = i\epsilon_{jkl}S_l, \quad [R_{\alpha j}, S_k] = i\epsilon_{jkl}R_{1\alpha l}, \\ [R_{\alpha j}, R_{\beta k}] &= i\epsilon_{\alpha\beta\gamma}\epsilon_{jkl}A_l \quad (\alpha \neq \beta), \quad [R_{\alpha j}, A_\beta] = i\epsilon_{\alpha\beta\gamma}R_{\gamma j}, \\ [S_j, A_\alpha] &= 0, \quad [A_\alpha, A_\beta] = i\epsilon_{\alpha\beta\gamma}A_\gamma. \end{aligned} \quad (2.47)$$

Casimir operators which impose kinematic constraint on the excitations are

$$\mathcal{C}_0 = \mathbf{S}^2 + \sum_{\alpha} \mathbf{R}_{\alpha}^2 + \sum_{\alpha} A_{\alpha}^2 = 5, \quad \mathcal{C}_{\alpha} = \mathbf{S} \cdot \mathbf{R}_{\alpha} = 0 \quad (2.48)$$

i.e. all vectors $\mathbf{R}_{\alpha}$ are orthogonal to the spin vector. Besides, one may construct higher order invariants like in the case of the n -dimensional hydrogen atom [274].

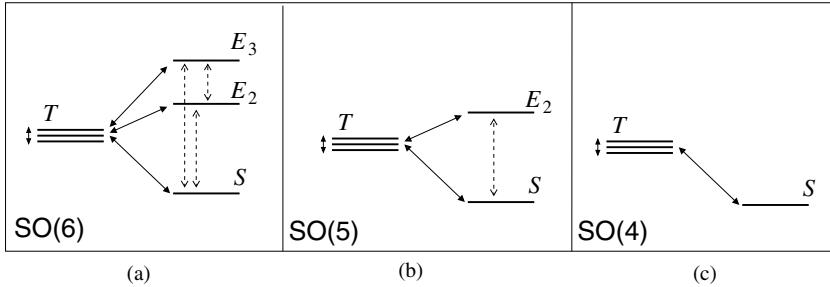


Fig. 2.2 (a) Scheme of the energy levels for $SO(6)$ dynamical symmetry group (triplet T and three singlets S, E_2, E_3); (b) the same for $SO(5)$ group (triplet T and two singlets S, E_2); (c) the same for $SO(4)$ group (triplet T and singlet S). Alternative notation S_1, S_2, S_3 for spin singlet states is used in subsequent chapters. Solid arrow denote vector generators $\mathbf{S}$ (transitions within spin triplet) and $\mathbf{R}_i$ (transitions between triplet and singlets). Dashed lines denote scalar generators A_i describing transitions between singlet states.

Let us now consider the well where only one exciton survives (the second one falls into the continuum spectrum and decays). Then we remain with a multiplet consisting of two singlets, (ground state S and exciton E_2) and the spin triplet T ,

Fig. 2.2(b). In this case, three irreducible vectors $\mathbf{S}, \mathbf{R}_1, \mathbf{R}_2$ and one scalar A_3 is enough to generate the supermultiplet from the ground state level. These operators give ten generators of the dynamical group $SO(5)$ with the algebra $o(5)$ which may be obtained from (2.47) by means of obvious reduction $\varepsilon_{\alpha\beta\gamma} \rightarrow \varepsilon_{\alpha\beta}$ and cancelling the last commutation relation. The Casimir constraint in this case is

$$\mathcal{C}_0 = \mathbf{S}^2 + \mathbf{R}_1^2 + \mathbf{R}_2^2 + A_3^2 = 4. \quad (2.49)$$

If the double-well trap is too shallow to retain excitons, we are left with the supermultiplet consisting of the ground state singlet G and the spin triplet, $T\mu$, Fig. 2.2(c). The dynamical symmetry of singlet/triplet supermultiplet is given by two vectors $\mathbf{S}$ and $\mathbf{R}_1$, and we return back to the group $SO(4)$, which describes its dynamical symmetry with the Casimir constraint

$$\mathcal{C}_0 = \mathbf{S}^2 + \mathbf{R}_1^2 = 3. \quad (2.50)$$

Here the vector $\mathbf{S}$ contains three generators of the symmetry group of the Schrödinger equation similarly to the vector $\mathbf{L}$ in cases of rigid rotator and hydrogen atom, whereas the vector $\mathbf{R}_1$ containing three operators of singlet/triplet transitions reveals the dynamical symmetry of spin supermultiplet and plays the same part as the vector $\mathbf{K}$ (2.11) in the problem of quantum rotator or the Runge – Lenz vector $\mathbf{F}$ (2.19) in the problem of Coulomb atom.

Next, the Hamiltonian (2.45) may be rewritten in terms of invariant operators with the help of expansions (2.46) and Casimir constraints. In particular, in case of singlet/triplet system obeying $SO(4)$ dynamical symmetry, the equality $\mathbf{R}_1^2 = 1 + 2X^{SS}$ follows from the normalization condition (2.6) and the Casimir constraint (2.50). Then the Hamiltonian may be represented in the form

$$\hat{H} = \frac{1}{2} (E_T \mathbf{S}^2 + E_S \mathbf{R}_1^2) + const \quad (2.51)$$

which reflects its $SO(4)$ dynamical symmetry.

In analogy with Eq. (9.16) one may introduce the operators

$$\mathbf{S}_1 = \frac{\mathbf{S} + \mathbf{R}}{2}, \quad \mathbf{S}_2 = \frac{\mathbf{S} - \mathbf{R}}{2} \quad (2.52)$$

with Casimir constraints

$$\mathbf{S}_1^2 + \mathbf{S}_2^2 = 3/2, \quad \mathbf{S}_1^2 - \mathbf{S}_2^2 = 0. \quad (2.53)$$

The simple quadratic form (2.51) for $\hat{H}$ exists only for $n = 4$. More universal representation uses the set of equalities

$$\mathbf{S}^2 = X^{11} + X^{00} + X^{\bar{1}\bar{1}}, \quad \mathbf{R}_\alpha^2 = \frac{\mathbf{S}^2}{2} + 3X^{E_\alpha E_\alpha} \quad (2.54)$$

valid for any $SO(n)$ with $n = 4, 5, 6$. These equalities are derived from Eqs. (2.46).

Then the Hamiltonian (2.45), which includes the system of triplet and three singlets possessing $SO(6)$ dynamical symmetry acquires the form

$$\hat{H} = \frac{1}{2} \left[E_T - \frac{1}{3} (E_S + E_{E_2} + E_{E_3}) \right] S^2 + \frac{1}{3} [E_S \mathbf{R}_1^2 + E_{E_2} \mathbf{R}_2^2 + E_{E_3} \mathbf{R}_3^2]. \quad (2.55)$$

In case of $SO(5)$ symmetry the terms $\sim E_3$ should be omitted, in case of $SO(4)$, only the terms $\sim E_1$ should be retained.

The scalars A_α do not enter explicitly in the Hamiltonian, but they play an essential part in the response of the system to perturbations which violate the dynamical symmetry of the Hamiltonian (see Chapters 7 and 8).

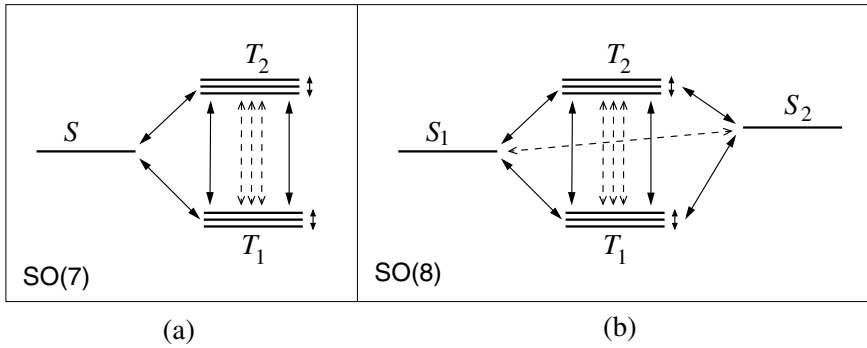


Fig. 2.3 (a) Scheme of the energy levels for $SO(7)$ dynamical symmetry group (two triplet T_1, T_2 and singlet S); (b) the same for $SO(8)$ group (two triplets T_1, T_2 and two singlets S_1, S_2); The meaning of the arrows is the same as in Fig. 2.2.

If the supermultiplet loses its invariance relative to rotations in spin space, its dynamical symmetry changes accordingly. Let us consider, for example, the set of triplet and two singlets [Fig. 2.2(b)] which has been shown above to obey the $SO(5)$ dynamical symmetry. If the nanoobject possesses an axial anisotropy, an additional term DS_z^2 added to the spin Hamiltonian results in splitting of spin triplet $E_{T,\pm 1} - E_{T,0} = D$. Due to this anisotropy, two more operators $X^{\bar{1}\bar{1}}$ and $X^{\bar{1}1}$ arise in the set of Hubbard operators. One may organize 16 operators of this extended

set into 15 generators of the $SU(4)$ group in accordance with the definition of Gell-Mann matrices λ_i for 4-dimensional spin space [397] [See Section 9.2.4, Eq. (9.41)]:

$$\begin{aligned}
 X_1 &= X^{\bar{1}1} + X^{1\bar{1}}, \quad X_2 = i(X^{\bar{1}1} - X^{1\bar{1}}), \quad X_3 = X^{11} - X^{\bar{1}\bar{1}}, \\
 X_4 &= X^{10} + X^{01}, \quad X_5 = i(X^{10} - X^{01}), \quad X_6 = X^{\bar{1}0} + X^{0\bar{1}}, \\
 X_7 &= i(X^{0\bar{1}} - X^{\bar{1}0}), \quad X_8 = \frac{1}{\sqrt{3}}(X^{11} + X^{\bar{1}\bar{1}} - 2X^{00}), \\
 X_9 &= X^{S1} + X^{1S}, \quad X_{10} = i(X^{S1} - X^{1S}), \quad X_{11} = X^{S\bar{1}} + X^{\bar{1}S}, \\
 X_{12} &= i(X^{S\bar{1}} - X^{\bar{1}S}), \quad X_{13} = X^{S0} + X^{0S}, \quad X_{14} = i(X^{S0} - X^{0S}), \\
 X_{15} &= \frac{1}{\sqrt{6}}(X^{11} + X^{\bar{1}\bar{1}} + X^{00} - 3X^{SS}).
 \end{aligned} \tag{2.56}$$

In the absence of spin singlet the problem is reduced to the well known model of single-ion anisotropy for spin 1, which possesses the $SU(3)$ symmetry [312, 313]. The algebra $u(3)$ is determined by the first eight operators $X_1 - X_8$ from the set (2.56), which are formed by means of the Gell-Mann matrices of the 3rd rank (9.35). These operators may be organized in the irreducible tensors $\mathcal{O}_\rho^{(r)}$ (2.8) in two different ways. In case of anisotropic spin 1 problem the physically reasonable way is to group these 8 operators in one vector and one tensor of 2nd rank [313] in accordance with recipe (9.40). The vector operator $\mathcal{O}^{(1)}$ is nothing but the spin 1 operator $\mathbf{S}$ defined in Eqs. (2.46), and the tensor operator $\mathcal{O}^{(2)}$ is the operator of quadrupole momentum $\hat{Q}^{(2)}$ with components

$$\begin{aligned}
 \hat{Q}_{+2}^{(2)} &= X^{1\bar{1}} \sim (S^+)^2, \quad \hat{Q}_{-2}^{(2)} = X^{\bar{1}1} \sim (S^-)^2, \\
 \hat{Q}_0^{(2)} &= (X^{11} + X^{\bar{1}\bar{1}}) - 2/3 \sim S_z^2 - 2/3, \\
 \hat{Q}_{+1}^{(2)} &= X^{10} - X^{0\bar{1}} \sim (S_z S^+ + S^+ S_z), \\
 \hat{Q}_{-1}^{(2)} &= X^{\bar{1}0} - X^{01} \sim (S_z S^- + S^- S_z).
 \end{aligned} \tag{2.57}$$

[see Eq. (9.40)].

Another mathematical possibility is to group them into two vectors and two scalars (see Section 9.2.4). Physical realization of such possibility was demonstrated in Ref. [245] for a three-level potential well occupied by 4 electrons. In that case the spin rotation invariance was broken by external magnetic field (see Section 4.3 for further details). More realizations used in quantum electronics (interaction of 3-level atomic systems with light) may be found in Ref. [160]

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

(2.58)

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 supermultiplet. The kinematic schemes of interlevel transitions corresponding to these groups are shown in Figs. 2.2 and 2.3.

One may construct similar hierarchy of dynamical symmetries starting from the problem of an electron in a trap with three minima (three-level system), then adding spin variable, increasing the number $\mathcal{N}$ etc. In this hierarchy the invariance group of the Schrödinger operator is $SU(3)$. Physical models possessing higher symmetries $SU(n)$ groups are also described in current literature [161, 310, 397, 398].

2.4 Hubbard atom and Fulde molecule

The method of projection operators for dynamical symmetry groups based on the expansion (2.8) allows one to construct operator algebras for more complicated cases where the states in the supermultiplet belong to adjacent charge sectors with electron numbers, $\mathcal{N} = \mathcal{N}_0, \mathcal{N}_0 \pm 1$. Let us demonstrate its abilities for a simplest case of $\mathcal{N}_0 = 1$, using as an example the elementary cell of the Hubbard Hamiltonian [169].

$$\hat{H}_{\text{Hub}} = \sum_i \hat{H}_i + \sum_{ij} \hat{H}_{ij} \quad (2.59)$$

where

$$\hat{H}_i = \varepsilon_d \sum_{\sigma=\uparrow,\downarrow} d_{i\sigma}^\dagger d_{i\sigma} + U n_{i\uparrow} n_{i\downarrow} \quad (2.60)$$

is the single-site Hamiltonian describing the states with variable occupation number $\mathcal{N}$ (“Hubbard atom”). In this “non-degenerate” version of the Hubbard model it is

supposed that each potential well contains only one level $\varepsilon_d < 0$. The second term is a sum of tunneling operators

$$\hat{H}_{ij} = t \sum_{\sigma} d_{i\sigma}^{\dagger} d_{j\sigma} \quad (2.61)$$

It describes the electron motion in a narrow band which emerges from atomic levels ε_d due to intersite tunneling with the amplitude t in presence of strong short-range repulsion U , which is a prototype of Coulomb blockade in tunneling through nanoobjects.

Here we are interested in the dynamical symmetry of the Hamiltonian $\hat{H}_i$ (2.60) diagonalized in accordance with (2.45). Since the tunneling motion changes the occupation numbers at any site i , this dynamical symmetry should include all states with $\mathcal{N} = 0, 1, 2$. The energy spectrum consists of four states $|\Lambda\rangle$ with $\Lambda = 0, \uparrow, \downarrow, 2$ corresponding to an empty site, $\mathcal{N} = 0$, singly occupied site, $\mathcal{N} = 1$ with electron spin projections $\uparrow, \downarrow$, and doubly occupied site, $\mathcal{N} = 2$, respectively. The energy levels E_{Λ} are

$$E_0 = 0, \quad E_1 \equiv E_{\uparrow} = E_{\downarrow} = \varepsilon_d, \quad E_2 = 2\varepsilon_d + U. \quad (2.62)$$

One can treat the parameter ε_d (electron binding energy in the Hubbard atom) as a control parameter regulating the occupation $\mathcal{N}$. If the energy differences

$$E_{01} = E_0 - E_1 = -\varepsilon_d, \quad E_{21} = E_2 - E_1 = \varepsilon_d + U \quad (2.63)$$

are positive, then the Hubbard atom is singly occupied in the ground state. Since the Hubbard atom in SCES is embedded into a macroscopic electron ensemble, the chemical potential μ may be introduced in the Hamiltonian. It is convenient to use μ as a reference level for addition/removal energies (2.63). In this case, changing occupation means change of the model parameters relative to the chemical potential. Practical realizations of this pattern in nanosystems are described in Chapter 3.

In accordance with our general approach to SCES, the Hamiltonian of the Hubbard atom may be represented in the diagonalized form (2.45) (Hubbard representation by means of X -operators. All interlevel transitions described by the Hubbard operators are shown in Fig. 2.4(a). The Hubbard operators in the space $(0, \uparrow, \downarrow, 2)$ arise as a result of expansion of electron creation annihilation operators

$$d_{\sigma}^{\dagger} = X^{\sigma 0} + \sigma X^{2\bar{\sigma}}, \quad d_{\sigma} = X^{0\sigma} + \sigma X^{\bar{\sigma} 2}. \quad (2.64)$$

This transformation is non-linear. Its inverse reads

$$\begin{aligned}
X^{\sigma 0} &= d_{\sigma}^{\dagger}(1 - n^{d\bar{\sigma}}), \quad X^{2\sigma} = \sigma d_{\bar{\sigma}}^{\dagger} n_{d\sigma}, \\
X^{\sigma\sigma} &= n_{d\sigma}(1 - n_{d\bar{\sigma}}), \quad X^{00} = (1 - n_{d\sigma})(1 - n_{d\bar{\sigma}}), \quad X^{22} = n_{d\sigma} n_{d\bar{\sigma}}, \\
X^{\sigma\bar{\sigma}} &= d_{\sigma}^{\dagger} d_{\bar{\sigma}}, \quad X^{20} = \sigma d_{\sigma}^{\dagger} d_{\bar{\sigma}}^{\dagger}.
\end{aligned} \tag{2.65}$$

Unlike the models discussed above, the X -operators for the Hubbard atom connect the states belonging to different charge and spin sectors. Hence the operators $X^{\Lambda\Lambda'}$ obey the *superalgebra* (2.7) which includes both commutation and anticommutation relations, because the full set $\{X^{\Lambda\Lambda'}\}$ contains operators which connect the states with different $\mathcal{N}$, so that the difference $\mathcal{N}_{\Lambda} - \mathcal{N}_{\Lambda'}$ acquires the values $0, \pm 1, \pm 2$. Besides, the spin variable of these excitations acquires both integer values $0, 1$ for Bose-like transitions and half-integer values $\pm 1/2$ for Fermi-like transitions. However, these operators may be grouped in combinations, which obey the $u(4)$ algebra of the Gell-Mann matrices (9.41) similarly to the supermultiplet $(S, 0, \pm 1)$ discussed above. To find these combinations, one should change the indices $(1, \bar{1}, 0, S,) \rightarrow (\uparrow, \downarrow, 0, 2)$ in the system (2.56), that is

$$\begin{aligned}
X_1 &= X^{\uparrow\downarrow} + X^{\downarrow\uparrow}, \quad X_2 = i(X^{\downarrow\uparrow} - X^{\uparrow\downarrow}), \quad X_3 = X^{\uparrow\uparrow} - X^{\downarrow\downarrow}, \\
X_4 &= X^{\uparrow 0} + X^{0\uparrow}, \quad X_5 = i(X^{\uparrow 0} - X^{0\uparrow}), \quad X_6 = X^{\downarrow 0} + X^{0\downarrow}, \\
X_7 &= i(X^{0\downarrow} - X^{\downarrow 0}), \quad X_8 = \frac{1}{\sqrt{3}}(X^{\uparrow\uparrow} + X^{\downarrow\downarrow} - 2X^{00}), \\
X_9 &= X^{2\uparrow} + X^{\uparrow 2}, \quad X_{10} = i(X^{2\uparrow} - X^{\uparrow 2}), \quad X_{11} = X^{2\downarrow} + X^{\downarrow 2}, \\
X_{12} &= i(X^{2\downarrow} - X^{\downarrow 2}), \quad X_{13} = X^{20} + X^{02}, \quad X_{14} = i(X^{20} - X^{02}), \\
X_{15} &= \frac{1}{\sqrt{6}}(X^{\uparrow\uparrow} + X^{\downarrow\downarrow} + X^{00} - 3X^{22}).
\end{aligned} \tag{2.66}$$

In the limit of $U \rightarrow \infty$ the “polar” state $\Lambda = 2$ is projected out from the effective Fock space and the dynamical symmetry $SU(4)$ reduces to $SU(3)$ in accordance with this isomorphism. Eight generators of this group are formed by means of Gell-Mann matrices $X_1 - X_8$ in the subspace $(\uparrow, \downarrow, 0)$.

Thus, the model of two-electron double quantum well with uniaxial spin anisotropy is isomorphous to the Hubbard atom model from the point of view of dynamical symmetry of their energy levels, although another type of expansion over the irreducible tensors should be used in this model (see below).

Although part of the operators forming $SU(4)$ and $SU(3)$ groups are “Bose-like” ($X_1 - X_3, X_8, X_{13} - X_{15}$), and the rest are “Fermi-like” ($X_4 - X_7, X_9 - X_{12}$) in the sense of commutation relations (2.7), they commute in accordance with the Gell-Mann

algebra (9.37). To understand this mapping in more details it is convenient to express the Hubbard operators and the Hubbard Hamiltonian $\hat{H}_i$ (2.60) via the irreducible operators T, U, V, W, Y, Z given by Eqs. (9.38) and (9.42):

$$\begin{aligned}
 T^+ &= X^{\uparrow\downarrow}, \quad T^- = X^{\downarrow\uparrow}, \quad T_z = X^{\uparrow\uparrow} - X^{\downarrow\downarrow} \\
 V^+ &= X^{\uparrow 0}, \quad V^- = X^{0\uparrow}, \quad V_z = X^{\uparrow\uparrow} - X^{00} \\
 U^+ &= X^{\downarrow 0}, \quad U^- = X^{0\downarrow}, \quad U_z = X^{\downarrow\downarrow} - X^{00} \\
 W^+ &= X^{\uparrow 2}, \quad W^- = X^{2\uparrow}, \quad W_z = X^{\uparrow\uparrow} - X^{22} \\
 Y^+ &= X^{\downarrow 2}, \quad Y^- = X^{2\downarrow}, \quad Y_z = X^{\downarrow\downarrow} - X^{22} \\
 Z^+ &= X^{02}, \quad Z^- = X^{20}, \quad Z_z = X^{00} - X^{22}
 \end{aligned} \tag{2.67}$$

Equations (2.67) realize the general expansion scheme (2.8) for the irreducible vector operators in the group $SU(4)$. The triad T is nothing but the set of spin 1/2 operators ($S^+, S^-, 2S_z$) acting in the charge sector $\mathcal{N} = 1$. The triad Z describes two-particle excitations ($\mathcal{N} = 0 \leftrightarrow \mathcal{N} = 2$). The rest four triads describe transitions between different charge sectors ($\mathcal{N} = 1 \leftrightarrow \mathcal{N} = 0, 2$).

The dual nature of Hubbard operators manifested in the commutation relations (2.7) allows one to use them for construction of $su(3)$ algebra formed by spin and pseudospin operators with commutation relations (9.43), (9.44). These commutation relations ensure complex dynamical properties of Hubbard-like SCES.

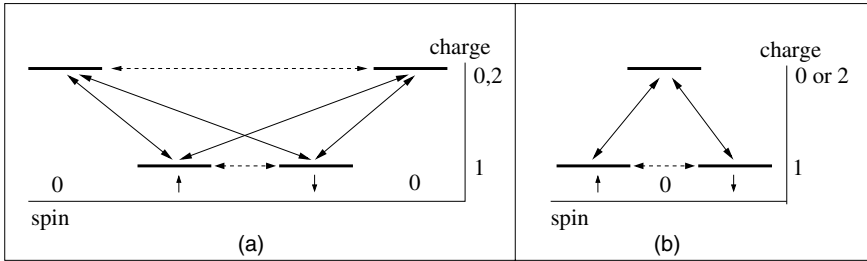


Fig. 2.4 (a): Scheme of energy levels for a Hubbard atom with $SU(4)$ dynamical symmetry describing transitions between the states with occupation $\mathcal{N} = 0, 1, 2$. (b) The same for a reduced spectrum with $SU(3)$ dynamical symmetry describing transitions between the states with $\mathcal{N} = 0$ or 2 and $\mathcal{N} = 1$. Bose-like transitions with even $\delta\mathcal{N} = 0, \pm 2$ are shown by dashed lines, Fermi-like transitions with odd $\delta\mathcal{N} = \pm 1$ are shown by solid lines.

It is expedient to rewrite the original Hamiltonian (2.60) in terms of generators of the group $SU(4)$ in the case where all four eigenstates (2.62) shown in Fig. 2.4(a) are taken into account, and in terms of $SU(3)$ generators in the case when the polar

states with $\mathcal{N} = 2$ are frozen out [Fig. 2.4(b)]. Let us denote the Fock space in which the Gell-Mann matrices are defined as

$$\bar{\Phi}_4 = (\uparrow \downarrow 0 2), \quad \bar{\Phi}_3 = (\uparrow \downarrow 0) \text{ or } (\uparrow \downarrow 2) \quad (2.68)$$

for 4-level and 3-level cases, respectively.

In the general case of $SU(4)$ symmetry the Hamiltonian (2.60) rewritten in terms of Gell-Mann generators (2.66) acting in the space $\bar{\Phi}_4$ [see also (9.49)] reads

$$\begin{aligned} \hat{H}_i^{\text{SU}(4)} = & \frac{E_0}{4} \left(1 - \frac{4}{\sqrt{3}} X_8 + \frac{2}{\sqrt{6}} X_{15} \right) + \frac{E_2}{4} \left(1 - \sqrt{6} X_{15} \right) \\ & + \frac{E_1}{2} \left(1 + \frac{2}{\sqrt{3}} X_8 + \frac{2}{\sqrt{6}} X_{15} \right) \end{aligned} \quad (2.69)$$

Similarly

$$\hat{H}_i^{\text{SU}(3)} = \frac{E_p}{3} \left(1 - \sqrt{3} X_8 \right) + \frac{E_1}{3} \left(2 + \sqrt{3} X_8 \right), \quad (2.70)$$

where $p = 0, 2$ for two cases of $SU(3)$ symmetry in the subspace $\bar{\Phi}_3$ where the states E_2 or E_0 , respectively, are frozen [see Eq. (9.51)].

In terms of the irreducible operators (2.67) the Hamiltonian $\hat{H}_i$ acquires more transparent form. In a chosen representation the z -components of the irreducible operators may be diagonalized, so that the equations $\hat{H}_i \mathcal{O}_z = \varepsilon_z \mathcal{O}_z$ are valid. In case of $SU(4)$ space $\bar{\Phi}_4$ there are three such operators that can be diagonalized simultaneously. One may choose these operators as T_z , $Q_z = U_z + V_z$ and $P_z = W_z + Z_z$. Then adding the Zeeman term with external magnetic field $h = g\mu_B B$, we represent $\hat{H}_i$ as

$$\begin{aligned} \hat{H}_i^{\text{SU}(4)} = & \frac{E_{10}}{8} \cdot Q_z + \frac{E_{12}}{8} \cdot P_z \\ & + \frac{E_{20}}{4} \cdot (Q_z - P_z) + \frac{h}{2} \cdot T_z + C_4 \cdot 1. \end{aligned} \quad (2.71)$$

Here $E_{pp'} = E_p - E_{p'}$, the constant $C_4 = (E_0 + E_2 + 2E_1)/4$ and 1 is the unit matrix of 4-th rank. Thus, the eigen operators for a general $SU(4)$ Hubbard atom are

$$\frac{T_z}{2}, \frac{Q_z}{8}, \frac{P_z}{8}, \frac{Q_z - P_z}{4}, \quad (2.72)$$

with eigenvalues ε_z equal to

$$\pm h, \pm E_{10}, \pm E_{12}, \pm E_{20}, \quad (2.73)$$

These eigenvalues correspond to spin-flip excitations in the singly-occupied state $\mathcal{N} = 1$, hole addition/extraction, electron addition/extraction and two hole excitations, respectively [see Fig. 2.4(a)]. In the degenerate $SU(4)$ model with $E_0 = E_2$ only the two first operators from (2.72) are involved. In the reduced subspace $\bar{\Phi}_3$ only two operators $T_z/2$, $Q_z/3$ enter the Hamiltonian of the Hubbard atom

$$\hat{H}_i^{\text{SU}(3)} = \frac{E_{1p}}{3} \cdot Q_z + \frac{h}{2} \cdot T_z + C_3 \cdot 1 \quad (2.74)$$

where $p = 0$ or 2 , $C_3 = (E_0 + 2E_1)/3$ and 1 is the unit matrix of 3-rd rank. Here the eigenvalues of charge excitations are $\pm E_{01}$ or $\pm E_{02}$ [Fig. 2.4(b)].

Another prototypical model of elementary cell that demonstrates dynamical symmetry from which various many-particle effects emerge, is the so called "Fulde molecule" originally introduced to illustrate the origin of Kondo paradigm (complete screening of localized spin immersed in the sea of free metallic electrons due to multiple creation of electron-hole pairs in this Fermi bath [79, 119]). This artificial molecule consists of two orbitals centered around two adjacent sites. One of these orbitals is localized in a deep energy level ε_d within a narrow potential well, another one occupies a shallow level ε_s in a wide potential well. The tunneling V between these levels is allowed. The Hamiltonian of the system is

$$\hat{H}_{\text{FM}} = \varepsilon_d \sum_{\sigma} d_{\sigma}^{\dagger} d_{\sigma} + \varepsilon_s \sum_{\sigma} c_{\sigma}^{\dagger} c_{\sigma} + V \sum_{\sigma} (d_{\sigma}^{\dagger} c_{\sigma} + c_{\sigma}^{\dagger} d_{\sigma}) + U n_{d\uparrow} n_{d\downarrow}. \quad (2.75)$$

The last term in the Hamiltonian (2.75) is the repulsion interaction introduced in the Hubbard model. It is assumed that this repulsion is strong for d-electrons and negligible for s-electrons. In fact this model is an extremely asymmetric version of the TLS with $\mathcal{N} = 2$ considered in Section 2.3 [see Eq. (2.45) and discussion below]. In this limit the strong Hubbard repulsion suppresses the "polar" states with two electrons in the d-well, In case of weak tunneling, $V \ll (\varepsilon_s - \varepsilon_d)$, the two-electron spectrum consists of five levels

$$E_S = \varepsilon_s + \varepsilon_d - \frac{2V^2}{\varepsilon_s - \varepsilon_d}, \quad E_T = \varepsilon_s + \varepsilon_d, \quad E_E = 2\varepsilon_l + \frac{2V^2}{\varepsilon_s - \varepsilon_d}. \quad (2.76)$$

The second-order correction to the positions of singlet levels E_S and E_E is the indirect exchange of Anderson type, which favors antiparallel orientation of spins in the ground state of the Fulde molecule. Thus, we come to the familiar case of the supermultiplet with $SO(5)$ dynamical symmetry which contains the subgroup

$SO(4)$ of low-lying spin singlet – spin triplet set. The latter symmetry survives in the excitation spectrum of Anderson-Kondo model, where the localized d-electron is hybridized with non-interacting Fermi continuum [119].

2.4.1 Three-fold way for Hubbard atom

As was noticed in the sixties [127], various families of hadrons are classified in accordance with the irreducible representations of the $SU(3)$ group (see also [92]). In particular, 18 baryons form two multiplets corresponding to representations $D^{(11)}$ (octet of baryons with spin 1/2) and $D^{(30)}$ (decuplet of baryons with spin 3/2); octet of spinless mesons also transforms along the representation $D^{(11)}$. The higher representations of $SU(3)$ are realized in the physics of strong interaction because these "elementary" particles possess not only spin and charge but also isospin and hypercharge quantum numbers. Really the elementary particles representing $SU(3)_{\text{color}}$ symmetries are quarks with their fractional charge and other quantum numbers. The $SU(3)$ symmetry in the hadron multiplets under strong interaction is satisfied only approximately due other types of interaction, so that this symmetry may be treated as a dynamical symmetry in the original sense of this notion.

The Hubbard atom with frozen doubly occupied states possesses only two quantum numbers, namely spin and charge. Therefore, the multiplet of Hubbard states is described by the lowest irreducible representation $D^{(10)}$ of $SU(3)$ group. To show this one should recollect that only two of the eight Gell-Mann matrices can be diagonalized simultaneously. Following Eq. (2.74) (see also [92]), we choose the representation with diagonal matrices T_z and Q_z . Then the set of allowed states is defined by two integer numbers λ, μ so that the eigenstates are determined as

$$M_T = \lambda + \mu, \quad M_Q = \frac{1}{3}(\lambda - \mu). \quad (2.77)$$

The whole set of eigenstates form a two-dimensional triangular lattice on the plane (M_T, M_Q) . Each irreducible representation $D^{\bar{\lambda}\bar{\mu}}$ is marked by the indices $\bar{\lambda}, \bar{\mu}$ corresponding to the state with maximum eigenvalue $\bar{M}_Q$ and the maximum value of $\bar{M}_T$ possible at this $\bar{M}_Q$. Then the other states forming this irreducible representation are constructed by means of the ladder operators $T^\pm, U^\pm, V^\pm$ acting on the state $|\bar{M}_Q, \bar{M}_T\rangle$.

This procedure results in construction of the stars of basis vectors $\mathbf{D}^{\lambda\mu}$ and polygons connecting the points generated by the ladder operators subsequently acting

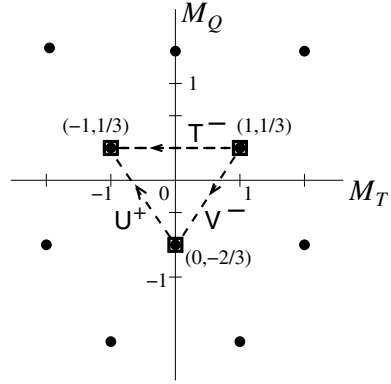


Fig. 2.5 Irreducible representation $D^{(10)}$ of $SU(3)$ group for the Hubbard atom with infinite U (see text for detailed explanation).

on the point $(\bar{M}_Q, \bar{M}_T)$. In case of baryon family the corresponding multiplets are hexagon with doubly degenerate central point for representation $D^{(11)}$ and triangle with ten point in its vertices and on its sides for representation $D^{(30)}$. In Hubbard atom the multiplet is represented by a triangle (Fig. 2.5) labeled in accordance with the state with highest quantum numbers $\lambda = 1, \mu = 0$, which correspond to the state $|\mathcal{N}, \sigma\rangle = |1, \uparrow\rangle$ of the Hubbard atom. Two other components of the multiplet $\bar{\Phi}_3$ may be generated from the state $|1, \uparrow\rangle$ by means of the ladder operators $T^- = X^{\downarrow\uparrow}$ and $V^- = X^{0\uparrow}$. The first of this operators corresponds to a "Bose-like" excitation with spin 1, and the second one is the "Fermi-like" excitation with spin 1/2. The triangle $D^{(10)}$ is closed by means of the operator $U^+ = X^{0\downarrow}$. Interrelations between the values of the parameters λ, μ , the eigenvalues of the operators T_z and Q and the eigenvalues $|\Lambda\rangle$ of the Hubbard Hamiltonian are presented in (2.78):

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

(2.78)

Here the notations u, d, h are used for the spin up, spin down and hole states, respectively. The basis vectors in the plane (M_T, M_Q) are $\mathbf{D}^{10}, \mathbf{D}^{0\bar{1}}, \mathbf{D}^{\bar{1}1}$.

In spite of formal analogy with the $SU(3)$ description of elementary particles, in case of the Hubbard atom where spin and charge are the only quantum numbers this symmetry is realized only as a dynamical symmetry of interlevel transitions induced due to interaction with the bath. This means that the diagonal components of the group generators V_z and U_z describe interlevel transitions (excitations) rather than the eigenstates of the Hamiltonian. The ladder operators $V^\pm$ and $U^\pm$, describe

excitations corresponding to transitions between adjacent charge sectors. These operators enter the interaction Hamiltonian which describes coupling between the nanoobject and the bath. Various forms of this interaction will be discussed in Chapter 4. In analogy with the term offered by Gell-Mann and Ne’eman for the multiplet of light hadrons, one may use the term ”three-fold” way for the SCES with approximate $SU(3)$ symmetry. This formal analogy does not imply physical analogy. In case of hadron octet the ladder operators describe transition from one set of quarks to another. Since $SU(3)$ symmetry is only approximate the energy levels in the octet characterized by spin, charge, isospin and hypercharge are split (masses of “elementary” particles are different), and the lowest state is occupied by proton. Interlevel transitions (conversion of a hadron into another one or its decay) are induced by electroweak interactions. The basic symmetry is the $SU(3)_{\text{color}}$ symmetry of u, d, s quarks,

In the Hubbard atom one deals only with spin and charge, and the ladder operators mean transitions between the charge sectors $(\mathcal{N} = 0) \leftrightarrow (\mathcal{N} = 1)$ and between spin states within the charge sector $\mathcal{N} = 1$, so its dynamical symmetry is described by the lowest irreducible representation $D^{(10)}$. The kinematical scheme shown in Fig. 2.5 corresponds to the scheme of interlevel transitions for the $SU(3)$ group [Fig. 2.4(b)]. Similar scheme for the group $SU(4)$ [Fig. 2.4(a)] have a form of pyramid in the corresponding 3D space (see below).

2.5 Fock – Darwin atom

The problem of discrete states of an electron in a parabolic (harmonic) potential was solved at the early stage of quantum mechanical studies by V.A. Fock [110] and C.G. Darwin [72]. 70 years later the Fock – Darwin atom became the physical reality because it turned out that the confining electrostatic potential in so called vertical quantum dots [238] has nearly parabolic shape (see Section 3.3). Having in mind this physical realization, we consider here the two-dimensional Fock – Darwin model for an electron confined in parabolic well in a perpendicular magnetic field $\mathbf{B}$ with vector potential gauged as $\mathbf{A} = \frac{B}{2}(-y, x)$. The 2D Fock – Darwin Hamiltonian then has the following form

$$\hat{H}_{\text{FD}} = \frac{1}{2m} \left(\mathbf{p}^2 - \frac{e}{c} \mathbf{A} \right)^2 + \frac{m}{2} \omega_0^2 \mathbf{r}^2 - \mu_B \boldsymbol{\sigma} \cdot \mathbf{B}, \quad (2.79)$$

where ω_0 is an eigenenergy of parabolic potential. Let us first ignore the last term which describes the Zeeman splitting of electron levels in magnetic field and rewrite the Hamiltonian as

$$\hat{H}_{\text{FD}} = \frac{\mathbf{p}^2}{2m} + \left(\omega_0^2 + \frac{\omega_c^2}{4} \right) \frac{m\mathbf{r}^2}{2} + \frac{\omega_c}{2} l_z. \quad (2.80)$$

where $\omega_c = eB/mc$ is the cyclotron frequency. The first two terms in (2.80) is the Hamiltonian of an electron in harmonic potential with the confinement frequency $\Omega = \sqrt{\omega_0^2 + \omega_c^2/4}$ and the third one is the energy of angular motion in magnetic field. Then it is clear that the dynamical symmetry of the Fock – Darwin atom is closely related with the dynamical symmetry of quantum oscillator. The latter was revealed in Refs. [40, 145, 173].

One may construct the algebra $o(2, 1)$ of the non-compact Lorentz Group $SO(2, 1)$ in 2+1 dimensions for the operators generating transitions between the eigenstates of harmonic 1D oscillator. This group is locally isomorphic to the unitary group $SU(1, 1)$, i.e., $SO(2, 1) = SU(1, 1)/Z_2$, where $Z_2 = \{1, -1\}$. The generators of the Lorentz group in D=2+1 act in the Hilbert space where the basis functions $|\Lambda\rangle = |n\rangle$

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle \quad (2.81)$$

are built from the ground state $|0\rangle = \pi^{-1/4} \exp(-x^2/2)$ by means of creation operators $a^\dagger = (x - \partial/\partial x)/\sqrt{2}$.

In accordance with the general definitions given in Section 9.2.2, the Lie algebra $o(2, 1)$ is given by three generators L_1, K_1, K_2 with commutation relations

$$[K_1, L_1] = -iK_2, \quad [K_2, L_1] = -iK_1, \quad [K_1, K_2] = iL_1 \quad (2.82)$$

and the Casimir operator

$$\mathcal{C} = L_1^2 - K_1^2 - K_2^2 \quad (2.83)$$

so that L_1 is generator of geometric rotations, and K_1, K_2 perform Lorentz transformations. The ladder operators are introduced as $K^\pm = (iK_1 \pm K_2)/\sqrt{2}$. Then the $o(2, 1)$ algebra may be realized on the basis of Bose operators $a, a^\dagger$ in the following way [39]:

$$\begin{aligned} K^+ &= -\frac{a^\dagger}{\sqrt{2}} \sqrt{a^\dagger a + 1}, \quad K^- = \frac{a}{\sqrt{2}} \sqrt{a^\dagger a}, \\ L_1 &= a^\dagger a + 1/2. \end{aligned} \quad (2.84)$$

The matrix elements of interlevel transitions described by the operators $K^\pm, L_1$ (2.84) are

$$\begin{aligned}\langle m|K^+|n\rangle &= -\frac{n+1}{\sqrt{2}}\delta_{m,n+1}, \quad \langle m|K^-|n\rangle = \frac{n}{\sqrt{2}}\delta_{m,n-1}, \\ \langle m|L_1|n\rangle &= (n+1/2)\delta_{m,n}.\end{aligned}\quad (2.85)$$

Another realization [145] of the same algebra is obviously given by

$$K^+ = \sqrt{a^\dagger a} a^\dagger, \quad K^- = a \sqrt{a^\dagger a}, \quad L_1 = a^\dagger a + 1/2. \quad (2.86)$$

Thus, the non-compact group $SO(2, 1)$ with the Casimir operator $\mathcal{C} = -1/4$ is indeed the dynamical group, which realizes the single irreducible representation for all levels of one-dimensional harmonic oscillator. Discussion of dynamical symmetries which are realized in D-dimensional oscillators may be found in Refs. [40, 173].

Now we return to the Fock – Darwin atom with the Hamiltonian (2.80). This is the two-dimensional system, and the basis functions realizing the dynamical algebra should consist of two sets of oscillator states [152, 188, 274, 423]. For this sake, we turn from the Cartesian coordinates x, y to the complex coordinate ξ, ξ^* :

$$\xi = \frac{x+iy}{2}\sqrt{m\Omega}, \quad \xi^* = \frac{x-iy}{2}\sqrt{m\Omega}. \quad (2.87)$$

Then two pairs of boson operators are introduced as

$$\begin{aligned}a &= -(i/\sqrt{2})(\xi + \partial/\partial\xi^*), \quad a^\dagger = (i/\sqrt{2})(\xi^* - \partial/\partial\xi) \\ b &= (1/\sqrt{2})(\xi^* + \partial/\partial\xi), \quad b^\dagger = (1/\sqrt{2})(\xi - \partial/\partial\xi^*).\end{aligned}\quad (2.88)$$

As a result of this transformation the Fock – Darwin Hamiltonian is reduced to the Hamiltonian of two-dimensional anisotropic oscillator. The basis functions

$$|\Lambda\rangle = |n, m\rangle = \frac{(a^\dagger)^n (b^\dagger)^m}{\sqrt{n!m!}}|0, 0\rangle \quad (2.89)$$

are built from the ground state function $|0, 0\rangle = \sqrt{m\Omega/2\pi}\exp(-|\xi|^2)$. The Fock – Darwin Hamiltonian is readily rewritten in terms of boson operators

$$\hat{H}_{\text{FD}} = \Omega_+ \left(\hat{n}_a + \frac{1}{2} \right) + \Omega_- \left(\hat{n}_b + \frac{1}{2} \right) \quad (2.90)$$

where $\Omega_\pm = \Omega \pm \omega_c/2$, $\hat{n}_a = a^\dagger a$, $\hat{n}_b = b^\dagger b$.

The energy spectrum of a confined electron in terms of boson occupation numbers n, m is given by

$$E_{n,m} = \Omega(n + m + 1) + \frac{\omega_c}{2}(n - m) \quad (2.91)$$

Thus, we come to a conclusion that the dynamical symmetry of the Fock – Darwin atom is the direct product $SO(2, 1) \times SO(2, 1)$ in accordance with general prescription of the theory of d -dimensional quantum oscillator [40]. The energy spectrum (2.91) interpolates smoothly between the two limiting cases. In zero field, $\omega_c = 0$ it gives the eigenvalues of the 2D harmonic oscillator, and in the extremely strong magnetic field $\omega_c \gg \omega_0$ it describes the Landau levels of a free electron in magnetic field, because in this limit the radius of magnetic confinement is much smaller than that of the potential confinement. But the dynamical symmetry of quantum oscillator is realized in all cases.

Another way of treating this problem is to express the Fock – Darwin states in terms of effective momentum operators. Now we restore the last term in the Hamiltonian (2.79), so that the state vectors are determined by three quantum numbers, $|\Lambda\rangle = |nm\sigma\rangle$. Then the total angular momentum is a result of addition of the orbital momentum and the electron spin. The former is given by the operator $\hat{l} = \hat{n}_a - \hat{n}_b$ [cf. Eqs. (2.80) and (2.90)], the latter is the usual spin 1/2 operator. To build the total moment, one has to turn to the spinor representation for boson operators,

$$\bar{\chi} = (a^\dagger \ b^\dagger), \quad \chi = \begin{pmatrix} a \\ b \end{pmatrix}.$$

Then two spinor operators may be constructed

$$\hat{j} = \bar{\chi} \sigma_0 \chi, \quad \mathbf{J} = \bar{\chi} \boldsymbol{\sigma} \chi, \quad (2.92)$$

and the Fock – Darwin Hamiltonian acquires the form

$$\hat{H}_{\text{FD}} = \Omega \left(\hat{j} + \frac{1}{2} \right) + \omega_c J_z, \quad (2.93)$$

so that the spectrum of the Fock Darwin atom in magnetic field is characterized by additional dynamical symmetry $SU(2)$ given by the ladder operators $J^\pm$. Other possibilities of revealing dynamical symmetries of electron states in oscillator-like problems are discussed in the books [80, 274].

2.6 Dynamical symmetry and supersymmetry

The supersymmetry group is a group which unites in a special way the continuous Lie transformations with discrete reflection-like even-odd transformations. Specifically this is a group generated by an algebra, which covers the algebra of anticommuting fermionic operators

$$\{f_i, f_j^\dagger\} = \delta_{ij} \quad (2.94)$$

and commuting bosonic operators

$$[b_i, b_j^\dagger] = \delta_{ij} \quad (2.95)$$

with $[b_i, f_j] = 0$.

The supersymmetry algebra and the corresponding supergroup have been constructed in Refs. [141, 412, 424]. Within several years the supersymmetrical formulation of quantum mechanics was proposed [430]. Supersymmetric operations describe transitions between the states with different numbers of bosons and fermions and in this sense the supersymmetry is closed to dynamical symmetries discussed above. In this section we will present the basic ideas of supersymmetry following the review [128] and then apply these ideas to some of integrable models introduced in the preceding sections.

The supersymmetric generators are defined in a Fock space defined by the basis vectors

$$|n_B, n_F\rangle, \quad n_B = 0, 1, 2, \dots, \infty, \quad n_F = 0, 1. \quad (2.96)$$

Transformation of a boson into fermion and v.v. is defined by the *supercharge* operators

$$Q_+ = qb f^\dagger, Q_- = qb^\dagger f \quad (2.97)$$

where q is c -number. In the space (2.96) these operators act as

$$\begin{aligned} Q_+ |n_B, n_F\rangle &= q |n_B - 1, n_F + 1\rangle, \\ Q_- |n_B, n_F\rangle &= q |n_B + 1, n_F - 1\rangle. \end{aligned} \quad (2.98)$$

It is convenient to introduce two Hermitian combinations of the operators (2.97):

$$Q_1 = Q_+ + Q_-, \quad Q_2 = -i(Q_+ - Q_-). \quad (2.99)$$

These operators anticommute,

$$\{Q_1, Q_2\} = 0. \quad (2.100)$$

because the operators $Q_{\pm}$ are nilpotent,

$$Q_+^2 = Q_-^2 = 0. \quad (2.101)$$

Besides,

$$Q_1^2 = Q_2^2 = \{Q_+, Q_-\}. \quad (2.102)$$

In order to construct closed supersymmetric algebras one should define the supersymmetric Hamiltonian written in terms of supersymmetric operators. This fundamental property of supersymmetric systems is formulated as

$$[\hat{H}, Q] = 0, \quad (2.103)$$

where Q is any of the operators from the set (2.97) or (2.99). The simplest toy Hamiltonian characterized by the supersymmetry group $S(2)$ is

$$\hat{H} = Q_1^2 = Q_2^2 = \{Q_+, Q_-\}. \quad (2.104)$$

In this way we come to the simplest Lie superalgebra $s(2)$ including commutation and anticommutation relations:

$$\begin{aligned} \{Q_i, Q_j\} &= 2\hat{H}\delta_{ij}, \\ [Q_i, \hat{H}] &= 0, \quad i, j = 1, 2. \end{aligned} \quad (2.105)$$

Supersymmetric Lie algebras are Z_2 graded, i.e. the constituent generators are classified in accordance with some parity as even operators $\mathcal{O}_e$ and odd operators $\mathcal{O}_o$. The structure of the Lie superalgebra is as follows:

$$\begin{aligned} [\mathcal{O}_e, \mathcal{O}_e] &\rightarrow \mathcal{O}_e, \\ [\mathcal{O}_e, \mathcal{O}_o] &\rightarrow \mathcal{O}_o, \\ \{\mathcal{O}_o, \mathcal{O}_o\} &\rightarrow \mathcal{O}_e. \end{aligned} \quad (2.106)$$

In the above example (2.105) the only even operator is the Hamiltonian $\hat{H}$ and two odd operators are Q_i .

To reveal the sense of “parity” ascribed to the supersymmetric operators, one has to define the variation of some operator $\mathcal{O}$ under transformation generated by another operator $\mathcal{P}$. In case of conventional Lie algebras this variation is

$$\delta\theta \sim [\varepsilon\mathcal{P}, \theta], \quad (2.107)$$

where ε is the transformation parameter. In case of superalgebras ε is not a c -number. This parameter should commute with Bose operators and anticommute with Fermi operators. Namely, choosing $\mathcal{P} = Q$, one demands

$$\begin{aligned} \delta b &\sim [\varepsilon Q, b] = \varepsilon[Q, b] \sim \varepsilon f, \\ \delta f &\sim [\varepsilon Q, f] = \varepsilon\{Q, f\} \sim \varepsilon b. \end{aligned} \quad (2.108)$$

This definition means that the parameters ε also possess definite parity: even parameters ε_e are c -numbers commuting with all operators and parameters, while odd parameters ε_o commute with even quantities and anticommute with odd ones.

The above definition of supersymmetric operators and parameters may be unified. Let us change the normalization of the Q -operators:

$$q_i = \frac{Q_i}{\sqrt{E}}, \quad (2.109)$$

where E is an eigenstate of the Hamiltonian $\hat{H}$. Then $\hat{H}$ transforms into the unit operator $\hat{1}$ in the superspace (2.96), and the algebra defined by Eqs. (2.105) reads

$$\{q_i, q_k\} = 2\delta_{ik} \quad (2.110)$$

These relations define the Clifford algebra with generators q_i .

On the other hand, odd parameters ε anticommute with each other and each of them anticommutes with itself, which means $\varepsilon^2 = 0$. These relations may be summarized as

$$\{\varepsilon_i, \varepsilon_j\} = 0. \quad (2.111)$$

Thus, the odd parameters form a Grassmann algebra, and each Grassmann algebra with N constituents is associated with Clifford algebra for $2N$ constituents.

Now let us find out what kind of physical object is described by the toy Hamiltonian (2.104). Using the definition (2.97), one may rewrite (2.104) as

$$\hat{H} = \{Q_+, Q_-\} = q^2(b^\dagger b + f^\dagger f) = q^2\left(n_B + \frac{1}{2}\right) + q^2\left(n_F - \frac{1}{2}\right). \quad (2.112)$$

This is a sum of non-interacting systems of bosonic and fermionic oscillators with the same frequency $\Omega = q^2$:

$$\hat{H} = \hat{H}_B + \hat{H}_F, \quad (2.113)$$

$$\begin{aligned}\hat{H}_B &= q^2 \left(b^\dagger b + \frac{1}{2} \right), \quad E_B = \Omega \left(n_B + \frac{1}{2} \right), \quad n_B = 0, 1, \dots, \infty, \\ \hat{H}_F &= q^2 \left(f^\dagger f - \frac{1}{2} \right), \quad E_F = \Omega \left(n_F - \frac{1}{2} \right), \quad n_F = 0, 1.\end{aligned}$$

Thus, the energy spectrum of the supersymmetric system is non-negative and doubly degenerate,

$$E_{\{n_B, n_F\}} = \Omega(n_B + n_F). \quad (2.114)$$

This spectrum is shown in Fig. 2.6. The operators $Q_\pm$ generate “rotations” boson $\leftrightarrow$ fermion in a supersymmetric Fock space without changing the energy of the system,

$$E_{\{n_B, 0\}} = E_{\{n_B - 1, 1\}}. \quad (2.115)$$

The ground state energy of the supersymmetric system is zero, because the zero vibration energies of bosonic and fermionic excitations compensate each other. One may say that the zero vacuum energy of the supersymmetric state is split into negative and positive infinite vacuum energies of Fermi- and Bose-sectors of the system.

Supersymmetric operators may be represented in a spinor form due to the fact that the fermionic wave function is a spinor of second rank in a subspace $n_F = 1, 0$:

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix}, \quad (2.116)$$

where $\psi_{1,0}$ corresponds to $n_F = 1, 0$. Respectively, the fermionic creation and annihilation operators are realized as Pauli matrices (9.3) in this representation, $f^+ = \tau^+, f = \tau^-$. Then the supercharge operators acquire the form

$$\begin{aligned}Q_1 &= q(b^\dagger \tau^- + b \tau^+) = B_1 \tau_1 + B_2 \tau_2, \\ Q_2 &= -i(b^\dagger \tau^- - b \tau^+) = -B_2 \tau_1 + B_1 \tau_2\end{aligned} \quad (2.117)$$

where

$$B_1 = q(b + b^\dagger), \quad B_2 = iq(b - b^\dagger)$$

In this representation the supersymmetric Hamiltonian (2.104) is

$$\hat{H} = \frac{1}{2} \{B^-, B^+\} + [B^-, B^+] \tau_0 \quad (2.118)$$

with $B^\pm = B_1 \pm iB_2$.

2.6.1 Manifestations of supersymmetry in atomic models

Some of the model Hamiltonians with definite dynamical symmetries considered in the preceding sections also may be treated in terms of the group $S(2)$ of supersymmetric transformations. In particular, the minimal model (2.104) with the spectrum (2.114) is related to the limiting case of the Fock – Darwin model (Section 2.5) with $\omega_c \gg \omega_0$. As was mentioned above, in strong magnetic field spatial confinement of electrons in the Fock – Darwin atom is determined by the magnetic length, and then the electrons at Landau levels acquire the supersymmetry [128].

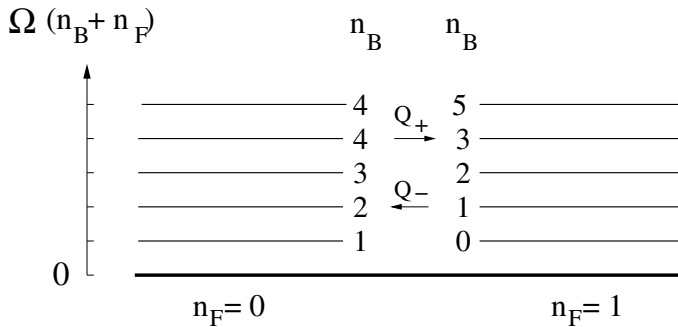


Fig. 2.6 Supersymmetric spectrum (2.119) of Fock – Darwin atom at $\omega_0/\omega_c \rightarrow 0$. Transitions with changing occupation numbers n_B and n_F are marked by arrows, $\Omega = \omega_c$.

Indeed, in the limit $\omega_0/\omega_c \rightarrow 0$, where $\Omega_+ \rightarrow \omega_c$, $\Omega_- \rightarrow 0$, instead of two-boson representation (2.90) one may turn to a mixed fermion-boson representation, where the spectrum of Landau states for spinful electrons may be represented as

$$E = \omega_c \left(n + \frac{1}{2} \right) \pm \frac{\omega_c}{2} = \omega_c \left[\left(n_B + \frac{1}{2} \right) + \left(n_F - \frac{1}{2} \right) \right]. \quad (2.119)$$

In this representation bosonic degrees of freedom describe quantized orbital motion of Landau electrons and fermionic degrees of freedom correspond to electron spin states split due to the Zeeman effect. Looking at the spectrum of Landau levels rearranged in accordance with Fig. 2.6, we see that the supersymmetric transformation corresponds to a spin flip accompanied by simultaneous transition from a given Landau level to adjacent one. Choosing one of two cartesian coordinates forming the basis $\{\xi, \xi^*\}$ (2.87) as a continuous variable and spin projection as a discrete variable, we conclude that the supersymmetry of Landau electrons is a result of

interplay between continuous orbital motion and discrete spin “reflection” in accordance with general properties of supersymmetric systems.

Intimate relation between dynamical symmetry and supersymmetry is clearly seen in this system: the supersymmetry is realized as *interstate transitions* generated by the supercharge operators $Q_{\pm}$ (2.97) involving both bosonic and fermionic sectors of Fock superspace. At the same time the dynamical $SO(2, 1)$ symmetry is realized as *interstate transitions* within the bosonic sector generated by the operators $K^{\pm}, L_1$ (2.84). At finite ratio ω_0/ω_c the Fermi-Bose supersymmetry of the electron spectrum breaks because the confinement potential of Fock – Darwin atom $\sim \omega_0^2$ violates the equivalence of boson and fermion frequencies in the spectrum (2.119), but the dynamical $SO(2, 1)$ symmetry still exists.

Supersymmetry is also a generic feature of an electron in the Coulomb potential (Section 2.2). To reveal this supersymmetry [236, 394], one has to add a discrete spin variable to the set of continuous operators $\mathbf{L}$ and $\mathbf{F}$ (2.19) responsible for the $SO(4)$ symmetry of the spinless problem determined by Eqs. (2.21). The projection of the Runge – Lenz vector $\mathbf{F}$ onto the electron spin direction plays the part of the supercharges $Q_{1,2}$ in this model. To find these supercharges, we construct the invariants for the group $SO(4) \times SU(2)$ which arise as a result of adding the orbital and spin moments of an electron in the total moment $\mathbf{J} = \mathbf{L} + \mathbf{S}$. The set of observables is given by the operators $\hat{H}, \mathbf{L}^2, \mathbf{J}^2, J_z$ with eigenvalues $E, l(l+1), j(j+1), m$, respectively. It is convenient to introduce the scalar operator $\mathcal{K}$ with eigenvalues $\pm\kappa$ in such a way that the states with fixed j and $l = j \pm \frac{1}{2}$ correspond to the same $|\kappa|$ but to opposite “projections” $\pm\kappa$. This aim is achieved by introducing $\mathbf{J}^2 - \mathbf{L}^2 = -(1 + \mathcal{K})$ so that

$$\mathbf{L}^2 = \mathcal{K}(\mathcal{K} + 1) \Rightarrow l(\kappa) = |\kappa| + \frac{1}{2}(\text{sgn}\kappa - 1), \quad (2.120)$$

$$\mathbf{J}^2 = \mathcal{K}^2 - 1 \Rightarrow j(\kappa) = |\kappa| - \frac{1}{2},$$

It is clear that the index κ labels transitions in graded superspace. Indeed, the scalar operator $\mathcal{K}$ plays the key part in the construction of supercharges. The parity operator with eigenvalues $\pm\text{sgn}\kappa$ is

$$P_{\kappa} = \frac{\mathcal{K}}{|\kappa|}. \quad (2.121)$$

This operator controls the Z_2 grading of superalgebra.

The scalar $(\mathbf{S} \cdot \mathbf{A})$ is an odd operator in the supersymmetric sense, and its square is an even operator connected with the even operator $\hat{H}$ entering the superalgebra by the following relation

$$(\mathbf{S} \cdot \mathbf{A})^2 = \frac{1}{2} \left(\hat{H} \mathcal{K}^2 + \frac{1}{2} \right). \quad (2.122)$$

[see Eqs. (2.22)-(2.25)]. Restricting ourselves to the subspace of fixed $|\kappa| \equiv k$, we rewrite (2.122) as

$$2 \left(\frac{(\mathbf{S} \cdot \mathbf{A})^2}{k} \right) = \hat{H} + \frac{1}{2k^2} = \hat{H}'. \quad (2.123)$$

Then we introduce two supercharge operators

$$Q_{\pm} = \frac{1}{\sqrt{2}k} (\mathbf{S} \cdot \mathbf{A}) (1 \mp P_{\kappa}), \quad (2.124)$$

(see Eq. 2.20) and their Hermitian combinations are

$$Q_1 = \frac{(\mathbf{S} \cdot \mathbf{A})}{k}, \quad Q_2 = iQ_1 P_{\kappa} = \frac{i}{k^2} (\mathbf{S} \cdot \mathbf{A}) \quad (2.125)$$

These two operators together with “shifted” operator $\hat{H}'$ (2.123) generate the $s(2)$ algebra (2.100) - (2.105). Substituting $\mathbf{A}$ for $\mathbf{F}$ in Eqs. (2.123) - (2.125), we come to the Clifford algebra (2.110).

The energy levels of a nonrelativistic particle with spin 1/2 in a Coulomb field involved in supersymmetric degeneracy are those with fixed quantum numbers j, m and $l = j \pm 1/2$ (see Fig. 2.7). Like in the above example, the $S(2)$ supersymmetry complements other symmetries characterizing the supermultiplet of the energy levels: the hidden symmetry of the atom is characterized by continuous $SO(4)$ or $SO(4, 2)$ groups describing transitions between the states with given parity κ , while transitions with changing parity initiated by the operator $(\mathbf{S} \cdot \mathbf{A})/k$ are involved in the supersymmetry group $S(2)$.

More detailed analysis of this problem including description of irreducible representations of the $S(2)$ group may be found in Ref. [128]. The supersymmetric quantum mechanical description of a spinful particle in a $1/r$ potential in arbitrary dimension d is given in Ref. [212].

To close the discussion of supersymmetric properties of real and artificial atoms, we consider in brief the prospects of supersymmetric description of SCES models with a Hubbard atom or a grid of Hubbard atoms as zero-order approximation.

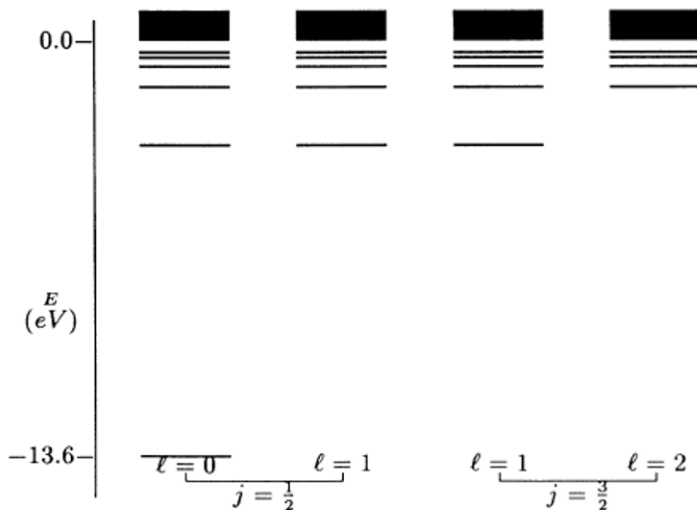


Fig. 2.7 Supersymmetric spectrum of hydrogen atom. All levels of equal j and m are connected by an $S(2)$ supersymmetry (after [394])

We have noted above that the dynamical symmetry $SU(3)$ unites "Bose-like" and "Fermi-like" excitations into the a supermultiplet shown in Fig. 2.4(b). It is a tempting prospect to look for relation between this symmetry and supersymmetry $S(2)$. The theoretical grounds of such prospect can be looked for in various fermionization and bosonizations procedures available for Hubbard operators $X^{\Lambda\Lambda'}$. In particular, the operators from the triads U, V, W, Y (2.67) may be expressed via products of Fermi- and Bose operators in slave-boson [37, 60, 237, 350] and slave-fermion [30, 122, 433] representations. Spin operators from the triad T may be represented as products of spin-fermions [1, 335], Popov-Fedotov semi-fermions [214, 337] or Majorana fermions [271, 429]. Representations of these operators via products of Bose operators are also available [278]. Existing fermionization/bosonization procedures for Hubbard operators are described in Section 9.3. Here we are interested in mixed fermion-boson representations which formally remind those used in the definition of supercharge operators Q_i (2.97), (2.99).

In order to reveal the hidden extension of the Fock space of Hubbard atom (2.60) with the energy spectrum (2.62), we work in adjacent charge sectors $\mathcal{N} = 1, 2$, Fig. 2.4(b). Following the general scheme of the $s(2)$ algebra we represent the off-diagonal operators from the triads W, Y (2.67) as supercharge operators using slave-boson representation [cf. Eqs. (9.83)]

$$Q_{\sigma}^{+} = X^{2\sigma} = b^{\dagger} f_{\sigma}, \quad Q_{\sigma}^{-} = X^{\sigma 2} = b f_{\sigma}^{\dagger}. \quad (2.126)$$

Respectively,

$$Q_{1\sigma} = Q_{\sigma}^{+} + Q_{\sigma}^{-} = X^{2\sigma} + X^{\sigma 2} \quad (2.127)$$

$$Q_{2\sigma} = -i(Q_{\sigma}^{+} - Q_{\sigma}^{-}) = -i(X^{2\sigma} - X^{\sigma 2})$$

Then

$$Q_{1\sigma}^2 = Q_{2\sigma}^2 = \{Q_{\sigma}^{+}, Q_{\sigma}^{-}\} = X^{\sigma\sigma} + X^{22} = n_{F\sigma} + n_B. \quad (2.128)$$

Here Bose operators $b, b^{\dagger}$ stand for “doublon” states in doubly occupied Hubbard atom [237]. The supercharge operators transforms the system from the charge sector $\mathcal{N} = 2$ with zero spin into the charge sector $\mathcal{N} = 1$ with spin 1/2, and thus connect fermionic and bosonic sectors of the Fock space $\bar{\Phi}_3(\uparrow, \downarrow, 2)$. The Hamiltonian $\hat{H}_i^{\text{SU}(3)}$ rewritten in terms of the supercharge operators (2.126), acquires the form

$$H_i = \varepsilon_1 \sum_{\sigma} X^{\sigma\sigma} + (2\varepsilon_1 + U)X^{22} = \varepsilon_1 \sum_{\sigma} Q_{\sigma}^2 + UX^{22} \quad (2.129)$$

with $Q_{\sigma}^2 = Q_{1\sigma}^2 = Q_{2\sigma}^2$. Renormalizing the operator

$$\hat{H}_i \rightarrow \varepsilon_1 \sum_{\sigma} \hat{H}_{\sigma},$$

one arrives at two $s(2)$ superalgebras (2.105) for the operators $\hat{H}_{\sigma}, Q_{1\sigma}, Q_{2\sigma}$ in the limit $r = U/\varepsilon_1 \rightarrow \infty$, where two spin sectors are disentangled. At finite r any interaction with the bath $\mathcal{B}$ initiates spin-flip transitions, which merge two spin subsectors via the anticommutation relation

$$\{Q_{1\sigma}, Q_{2\bar{\sigma}}\} = -i(f_{\sigma}^{\dagger} f_{\bar{\sigma}} - f_{\bar{\sigma}}^{\dagger} f_{\sigma}). \quad (2.130)$$

One should emphasize that the existence of $s(2)$ superalgebra does not imply supersymmetry of the Hubbard atom in the classical meaning of this term, because the original Hamiltonian $\hat{H}_i^{\text{SU}(3)}$ describes fully discrete system with the constraint (2.6), which in the fermion-boson representation reads as

$$\sum_{\sigma} n_{F\sigma} + n_B = 1. \quad (2.131)$$

so that the physical sector of phase space consists of three states

$$|n_B, n_{F\uparrow}, n_{F\downarrow}\rangle = |1, 0, 0\rangle, |0, 1, 0\rangle, |0, 0, 1\rangle \quad (2.132)$$

instead of (2.96). Thus, the boson-fermion transformation

$$Q_{\uparrow}^+ |1, 0, 0\rangle = |0, 1, 0\rangle$$

reveals only internal symmetry of the $SU(3)$ Hubbard atom. To make the Bose states continuous or quasicontinuous, this toy model should be generalized. In particular, one may introduce “ N -colored” model with N orbitals [5] and ascribe additional index $m = 1, 2 \dots N$ to slave bosons, i.e. introduce Bose operators as $X^{\sigma m, 2} = f_{\sigma}^{\dagger} b_m$ etc. In case of $N \rightarrow \infty$ this supersymmetric model with slave-boson continuum is exactly solvable, and one may hope that the supersymmetric approach will give reasonable description of excitations in Hubbard atom at finite N [61, 167]. This mathematical trick does not look too promising for the description of realistic physical models. More attractive is the use of slave-fermion approach, where the Hubbard operators are expressed via spinless charged fermion operators g and Schwinger boson operators a, b (see Section 9.3). For example, in the subspace $\bar{\Phi}_3 = 0, \uparrow, \downarrow$ one introduces the supercharge operators

$$Q_{\uparrow}^{\dagger} = X^{\uparrow 0} = a^{\dagger} g, \quad Q_{\downarrow}^{\dagger} = X^{\downarrow 0} = b^{\dagger} g, \quad (2.133)$$

Then the Schwinger bosons describe local spin fluctuations by means of bosonized operators from the triad T [see Eqs. (2.67), (9.56)]. Introducing N -component Schwinger representation, one transforms the Bose branch into continuous two-dimensional harmonic oscillator at large N . Such continuous mode arises naturally, if the bath $\mathcal{B}$ is chosen in a form of local spin environment like in molecular magnets with large total spin (see Section 5.2). In any case, supersymmetric aspects of Hubbard-like and Anderson-like models need further investigation (see [98] for further discussion of supersymmetric description of periodic Hubbard model).

The theory of mesoscopic objects also has benefited from the supersymmetry ideas [88]. Supersymmetric approach reveals hidden symmetries in disordered and chaotic systems, including the fundamental problem of electron localization. This fructiferous offshoot of supersymmetry is, however, beyond the scope of our book.

2.7 Quasienergy spectrum for periodical time-dependent problems

In some practical applications devices consisting of nanoobjects, electrodes and contacts are subject to periodic perturbation

$$\hat{H}(\mathbf{x}, t) = \hat{H}_0(\mathbf{x}) + \hat{H}'(\mathbf{x}, t), \quad (2.134)$$

where $\mathbf{x}$ stand for spatial coordinates, t is real time, $\hat{H}'(\mathbf{x}, t + T) = \hat{H}'(\mathbf{x}, t)$ and $T = 2\pi/\Omega$ is a period of perturbing potential. There is no stationary solutions

$$\Psi(\mathbf{x}, t) = \sum_{\alpha} c_{\alpha} \psi_{\alpha}(\mathbf{x}) \exp(-i\varepsilon_{\alpha} t)$$

of the Schrödinger equation

$$i \frac{d}{dt} \Psi(\mathbf{x}, t) = \hat{H} \Psi(\mathbf{x}, t) \quad (2.135)$$

characterized by the energy states ε_{α} . However, in case of strictly periodic in time perturbation one may introduce a set of functions $\psi_{\alpha}(\mathbf{x}, t)$ and corresponding *quasienergy* states f_{α} which inherit the quantum numbers α from the eigenstates of the time-independent Hamiltonian $\hat{H}_0$,

$$\Psi(\mathbf{x}, t) = \sum_{\alpha} c_{\alpha} \psi_{\alpha}(\mathbf{x}, t) \exp(-if_{\alpha} t) \quad (2.136)$$

Moreover, the spectrum of quasienergies possesses the dynamical symmetry in the same mathematical sense as the spectrum of eigenenergies ε_{α} for $\hat{H}_0$.

Theoretical description of quasienergy states is based on appropriate modification of the basis wave functions, which explicitly takes into account the periodicity in time domain [352, 378, 439, 440]. Indeed, the periodicity in time implies

$$\psi_{\alpha}(\mathbf{x}, t + T) = e^{-if_{\alpha} T} \psi_{\alpha}(\mathbf{x}, t) \quad (2.137)$$

This means that the wave function may be represented in the form

$$\psi_{\alpha}(\mathbf{x}, t) = e^{-if_{\alpha} t} u_{\alpha}(\mathbf{x}, t) \quad (2.138)$$

in accordance with the Floquet – Bloch theorem. The Floquet amplitude is periodic in time, $u_{\alpha}(t + T) = u_{\alpha}(t)$. The quantity f_{α} plays the same part as the quasimomentum k_{α} in the Bloch wave function periodic in space. Basing on this analogy,

Nikishov and Ritus [298] introduced the concept of four-dimensional quasimomentum, where the factor f_α in the exponent in Eqs. (2.137), (2.138) plays part of *quasienergy*.

It is natural to choose for the basis functions $\phi_\alpha(\mathbf{x}, t)$ for the quasienergy states those, which evolve from the eigenfunctions of the Hamiltonian $\hat{H}_0$. In principle, each eigenstate of the Hamiltonian $\hat{H}_0$ may be put in correspondence to some quasienergy state. To verify this statement, one may introduce the perturbation $\lambda(t)\hat{H}_p$ and trace the variation of the solutions when λ varies slowly from 0 to 1 during a time much longer than the period T .

Due to periodicity in time, the variable t may be eliminated from the calculation of quasienergy spectrum by means of the expansion of the wave functions $\psi_\alpha(\mathbf{x}, t)$ in a Fourier series,

$$\psi_\alpha(\mathbf{x}, t) = \sum_{m=-\infty}^{+\infty} u_{m\alpha}(\mathbf{x}) e^{-i(f_\alpha + m\Omega)t}. \quad (2.139)$$

Then the Fourier transformation of the Schrödinger equation $[id/dt - H(t)]\psi(t)$ results in an infinite system of equations for the Fourier components $u_{m\alpha}$:

$$(f_\alpha + m\Omega - \varepsilon_\alpha)u_{m\alpha} = \sum_{n\beta} H_{\alpha\beta}^{mn} u_{n\beta}, \quad (2.140)$$

$$H_{\alpha\beta}^{mn} = \frac{1}{T} \int_{-T/2}^{+T/2} dt \langle \alpha n | \hat{H}(t) | \beta m \rangle e^{i(m-n)\Omega t} \quad (2.141)$$

We learn from this system that the quasienergy is not conserved in a periodic field: if the state f_α is replaced by $f_\alpha + m'\Omega$, the secular equation

$$|(f_\alpha - \varepsilon_\alpha + m\Omega)\delta_{\alpha\beta}\delta_{mn} - H_{\alpha\beta}^{mn}| = 0 \quad (2.142)$$

which determines the solutions of Eq. (2.140) remains unchanged. The satellites at $m\Omega$ arise in the quasienergy spectrum in the same sense as the Umklapp vectors $m\mathbf{G}$ accompany the quasimomenta in Bloch states, i.e. the quasienergy f_α in accordance with the Fourier expansion (2.139) is defined up to the additive constant, $f_{\alpha n} - f_{\alpha m} = (n - m)\Omega$.

The composite Hilbert space $\mathbb{S}$ for the Hamiltonian $\hat{H}(x, t)$ (2.134) is made up of the subspace $\mathbb{R}$ of square integrable functions in configuration space and subspace $\mathbb{T}$ of functions periodic in time, $\mathbb{S} = \mathbb{R} \otimes \mathbb{T}$. The orthogonal basis functions for the temporal subspace $\mathbb{T}$ are the exponents $\exp(im\Omega t)$, and the functions

$$\Phi_{\alpha m}(\mathbf{x}, t) = u_\alpha(\mathbf{x}, t) \exp(im\Omega t) \quad (2.143)$$

taken at a given moment t are orthogonal,

$$\langle\langle\Phi_{\alpha m}|\Phi_{\beta n}\rangle\rangle = \frac{1}{T} \int_0^T \int_{-\infty}^{\infty} \Phi_{\alpha m}^*(\mathbf{x}, t) \Phi_{\beta n}(\mathbf{x}, t) = \delta_{\alpha\beta} \delta_{mn}. \quad (2.144)$$

They form a complete set of basis functions for a time-dependent Schrödinger equation with the Hamiltonian (2.134). One may treat conversion of the energy spectrum ε_α into the quasi-energy spectrum $f_{\alpha m}$ as a manifestation of the dynamical symmetry $SO(2)$ of Fourier transformation using the basis $e^{-im\Omega t}$ in the Fock subspace $\mathbb{T}$. indexdynamical symmetry groups! – $SO(2)$ group In this special case we deal with real dynamics of quantum mechanical states in time. Due to Floquet theorem, this dynamics results in (a) transformation of stationary states with definite energies ε_α into quasienergy states $f_{\alpha m}$ and (b) initiation of transitions between these states given by the non-diagonal matrix elements (2.141).

The key features of quasienergy spectrum may be demonstrated on the elementary example of two-level systems discussed above in Section II.3. Let us assume that the tunneling term in the Hamiltonian (2.37) is periodic in time in accordance with a simple law $W(t) = V \cos \Omega t$. In this case, the spectrum of stationary states consists of two levels $\varepsilon_{1,2}$, perturbation $\hat{H}_p(t)$ contains a single harmonics $\pm\Omega$, and the secular equation (2.142) has the following structure

$$\begin{vmatrix} \ddots & & & & & & & \\ & F_2 - 2\Omega & V & 0 & 0 & 0 & 0 & 0 \\ & V & F_1 - \Omega & 0 & 0 & V & 0 & 0 \\ & 0 & 0 & F_2 - \Omega & V & 0 & 0 & 0 \\ & 0 & 0 & V & F_1 & 0 & 0 & V \\ & 0 & V & 0 & 0 & F_2 & V & 0 \\ & 0 & 0 & 0 & 0 & V & F_1 + \Omega & 0 \\ & 0 & 0 & 0 & V & 0 & 0 & F_2 + \Omega \\ & 0 & 0 & 0 & 0 & 0 & V & F_1 + 2\Omega \\ & & & & & & & \ddots \end{vmatrix} = 0 \quad (2.145)$$

($F_i = f_i - \varepsilon_i$). This equation illustrates transformation of the stationary spectrum $F_i = 0$ into a set of two interconnected ladders of quasienergy states. The temporal dynamics of a particle in such a double well is determined by the evolution operator

$$U(t, t') = \hat{\Psi}(t) \hat{\Psi}^{-1}(t') \quad (2.146)$$

This dynamics is given by transitions between two quasienergy ladders.

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2012, XIII, 351 p. 129 illus., Hardcover

ISBN: 978-3-211-99723-9