Chapter 2
Time Reversal and Unitary Symmetries

2.1 Autonomous Classical Flows

A classical Hamiltonian system is called time-reversal invariant if from any given solution $\boldsymbol{x}(t),\ \boldsymbol{p}(t)$ of Hamilton's equations an independent solution $\boldsymbol{x}'(t'),\ \boldsymbol{p}'(t')$, is obtained with $t' = -t$ and some operation relating $\boldsymbol{x}'$ and $\boldsymbol{p}'$ to the original coordinates $\boldsymbol{x}$ and momenta $\boldsymbol{p}$. The simplest such invariance, to be referred to as conventional, holds when the Hamiltonian is an even function of all momenta,

$$t \to -t,\quad \boldsymbol{x} \to \boldsymbol{x},\quad \boldsymbol{p} \to -\boldsymbol{p},\quad H(\boldsymbol{x},\boldsymbol{p}) = H(\boldsymbol{x},-\boldsymbol{p}). \tag{2.1.1}$$

This is obviously not a canonical transformation since the Poisson brackets $\{p_i, x_j\} = \delta_{ij}$ are not left intact. The change of sign brought about for the Poisson brackets is often acknowledged by calling classical time reversal anticanonical. We should keep in mind that the angular momentum vector of a particle is bilinear in $\boldsymbol{x}$ and $\boldsymbol{p}$ and thus odd under conventional time reversal.

The motion of a charged particle in an external magnetic field is not invariant under conventional time reversal since the minimal-coupling Hamiltonian $(\boldsymbol{p} - (e/c)\boldsymbol{A})^2/2\,\mathrm{m}$ is not even in $\boldsymbol{p}$. Such systems may nonetheless have some other, nonconventional time-reversal invariance, to be explained in Sect. 2.9.

Hamiltonian systems with no time-reversal invariance must not be confused with dissipative systems. The differences between Hamiltonian and dissipative dynamics are drastic and well known. Most importantly from a theoretical point of view, all Hamiltonian motions conserve phase-space volumes according to Liouville's theorem, while for dissipative processes such volumes contract in time. The difference between Hamiltonian systems with and without time-reversal invariance, on the other hand, is subtle and has never attracted much attention in the realm of classical physics. It will become clear below, however, that the latter difference plays an important role in the world of quanta [1–3].

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2.2 Spinless Quanta

The Schrödinger equation

$$\mathrm{i}\hbar\dot{\psi}(\boldsymbol{x}, t) = H\psi(\boldsymbol{x}, t) \tag{2.2.1}$$

is time-reversal invariant if, for any given solution $\psi(\boldsymbol{x}, t)$, there is another one, $\psi'(\boldsymbol{x}, t')$, with $t' = -t$ and ψ' uniquely related to ψ. The simplest such invariance, again termed conventional, arises for a spinless particle with the real Hamiltonian

$$H(\boldsymbol{x}, \boldsymbol{p}) = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{x}), \quad V(\boldsymbol{x}) = V^*(\boldsymbol{x}), \tag{2.2.2}$$

where the asterisk denotes complex conjugation. The conventional reversal is

$$\begin{aligned} &t \;\to\; -t, \quad \boldsymbol{x} \;\to\; \boldsymbol{x}, \quad \boldsymbol{p} \;\to\; -\boldsymbol{p}, \\ &\psi(\boldsymbol{x}) \;\to\; \psi^*(\boldsymbol{x}) = K\psi(\boldsymbol{x}). \end{aligned} \tag{2.2.3}$$

In other words, if $\psi(\boldsymbol{x}, t)$ solves (2.2.1) so does $\psi'(\boldsymbol{x}, t) = K\psi(\boldsymbol{x}, -t)$. The operator K of complex conjugation obviously fulfills

$$K^2 = 1, \tag{2.2.4}$$

i.e., it equals its inverse, $K = K^{-1}$. Its definition also implies

$$K\left(c_1\psi_1(\boldsymbol{x}) + c_2\psi_2(\boldsymbol{x})\right) = c_1^* K\psi_1(\boldsymbol{x}) + c_2^* K\psi_2(\boldsymbol{x}), \tag{2.2.5}$$

a property commonly called antilinearity. The transformation $\psi(\boldsymbol{x}) \to K\psi(\boldsymbol{x})$ does not change the modulus of the overlap of two wave functions,

$$|\langle K\psi|K\phi\rangle|^2 = |\langle\psi|\phi\rangle|^2, \tag{2.2.6}$$

while the overlap itself is transformed into its complex conjugate,

$$\langle K\psi|K\phi\rangle = \langle\psi|\phi\rangle^* = \langle\phi|\psi\rangle. \tag{2.2.7}$$

The identity (2.2.7) defines the property of antiunitarity which implies antilinearity [1] (Problem 2.4).

It is appropriate to emphasize that I have defined the operator K with respect to the position representation. Dirac's notation makes this distinction of K especially obvious. If some state vector $|\psi\rangle$ is expanded in terms of position eigenvectors $|x\rangle$,

$$|\psi\rangle = \int d\boldsymbol{x}\,\psi(\boldsymbol{x})|\boldsymbol{x}\rangle, \tag{2.2.8}$$

the operator K acts as

$$K|\psi\rangle = \int d\boldsymbol{x}\,\psi^*(\boldsymbol{x})|\boldsymbol{x}\rangle, \tag{2.2.9}$$

i.e., as $K|\boldsymbol{x}\rangle = |\boldsymbol{x}\rangle$. A complex conjugation operator K' can of course be defined with respect to any representation. It is illustrative to consider a discrete basis and introduce

$$K'|\psi\rangle = K'\sum_\nu \psi_\nu|\nu\rangle = \sum_\nu \psi_\nu^*|\nu\rangle. \tag{2.2.10}$$

Conventional time reversal, i.e., complex conjugation in the position representation, can then be expressed as

$$K = UK' \tag{2.2.11}$$

with a certain symmetric unitary matrix U, the calculation of which is left to the reader as problem 2.5. Unless otherwise stated, the symbol K will be reserved for complex conjugation in the coordinate representation, as far as orbital wave functions are concerned. Moreover, antiunitary time-reversal operators will, for the most part, be denoted by T. Only the conventional time-reversal for spinless particles has the simple form $T = K$.

2.3 Spin-1/2 Quanta

All time-reversal operators T must be antiunitary

$$\langle T\psi|T\phi\rangle = \langle\phi|\psi\rangle, \tag{2.3.1}$$

because of (i) the explicit factor i in Schrödinger's equation and (ii) since they should leave the modulus of the overlap of two wave vectors invariant. It follows from the definition (2.3.1) of antiunitarity that the product of two antiunitary operators is unitary. Consequently, any time-reversal operator T can be given the so-called standard form

$$T = UK, \tag{2.3.2}$$

where U is a suitable unitary operator and K the complex conjugation with respect to a standard representation (often chosen to be the position representation for the orbital part of wave functions).

Another physically reasonable requirement for every time-reversal operator T is that any wave function should be reproduced, at least to within a phase factor, when acted upon twice by T,

$$T^2 = \alpha, \quad |\alpha| = 1. \tag{2.3.3}$$

Inserting the standard form (2.3.2) in (2.3.3) yields[1] $UKUK = UU^*K^2 = UU^* = \alpha$, i.e., $U^* = \alpha U^{-1} = \alpha U^\dagger = \alpha \tilde{U}^*$. The latter identity once iterated gives $U^* = \alpha^2 U^*$, i.e., $\alpha^2 = 1$ or

$$T^2 = \pm 1. \tag{2.3.4}$$

The positive sign holds for conventional time reversal with spinless particles. It will become clear presently that $T^2 = -1$ in the case of a spin-1/2 particle. See also Problem 2.9.

A useful time-reversal operation for a spin-1/2 results from requiring that

$$T\boldsymbol{J}T^{-1} = -\boldsymbol{J} \tag{2.3.5}$$

holds not only for the orbital angular momentum but likewise for the spin. With respect to the spin, however, T cannot simply be the complex conjugation operation since all purely imaginary Hermitian 2×2 matrices commute with one another. The more general structure (2.3.2) must therefore be considered. Just as a matter of convenience, I shall choose K as the complex conjugation in the standard representation where the spin operator $\boldsymbol{S}$ takes the form

$$\begin{aligned} &\boldsymbol{S} = \tfrac{\hbar}{2}\boldsymbol{\sigma}, \\ &\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned} \tag{2.3.6}$$

The matrix U is then constrained by (2.3.5) to obey

$$\begin{aligned} T\sigma_x T^{-1} &= UK\sigma_x KU^{-1} = U\sigma_x U^{-1} = -\sigma_x \\ T\sigma_y T^{-1} &= UK\sigma_y KU^{-1} = -U\sigma_y U^{-1} = -\sigma_y \\ T\sigma_z T^{-1} &= UK\sigma_z KU^{-1} = U\sigma_z U^{-1} = -\sigma_z, \end{aligned} \tag{2.3.7}$$

i.e., U must commute with σ_y and anticommute with σ_x and σ_z. Because any 2×2 matrix U can be represented as a sum of Pauli matrices, we can write

$$U = \alpha\sigma_x + \beta\sigma_y + \gamma\sigma_z + \delta. \tag{2.3.8}$$

The first of the Eq. (2.3.7) immediately gives $\alpha = \delta = 0$; the second yields $\gamma = 0$, whereas β remains unrestricted by (2.3.7). However, since U is unitary, β must have unit modulus. It is thus possible to choose $\beta = \mathrm{i}$ whereupon the time-reversal operation reads

[1] Matrix transposition will always be represented by a tilde, while the dagger † will denote Hermitian conjugation.

$$T = \mathrm{i}\sigma_y K = \mathrm{e}^{\mathrm{i}\pi\sigma_y/2} K. \tag{2.3.9}$$

This may be taken to include, if necessary, the time reversal for the orbital part of wave vectors by interpreting K as complex conjugation both in the position representation and in the standard spin representation. In this sense I shall refer to (2.3.9) as conventional time reversal for spin-1/2 quanta.

The operation (2.3.9) squares to minus unity, in contrast to conventional time reversal for spinless particles. Indeed, $T^2 = \mathrm{i}\sigma_y K \mathrm{i}\sigma_y K = (\mathrm{i}\sigma_y)^2 = -1$.

If one is dealing with N particles with spin 1/2, the matrix U must obviously be taken as the direct product of N single-particle matrices,

$$\begin{aligned} T &= \mathrm{i}\sigma_{1y}\mathrm{i}\sigma_{2y} \ldots \mathrm{i}\sigma_{Ny} K \\ &= \exp\left[\mathrm{i}\frac{\pi}{2}\left(\sigma_{1y} + \sigma_{2y} + \ldots + \sigma_{Ny}\right)\right] K = \exp\left(\mathrm{i}\pi \frac{S_y}{\hbar}\right) K, \end{aligned} \tag{2.3.10}$$

where S_y now is the y-component of the total spin $\boldsymbol{S} = \hbar(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2 + \ldots + \boldsymbol{\sigma}_N)/2$. The square of T depends on the number of particles according to

$$T^2 = \begin{cases} +1 & N \text{ even} \\ -1 & N \text{ odd.} \end{cases} \tag{2.3.11}$$

I shall ocasionally refer to "kicked tops", dynamical systems involving only components of an angular momentum $\boldsymbol{J} = (J_x, J_y, J_z)$ as dynamical variables. The square $\boldsymbol{J}^2$ is then conserved and the Hilbert space can be chosen as the $2j+1$ dimensional space with $\boldsymbol{J}^2 = j(j+1)$ spanned the eigenvectors $|j, m\rangle$ of, say, J_z with $m = -j, -j+1, \ldots, j$. The standard time reversal operator is the given by (2.3.10) as $T = \mathrm{e}^{\mathrm{i}\pi J_z/\hbar} K$ with $K|j, m\rangle = |j, m\rangle$ and squares to $+1$ or -1 when the qantum number j is integer and half-integer, respectively.

2.4 Hamiltonians Without *T* Invariance

All Hamiltonians can be represented by Hermitian matrices. Before proceeding to identify the subclasses of Hermitian matrices to which time-reversal invariant Hamiltonians belong, it is appropriate to pause and make a few remarks about Hamiltonians unrestricted by antiunitary symmetries.

Any Hamiltonian becomes real in its eigenrepresentation, diag $(E_1, E_2, \ldots)$. Under a unitary transformation U,

$$H_{\mu\nu} = U_{\mu\lambda} E_\lambda U^\dagger_{\lambda\nu} = U_{\mu\lambda} E_\lambda U^*_{\nu\lambda}, \tag{2.4.1}$$

H preserves Hermiticity, $(H_{\mu\nu})^* = \tilde{H}_{\mu\nu} = H_{\nu\mu}$, but ceases, in general, to be real.

Now, I propose to construct the class of "canonical transformations" that change a Hamiltonian matrix without destroying its Hermiticity and without altering its eigenvalues. To this end it is important to look at each irreducible part of the matrix H separately, i.e., to think of good quantum numbers related to a complete set of mutually commuting conserved observables (other than H itself) as fixed. Eigenvalues are preserved under a similarity transformation with an arbitrary nonsingular matrix A. To show that $H' = A\, HA^{-1}$ has the same eigenvalues as H, it suffices to write out H' in the H representation,

$$H'_{\mu\nu} = \sum_{\lambda} A_{\mu\lambda} E_{\lambda} \left(A^{-1}\right)_{\lambda\nu}, \tag{2.4.2}$$

and to multiply from the right by A. The columns of A are then recognized as eigenvectors of H', and the eigenvalues of H turn out to be those of H' as well.

For A to qualify as a canonical transformation, H' must also be Hermitian,

$$\left(A\, HA^{-1}\right)^{\dagger} = A\, HA^{-1} \;\Leftrightarrow\; \left[H, A^{\dagger}A\right] = 0. \tag{2.4.3}$$

Excluding the trivial solution where $A^{\dagger}A$ is a function of H and recalling that all other mutually commuting conserved observables are multiples of the unit matrix in the space considered, one concludes that $A^{\dagger}A$ must be the unit matrix, at least to within a positive factor. That factor must itself be unity if A is subjected to the additional constraint that it should preserve the normalization of vectors,

$$A^{\dagger}A = \mathbb{1}. \tag{2.4.4}$$

The class of canonical transformations of Hamiltonians unrestricted by antiunitary symmetries is thus constituted by unitary matrices. Obviously, for an N-dimensional Hilbert space that class is the group $U(N)$.

It is noteworthy that Hamiltonian matrices unrestricted by antiunitary symmetries are in general complex. They can, of course, be given real representations, but any such representation will become complex under a general canonical (i.e., unitary) transformation.

A few more formal remarks may be permissible. The time evolution operators $U = \mathrm{e}^{-\mathrm{i}Ht/\hbar}$ generated by complex Hermitian Hamiltonians form the Lie group $U(N)$. The Hamiltonians themselves can be associated with the generators $X = \mathrm{i}H$ of the Lie algebra $u(N)$, the tangent space to the group $U(N)$. — Moreover, Eq. (2.4.1) reveals that a general complex Hermitian $N{\times}N$ Hamiltonian can be diagonalized by a unitary transformation. Once such a diagonalizing transformation U is found, others can be obtained by splitting off an arbitrary diagonal unitary matrix as $U\mathrm{diag}\,(\mathrm{e}^{-\mathrm{i}\phi_1}, \dots \mathrm{e}^{-\mathrm{i}\phi_N})$. By identifying all such matrices one arrives at the coset space $U(N)/U(1)^N$. — For all of these reasons, complex Hermitian Hamiltonians are said to form the "unitary symmetry class".

2.5 T Invariant Hamiltonians, $T^2 = 1$

When we have an antiunitary operator T with

$$[H, T] = 0, \quad T^2 = 1 \tag{2.5.1}$$

the Hamiltonian H can always be given a real matrix representation and such a representation can be found without diagonalizing H.

As a first step toward proving the above statement, I demonstrate that, with the help of an antiunitary T squaring to plus unity, T invariant basis vectors ψ_ν can be constructed. Take any vector ϕ_1 and a complex number a_1. The vector

$$\psi_1 = a_1\phi_1 + Ta_1\phi_1 \tag{2.5.2}$$

is then T invariant, $T\psi_1 = \psi_1$. Next, take any vector ϕ_2 orthogonal to ψ_1 and a complex number a_2. The combination

$$\psi_2 = a_2\phi_2 + Ta_2\phi_2 \tag{2.5.3}$$

is again T invariant. Moreover, ψ_2 is orthogonal to ψ_1 since

$$\begin{aligned}\langle\psi_2|\psi_1\rangle &= a_2^*\langle\phi_2|\psi_1\rangle + a_2\langle T\phi_2|\psi_1\rangle \\ &= a_2\left\langle T^2\phi_2|\psi_1\right\rangle^* = a_2\langle\phi_2|\psi_1\rangle^* = 0.\end{aligned} \tag{2.5.4}$$

By so proceeding we eventually arrive at a complete set of mutually orthogonal vectors. If desired, the numbers a_ν can be chosen to normalize as $\langle\psi_\mu|\psi_\nu\rangle = \delta_{\mu\nu}$.

With respect to a T invariant basis, the Hamiltonian $H = THT$ is real,

$$\begin{aligned}H_{\mu\nu} &= \langle\psi_\mu|H\psi_\nu\rangle = \langle T\psi_\mu|TH\psi_\nu\rangle^* \\ &= \langle\psi_\mu|THT^2\psi_\nu\rangle^* = \langle\psi_\mu|THT\psi_\nu\rangle^* = H_{\mu\nu}^*.\end{aligned} \tag{2.5.5}$$

Note that the Hamiltonians in question can be made real without being diagonalized first. It is therefore quite legitimate to say that they are generically real matrices. The canonical transformations that are admissible now form the Lie group $O(N)$ of real orthogonal matrices O, $O\tilde{O} = 1$. Beyond preserving eigenvalues and Hermiticity, an orthogonal transformation also transforms a real matrix H into another real matrix $H' = OH\tilde{O}$. The orthogonal group is obviously a subgroup of the unitary group considered in the last section. A T invariant $N \times N$ Hamiltonian can be diagonalized by a matrix from the yet smaller group $SO(N)$ of unit-determinant orthogonal matrices if $T^2 = 1$. It is therefore customary to say that the Hamiltonians under scrutiny form the "orthogonal symmetry class".

It may be worthwhile to look back at Sect. 2.2 where it was shown that the Schrödinger equation of a spinless particle is time-reversal invariant provided the Hamiltonian is a real operator in the position representation. The present section generalizes that previous statement.

The time evolution operators for the orthogonal class can be characterized from the point of view of Lie groups, in analogy to $\mathrm{e}^{-\mathrm{i}Ht/\hbar} \in U(N)$ for the unitary class. To that end I argue that $H = \tilde{H}$ entails $\mathrm{e}^{-\mathrm{i}Ht/\hbar}$ to be symmetric as well. The time evolution operators can thus be written as $U\tilde{U}$ with $U \in U(N)$. Now the product $U\tilde{U}$ remains unchanged when U is replaced by UO with O any orthogonal matrix, and therefore the coset space $U(N)/O(N)$ houses the time evolution operators from the orthogonal class.

2.6 Kramers' Degeneracy

For any Hamiltonian invariant under a time reversal T,

$$[H, T] = 0, \tag{2.6.1}$$

i.e., if ψ is an eigenfunction with eigenvalue E, so is $T\psi$. As shown above, we may choose the equality $T\psi = \psi$ without loss of generality if $T^2 = +1$. Here, I propose to consider time-reversal operators squaring to minus unity,

$$T^2 = -1. \tag{2.6.2}$$

In this case, ψ and $T\psi$ are orthogonal,

$$\langle\psi|T\psi\rangle = \left\langle T\psi|T^2\psi\right\rangle^* = -\langle T\psi|\psi\rangle^* = -\langle\psi|T\psi\rangle = 0, \tag{2.6.3}$$

and therefore all eigenvalues of H are doubly degenerate. This is Kramers' degeneracy. It follows that the dimension of the Hilbert space must, if finite, be even. This fits with the result of Sect. 2.3 that $T^2 = -1$ is possible only if the number of spin-$1/2$ particles in the system is odd; the total-spin quantum number s is then a half-integer and $2s + 1$ is even.

In the next two sections, I shall discuss the structure of Hamiltonian matrices with Kramers' degeneracy, first for the case with additional geometric symmetries and then for the case in which T is the only invariance.

2.7 Kramers' Degeneracy and Geometric Symmetries

As an example of geometric symmetry, let us consider a parity such that

$$[R_x, H] = 0, \quad [R_x, T] = 0, \quad R_x^2 = -1. \tag{2.7.1}$$

This could be realized, for example, by a rotation through π about, say, the x-axis, $R_x = \exp(\mathrm{i}\pi J_x/\hbar)$; note that since $T^2 = -1$ only half-integer values of the total angular momentum quantum number are admitted.

To reveal the structure of the matrix H, it is convenient to employ a basis ordered by parity,

$$R_x|n\pm\rangle = \pm\mathrm{i}|n\pm\rangle. \tag{2.7.2}$$

Moreover, since T changes the parity,

$$R_x T|n\pm\rangle = T R_x|n\pm\rangle = \mp\mathrm{i}T|n\pm\rangle, \tag{2.7.3}$$

the basis can be organized such that

$$T|n\pm\rangle = \pm|n\mp\rangle. \tag{2.7.4}$$

For the sake of simplicity, let us assume a finite dimension $2N$. The matrix H then falls into four $N \times N$ blocks

$$H = \begin{pmatrix} H^+ & 0 \\ 0 & H^- \end{pmatrix} \tag{2.7.5}$$

two of which are zero since H has vanishing matrix elements between states of different parity. Indeed, $\langle m+|R_x H R_x^{-1}|n-\rangle$ is equal to $+\langle m+|H|n-\rangle$ due to the invariance of H under R_x and equal to $-\langle m+|H|n-\rangle$ because of (2.7.2). The T invariance relates the two blocks $H^\pm$:

$$\begin{aligned}\langle m+|H|n+\rangle &= \left\langle m+\left|THT^{-1}\right|n+\right\rangle \\ &= -\langle m+|TH|n-\rangle = -\langle T(m+)|T^2 H|n-\rangle^* \\ &= +\langle m-|H|n-\rangle^* = \langle n-|H|m-\rangle.\end{aligned} \tag{2.7.6}$$

At this point Kramers' degeneracy emerges: Since they are the transposes of one another, H^+ and H^- have the same eigenvalues. Moreover, they are in general complex and thus have $U(N)$ as their group of canonical transformations.

Further restrictions on the matrices $H^\pm$ arise from additional symmetries. It is illustrative to admit one further parity R_y with

$$\left[R_y, H\right] = 0, \quad \left[R_y, T\right] = 0, \quad R_x R_y + R_y R_x = 0, \quad R_y^2 = -1 \tag{2.7.7}$$

which might be realized as $R_y = \exp(\mathrm{i}\pi J_y/\hbar)$. The anticommutativity of R_x and R_y immediately tells us that R_y changes the R_x parity, just as T does, $R_x R_y|m\pm\rangle = \mp\mathrm{i}R_y|m\pm\rangle$. The basis may thus be chosen according to

$$R_y|n\pm\rangle = \pm|n\mp\rangle \tag{2.7.8}$$

which is indeed the same as (2.7.4) but with R_y instead of T. Despite this similarity, the R_y invariance imposes a restriction on H that goes beyond those achieved by T precisely because R_y is unitary while T is antiunitary. The R_y invariance implies, together with (2.7.8), that

$$\begin{aligned}\langle m+|H|n+\rangle &= \langle m+|R_y H R_y^{-1}|n+\rangle \\ &= \langle m-|H|n-\rangle,\end{aligned} \tag{2.7.9}$$

i.e., $H^+ = H^-$ while the T invariance had given $H^+ = (H^-)^*$ [see (2.7.6)]. Thus we have the result that H^+ and H^- are identical real matrices. Their group of canonical transformation is reduced by the new parity from $U(N)$ to $O(N)$.

As a final illustration of the cooperation of time-reversal invariance with geometrical symmetries, the case of full isotropy, $[H, \boldsymbol{J}] = 0$, deserves mention. The appropriate basis here is $|\alpha jm\rangle$ with $\hbar m$ and $\hbar^2 j(j+1)$ the eigenvalues of J_z and $\boldsymbol{J}^2$, respectively. The Hamiltonian matrix then falls into blocks given by

$$\left\langle \alpha jm|H|\beta j'm'\right\rangle = \delta_{jj'}\delta_{mm'}\left\langle \alpha\left|H^{(j,m)}\right|\beta\right\rangle,$$

$$j = \tfrac{1}{2}, \frac{3}{2}, \tfrac{5}{2}, \ldots, \quad m = \pm\tfrac{1}{2}, \pm\tfrac{3}{2}, \ldots, \pm j. \tag{2.7.10}$$

It is left to the reader as Problem 2.10 to show that

(i) due to T invariance, for any fixed value of j, the two blocks with differing signs of m are transposes of one another,

$$H^{(j,m)} = \tilde{H}^{(j,-m)}, \tag{2.7.11}$$

and thus have identical eigenvalues (Kramers' degeneracy!), and

(ii) invariance of H under rotations about the y-axis makes the two blocks equal.

The two statements above imply that the blocks $H^{(j,m)}$ are all real and thus have the orthogonal transformations as their canonical transformations.

To summarize, unitary transformations are canonical both when there is no time-reversal invariance and when a time-reversal invariance with Kramers' degeneracy ($T^2 = -1$) is combined with one parity. Orthogonal transformations constitute the canonical group when time-reversal invariance holds, either with or without Kramers' degeneracy, in the first case, however, only in the presence of certain geometric symmetries. An altogether different group of canonical transformations will be encountered in Sect. 2.8.

2.8 Kramers' Degeneracy Without Geometric Symmetries

When a time reversal with $T^2 = -1$ is the only symmetry of H, it is convenient to adopt a basis of the form

$$|1\rangle\,,\ T|1\rangle\,,\ |2\rangle\,,\ T|2\rangle\,,\ \ldots\ |N\rangle\,,\ T|N\rangle. \tag{2.8.1}$$

[Note that in (2.7.5) another ordering of states $|n+\rangle$ and $T|n+\rangle = |n-\rangle$ was chosen.] Sometimes I shall write $|Tn\rangle$ for $T|n\rangle$ and $\langle Tn|$ for the corresponding Dirac bra. For the sake of simplicity, the Hilbert space is again assumed to have the finite dimension $2N$.

If the complex conjugation operation K is defined relative to the basis (2.8.1), the unitary matrix U in $T = UK$ takes a simple form which is easily found by letting T act on an arbitrary state vector

$$\begin{aligned} |\psi\rangle &= \sum_m (\psi_{m+}|m\rangle + \psi_{m-}|Tm\rangle)\,, \\ T|\psi\rangle &= \sum_m \left(\psi^*_{m+}|Tm\rangle - \psi^*_{m-}|m\rangle\right). \end{aligned} \tag{2.8.2}$$

Clearly, in each of the two-dimensional subspaces spanned by $|m\rangle$ and $|Tm\rangle$, the matrix U, to be called Z from now on, takes the form

$$Z_{mm} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \equiv \tau_2 \tag{2.8.3}$$

while different such subspaces are unconnected,

$$Z_{mn} = 0 \ \text{ for } \ m \neq n. \tag{2.8.4}$$

The $2N \times 2N$ matrix Z is obviously block diagonal with the 2×2 blocks (2.8.3) along the diagonal. In fact it will be convenient to consider Z as a diagonal $N \times N$ matrix, whose nonzero elements are themselves 2×2 matrices given by (2.8.3).

Similarly, the two pairs of states $|m\rangle$, $T|m\rangle$, and $|n\rangle$, $T|n\rangle$ give a 2×2 submatrix of the Hamiltonian

$$\begin{pmatrix} \langle m|H|n\rangle & \langle m|H|Tn\rangle \\ \langle Tm|H|n\rangle & \langle Tm|H|Tn\rangle \end{pmatrix} \equiv h_{mn}. \tag{2.8.5}$$

The full $2N \times 2N$ matrix H may be considered as an $N \times N$ matrix each element of which is itself a 2×2 block h_{mn}. The reason for the pairwise ordering of the basis (2.8.1) is, as will become clear presently, that the restriction imposed on H by time-reversal invariance can be expressed as a simple property of h_{mn}.

As is the case for any 2×2 matrix, the block h_{mn} can be represented as a linear combination of four independent matrices. Unity and the three Pauli matrices $\boldsymbol{\sigma}$ may come to mind first, but the condition of time-reversal invariance will take a nicer form if the anti-Hermitian matrices $\boldsymbol{\tau} = -\mathrm{i}\boldsymbol{\sigma}$ are employed,

$$\begin{aligned}&\tau_1 = \begin{pmatrix} 0 & -\mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix}, \quad \tau_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \tau_3 = \begin{pmatrix} -\mathrm{i} & 0 \\ 0 & +\mathrm{i} \end{pmatrix} \\ &\tau_i\tau_j = \varepsilon_{ijk}\tau_k, \quad \tau_i\tau_j + \tau_j\tau_i = -2\delta_{ij}.\end{aligned} \tag{2.8.6}$$

Four coefficients $h_{mn}^{(\mu)}$, $\mu = 0, 1, 2, 3$, characterize the block h_{mn},

$$h_{mn} = h_{mn}^{(0)}1 + \boldsymbol{h}_{mn} \cdot \boldsymbol{\tau}. \tag{2.8.7}$$

Now, time-reversal invariance gives

$$\begin{aligned} h_{mn} &= \left(THT^{-1}\right)_{mn} \\ &= \left(ZKHKZ^{-1}\right)_{mn} \\ &= \left(ZH^*Z^{-1}\right)_{mn} \\ &= -\tau_2 h_{mn}^* \tau_2 \\ &= -\tau_2 \left\{h_{mn}^{(0)^*} 1 + \boldsymbol{h}_{mn}^* \cdot \boldsymbol{\tau}^*\right\} \tau_2 \\ &= h_{mn}^{(0)^*} 1 + \boldsymbol{h}_{mn}^* \cdot \boldsymbol{\tau}, \end{aligned} \tag{2.8.8}$$

which simply means that the four amplitudes $h_{mn}^{(\mu)}$ are all real:

$$h_{mn}^{(\mu)} = h_{mn}^{(\mu)^*}. \tag{2.8.9}$$

For historical reasons, matrices with the property (2.8.9) are called "quaternion real". Note that this property does look nicer than the one that would have been obtained if we had used Pauli's triple $\boldsymbol{\sigma}$ instead of the anti-Hermitian $\boldsymbol{\tau}$.

The Hermiticity of H implies the relation

$$h_{mn} = h_{nm}^{\dagger}, \tag{2.8.10}$$

which in turn means that the four real amplitudes $h_{mn}^{(\mu)}$ obey

$$\begin{aligned} h_{mn}^{(0)} &= h_{nm}^{(0)} \\ h_{mn}^{(k)} &= -h_{nm}^{(k)}, \quad k = 1, 2, 3. \end{aligned} \tag{2.8.11}$$

It follows that the $2N \times 2N$ matrix H is determined by $N(2N - 1)$ independent real parameters.

With the structure of the Hamiltonian now clarified, it remains to identify the canonical transformations that leave this structure intact. To that end we must find the subgroup of unitary matrices that preserve the form $T = ZK$ of the time-reversal operator. In other words, the question is to what extent there is freedom in choosing a basis with the properties (2.8.1). The allowable unitary basis transformations S have to obey

$$T = STS^{-1} = SZKS^{-1} = SZ\tilde{S}K \quad \Longrightarrow \quad SZ\tilde{S} = Z. \tag{2.8.12}$$

The requirement $SZ\tilde{S} = Z$ defines the Lie group $Sp(2N)$, see Problem 2.12.

The symplectic transformations just found are in fact the relevant canonical transformations since they leave a quaternion real Hamiltonian quaternion real. To prove that statement, I shall show that if H is T invariant, then so is SHS^{-1}: With the help of the identities $ZS^* = SZ$ and $\tilde{S}Z = ZS^{-1}$, both of which reformulations of (2.8.12), I have

$$\begin{aligned} TSHS^{-1}T^{-1} &= ZKSHS^{-1}KZ^{-1} = ZS^*KHK\left(S^{-1}\right)^* Z^{-1} \\ &= SZKHK\tilde{S}(-Z) = SZKHK(-Z)S^{-1} \\ &= STHT^{-1}S^{-1} = SHS^{-1}. \end{aligned} \tag{2.8.13}$$

Of course, a T invariant $2N \times 2N$ Hamiltonian is diagonalizable by a symplectic transformation from $Sp(2N)$ if $T^2 = -1$.

Time reversal invariant Hamiltonians with $T^2 = -1$ are said to form the "symplectic symmetry class". Some readers may want to check that the pertinent time evolution operators live in the coset space $U(2N)/Sp(2N)$.

2.9 Nonconventional Time Reversal

We have defined conventional time reversal by

$$\begin{aligned} T\boldsymbol{x}T^{-1} &= \boldsymbol{x} \\ T\boldsymbol{p}T^{-1} &= -\boldsymbol{p} \\ T\boldsymbol{J}T^{-1} &= -\boldsymbol{J} \end{aligned} \tag{2.9.1}$$

and, for any pair of states,

$$\begin{aligned} &\langle T\phi|T\psi\rangle = \langle\psi|\phi\rangle \\ &T^2 = \pm 1. \end{aligned} \tag{2.9.2}$$

The motivation for this definition is that many Hamiltonians of practical importance are invariant under conventional time reversal, $[H, T] = 0$. An atom and a molecule in an isotropic environment, for instance, have Hamiltonians of that symmetry. But, as already mentioned in Sect. 2.1, conventional time reversal is broken by an external magnetic field.

In identifying the canonical transformations of Hamiltonians from their symmetries in Sects. 2.5, 2.6, 2.7, and 2.8, extensive use was made of (2.9.2) but none, as the reader is invited to review, of (2.9.1). In fact, and indeed fortunately, the validity of (2.9.1) is not at all necessary for the above classification of Hamiltonians according to their group of canonical transformations.

Interesting and experimentally realizable systems often have Hamiltonians that commute with some antiunitary operator obeying (2.9.2) but not (2.9.1). There is nothing strange or false about such a "nonconventional" time-reversal invariance: it associates another, independent solution, $\psi'(t) = T\psi(-t)$, with any solution $\psi(t)$ of the Schrödinger equation, and is thus as good a time-reversal symmetry as the conventional one.

An important example is the hydrogen atom in a constant magnetic field [4, 5]. Choosing that field as $\boldsymbol{B} = (0, 0, B)$ and the vector potential as $\boldsymbol{A} = \boldsymbol{B} \times \boldsymbol{x}/2$ and including spin-orbit interaction, one obtains the Hamiltonian

$$H = \frac{\boldsymbol{p}^2}{2m} - \frac{e^2}{r} - \frac{eB}{2mc}(L_z + gS_z) + \frac{e^2B^2}{8mc^2}\left(x^2 + y^2\right) + f(r)\boldsymbol{LS}. \tag{2.9.3}$$

Here $\boldsymbol{L}$ and $\boldsymbol{S}$ denote orbital angular momentum and spin, respectively, while the total angular momentum is $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$. This Hamiltonian is not invariant under conventional time reversal, T_0, but instead under

$$T = \mathrm{e}^{\mathrm{i}\pi J_x/\hbar} T_0. \tag{2.9.4}$$

If spin is absent, $T^2 = 1$, whereas $T^2 = -1$ with spin. In the subspaces of constant J_z and $\boldsymbol{J}^2$, one has the orthogonal transformations as the canonical group in the first case (Sect. 2.2) and the unitary transformations in the second case (Sect. 2.7 and Problem 2.11).

When a homogeneous electric field $\boldsymbol{E}$ is present in addition to the magnetic field, the operation T in (2.9.4) ceases to be a symmetry of H since it changes the electric-dipole perturbation $-e\boldsymbol{x} \cdot \boldsymbol{E}$. But $T = RT_0$ is an antiunitary symmetry where the unitary operator R represents a reflection in the plane spanned by $\boldsymbol{B}$ and $\boldsymbol{E}$. Note that the component of the angular momentum lying in this plane changes sign under that reflection since the angular momentum is a pseudo-vector. While the Zeeman term in H changes sign under both conventional time reversal and under the reflection in question, it is left invariant under the combined operation. The electric-dipole term as well as all remaining terms in H are symmetric with respect to both T_0 and R such that $[H, RT_0] = 0$ indeed results.

As another example *Seligman* and *Verbaarschot* [6] proposed two coupled oscillators with the Hamiltonian

$$\begin{aligned} H = {} & \tfrac{1}{2}\left(p_1 - a\,x_2^3\right)^2 + \tfrac{1}{2}\left(p_2 + a\,x_1^3\right)^2 \\ & + \alpha_1 x_1^6 + \alpha_2 x_2^6 - \alpha_{12}(x_1 - x_2)^6. \end{aligned} \tag{2.9.5}$$

Here, too, T_0 invariance is violated if $a \neq 0$. As long as $\alpha_{12} = 0$, however, H is invariant under

$$T = \mathrm{e}^{\mathrm{i}\pi L_2/\hbar} T_0 \tag{2.9.6}$$

and thus representable by a real matrix. The geometric symmetry TT_0^{-1} acts as $(x_1, p_1) \to (-x_1, -p_1)$ and $(x_2, p_2) \to (x_2, p_2)$ and may be visualized as a rotation through π about the 2-axis if the two-dimensional space spanned by x_1 and x_2 is imagined embedded in a three-dimensional Cartesian space. However, when $a \neq 0$ and $\alpha_{12} \neq 0$, the Hamiltonian (2.9.5) has no antiunitary symmetry left and therefore is a complex matrix. (Note that H is a complex operator in the position representation anyway.)

2.10 Stroboscopic Maps for Periodically Driven Systems

Time-dependent perturbations, especially periodic ones, are characteristic of many situations of experimental interest. They are also appreciated by theorists inasmuch as they provide the simplest examples of classical nonintegrability: Systems with a single degree of freedom are classically integrable, if autonomous, but may be nonintegrable if subjected to periodic driving.

Quantum mechanically, one must tackle a Schrödinger equation with an explicit time dependence in the Hamiltonian,

$$\mathrm{i}\hbar\dot{\psi}(t) = H(t)\psi(t). \tag{2.10.1}$$

The solution at $t > 0$ can be written with the help of a time-ordered exponential

$$U(t) = \left\{\exp\left[\frac{-\mathrm{i}}{\hbar}\int_0^t dt' H(t')\right]\right\}_+ \tag{2.10.2}$$

where the “positive” time ordering requires

$$\left[A(t)B(t')\right]_+ = \begin{cases} A(t)B(t') & \text{if } t > t' \\ B(t')A(t) & \text{if } t < t' \end{cases}. \tag{2.10.3}$$

Of special interest are cases with periodic driving,

$$H(t + n\tau) = H(t), \quad n = 0, \pm 1, \pm 2, \ldots . \tag{2.10.4}$$

The evolution operator referring to one period τ, the so-called Floquet operator

$$U(\tau) \equiv F, \tag{2.10.5}$$

is worthy of consideration since it yields a stroboscopic view of the dynamics,

$$\psi(n\tau) = F^n \psi(0). \tag{2.10.6}$$

Equivalently, F may be looked upon as defining a quantum map,

$$\psi\left([n+1]\tau\right) = F\psi(n\tau). \tag{2.10.7}$$

Such discrete-time maps are as important in quantum mechanics as their Newtonian analogues have proven in classical nonlinear dynamics.

The Floquet operator, being unitary, has unimodular eigenvalues (involving eigenphases alias quasi-energies) and mutually orthogonal eigenvectors,

$$\begin{aligned} F\Phi_\nu &= \mathrm{e}^{-\mathrm{i}\phi_\nu}\Phi_\nu, \\ \left\langle\Phi_\mu|\Phi_\nu\right\rangle &= \delta_{\mu\nu}. \end{aligned} \tag{2.10.8}$$

I shall in fact be concerned only with normalizable eigenvectors. With the eigenvalue problem solved, the stroboscopic dynamics can be written out explicitly,

$$\psi(n\tau) = \sum_\nu \mathrm{e}^{-\mathrm{i}n\phi_\nu}\,\langle\Phi_\nu|\psi(0)\rangle\,\Phi_\nu. \tag{2.10.9}$$

Monochromatic perturbations are relatively easy to realize experimentally. Much easier to analyse are perturbations for which the temporal modulation takes the form of a periodic train of delta kicks,

$$H(t) = H_0 + \lambda V\sum_{n=-\infty}^{+\infty}\delta(t-n\tau). \tag{2.10.10}$$

The weight of the perturbation V in $H(t)$ is measured by the parameter λ, which will be referred to as the kick strength. The Floquet operator transporting the state vector from immediately after one kick to immediately after the next reads

$$F = \mathrm{e}^{-\mathrm{i}\lambda V/\hbar}\mathrm{e}^{-\mathrm{i}H_0\tau/\hbar}. \tag{2.10.11}$$

The simple product form arises from the fact that only H_0 is on between kicks, while H_0 is ineffective "during" the infinitely intense delta kick.

It may be well to conclude this section with a few examples. Of great interest with respect to ongoing experiments is the hydrogen atom exposed to a monochromatic electromagnetic field. Even the simplest Hamiltonian,

$$H = \frac{p^2}{2m} - \frac{e^2}{r} - Ez\cos\omega t, \tag{2.10.12}$$

defies exact solution. The classical motion is known to be strongly chaotic for sufficiently large values of the electric field E : A state that is initially bound (with respect to $H_0 = p^2/2m - e^2/r$) then suffers rapid ionization. The quantum modifications of this chaos-enhanced ionization have been the subject of intense discussion. See [7] for the early efforts, and for a brief sketch of the present situation, see Sect. 7.1.

A fairly complete understanding has been achieved for both the classical and quantum behavior of the kicked rotator [8], a system of quite some relevance for microwave ionization of hydrogen atoms. The Hamiltonian reads

$$H(t) = \frac{1}{2I}p^2 + \lambda \cos\phi \sum_{n=-\infty}^{+\infty} \delta(t - n\tau). \tag{2.10.13}$$

The classical kick-to-kick description is *Chirikov*'s standard map [9]. Most of the chapter on quantum localization will be devoted to that prototypical system.

Somewhat richer in their behavior are the kicked tops for which H_0 and V in (2.10.10) and (2.10.11) are polynomials in the components of an angular momentum $\boldsymbol{J}$. Due to the conservation of $\boldsymbol{J}^2 = \hbar^2 j(j+1)$, $j = \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$, kicked tops enjoy the privilege of a finite-dimensional Hilbert space. The special case

$$H_0 \propto J_x, \quad V \propto J_z^2 \tag{2.10.14}$$

has recently been realized experimentally [10].

2.11 Time Reversal for Maps

It is easy to find the condition which the Hamiltonian $H(t)$ must satisfy so that a given solution $\psi(t)$ of the Schrödinger equation

$$\mathrm{i}\hbar\dot{\psi}(t) = H(t)\psi(t) \tag{2.11.1}$$

yields an independent solution,

$$\tilde{\psi}(t) = T\psi(-t), \tag{2.11.2}$$

where T is some antiunitary operator. By letting T act on both sides of the Schrödinger equation,

$$-\mathrm{i}\hbar\frac{\partial}{\partial t}T\psi(t) = TH(t)T^{-1}T\psi(t) \tag{2.11.3}$$

or, with $t \to -t$,

$$\mathrm{i}\hbar\frac{\partial}{\partial t}T\psi(-t) = TH(-t)T^{-1}T\psi(-t). \tag{2.11.4}$$

For (2.11.4) to be identical to the original Schrödinger equation, $H(t)$ must obey

$$H(t) = TH(-t)T^{-1}, \tag{2.11.5}$$

a condition reducing to that studied previously for autonomous dynamics.

For periodically driven systems it is convenient to express the time-reversal symmetry (2.11.5) as a property of the Floquet operator. As a first step in searching for that property, we again employ the formal solution of (2.11.1). Distinguishing now between positive and negative times,

$$\psi(t) = \begin{cases} U_+(t)\psi(0)\,, & t > 0 \\ U_-(t)\psi(0)\,, & t < 0 \end{cases} \tag{2.11.6}$$

where $U_+(t)$ is positively time-ordered as explained in (2.10.2) and (2.10.3) while the negative time order embodied in $U_-(t)$ is simply the opposite of the positive one. Now, I assume $t > 0$ and propose to consider

$$\tilde{\psi}(t) = T\psi(-t) = TU_-(-t)\psi(0) = TU_-(-t)T^{-1}T\psi(0). \tag{2.11.7}$$

If $H(t)$ is time-reversal invariant in the sense of (2.11.5), this $\tilde{\psi}(t)$ must solve the original Schrödinger equation (2.11.1) such that

$$U_+(t) = TU_-(-t)T^{-1}. \tag{2.11.8}$$

The latter identity is in fact equivalent to (2.11.5). The following discussion will be confined to τ-periodic driving, and we shall take the condition (2.11.8) for $t = \tau$. The backward Floquet operator $U_-(-\tau)$ is then simply related to the forward one. To uncover that relation, we represent $U_-(-\tau)$ as a product of time evolution operators, each factor referring to a small time increment,

$$\begin{aligned} U_-(-\tau) &= \left\{\exp\left[-\frac{\mathrm{i}}{\hbar}\int_0^{-\tau} dt' H(t')\right]\right\}_- \\ &= \mathrm{e}^{\mathrm{i}\Delta t H(-t_n)/\hbar}\mathrm{e}^{\mathrm{i}\Delta t H(-t_{n-1})/\hbar}\ldots \\ &\quad \ldots \mathrm{e}^{\mathrm{i}\Delta t H(-t_2)/\hbar}\mathrm{e}^{\mathrm{i}\Delta t H(-t_1)/\hbar}. \end{aligned} \tag{2.11.9}$$

As illustrated in Fig. 2.1, we choose equidistant intermediate times between $t_{-n} = -\tau$ and $t_n = \tau$ with the positive spacing $t_{i+1} - t_i = \Delta t = \tau/n$.

The intervals $t_{i+1} - t_i$ are assumed to be so small that the Hamiltonian can be taken to be constant within each of them. Note that the positive sign appears in each of the n exponents in the second line of (2.11.9) since Δt is defined to be positive while the time integral in the negatively time-ordered exponential runs toward the

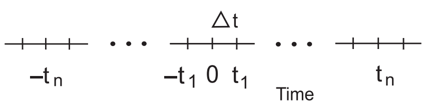

Fig. 2.1 Discretization of the time used to evaluate the time-ordered exponential in (2.11.9)

left on the time axis. Now, we invoke the assumed periodicity of the Hamiltonian, $H(-t_{n-i}) = H(t_i)$, to rewrite $U_-(-\tau)$ as

$$\begin{aligned} U_-(-\tau) = \; & \mathrm{e}^{\mathrm{i}\Delta t H(0)/\hbar} \mathrm{e}^{\mathrm{i}\Delta t H(t_1)/\hbar} \ldots \\ & \ldots \mathrm{e}^{\mathrm{i}\Delta t H(t_{n-2})/\hbar} \mathrm{e}^{\mathrm{i}\Delta t H(t_{n-1})/\hbar} = U_+(\tau)^\dagger \end{aligned} \tag{2.11.10}$$

which is indeed the Hermitian adjoint of the forward Floquet operator. Now, we can revert to a simpler notation, $U_+(\tau) = F$, and write the time-reversal property (2.11.8) for $t = \tau$ together with (2.11.10) as a time-reversal "covariance" of the Floquet operator

$$TFT^{-1} = F^\dagger = F^{-1}. \tag{2.11.11}$$

This is a very intuitive result indeed: The time-reversed Floquet operator TFT^{-1} is just the inverse of F.

An interesting general statement can be made about periodically kicked systems with Hamiltonians of the structure (2.10.10). If H_0 and V are both invariant under some time reversal T_0 (conventional or not), the Hamiltonian $H(t)$ is T_0-covariant in the sense of (2.11.5) provided the zero of time is chosen halfway between two successive kicks. The Floquet operator (2.10.11) is then not covariant in the sense (2.11.11) with respect to T_0, but it is with respect to

$$T = \mathrm{e}^{\mathrm{i}H_0\tau/\hbar} T_0. \tag{2.11.12}$$

The reader is invited, in Problem 2.13, to show that the Floquet operator defined so as to transport the wave vector by one period starting at a point halfway between two successive kicks is T_0-covariant.

The above statement implies that for the periodically kicked rotator defined by (2.10.13), F has an antiunitary symmetry of the type (2.11.12). Similarly, the Floquet operator of the kicked top (2.10.14) is covariant with respect to $T = \mathrm{e}^{\mathrm{i}H_0\tau/\hbar}$ where K is complex conjugation in the standard representation of angular momenta in which J_x and J_z are real and J_y is imaginary.

2.12 Canonical Transformations for Floquet Operators

The arguments presented in Sects. 2.4, 2.5, 2.7, and 2.8 for Hermitian Hamiltonians carry over immediately to unitary Floquet operators. We shall assume a finite number of dimensions throughout.

First, irreducible $N \times N$ Floquet matrices without any T covariance have $U(N)$ as their group of canonical transformations. Indeed, any transformation from that group preserves eigenvalues, unitarity, and normalization of vectors. The proof is analogous to that sketched in Sect. 2.4.

Next, when F is T covariant with $T^2 = 1$, one can find a T invariant basis in which F is symmetric. In analogy with the reasoning in (2.5.5), one takes matrix elements in $TF^\dagger T^{-1} = F$ with respect to T invariant basis states,

$$F_{\mu\nu} = \langle\psi_\mu \left|TF^\dagger T^{-1}\right| \psi_\nu\rangle = \langle T\psi_\mu \left|T^2 F^\dagger T\right| \psi_\nu\rangle^* \\ = \langle\psi_\mu \left|F^\dagger T\right| \psi_\nu\rangle^* = F_{\nu\mu}. \tag{2.12.1}$$

It is worth recalling that time-reversal invariant Hamiltonians were also found, in Sect. 2.5, to be symmetric if $T^2 = 1$. Of course, for unitary matrices $F = \tilde{F}$ does not imply reality. The canonical group is now $O(N)$, as was the case for $[H, T] = 0$, $T^2 = 1$. To see this, we assume that $F = \tilde{F}$ and that O is unitary, and require $OFO^\dagger$ to be symmetric,

$$OFO^\dagger = \tilde{O}^\dagger F \tilde{O}. \tag{2.12.2}$$

Multiplication from the left with $\tilde{O}$ and from the right with O gives

$$\tilde{O}OF = F\tilde{O}O. \tag{2.12.3}$$

Since F must be assumed irreducible, the product $O\tilde{O}$ must be unity, i.e., O must be an orthogonal matrix.

Finally, if F is T covariant with $T^2 = -1$, there is again Kramers' degeneracy. To prove this, let

$$F|\phi_\nu\rangle = \mathrm{e}^{-\mathrm{i}\phi_\nu}|\phi_\nu\rangle, \\ F^\dagger|\phi_\nu\rangle = \mathrm{e}^{\mathrm{i}\phi_\nu}|\phi_\nu\rangle \tag{2.12.4}$$

and let T act on the latter equation:

$$\mathrm{e}^{-\mathrm{i}\phi_\nu}T|\phi_\nu\rangle = TF^\dagger T^{-1}T|\phi_\nu\rangle = FT|\phi_\nu\rangle. \tag{2.12.5}$$

The orthogonality of $|\phi_\nu\rangle$ and $T|\phi_\nu\rangle$, following from $T^2 = -1$, has already been demonstrated in (2.6.3). The Hilbert space dimension must again be even.

Which group of transformations is canonical depends, as for time-independent Hamiltonians, on whether or not F has geometric invariances. Barring any such invariances for the moment, again we employ the basis (2.8.1), thus giving the time-reversal operator the structure

$$T = ZK. \tag{2.12.6}$$

The restriction imposed on F by T covariance can be found by considering the 2×2 block

$$
\begin{aligned}
F_{mn} &= \begin{pmatrix} \langle m|F|n\rangle & \langle m|F|Tn\rangle \\ \langle Tm|F|n\rangle & \langle Tm|F|Tn\rangle \end{pmatrix} \\
&= f_{mn}^{(0)}1 + \boldsymbol{f}_{mn}\cdot\boldsymbol{\tau}
\end{aligned}
\tag{2.12.7}
$$

which must equal the corresponding block of $TF^{\dagger}T^{-1}$. In analogy with (2.8.8),

$$
\begin{aligned}
f_{mn} &= \left(TF^{\dagger}T^{-1}\right)_{mn} = \left(ZKF^{\dagger}KZ^{-1}\right)_{mn} \\
&= -\left(Z\tilde{F}Z\right)_{mn} = -\tau_2\tilde{f}_{nm}\tau_2 \\
&= -\tau_2\left\{f_{nm}^{(0)}1 + \boldsymbol{f}_{nm}\cdot\tilde{\boldsymbol{\tau}}\right\}\tau_2 = f_{nm}^{(0)}1 - \boldsymbol{f}_{nm}\cdot\boldsymbol{\tau}.
\end{aligned}
\tag{2.12.8}
$$

Now, the restrictions in question can be read off as

$$
\begin{aligned}
f_{mn}^{(0)} &= f_{nm}^{(0)} \\
\boldsymbol{f}_{mn} &= -\boldsymbol{f}_{nm}.
\end{aligned}
\tag{2.12.9}
$$

They are identical in appearance to (2.8.11) but, in contrast to the amplitudes $h_{mn}^{(\mu)}$, the $f_{mn}^{(\mu)}$ are in general complex numbers.

The pertinent group of canonical transformation is the symplectic group defined by (2.8.12) since SFS^{-1} is T covariant if F is. Indeed, reasoning in parallel to (2.8.13),

$$
\begin{aligned}
TSFS^{-1}T^{-1} &= ZKSFS^{-1}KZ^{-1} = ZS^{*}KFK\tilde{S}Z^{-1} \\
&= SZKFKZ^{-1}S^{-1} = STFT^{-1}S^{-1} \\
&= SF^{\dagger}S^{-1} = \left(SFS^{-1}\right)^{\dagger}.
\end{aligned}
\tag{2.12.10}
$$

To complete the classification of Floquet operators by their groups of canonical transformations, it remains to allow for geometric symmetries in addition to Kramers' degeneracy. Since there is no difficulty in transcribing the considerations of Sect. 2.7, one can state without proof that the group in question is $U(N)$ when there is one parity R_x with $[T, R_x] = 0$, $R_x^2 = -1$, while additional geometric symmetries may reduce the group to $O(N)$, where the convention for N is the same as in Sect. 2.7.

We conclude this section with a few examples of Floquet operators from different universality classes, all for kicked tops. These operators are functions of the angular momentum components J_x, J_y, J_z and thus entail the conservation law $\boldsymbol{J}^2 = \hbar^2 j(j+1)$ with integer or half-integer j. The latter quantum number also defines the dimension of the matrix representation of F as $(2j+1)$.

The simplest top capable of classical chaos, already mentioned in (2.10.14), has the Floquet operator [11, 12]

$$
F = \mathrm{e}^{-\mathrm{i}\lambda J_z^2/(2j+1)\hbar^2}\mathrm{e}^{-\mathrm{i}pJ_x/\hbar}. \tag{2.12.11}
$$

Its dimensionless coupling constants p and λ may be said to describe a linear rotation and a nonlinear torsion. (For a more detailed discussion, see Sect. 7.6.) The quantum number j appears in the first unitary factor in (2.12.11) to give to the exponents of the two factors the same weight in the semiclassical limit $j \gg 1$. This simplest top belongs to the orthogonal universality class: Its F operator is covariant with respect to generalized time reversal

$$T = \mathrm{e}^{\mathrm{i}pJ_x/\hbar}\mathrm{e}^{\mathrm{i}\pi J_y/\hbar}T_0 \tag{2.12.12}$$

where T_0 is the conventional time reversal. By diagonalizing F, the level spacing distribution has been shown [11, 12] to obey the dictate of the latter symmetry, i.e., to display linear level repulsion (Chap. 3) under conditions of classical chaos.

An example of the unitary universality class is provided by

$$F = \mathrm{e}^{-\mathrm{i}\lambda' J_y^2/(2j+1)\hbar^2}\mathrm{e}^{-\mathrm{i}\lambda J_z^2/(2j+1)\hbar^2}\mathrm{e}^{-\mathrm{i}pJ_x/\hbar}. \tag{2.12.13}$$

Indeed, the quadratic level repulsion characteristic of this class (Chap. 3) is obvious from Fig. 1.2c that was obtained [13, 14] by diagonalizing F for $j = 500,\ p = 1.7$, $\lambda = 10,\ \lambda' = 0.5$.

Finally, the Floquet operator

$$\begin{aligned}
F &= \mathrm{e}^{-\mathrm{i}V}\mathrm{e}^{-\mathrm{i}H_0},\\
H_0 &= \lambda_0 J_z^2/j\hbar^2,\\
V &= \lambda_1 J_z^4/j^3\hbar^4 + \lambda_2\left(J_xJ_z + J_zJ_x\right)/\hbar^2 + \lambda_3\left(J_xJ_y + J_yJ_x\right)/\hbar^2
\end{aligned} \tag{2.12.14}$$

is designed so as to have no conserved quantity beyond $\boldsymbol{J}^2$ (i.e., in particular, no geometric symmetry) but a time-reversal covariance with respect to $T = \mathrm{e}^{-\mathrm{i}H_0}T_0$. Now, since $T^2 = +1$ and $T^2 = -1$ for j integer and half integer, respectively, the top in question may belong to either the orthogonal or the symplectic class. These alternatives are most strikingly displayed in Fig. 1.3b, d. Both graphs were obtained [13, 14] for $\lambda_0 = \lambda_1 = 2.5$, $\lambda_2 = 5$, $\lambda_3 = 7.5$, values which correspond to global classical chaos. The only parameter that differs in the two cases is the angular momentum quantum number: $j = 500$ (orthogonal class) for graph b and $j = 499.5$ (symplectic class) for d. The difference in the degree of level repulsion is obvious (Chap. 3). Such a strong reaction of the degree of level repulsion to a change as small as one part per thousand is really rather remarkable. No quantity with a well-defined classical limit could respond so dramatically.

2.13 Beyond Dyson's Threefold Way

We have been concerned with the orthogonal, unitary, and symplectic symmetry classes of Hamiltonians or Floquet operators. *Dyson* [15] deduced that classification from group theoretical arguments about complex Hermitian (or unitary) matrices. Much of the present book builds on Dyson's scheme.

During the nineties of the last century, work on the low-energy Dirac spectrum in chromodynamics [16] and on low-energy excitations in disordered superconductors has highlighted universal behavior not fitting Dyson's threefold way. In particular, *Zirnbauer* and his collegues [17–21] have argued that seven further symmetry classes exist and pointed to realizations in solid-state physics. The new classification corresponds to one given by *Cartan* for symmetric spaces.[2] However, the correspondence rests, in its present form, on the assumption of effective single-Fermion theories; there is thus room for further work on interactions as well as Bosonic particles.

More recently, the topic of nonstandard symmetry classes has reemerged in the relation of d dimensional topological insulators/superconductors to Anderson localization in $d-1$ dimensions [22, 23].

A short discussion of the new classes is in order. My aim is to introduce the reader to the essence of the new ideas without even trying to do justice to advanced solid-state topics or the underlying mathematics.

Most importantly, why does Dyson's scheme need extension? The following answer will be fully appreciated only with the help of elementary notions of level statistics to be developed in the following two chapters. A spectrum comprising many (possibly infinitely many) energy (or quasi-energy) levels can be characterized by a local density $\frac{\delta N}{\delta E}$ with δE just large enough to make for but small fluctuations of the ratio under shifts of the location on the energy axis by a few levels. Now if the spectrum affords a much larger range ΔE within which the local ratio undergoes small fluctuations about the mean but no systematic change, one can call the spectrum homogeneous over the range ΔE and work with $\frac{\Delta N}{\Delta E}$ as the mean density; the latter mean can still vary systematically on yet larger energy scales. For systems with homogeneous spectra the Dyson scheme is complete. On the other hand, a spectrum is non-homogeneous when near some distinguished point on the energy axis the local density $\frac{\delta N}{\delta E}$ displays systematic changes. For systems with non-homogeneous spectra additional symmetries yield symmetry classes beyond Dyson's scheme.

The seven new classes have energy spectra symmetric about a point on the energy axis which can be chosen as $E=0$. Near that spectral center, the local level densities display systematic variations. Such spectra are known e.g., for superconductivity and relativistic Fermions.

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[2] A symmetric space is a Riemannian manifold M with global invariance under a distance preserving geodesic inversion (sign change of all normal coordinates reckoned from any point on M). The curvature tensor is then constant. The scalar curvature can be positive, negative, or zero. The positive-curvature case deserves special interest since the pertinent compact symmetric spaces house the unitary quantum evolution operators. The set of evolution operators (or unitary matrices, in a suitable irreducible representation) can be shown to form a symmetric space, where the matrix inversion $U \mapsto U^{-1}$ yields geodesic inversion w.r.t. the identity as a distance preserving transformation (isometry), with $\mathrm{Tr}\,(U^{-1}dU)^2$ as the metric. For a discussion of the ten symmetry classes in terms of symmetric spaces see [20].

2.13.1 Normal-Superconducting Hybrid Structures

Four of the new universality classes are realizable in normal-superconducting hybrid structures, like a normal conductor of the form of a billiard with superconductors attached at the boundary. Chaos must be provided either by randomly placed scatterers or by the geometry of the sample.

A prominent effect distinguishing such hybrid structures from all-normal electronic billiards is Andreev scattering [24]: An electron leaving the normal conductor to enter a superconductor may there combine with another electron of (nearly) opposite velocity to form a Cooper pair. A hole with velocity (nearly) opposite to the lost electron must then enter the normal conductor and retrace the path of the lost electron, a small angular mismatch apart which is due to the small energy mismatch ϵ of a quasiparticle relative to the Fermi energy E_F. Roughly speaking, an electron of energy ϵ is scattered into a hole of energy $-\epsilon$. The hole picks up a scattering phase $\pi/2 - \phi$ where ϕ is the phase of the superconducting order parameter at the interface.

Due to Andreev scattering a non-vanishing Cooper-pair amplitude forms within the normal conductor, close to the interface with each superconductor, as the following rough argument indicates. When the hole "created" by Andreev scattering retraces the path of the original electron back to the interface with the same superconductor and becomes retroreflected as an electron again the coherent succession of two electrons appears like a Cooper pair. An observable consequence is a gap, called Andreev gap in the excitation spectrum.

The simplest description of the many-electron problem arises in the mean-field approximation which yields an effective single-particle theory. The pertinent second-quantized Bardeen-Cooper-Schrieffer (BCS) Hamiltonian involves annihilation operators c_α and creation operators $c_\alpha^\dagger$. The index α accounts for, say, N orbital single-particle states as well as two spin states such that $\alpha = 1, 2, \ldots 2N$. Electrons being Fermions these operators obey the anticommutation rules

$$c_\alpha c_\beta^\dagger + c_\beta^\dagger c_\alpha = \delta_{\alpha\beta} \,. \tag{2.13.1}$$

The Hamiltonian then reads

$$H = \sum_{\alpha\beta} \left(h_{\alpha\beta} c_\alpha^\dagger c_\beta + \frac{1}{2} \Delta_{\alpha\beta} c_\alpha^\dagger c_\beta^\dagger + \frac{1}{2} \Delta_{\alpha\beta}^* c_\beta c_\alpha \right) ; \tag{2.13.2}$$

herein the matrix h accounts for normal motion due to kinetic energy, single-particle potential, and possibly magnetic fields; the order-parameter matrix Δ brings in superconduction and coupling of electrons with holes. Hermiticity of H and Fermi statistics restrict the $2N \times 2N$-matrices h and Δ as

$$h_{\alpha\beta} = h_{\beta\alpha}^* \,, \qquad \Delta_{\alpha\beta} = -\Delta_{\beta\alpha} \,. \tag{2.13.3}$$

It is convenient to write the BCS Hamiltonian as row×matrix×column,

$$H = \frac{1}{2}(c^\dagger, c)\begin{pmatrix} h & \Delta \\ -\Delta^* & -\tilde{h} \end{pmatrix}\begin{pmatrix} c \\ c^\dagger \end{pmatrix} + \text{const}\,, \tag{2.13.4}$$

with const $= \frac{1}{2}\mathrm{Tr}\,h$, so as to associate the BCS-Hamitonian H with a Hermitian $4N \times 4N$ matrix

$$\mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -\tilde{h} \end{pmatrix} \tag{2.13.5}$$

known as the Bogolyubov-deGennes (BdG) Hamiltonian. The "physical space" spanned by the orbital and spin states is thus enlarged by a two-dimensional "particle-hole space."[3] The restrictions (2.13.3) take the form[4]

$$\mathcal{H} = -\Sigma_x \mathcal{H}^* \Sigma_x\,, \qquad \Sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{2.13.6}$$

It is immediately clear, then, that if ψ is an eigenvector of $\mathcal{H}$ and ω the associated eigenvalue, $\Sigma_x\psi^*$ is an eigenvector with eigenvalue $-\omega$. The announced symmetry of the spectrum about $E = 0$ is thus manifest.

One might view the restriction (2.13.6) as a "particle-hole symmetry" (PHS) since it reflects the easily checked invariance of the BCS Hamiltonian (2.13.2) under the interchange $c \leftrightarrow c^\dagger$ of creation and annihilation operators, combined with complex conjugation; note $\Sigma_x \binom{c}{c^\dagger} = \binom{c^\dagger}{c}$. Moreover, that PHS could be associated with an antiunitary operator of charge conjugation,

$$\mathcal{C} = \Sigma_x K\,, \quad \mathcal{C}^2 = 1\,, \qquad \mathcal{C}\mathcal{H}\mathcal{C}^{-1} = -\mathcal{H} \quad \Longleftrightarrow \quad \mathcal{C}\mathcal{H} + \mathcal{H}\mathcal{C} = 0\,. \tag{2.13.7}$$

I would like to warn the reader, however, that the foregoing restriction of the BdG Hamiltonian is not a symmetry in the usual sense since $\mathcal{H}$ and $\mathcal{C}$ do not commute but *anticommute*.

Imaginary Hermitian matrices (which must be odd under transposition) also have spectra symmetric about zero. In fact, every BdG Hamiltonian becomes imaginary when conjugated with the unitary $4N \times 4N$ matrix

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ \mathrm{i} & -\mathrm{i} \end{pmatrix} \tag{2.13.8}$$

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[3] No extra states are introduced here even though the BdG jargon does invite such misunderstanding; the $2N$ single-electron states acted upon by the matrix h may have their energies above or below the Fermi energy; BdG jargon terms them "particle states" and even indulges in speaking about "hole states" acted upon by the matrix $-\tilde{h}$; the BdG hole states are in fact identical copies of the BdG particle states.

[4] A cleaner notation would be $\Sigma_x = \sigma_x \otimes \mathbf{1}_2 \otimes \mathbf{1}_N$ with σ_x the familiar Pauli matrix operating in particle-hole space, the second factor refering to spin space, and the third factor refering to orbital space.

as is readily verified by doing the matrix multiplications in

$$\mathcal{H}_U = U\mathcal{H}U^{-1} = -\mathcal{H}_U^* = -\tilde{\mathcal{H}}_U. \tag{2.13.9}$$

The isospectral representative $\mathcal{H}_U$ of $\mathcal{H}$ is diagonalized by an $SO(4N)$ matrix g, $g\mathcal{H}_U g^{-1} = \mathrm{diag}(\omega_1, \omega_2, \ldots, \omega_{2N}, -\omega_1, -\omega_2, \ldots, -\omega_{2N})$. The BdH Hamiltonian itself is then diagonalized by gU.

Symmetry class D. In the absence of any symmetries beyond the particle-hole symmetry, BdG Hamiltonians form the new symmetry class D. The group $SO(4N)$ is the pertinent group of canonical transformations since conjugation of the imaginary representative $\mathcal{H}_U$ of $\mathcal{H}$ with any $SO(4N)$ matrix yields a new version of the Hamiltonian with imaginary matrix elements and the same spectrum. The set of Hamiltonians spanning the new symmetry class is most naturally characterized by looking at the real anti-Hermitian matrices[5] $X_U = \mathrm{i}\mathcal{H}_U = X_U^*$ which form the Lie algebra $so(4N)$; their exponentials are orthogonal matrices forming the Lie group $SO(4N)$.

AntiHermitian representatives $X = \mathrm{i}\mathcal{H}$ of Hamiltonians will remain with us throughout the discussion of the new symmetry classes. A further word on them is thus in order in the simplest context of class D where no symmetries reign, beyond the particle-hole symmetry as expressed in (2.13.6) and (2.13.7) for $\mathcal{H}$ or

$$-X^\dagger = X = -\Sigma_x \tilde{X} \Sigma_x \,. \tag{2.13.10}$$

The algebra formed by the $X = \mathrm{i}\mathcal{H}$ is isomorphic to that formed by the $X_U = \mathrm{i}\mathcal{H}_U = X_U^*$, $so(4N)$. The name "D" for the present class is chosen in respect to Cartan.

Symmetry class DIII. I proceed to BdG Hamiltonians enjoying time reversal invariance, $[T, \mathcal{H}] = 0$. Since an effective single-electron theory is at issue the time reversal operator (2.3.9) must be employed,

$$T = \mathrm{i}\sigma_y K \,, \tag{2.13.11}$$

where the 2×2 matrix σ_y operates in spin space; mustering more cleanliness of notation I write $T = \mathbf{1}_2 \otimes \mathrm{i}\sigma_y \otimes \mathbf{1}_N K \equiv \tau\, K$. The time reversal invariance of the Hamiltonian can be noted as

$$\mathcal{H} = \tau\mathcal{H}^*\tau^{-1}, \quad \tau = \begin{pmatrix} \mathrm{i}\sigma_y & 0 \\ 0 & \mathrm{i}\sigma_y \end{pmatrix}. \tag{2.13.12}$$

Kramers' degeneracy arises as a further property of the spectrum since $T^2 = -1$.

To characterize the class of Hamiltonians so restricted it is again convenient to argue with the antiHermitian matrices $X = \mathrm{i}\mathcal{H} = -X^\dagger$, simply because these form

[5] Note that the imaginary Hermitian matrices do not form a closed algebra under commutation since the commutator of any two such is antiHermitian.

a closed algebra under commutation; for class D, that algebra was just revealed as (isomorphic to) $so(4N)$. The restriction (2.13.6) of $\mathcal{H}$ due to Hermiticity and Fermi statistics and the property (2.13.12) due to time reversal invariance translate into the following restrictions of the representative $X = -X^\dagger$ of $\mathcal{H}$,

$$-X^\dagger = X = -\Sigma_x \tilde{X} \Sigma_x \quad \text{and} \\ X = \tau \tilde{X} \tau^{-1} . \tag{2.13.13}$$

In search is the set $\mathcal{P}$ of solutions of the latter conditions within $so(4N)$. That set does not close under commutation. Indeed, for two members of $\mathcal{P}$ we have[6] $[X_1, X_2] = \tau[\tilde{X}_1, \tilde{X}_2]\tau^{-1} = -\tau[X_1, X_2]^T\tau^{-1}$, with the minus sign signalling disobedience of the commutator to (2.13.13). We can, however, easily identify an auxiliary set $\mathcal{K}$, complementary to $\mathcal{P}$ in $so(4N)$, such that $\mathcal{K}$ does from a subalgebra of $so(4N)$. I define the members Y of $\mathcal{K}$ by replacing the condition (2.13.13) with the complementary one, $Y = -\tau\tilde{Y}\tau^{-1}$. Indeed, the set $\mathcal{K}$ does close under commutation and therefore forms a subalgebra of $so(4N)$. The complementarity in play is owed to the fact that the condition (2.13.13) involves an involution, $X \mapsto I(X)$ with $I(I(X)) = X$. The $so(4N)$ matrices can be chosen such that each of them is either even or odd under I; the even ones are the X's forming $\mathcal{P}$ while the odd ones are the Y's forming $\mathcal{K}$. We may write $so(4N) = \mathcal{P} + \mathcal{K}$ and hold fast to $\mathcal{K}$ being a subalgebra of $so(4N)$.

The equations for $\mathcal{K}$ can be rewritten as

$$-Y^\dagger = Y = -\Sigma_x \tilde{Y} \Sigma_x = +(\Sigma_x\tau)Y(\Sigma_x\tau)^{-1} . \tag{2.13.14}$$

The conjugation $U^{-1}YU \equiv Y_U$ with the unitary matrix

$$U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & \mathrm{i}\sigma_y \\ \sigma_y & -\mathrm{i} \end{pmatrix} \tag{2.13.15}$$

(in cleaner notation, $U = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathbf{1}_2 & \mathrm{i}\sigma_y \\ \sigma_y & -\mathrm{i}\mathbf{1}_2 \end{pmatrix} \otimes \mathbf{1}_N$) turns the equations for $\mathcal{K}$ into

$$-Y_U^\dagger = Y_U = -\Sigma_x \widetilde{Y_U} \Sigma_x = +\Sigma_z Y_U \Sigma_z^{-1} \tag{2.13.16}$$

where $\Sigma_z = \sigma_z \otimes \mathbf{1}_2 \otimes \mathbf{1}_N$ with the Pauli matrix σ_z acting in particle-hole space. The set of solutions is now easy to ascertain. Since Y_U is required to commute with Σ_z it must be diagonal in particle-hole space, $Y_U = \begin{pmatrix} Z_{pp} & 0 \\ 0 & Z_{hh} \end{pmatrix}$. The condition $Y_U = -\Sigma_x \widetilde{Y_U} \Sigma_x$ relates the two $2N \times 2N$ blocks as $Z_{hh} = -\widetilde{Z_{pp}}$, and the antiHermiticity of Y_U carries over to both blocks. Scratching off indices I write $Y_U = \mathrm{diag}(Z, -\tilde{Z})$ and can recognize $\mathcal{K}$ as isomorphic to the Lie algebra of antiHermitian $2N \times 2N$

[6] Matrix transposition is mostly denoted by a tilde but typographical reasons occasionally suggest to employ a right superscript "T".

matrices, $\mathcal{K} \simeq u(2N)$. The space $\mathcal{P}$ of (the antiHermitian representatives $X = \mathrm{i}\mathcal{H}$ of) time reversal invariant BdG Hamiltonians is obtained from $so(4N)$ by removing a $u(2N)$ algebra. Being the complement of $u(2N)$ in $so(4N)$, the space $\mathcal{P}$ can be seen as the tangent space of the quotient $SO(4N)/U(2N)$ of the corresponding Lie groups. The latter quotient is the symmetric space termed DIII by Cartan; hence the name DIII for the symmetry class of time reversal invariant BdG Hamiltonians.

Symmetry class C. Next come BdG Hamiltonians without time reversal symmetry but with isotropy in spin space. The generators of spin rotations J_k $(k = x, y, z)$ then commute with the Hamiltonian. To write out the familiar second-quantization form of these generators I must split the double index into an orbital and a spin part, $\alpha = qs$ with $q = 1, 2, \ldots, N$ and $s =\uparrow, \downarrow$; the spin label $\uparrow$ indicates the eigenvalue $+\frac{\hbar}{2}$ for the z component of the spin angular momentum. The angular momenta take the form $J_k = \frac{\hbar}{2} \sum_{qss'} c_{qs}^{\dagger} \sigma_{kss'} c_{qs}$ where σ_k, $k = x, y, z$ are the Pauli matrices. In line with the "row×matrix×column" notation (2.13.5) for the BdG Hamiltonian I represent the angular momenta by the $4N \times 4N$ matrices

$$J_k = \frac{\hbar}{4} \begin{pmatrix} \sigma_k & 0 \\ 0 & -\tilde{\sigma_k} \end{pmatrix} \otimes \mathbf{1}_N \,. \tag{2.13.17}$$

The spin isotropy for the antiHermitian representative $X = \mathrm{i}\mathcal{H}$ of the BdG Hamiltonian, $[X, J_k] = 0$, is easily seen to restrict the four $2N \times 2N$ blocks of X in particle-hole space as

$$\begin{aligned} X_{pp} &= \mathrm{i}h = \mathbf{1}_2 \otimes a \,, & X_{ph} &= \mathrm{i}\Delta = \mathrm{i}\sigma_y \otimes b \,, \\ X_{hp} &= -\mathrm{i}\Delta^* = -\mathrm{i}\sigma_y \otimes c \,, & X_{hh} &= -\mathrm{i}\tilde{h} = -\mathbf{1}_2 \otimes \tilde{a} \,. \end{aligned} \tag{2.13.18}$$

In terms of $N \times N$ (orbital) blocks the generator X reads

$$X = \begin{pmatrix} a & 0 & 0 & b \\ 0 & a & -b & 0 \\ 0 & -c & -\tilde{a} & 0 \\ c & 0 & 0 & -\tilde{a} \end{pmatrix} \tag{2.13.19}$$

and decomposes into two commuting subblocks. One (the outer one) corresponds to spin-up particles and spin-down holes, the other (the inner one) to spin-down particles and spin-up holes. Because the two subblocks are uniquely related by $b \to -b$, $c \to -c$ it suffices to focus on one of them, say

$$X_{\uparrow} = \begin{pmatrix} a & b \\ c & -\tilde{a} \end{pmatrix} . \tag{2.13.20}$$

It remains to reveal the restrictions (of AntiHermiticity and Fermi statistics) (2.13.10) for the new subblock $X_{\uparrow}$. Since $X_{ph} = -\widetilde{X_{ph}}$ the equation $X_{pp} = \mathrm{i}\sigma_y \otimes b$ entails $b = \tilde{b}$. Similar reasoning yields $c = \tilde{c}$. AntiHermiticity requires $a = -a^{\dagger}$ and $c = -b^{\dagger}$. All these conditions are summarized by

$$-X_\uparrow^\dagger = X_\uparrow = -\Sigma_y \tilde{X}_\uparrow \Sigma_y\,, \qquad \Sigma_y = \sigma_y \otimes \mathbf{1}_N\,. \tag{2.13.21}$$

This is the defining equation of the Lie algebra $sp(2N)$ of which the $X_\uparrow$'s under scrutiny thus turn out to be elements. The reader is kindly invited to crosscheck with the definition (2.8.12) of the symplectic group whose elements are the exponentials of the elements of the symplectic algebra. Of course, the canonical transformations for the present symmetry class are matrices from $Sp(2N)$ and diagonalization of $X_\uparrow$ can be achieved by such a matrix. In line with Cartan's notation for symmetric spaces the present symmetry class is called C.

I had played with characterizing the conditions of Hermiticity and Fermi statistics for BdG Hamiltonians as the behavior $\mathcal{HC}+\mathcal{CH}=0$ under charge conjugation, see (2.13.7). Indulging a bit further, I refine the definition of charge conjugation for the subblock $\mathcal{H}_\uparrow = -\mathrm{i}X_\uparrow$. The above condition (2.13.10) demands $\mathcal{H}_\uparrow\mathcal{C}_\uparrow + \mathcal{C}_\uparrow\mathcal{H}_\uparrow = 0$ with $\mathcal{C}_\uparrow = \Sigma_y K$ and $\mathcal{C}_\uparrow^2 = -1$. A corresponding definition can be made for the spin-down subblock, such that the overall charge conjugation $\mathcal{C} = \mathcal{C}_\uparrow \otimes \mathcal{C}_\downarrow$ squares to minus one for class C.

Symmetry class CI. The final class of BdG Hamiltonians is distinguished by invariance under both spin rotation and time reversal. Subjecting the representation (2.13.19) of the generator X in terms of orbital blocks to the further restriction (2.13.13) due to time reversal invariance we easily find that X becomes a symmetric matrix, $X = \tilde{X}$. That symmetry carries over to the two commuting subblocks, $X_\uparrow = \tilde{X}_\uparrow$. The universality class under consideration is thus formed by the set $\mathcal{P}$ of symmetric matrices in $sp(2N)$. Calling $\mathcal{K}$ the subalgebra of antisymmetric matrices in $sp(2N)$ we have $\mathcal{P} = sp(2N) - \mathcal{K}$. I propose to show that $\mathcal{K}$ is isomorphic to the Lie algebra $u(N)$. To that end I note that the solutions $Y \in \mathcal{K}$ of $-Y^\dagger = Y = -\Sigma_y \tilde{Y} \Sigma_y = -\tilde{Y}$ have the form $\mathbf{1_2} \otimes \mathrm{Re}A + \mathrm{i}\sigma_y \otimes \mathrm{Im}A \equiv Y(A)$ where A is an arbitrary antiHermitian $N \times N$ matrix, i.e., $A \in u(N)$. The function $Y(A)$, which maps a $u(N)$ matrix A to an antisymmetric matrix Y in $sp(2N)$, preserves the operation defining Lie algebras, commutation. Indeed, with two $u(N)$ matrices A_1 and A_2 we have $Y([A_1, A_2]) = [Y(A_1), Y(A_2)]$ and the latter commutator is again an antisymmetric $sp(2N)$ matrix The isomorphism $\mathcal{K} \simeq u(N)$ is thus established.

The complement $\mathcal{P}$ of $u(N)$ in $sp(2N)$ can be regarded as the tangent space of the coset space $Sp(2N)/U(N)$ which is a symmetric space of type CI à la Cartan, hence the name for the universality class of BdG Hamiltonians enjoying invariance under time reversal and spin rotation.

No change relative to the class C arises for the antiunitary charge conjugation operator $\mathcal{C}$; in particular, we still have $\mathcal{C}^2 = -1$.

2.13.2 Systems with Chiral Symmetry

The remaining three of the seven new symmetry classes have Hamiltonians (or, for relativistic electrons, Dirac operators) affording the block representation

$$H = \begin{pmatrix} 0 & Z \\ Z^\dagger & 0 \end{pmatrix}, \tag{2.13.22}$$

due to a “symmetry” of the form

$$H = -PHP^{-1}\,, \qquad PP^{\dagger} = 1\,, \qquad P^2 = 1\,. \tag{2.13.23}$$

No conserverved quantity comes with that “symmetry” since P anticommutes with H. The latter anticommutativity entails an energy spectrum symmetric about zero, as the particle-hole symmetry does for BdG Hamiltonians. In contrast to the antiunitary charge conjugation operator (2.13.7) associated with the particle-hole symmetry, the operator P now involved is unitary.

In complete analogy with the standard symmetry classes, the ensemble of chiral Hamiltonians without any further restrictions is called the *chiral unitary* class (in Cartan notation, AIII). By imposing time reversal invariance for half-integer spin, one gets the *chiral symplectic* class (CII, in Cartan notation). Finally, the presence of both time reversal invariance and full spin rotation invariance enforces $H = \tilde{H}$ and defines the *chiral orthogonal* class (BDI, in Cartan notation).

A solid-state realization of the chiral unitary class AIII is a disordered tight-binding model on a bipartite lattice with broken time reversal invariance, such as the random flux problem [25]. Moreover, the class AIII arises from BdG Hamiltonians with invariance under time reversal and spin rotation about the z axis in spin space [23]. For further solid-state applications of the chiral classes see [24]. Applications in chromodynamics have been discussed by *Verbaarschot* [16].

2.14 Problems

2.1 Consider a particle with the Hamiltonian $H = (\boldsymbol{p} - (e/c)\boldsymbol{A})^2/2m + V(|\boldsymbol{x}|)$ where the vector potential $\boldsymbol{A}$ represents a magnetic field $\boldsymbol{B}$ constant in space and time. Show that the motion is invariant under a nonconventional time reversal which is the product of conventional time reversal with a rotation by π about an axis perpendicular to $\boldsymbol{B}$. Give the general condition for $V(\boldsymbol{x})$ necessary for the given nonconventional T to commute with H.

2.2 Generalize the statement in Problem 2.1 to N particles with isotropic pair interactions.

2.3 Show that $K\boldsymbol{x}K^{-1} = \boldsymbol{x}$, $K\boldsymbol{p}K^{-1} = -\boldsymbol{p}$, and $K\boldsymbol{L}K^{-1} = -\boldsymbol{L}$, where $\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p}$ is the orbital angular momentum and K the complex conjugation defined with respect to the position representation.

2.4 (a) Show that antiunitary implies antilinearity. (b) Show that antilinearity and $|\langle K\psi|K\phi\rangle|^2 = |\langle\psi|\phi\rangle|^2$ together imply the antiunitarity of K.

2.5 Show that $U_{\mu\nu} = U_{\nu\mu} = \int dx \langle\mu|x\rangle\,\langle\nu|x\rangle$, $U^{\dagger} = U^{-1}$, for $K = U\tilde{K}$ where K and $\tilde{K}$ are the complex conjugation operations in the continuous basis $|x\rangle$ and the discrete basis $|\mu\rangle$, respectively.

2.6 Show that for spin-1 particles, time reversal can be simply complex conjugation.

2.7 Show that the unitary matrix U in $T = UK$ is symmetric or antisymmetric when T squares to unity or minus unity, respectively.

2.8 Show that $\langle\phi|\psi\rangle = \langle T\phi|T\psi\rangle^*$ for $T = UK$ with $U^\dagger = U^{-1}$.

2.9 Use the associative law $TT^2 = T^2T$ for the antilinear operator of time reversal to show that the unimodular number α in $T^2 = \alpha$ must equal ± 1.

2.10 Show that time-reversal invariance with $T^2 = -1$ together with full isotropy implies that the canonical transformations are given by the orthogonal transformations.

2.11 Find the group of canonical transformations for a Hamiltonian obeying $[T, H] = 0$, $T^2 = -1$ and having cylindrical symmetry.

2.12 Show that the symplectic matrices S defined by $SZ\tilde{S} = Z$ form a group.

2.13 Let H_0 and V commute with an antiunitary operator T. Show that $TFT^{-1} = F^\dagger$ with $F = \mathrm{e}^{-H_0\tau/2\hbar}\mathrm{e}^{-\mathrm{i}kV/\hbar}\mathrm{e}^{-\mathrm{i}H_0\tau/2\hbar}$.

2.14 What would be the analogue of $H(t) = TH(-t)T^{-1}$ if the Floquet operator were to commute with some T_0?

2.15 Show that the eigenvectors of unitary operators are mutually orthogonal.

2.16 Show that $U(N)$ is canonical for Floquet operators without any T covariance.

2.17 Show that $U(N) \otimes U(N)$ is canonical for Floquet operators with $TFT^{-1} = F^\dagger$, $T^2 = -1$, $[R_x, F] = 0$, $[T, R_x] = 0$, $R_x^2 = -1$.

2.18 Show that $O(N) \otimes O(N)$ is canonical if, in addition to the symmetries in Problem 2.16, there is another parity R_y commuting with F and T but anticommuting with R_x.

2.19 Give the group of canonical transformations for Floquet operators in situations of full isotropy.

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