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Time dependence in quantum mechanics – Floquet theory and the Berry phase.

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Abstract

We give a short review of some aspects of the dynamics of time-dependent quantum systems. In particular we discuss how to recast time-periodic quantum problems into an equivalent time-independent form, contrasting the results with those gained for a similar reformulation in the case of general time-dependence. This approach, usually known under the name of Floquet theory, can be used to clarify the structure of, for example, invariants of the given quantum system. We also apply it to the calculation of the Berry phase and show how it enables us to understand Berry phases for time-independent systems. This involves rewriting earlier work of the author in a coordinate-free fashion.

1 Introduction

When we allow the Hamiltonian of a quantum system to become time-dependent many complications arise. On the formal level, in the time-independent case the evolution is simply given in terms of an exponential; $U(t,s) = \exp\{-iH(t-s)\}$, where U is the operator of evolution from time s to time t. This result is known as Stone's theorem [Conway 1985, p269]. The direct analogy for time-dependent systems is the Dyson expansion [Scharf 1989, p9], where the exponential must be time ordered since in general $[H(t), H(t')] \neq 0$.

The addition of time-dependent terms to the Hamiltonian also causes deep qualitative changes to the nature of the evolution. A simple consequence of Stone's theorem is that an eigenstate of the Hamiltonian will stay in that eigenstate. Here the evolution merely multiplies the state by the time-dependent phase $e^{-iE(t-s)}$, where E is the energy of the state. It is for this reason that energy eigenstates are often called stationary states.

Now in the time-dependent case an initial eigenstate of $H(s)$ will in general leave the corresponding eigenspace of $H(t)$. However even when the evolution does preserve the eigenvectors, the so-called adiabatic case, it has undergone a profound qualitative change. One finds that the phase is no longer just given by the (instantaneous) energy, but contains a term which arises due to the "twisting" of the evolving state. This extra term is called the Berry phase [Berry 1984] and is a feature of all time-periodic Hamiltonians, not just adiabatic ones.

The aim of this work is to show that by recasting the time-dependent problem into an equivalent time-independent form we can gain some useful insights into the Berry phase. Thus, in a sense, tackling the first difficulty of time-dependent problems helps us with the second as well.

The price that must be paid to allow us to apply Stone's theorem directly to time-dependent systems is an enlargement of the system's Hilbert space. In this space the Hamiltonian is replaced by the Floquet Hamiltonian. Generically this operator will have a purely continuous spectrum [Flesia and Piron 1984], but this need not be the case for the important class of systems with time-periodic Hamiltonians. Here the analysis is called Floquet theory [Chu 1989]. We will see that the eigenvectors of the Floquet Hamiltonian, if they exist, provide us with the so-called cyclic initial states used in the discussion of Berry phases. Further one obtains a useful characterisation of the Berry phases themselves as expectation values of a certain self-adjoint operator.

The rest of this work is organised as follows. In section 2 the new Hilbert space $\mathcal{K}$

and Floquet Hamiltonian $\underline{K}$ are defined for the periodic case. On the other hand, the corresponding construction is sketched for the general case in section 3. In section 4 the cyclic initial states of the system are shown to be related to the eigenvectors of $\underline{K}$ and the corresponding Berry phases are calculated. Finally in section 5 some applications, such as the structure of invariants, are discussed.

2 The New Hilbert Space

Essentially we want to expand the Hilbert space $\mathcal{H}$ to include the initial time t. The most natural way to do this in the T-periodic case is to consider T-periodic maps from $\mathbf{R}$ into $\mathcal{H}$. The canonical inner product in this space is the integral of the corresponding inner product in $\mathcal{H}$ itself. Thus we need a set $\mathcal{S}$ of T-periodic maps such that for all $\xi, \xi' \in \mathcal{S}$ the integral $\int_0^T \langle \xi(t), \xi'(t) \rangle_{\mathcal{H}} \, \mathrm{d}t$ exists and is finite. One can show that the largest such set is comprised of those maps ξ for which the function $\|\xi(\cdot)\|^2_{\mathcal{H}}$ is integrable on the interval $[0, T]$ and the function $\langle \psi, \xi(\cdot) \rangle_{\mathcal{H}}$ is measurable for all $\psi \in \mathcal{H}$. Here "measurable" means Borel measurable and "integrable" means Lebesgue integrable. This measure is taken as its properties, such as being complete and translationally invariant, will become important in the following.

As in the case of $\mathrm{L}^2(\mathbf{R}, \mathrm{d}x)$, to get a Hilbert space we have to take equivalence classes; $\xi \sim \xi'$ if they differ only on a set of measure zero. This leads to the definition of the Hilbert space $\mathcal{K}$ as being the set of equivalence classes $[\xi]$ with the inner product $\langle\langle [\xi], [\xi'] \rangle\rangle = \frac{1}{T} \int_0^T \langle \xi(t), \xi'(t) \rangle_{\mathcal{H}} \, \mathrm{d}t$. The normalisation factor $\frac{1}{T}$ is introduced for convenience. On following the standard arguments for $\mathrm{L}^2(\mathbf{R}, \mathrm{d}x)$, one finds that $\mathcal{K}$ is separable with orthonormal basis $\{[\xi_{\alpha n}]\}$. Here $\xi_{\alpha n}(t) = \mathrm{e}^{in\omega t} \psi_\alpha$ for some orthonormal basis $\{\psi_\alpha\}$ of $\mathcal{H}$ and $\omega = 2\pi/T$. Note that the measurability of $\langle \psi, \xi_{\alpha n}(\cdot) \rangle_{\mathcal{H}}$ comes from the continuity of the exponential and the fact that our σ-algebra contains the open sets. Essentially this space is just the tensor product of $\mathcal{H}$ with $\mathrm{L}^2([0, T], \mathrm{d}t)$ and periodic boundary conditions. The Hilbert space $\mathcal{K}$ was introduced by Sambe [1973] in this context after initial work by Shirley [1965] in the matrix formulation.

We will have occasion to use several operators on $\mathcal{K}$. First of all define $\underline{T}(s)$ by setting $\underline{T}(s)[\xi] = [t(s)\xi]$ with $(t(s)\xi)(t) = \xi(t - s)$. Here the necessary integrability properties are simple consequences of the translation invariance of the measure. We call this operator the translation operator and note that it has eigenvectors $[\xi_{\alpha n}]$ with eigenvalues $e^{-in\omega s}$. As $\underline{T}(s)$ is a strongly continuous one-parameter unitary group it has a self-adjoint generator $\underline{D}$. This is just the differentiation operator, usually written $\underline{D} = -i\partial_t$.

Similarly we define an operator $\underline{W}(s)$ starting from the evolution $U(t,s)$ by setting $\underline{W}(s)[\xi] = [w(s)\xi]$, where $(w(s)\xi)(t) = U(t, t-s)\xi(t-s)$. The periodicity of the map $w(s)\xi$ follows from the fact that for periodic Hamiltonians $U(t+T, s+T) = U(t,s)$ which is a consequence of $\phi(t)$ and $\phi'(t) = \phi(t+T)$ satisfying the same Schrödinger equation. A quick calculation shows that $\underline{W}(s)$ is a strongly continuous one-parameter unitary group. We write $\underline{K}$ for its generator, called the Floquet Hamiltonian.

If we now write $\underline{H}$ for the lifting of the periodic Hamiltonian $H(t)$ to $\mathcal{K}$ we find the following result which is a consequence of Trotter's theorem [Flesia and Piron 1984];

Theorem 2.1 *If there is a dense linear manifold in $\mathcal{K}$ on which $\underline{K}$,$\underline{D}$ and $\underline{K} - \underline{D}$ are all essentially self-adjoint then the self-adjoint extension of $\underline{K} - \underline{D}$ is just $\underline{H}$. In this case the Floquet Hamiltonian $\underline{K}$ is the self-adjoint extension of $\underline{H} + \underline{D}$.*

This result is often expressed in the form $K(t) = H(t) - i\partial_t$, however we prefer the form above as it emphasises that the initial time t has now been absorbed into the structure of the new Hilbert space so that the operators $\underline{K}$, $\underline{D}$ and $\underline{H}$ are all "time-independent" in $\mathcal{K}$.

3 The General Case

If we want to treat the case of a general time-dependent Hamiltonian in this manner we must extend the interval $[0,T]$ to the whole real line. That is we must consider $\mathcal{S}$ as the set of those maps from $\mathbb{R}$ into $\mathcal{H}$ such that $\|\xi(\cdot)\|^2_{\mathcal{H}}$ is integrable over $\mathbb{R}$. Note that the measurability condition on $\langle\psi, \xi(\cdot)\rangle_{\mathcal{H}}$ remains the same. After taking equivalence classes we end up with the direct sum $\mathcal{K} = \oplus_t \mathcal{H}_t$. The major qualitative difference that this makes is that those maps with constant norm can no longer belong to $\mathcal{S}$.

In this case it can be shown that the Floquet Hamiltonian $\underline{K}$ has a purely continuous spectrum. There are many simple ways of showing this. For example if $[\xi]$ is an eigenvector of $\underline{K}$ with eigenvalue ϵ then $[\xi']$ with $\xi'(t) = e^{i\lambda t}\xi(t)$ is an eigenvector of $\underline{K}$ with eigenvalue

$\epsilon+\lambda$. As this holds for any $\lambda \in \mathsf{R}$, if $\underline{K}$ has any eigenvector at all then it has an uncountable number of them corresponding to different eigenvectors. As $\mathcal{K}$ is separable this cannot be the case. Note that the corresponding trick does not work in the periodic case as there we require ξ' to be T-periodic. This means that $\lambda = n\omega$, giving a countable set of linearly independent eigenvectors.

It is instructive to make some comment on two other methods of proving this result. The first of these relies on showing that the eigenvectors of $\underline{K}$ would have to have norm essentially constant in time, which is impossible as noted above. The second strategy is to show that $\underline{K}$ is unitarily equivalent to the operator $\underline{D}$, which has a purely continuous spectrum in the general case.

Let $[\xi]$ be an eigenvector of $\underline{K}$ with eigenvector ϵ so that $[\xi]$ is also an eigenvector of $\underline{W}(s)$ with eigenvalue $\mathrm{e}^{-i\epsilon s}$. Thus for any representative $\xi \in [\xi]$ we have that $\mathrm{e}^{-i\epsilon s}\xi \sim w(s)\xi$. This implies that for fixed s and almost all t the map ξ satisfies $\mathrm{e}^{-i\epsilon s}\xi(t) = w(s)\xi(t) = U(t,t-s)\xi(t-s)$. Hence for almost all t and fixed s we have that $\|\xi(t)\|^2_{\mathcal{H}} = \|\xi(t-s)\|^2_{\mathcal{H}}$. If this result held for an s-independent set of $t \in \mathsf{R}$ of full measure then the result would be proved, as the norm of $[\xi]$ in $\mathcal{K}$ could not be non-zero and finite.

As this is not necessarily the case we take the following indirect route. Take any fixed t^*. Then $\int_{t^*}^{t^*+s} \|\xi(t)\|^2_{\mathcal{H}}\, \mathrm{d}t = \int_{t^*}^{t^*+s} \|\xi(t-s)\|^2_{\mathcal{H}}\, \mathrm{d}t = \int_{t^*-s}^{t^*} \|\xi(t)\|^2_{\mathcal{H}}\, \mathrm{d}t$. Hence by induction we see that the integral of the instantaneous norm of $\xi(t)$ is constant on each interval $[ns,(n+1)s]$. Thus the integral over all time cannot be non-zero and finite. In this manner we see that the difference in behaviour in the general and periodic cases is due to the fact that states of essentially constant norm cannot belong to $\mathcal{S}$.

Now imagine that $\|U(t,t-s)\xi(t-s)\|_{\mathcal{H}}$ is measurable in the two variables s and t and there is a dense linear manifold on which $\underline{K}$, $\underline{D}$ and $\underline{H}$ are essentially self-adjoint. Then a quick calculation shows that $\underline{R}(t_0)\underline{K}\,\underline{R}(t_0)^* = \underline{D}$, where $\underline{R}(t_0)[\xi] = [\xi']$ for $\xi'(t) = U(t,t_0)^*\xi(t)$. To demonstrate this result it is simplest to show that $\underline{R}(t_0)\underline{W}(s)\underline{R}(t_0)^* = \underline{T}(s)$, the translation operator defined in section 2. The result then follows as $\underline{K}$ is the generator of $\underline{W}(s)$ and $\underline{D}$ is the generator of $\underline{T}(s)$. Hence as $\underline{D}$ has a purely continuous spectrum so does $\underline{K}$.

Physically the operator $\underline{R}(t_0)$ transforms the system into the Heisenberg picture at time t_0. This fact can be used to show that the general method discussed here is simply a direct application of Lax-Phillips scattering theory to quantum mechanics, with the scattering operator being given by $\underline{S}(\rho_-, \rho_+) = \underline{R}(\rho_+)\underline{R}(\rho_-)^*$ for $0 < \rho_+$ and $\rho_- < 0$ [Flesia and Piron 1984].

Now let us try to apply this result to the periodic case. First in this case the operator $\underline{D}$ has a pure point spectrum with eigenvalues $n\omega$. Hence if the result were true it would mean that the Floquet Hamiltonian was always diagonalisable. However we also find that the theorem fails as $\underline{R}(t_0)$ is not in general an operator on $\mathcal{K}$, its induced action on $\mathcal{S}$ not preserving periodicity. In fact for $\xi'(t) = U(t,t_0)^*\xi(t)$ we have $\xi'(t+T) = U(t+T,t_0)^*\xi(t)$ where we have used the fact that $\xi(t+T) = \xi(t)$. However $U(t+T,t_0) = U(t+T,t)U(t,t_0)$ so that for a periodic $\underline{R}$ we would need $U(t+T,t) = 1$ for all t which is not necessarily the case. Note that this last condition can easily be shown to be equivalent to $U(T,0) = 1$.

Finally the difference between the formalism in the general and periodic case has an exact analogue in the quantum mechanics of a particle on a line. Let us consider the differentiation operator on various subsets of R [Akhiezer and Glazman 1981]. First, on the whole axis the domain of the differentiation operator is simply all those elements $\phi(x)$ of $\mathrm{L}^2(\mathsf{R}, \mathrm{d}x)$ which are absolutely continuous and such that $\phi'(x) \in \mathrm{L}^2(\mathsf{R}, \mathrm{d}x)$. The condition of absolute continuity is needed so that we may integrate by parts. This leads to the differentiation operator being self-adjoint. One finds that this operator, the analogue of $\underline{D}$ in the general case, has a purely continuous spectrum.

We now look at the operator in a finite interval $[a,b]$. Here we need more than the conditions stated above. This is because integrating by parts leaves a surface term. This was zero in the case above as the functions vanished at infinity. However for the finite interval the condition of vanishing surface term, necessary for the differentiation operator to be symmetric, provides an independent constraint on the domain. One finds that we must require $\phi(b) = \mathrm{e}^{\mathrm{i}\theta}\phi(a)$ for some fixed θ. This parameter θ then labels a continuous set of possible self-adjoint differentiation operators, all of which having pure point spectrum.

Effectively what we do in Floquet theory is pick the case $\theta = 0$ corresponding to periodic vectors, however in theory we could have made any other choice. Our reason for choosing $\theta = 0$ is that any other choice would lead to a more complicated expression for the Berry phase without giving any compensatory advantages. One can also discuss the differentiation operator on the semi-finite interval $[0, \infty)$, taking $\phi(0) = 0$ so that the operator is symmetric. However in this case we find that the differentiation operator is not self-adjoint, and further has no self-adjoint extensions. This is because the deficiency indices of the operator are different. Hence any attempt to create a formalism akin to the two above will be hampered by severe technical problems.

4 Cyclic Initial States

From the analysis in the last section we can expect to find a range of spectral properties for the Floquet Hamiltonian depending on the particular periodic Hamiltonian chosen. Our next task is to give some physical meaning to these states, if indeed they exist. This leads us to the definition of cyclic initial states.

Consider the evolution $U(t,s)$ generated by a T-periodic Hamiltonain $H(t)$ in the Hilbert space $\mathcal{H}$. Now two vectors ψ and ψ' that differ by only a multiplicative phase, $\psi' = e^{i\theta}\psi$, have the same expectation values for all linear operators and so they represent the same state. Hence the real state space of the system is the projective Hilbert space $\mathcal{P} = \mathcal{H}/\sim$, where $\psi \sim \psi'$ if there exists $\alpha \in \mathrm{C}$ such that $\psi' = \alpha\psi$. The reason one habitually works with $\mathcal{H}$ is that the linear structure on $\mathcal{H}$ greatly simplifies any calculation, however we must bear in mind that there is then an overall phase arbitrariness in ψ and so only relative phases are physically meaningful.

Bearing these considerations in mind we are lead to call an initial state $\phi(0)$ cyclic if $\phi(T) = e^{i\chi}\phi(0)$ for some χ, that is if the initial and final rays in the Hilbert space are the same. We will call the number χ (mod 2π) the overall phase of the system, although some care must be taken in ascribing physical reality to this phase, nominally the relative phase difference of the initial and final states. This is because it is most natural to describe the time as a continuous superselection rule which therefore indexes the Hilbert space. Hence to compare $\phi(0) \in \mathcal{H}_0$ with $\phi(t) \in \mathcal{H}_t$ we must identify the two Hilbert spaces which leads to some conventionality. This is just the choice of picture – either Schrödinger, Heisenberg or some form of interaction.

The justification for choosing the Schrödinger picture, which corresponds to simply identifying $\mathcal{H}_0$ and $\mathcal{H}_t$ is the following. In other pictures the periodicity of the system is partially contained in the time-dependence of the operators involved, and so the resulting analysis is more complicated. Hence our choice is a matter of convenience rather than logical necessity. Of course the clearest experiments designed to measure such phases avoid the problem by starting with a linear superposition of two cyclic initial states and looking at the internal interference of the two components at a later time. This internal interference is manifest in, for example, the rotation of the plane of polarised light as it propagates through a helically wound optical fibre [Chiao and Wu 1986].

The link between the eigenvectors $[\xi]$ of $\underline{K}$ in the Hilbert space $\mathcal{K}$ and the cyclic initial states $\phi(0)$ of the Hamiltoinian $H(t)$ in the Hilbert space $\mathcal{H}$ is contained in the following two results.

Theorem 4.1 *Each cyclic initial state $\phi(0)$ with overall phase $\chi = -\epsilon T$ generates an eigenvector $[\xi]$ of $\underline{K}$ with eigenvalue ϵ.*

Proof: Let $\phi(0)$ be a cyclic initial state with overall phase $\chi = -\epsilon T$ so that $U(T,0)\phi(0) = \mathrm{e}^{-\mathrm{i}\epsilon T}\phi(0)$. Define $\xi(t) = \mathrm{e}^{\mathrm{i}\epsilon t}U(t,0)\phi(0)$. One can easily show that $\xi \in \mathcal{S}$ using the unitarity of U and the fact that $U(t+T,T) = U(t,0)$. Then $(w(s)\xi)(t) = U(t,t-s)\xi(t-s) = \mathrm{e}^{-\mathrm{i}\epsilon s}\xi(t)$ so that $[\xi]$ is an eigenvector of $\underline{W}(s)$ with eigenvector $\mathrm{e}^{-\mathrm{i}\epsilon s}$ and so an eigenvector of $\underline{K}$ with eigenvalue ϵ. ∎

Note that each $\phi(0)$ generates a countable set of eigenvectors $[\xi_n]$ whose eigenvalues differ by an integral multiple of ω.

Theorem 4.2 *Each eigenvector $[\xi]$ of $\underline{K}$ with eigenvalue ϵ generates a cyclic initial state $\phi(0)$ with overall phase $\chi = -\epsilon T$.*

Proof: Let $[\xi]$ be an eigenvector of $\underline{K}$ with eigenvalue ϵ so that $[\xi]$ is also an eigenvector of $\underline{W}(s)$ with eigenvalue $\mathrm{e}^{-\mathrm{i}\epsilon s}$. Then if $\xi \in [\xi]$ and putting $s = T$ we have that $w(T)\xi \sim \mathrm{e}^{-\mathrm{i}\epsilon T}\xi$. Hence there is at least one time t^* for which $U(t^*, t^* - T)\xi(t^* - T) = (w(T)\xi)(t^*) = \mathrm{e}^{-\mathrm{i}\epsilon T}\xi(t^*)$. Let $\phi(0) = U(0,t^*)\xi(t^*)$. Then using the fact that ξ is periodic and $U(T,t^*) = U(0,t^* - T)$ we have $U(T,0)\phi(0) = \mathrm{e}^{-\mathrm{i}\epsilon T}\phi(0)$, so that $\phi(0)$ is a cyclic initial state with overall phase $\chi = -\epsilon T$. ∎

If one asks about the nature of the overall phase one is lead to the discovery that χ is the sum of two qualitatively different parts. This discovery was made by Berry [1984] in the case of adiabatic evolution, although it was implicit in earlier work [Berry 1990]. The generalisation to non-adiabatic evolution soon followed [Aharonov and Anandan 1987]. The first part of the overall phase is given by $\delta = -\int_0^T \langle \phi(t), H(t)\phi(t)\rangle_{\mathcal{H}}\, dt$ and is called the dynamical phase, while the rest is called the Berry phase. Note that if we add a time-dependent ground state energy to the Hamiltonian, the only change suffered by the evolving state is a time-dependent rephasing. Thus the path followed by the system in the projective Hilbert space remains the same. Now it can easily be shown that this rephasing contributes only to the dynamical phase. This means that the Berry phase only depends on the path followed by the system in the projective Hilbert space, a fact that has lead to it being called the geometrical phase by many authors

Since its discovery the Berry phase has been the subject of much study (see for example the reviews by Mead [1992], Moore [1991] and Zwanziger, Koenig and Pines [1990]), most of which addressing one of the two following questions. Firstly much effort has been spent on elucidating the geometrical nature of Berry phases. As it only depends on the path in projective Hilbert space, it is natural to ask whether the Berry phase can be expressed as the holonomy of a connection in the canonical fibre bundle $\pi : \mathcal{H} \rightarrow \mathcal{P}$. Indeed this is so, with the desired connection being the natural one induced by the inner product on $\mathcal{H}$; that is a path $\psi(t)$ is parallel transported if $\langle \psi, \dot{\psi} \rangle = 0$ [Simon 1983]. Extensions of this idea have been made in various directions, for example to the case of a multi-dimensional cyclic initial space [Giler *et. al.* 1989] and the evolution of density operators [Uhlmann 1989]. An explicit form for the Berry phase in terms of a coordinatisation of the projective Hilbert space has also been given [Page 1987].

The other major area of interest has been the use of the Berry phase to unify various phenomena in physics. For example Hamiltonian anomalies [Nelson and Alvarez-Gaumé 1985], the Rabi oscillation in quantum optics [Moore 1990b, Tewari 1989] and electron diffraction from a screw dislocation [Bird and Preston 1988] have all been interpreted as arising due to the existence of non-zero Berry phases.

We now show how the Berry phases can be expresssed in terms of the Floquet formalism. This can be thought of as a "coordinate free" recasting of the results of Moore [1990a]. Let $[\xi]$ be an eigenvector of the Floquet Hamiltonian corresponding to the cyclic initial state $\phi(0)$. Then the overall phase is given by $\chi = -\epsilon T = -T\langle\langle[\xi], \underline{K}[\xi]\rangle\rangle$ and the dynamical phase is given by $\delta = -\int_0^T \langle\phi(t), H(t)\phi(t)\rangle_{\mathcal{H}}\, \mathrm{d}t$. Now the corresponding eigenvector $[\xi]$ contains the represntative $\xi(t) = \mathrm{e}^{i\epsilon t}\phi(t)$ so that $\delta = -\int_0^T \langle\xi(t), H(t)\xi(t)\rangle_{\mathcal{H}}\, \mathrm{d}t = -T\langle\langle[\xi], \underline{H}[\xi]\rangle\rangle$. This means that $\gamma = \chi - \delta = -T\langle\langle[\xi], (\underline{K} - \underline{H})[\xi]\rangle\rangle$ and so we have proved the following result ,

Theorem 4.3 *Let $\phi(0)$ be a cyclic initial state and $[\xi]$ a corresponding eigenvector of the Floquet Hamiltonian. Then the corresponding Berry phase is given by $\gamma = -T\langle\langle[\xi], \underline{D}[\xi]\rangle\rangle$.*

This approach can also be extended to the systems with an underlying non-adiabatic periodicity subjected to an adiabatic perturbation, as here the Floquet Hamiltonian behaves in many respects as a normal adiabatic Hamiltonian. We find that the Berry phase is naturally split into an overall adiabatic phase and a sum of non-adiabatic Berry phases, one for each of the many non-adiabatic periods that form part of one adiabatic period [Moore and Stedman 1990, Breuer *et. al.* 1990].

5 Applications

We now give a brief survey of several applications of the above theory. First we discuss the use of Floquet theory to give a geometric characterisation of the set of quasi-periodic initial states, that is those initial states which are linear combinations of cyclic inital states. Next the case of the existence of non-zero Berry phases for time-independent Hamiltonians is considered and finally we comment on the structure of invariants in the Hilbert space $\mathcal{K}$.

A deep geometric characterisation of the point and continuous spectral subspaces of the Floquet Hamiltonian is provided by a generalisation of the RAGE theorem to the time-periodic case [Enss and Veselić 1983, Yajima and Kitada 1983, Bunimovich *et. al.* 1991]. Let the system of interest have Hilbert space $\mathrm{L}^2(\mathrm{R}^n, \mathrm{d}x^n)$ and $\mathcal{M}$ be a subset of R^n. We define the operator $F(\mathcal{M})$ to be the operator of multiplication by the characteristic function of $\mathcal{M}$. Then an initial state $\phi(0)$ is called bound if $\lim_{R\to\infty} \sup_{t>0} \|F(|x| >$

$R)U(t,0)\phi(0)\|_{\mathcal{H}} = 0$. In contrast, the state $\phi(0)$ is called propagating if for all R, $\lim_{T\to\infty} \frac{1}{T}\int_0^T \|F(|x| < R)U(t,0)\phi(0)\|_{\mathcal{H}}\, dt = 0$.

We then find that, as long as a certain subsidiary condition is met, the subspace of bound states is precisely that space spanned by the cyclic initial states. Hence if all states are bound then the system has a complete set of cyclic initial states. Intuitively this means that the only non-quasiperiodic states, that is initial states that are not linear combinations of cyclic initial states, are those that in a sense go to infinity as time passes.

As an example of the type of subsidiary technical condition needed, we note that it is sufficient for the Hamiltonian to have the form $H(t) = -\frac{1}{2}\nabla^2 + V_1(t) + V_2(t)$. Here V_1 and V_2 are symmetric, V_1 is continuously differentiable and bounded, and V_2 is the multiplication operator by an $\mathrm{L}^p(\mathrm{R}^n) \cap \mathrm{L}^q(\mathrm{R}^n)$ function with $1 \le p < \frac{n}{2} < q \le \infty$ [Yajima and Kitada 1983]. Note that this condition is not met, for example, for a particle trapped inside a box and subjected to an external periodic force.

This approach has been used to show that Hamiltonians of the form $H(t) = \alpha(t)p^2 + \beta(t)(p\cdot q + q\cdot p) + \gamma(t)q^2 + \delta(t)p + \epsilon(t)q + \eta(t)$ either have a complete set of cyclic initial states or none at all [Hagedorn *et. al.* 1986]. The result is even more striking for the special case $H(t) = \omega a^* a + \overline{f}(t)a + f(t)a^* + \beta(t)$, where f and β have period $2\pi/\omega$. Here either all states are cyclic or none are [Moore 1990b]. This can best be seen by noting that the forced harmonic oscillator Hamiltonian preserves coherence and that no two coherent states are orthogonal or collinear.

There has been much interest in the literature in the characterisation of such states, particularly in relation to the notion of quantum chaos. For example Seba [1990] has discussed the quasi-energy spectrum for a particle moving between two rigid walls, one of which periodically oscillates in time and Casati and Guarneri [1984] have discussed the motion of a quantum rotator under an external periodic perturbation. Note also that Howland [1989] has shown how to use Floquet theory probabilistically to look at the perturbative stability of the spectral properties of the Floquet Hamiltonian.

We next consider the Berry phases for time-independent Hamiltonians. To guarantee the existence of an evolution operator it is usual to require that the family $H(t)$ has a common domain. Choosing some basis $\{\psi_\alpha\}$ of $\mathcal{H}$ in this dense linear manifold leads to the construction of a basis $[\xi_{\alpha n}]$ of $\mathcal{K}$ contained in the domain of the lifting $\underline{H}$. Using this basis one can show that $H(t)$ is time-independent if and only if $[\underline{H},\underline{D}]=0$. In fact one can go further and show that $H(t)$ is time-independent if and only if the seemingly weaker condition that $[\underline{H},[\underline{H},\underline{D}]]=[\underline{D},[\underline{H},\underline{D}]]=0$ holds. To do this it suffices to show by explicit calculation that if we write $\underline{H}[\xi_{\alpha n}]=\sum_{\alpha' n'} a_{\alpha' n'}[\xi_{\alpha' n'}]$ and require either of the above two conditions then $a_{\alpha' n'}=0$ if $n\neq n'$. Hence the two cases where the exponential $\exp\{-i(\underline{H}+\underline{D})\}$ can easily be evaluated both require time-independent Hamiltonians.

The fact that we then have $[\underline{D},\underline{K}]=0$ allows us to specify completely when non-zero Berry phases for such systems can occur. Let $\mathcal{M}$ be the eigenspace of $\underline{K}$ corresponding to the eigenvalue ϵ. Then $\mathcal{M}$ has a basis $\{[\xi_\lambda]\}$, each member of which is an eigenvector of $\underline{D}$ with eigenvalue $n_\lambda\omega$. But then $\gamma_\lambda=-T\langle\langle[\xi_\lambda],\underline{D}[\xi_\lambda]\rangle\rangle=0 \pmod{2\pi}$. Hence non-zero Berry phases can occur only for those elements of $\mathcal{M}$ which have non-zero components for basis elements with different n_λ. Such a situation is called quasi-degeneracy [Moore 1990b].

Finally we discuss the structure of invariants in the context of the Hilbert space $\mathcal{K}$. Let $I(t)$ be a family of self-adjoint operators with domain $\mathcal{D}(t)$ such that $U(t,0)$ maps $\mathcal{D}(0)$ onto $\mathcal{D}(t)$. Then $I(t)$ is called an invariant if $U(t,0)I(0)=I(t)U(t,0)$. Such invariants can be used, for example, to construct a rigorous proof of the adiabatic theorem [Avron *et. al.* 1987]. It is easily shown that invariants are exactly those families of operators satisfying the differential equation $i\dot{I}(t)=[H(t),I(t)]$.

The reason such operators are called invariants is that if any one of the $I(t)$ has an eigenvector then we can construct a corresponding eigenvector with the same eigenvalue for all other times. For example, if $I(0)\psi=\alpha\psi$ then $I(t)\psi'=\alpha\psi'$ where $\psi'=U(t,0)\psi$. Now imagine that there exists a periodic invariant $I(t)$ for which $I(0)$ has an n-dimensional eigenspace. One can then shown that this space reduces the monodromy operator $U(T,0)$, so that there are at least n linearly independent cyclic initial states.

If the invariant I is periodic we can consider it as being an operator $\underline{I}$ on $\mathcal{K}$, which can then be seen to commute with $\underline{K}$. On the other hand, consider a decomposable operator on $\mathcal{K}$, that is an operator $\underline{X}$ which can also be considered a periodic operator on $\mathcal{H}$. For example $\underline{H}$ is decomposable while $\underline{D}$ is not. This latter fact is due to the derivative depending on the values of $\xi(t)$ in a *neighbourhood* of the time of interest. If our chosen decomposable operator commutes with the Floquet Hamiltonian, then one can easily show that it gives an invariant when considered as a family of operators on $\mathcal{H}$. Hence the structure of periodic invariants is completely contained in their commutation properties with the Floquet Hamiltonian.

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