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 $G_S$ 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 $G_S$.

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 $|l\lambda\rangle$ of a Schrödinger equation

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

describing quantum system $\mathcal{S}$. Here $l$ is the index of irreducible representation and $\lambda$ enumerates the lines of this representation. Projection operators for an irreducible
representation \( l \)
\[
X_{(l)}^\lambda \mu = |l\lambda\rangle \langle l\mu| \tag{2.2}
\]
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
\[
X_{(l)}^\lambda \mu |l'\nu\rangle = \delta_{l\mu} \delta_{\mu
u} |l\lambda\rangle. \tag{2.3}
\]
These operators are useful for construction of basis functions for irreducible representations of \( G_{\mathcal{S}} \). Group generators obeying algebra \( g_{\mathcal{S}} \) 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
\[
X_{(l')}(l) = |l\lambda\rangle \langle l'\mu| \tag{2.4}
\]
which project the states belonging to different irreducible representations \((l \neq l')\) of the group \( G_{\mathcal{S}} \) one onto another. Unifying the notations \(|l\lambda\rangle = |\Lambda\rangle\), one may write the commutation relation
\[
[X^{\Lambda\Lambda'}, \hat{H}] = (E_{\Lambda'} - E_{\Lambda}) \hat{H} \tag{2.5}
\]
The right hand side of this relation turns into zero provided the states \( \Lambda \) and \( \Lambda' \) belong to the same irreducible representation of the group \( G_{\mathcal{S}} \).

If one succeeds in constructing a closed algebra \( d_{\mathcal{S}} \) 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
\[
\sum_{\lambda} X^{\lambda\lambda} = 1 \tag{2.6}
\]
and the commutation relations for the operators \( X^{\kappa\lambda} \). In general case these relations may be presented in the following form [170]
\[
[X^{\kappa\lambda}, X^{\mu\nu}] = X^{\kappa\nu} \delta_{\lambda\mu} \mp X^{\mu\lambda} \delta_{\kappa\nu}\tag{2.7}
\]
“General case” means that the Fock space includes states which may belong to different charge sectors, where changing the state \( \lambda \) for the state \( \kappa \) implies changing the number of fermions \( N_{\lambda} \to N_{\kappa} \) 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.