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LETTER TO THE EDITOR

Floquet theory and the non-adiabatic Berry phase

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Abstract. An efficient calculational algorithm is provided for the operator decomposition approach to non-adiabatic Berry phases for systems with periodic Hamiltonians.

There has been much interest recently in the phase acquired by a system's wavefunction upon cyclic evolution in projective Hilbert space. We will call this phase the Berry phase although some authors prefer the term Aharonov–Anandan phase (Bouchiat and Gibbons 1988). Theoretical studies of the Berry phase have looked at the formulation of the problem in general (Berry 1984, Simon 1983, Aharonov and Anandan 1987, Jordan 1988) and the relationship of the Berry phase to other fields of physics such as field theoretic anomalies (Jackiw 1988) and Jahn–Teller problems (Chancey and O'Brien 1988, Ham 1987). Experimental studies have verified the existence of the Berry phase for photons travelling down helically wound optical fibres (Tomita and Chiao 1986) and investigated its implications in such fields as ESR spectroscopy (Gamliel and Freed 1989).

In the past there have been two distinct ways of looking at the Berry phase. Berry used the adiabatic theorem to guarantee the cyclic evolution of an initial eigenstate of a Hamiltonian varying slowly with time, while Aharonov and Anandan considered a general cyclic evolution essentially without reference to the Hamiltonian that generated it. In a recent paper (Moore and Stedman 1990b) it was shown that the adiabatic assumption in Berry's work can be removed by a suitable choice of cyclic initial states, thereby putting the two approaches on an even footing. Further an operator decomposition formalism was developed to calculate the cyclic initial states and their Berry phases. However as it stands this calculation takes more labour than a direct calculation from the evolution operator so that the formulation provided no computational advantage. The purpose of this letter is to show that the early work of Shirley on Floquet theory (Shirley 1965) provides a way of obtaining results from Moore and Stedman's formalism with less work than is required for a direct calculation, thereby making the operator decomposition scheme of some practical importance.

First we need some results concerning fundamental matrices. Proofs can be found in Cronin (1980). Let H be a time-dependent matrix. A non-singular matrix A is a called a fundamental matrix of the system of ordinary differential equations $\mathrm{i}\dot{\phi} = H\phi$ if $\mathrm{i}\dot{A} = HA$. The following lemmas are of pivotal importance.

Lemma 1. Let A and A' be fundamental matrices of $\mathrm{i}\dot{\phi} = H\phi$. Then there exists a constant non-singular matrix X such that $A' = AX$.

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Lemma 2. Let A be a fundamental matrix of $\mathrm{i}\dot{\phi} = H\phi$, where H is $\tilde{t}$-periodic. Then A' with $A'(t) = A(t+\tilde{t})$ is also a fundamental matrix of $\mathrm{i}\dot{\phi} = H\phi$.

We can use these two lemmas to give Floquet's theorem.

Theorem 1. Let A be a unitary fundamental matrix of $\mathrm{i}\dot{\phi} = H\phi$, where H is Hermitian and $\tilde{t}$-periodic. Then there exists a unitary $\tilde{t}$-periodic B and a constant Hermitian C such that $A = B\,\mathrm{e}^{\mathrm{i}Ct}$.

In this case we can obviously take H to be the Hamiltonian of some quantum mechanical system whose evolution is governed by the time-dependent Schrödinger equation

$$\mathrm{i}\dot{\phi} = H\phi \tag{1}$$

where we have taken $\hbar = 1$ for simplicity. There are two unitary fundamental matrices of particular importance. The first is the unique fundamental matrix U satisfying $U(0) = I$, this is called the evolution matrix. We write its decomposition as $U = Z\mathrm{e}^{\mathrm{i}Mt}$. The second is the fundamental matrix $F = P\,\mathrm{e}^{\mathrm{i}Qt}$, discussed by Shirley, that has Q real and diagonal in some convenient basis $\{|\alpha\rangle\}$, say an eigenbasis of $H(0)$. Moore and Stedman used Z and M to calculate the Berry phase for the evolution (1) while Shirley used H to calculate P and Q. Now as U and F are both fundamental matrices of (1) there exists a constant invertible matrix X with $U = FX$ by lemma 1. Using the fact that $U(0) = I$ it is easy to see that $X = F^{\dagger}(0)$ so that $U(t) = F(t)F^{\dagger}(0)$. In the following we use this relationship to combine Shirley's approach with that of Moore and Stedman to derive an efficient way of calculating Berry phases from the Hamiltonian H. We note that Layton *et al* (1990) also use Floquet theory to study Berry phases; however they only use it to calculate the evolution matrix.

First we summarise the two formalisms. Moore and Stedman showed that the cyclic initial states $\{|\phi_\alpha(0)\rangle\}$ for the evolution in question are precisely the eigenvectors of M and that their Berry phases are given by

$$\gamma_\alpha = \mathrm{i}\int_0^{\tilde{t}} \langle\phi_\alpha(0)|Z^{\dagger}\dot{Z}|\phi_\alpha(0)\rangle\,\mathrm{d}t. \tag{2}$$

Thus we need to calculate Z and M. In fact it is sufficient to calculate Z as we can then find M from the relationship

$$M = -H(0) + \mathrm{i}\dot{Z}(0). \tag{3}$$

On the other hand, Shirley calculated the terms in the Fourier expansion

$$P = \sum_{n=-\infty}^{\infty} P^{(n)}\,\mathrm{e}^{\mathrm{i}n\omega t} \tag{4}$$

of P, where $\omega = 2\pi/\tilde{t}$, from the Fourier expansion

$$H = \sum_{n=-\infty}^{\infty} H^{(n)}\,\mathrm{e}^{\mathrm{i}n\omega t} \tag{5}$$

of H, $H^{(n)}$ being readily calculable using $H^{(n)} = (1/\tilde{t})\int_0^{\tilde{t}} H\,\mathrm{e}^{-\mathrm{i}n\omega t}\,\mathrm{d}t$. For convenience we introduce the product Hilbert space $\mathscr{H}\oplus\mathscr{T}$ where the spatial part $\mathscr{H}$ is spanned by the kets $|\alpha\rangle$ and the temporal part $\mathscr{T}$ is spanned by the kets $|n\rangle$ with $\langle t|n\rangle = \mathrm{e}^{\mathrm{i}n\omega t}$ (Sambe 1973). A basis ket in $\mathscr{H}\oplus\mathscr{T}$ is written $|\alpha n\rangle$. Let H_{F} be the Floquet Hamiltonian acting on $\mathscr{H}\oplus\mathscr{T}$ defined by the matrix elements

$$\langle\alpha n|H_{\mathrm{F}}|\beta m\rangle = H_{\alpha\beta}^{(n-m)} + n\omega\delta_{\alpha\beta}\delta_{nm} \tag{6}$$

where the $H_{\alpha\beta}^{(n)}$ are the matrix elements of $H^{(n)}$ in the basis $\{|\alpha\rangle\}$. Further let H_F have eigenvectors $|\varepsilon_{\alpha n}\rangle$ and eigenvalues $\varepsilon_{\alpha n}$. Shirley showed that the matrix elements of Q and the Fourier coefficients of P are given by

$$Q_{\alpha\beta} = -\varepsilon_{\alpha 0}\delta_{\alpha\beta} \tag{7}$$

$$P_{\alpha\beta}^{(n)} = \langle \alpha n | \varepsilon_{\beta 0}\rangle. \tag{8}$$

For a review of several modern applications of this theory see Chu (1989).

We now show how to combine these two formalisms. Using the fact that $U(t) = F(t)F^{\dagger}(0)$ and $F = P\,\mathrm{e}^{\mathrm{i}Qt}$ we find that $U(t) = P(t)P^{\dagger}(0)\exp\{\mathrm{i}P(0)QP^{\dagger}(0)\}$ and so, as $P(t)p^{\dagger}(0)$ is $\tilde{t}$-periodic and $P(0)QP^{\dagger}(0)$ is constant, we can make the identifications

$$Z(t) = P(t)P^{\dagger}(0) \tag{9}$$

$$M = P(0)QP^{\dagger}(0). \tag{10}$$

Now the eigenvectors of M are given by

$$|\phi_\alpha(0)\rangle = P(0)|\alpha\rangle \tag{11}$$

and combining this with equation (2) we find that

$$\gamma_\alpha = \left\langle \alpha \middle| \int_0^{\tilde{t}} \mathrm{i}P^{\dagger}\dot{P}\,\mathrm{d}t \middle| \alpha \right\rangle. \tag{12}$$

We can evaluate the integral using the orthogonality relations

$$\int_0^{\tilde{t}} \mathrm{e}^{\mathrm{i}(n-m)\omega t}\,\mathrm{d}t = \tilde{t}\delta_{nm} \tag{13}$$

as follows. From the fourier expansion (4) of P we have that

$$\mathrm{i}P^{\dagger}\dot{P} = \sum_{n,m=-\infty}^{\infty} (-n\omega)P^{\dagger(m)}P^{(n)}\,\mathrm{e}^{\mathrm{i}(n-m)\omega t} \tag{14}$$

so that

$$\gamma_\alpha = \left\langle \alpha \middle| \sum_{n=-\infty}^{\infty} -2\pi n P^{\dagger(n)}P^{(n)} \middle| \alpha \right\rangle. \tag{15}$$

Thus we can calculate the cyclic initial states and their Berry phases directly from the Fourier expansion of the Hamiltonian and less work than is required for calculating them from the evolution matrix.

Here we discuss an elementary example using the above formalism. Consider the two-dimensional $2\pi/\omega$-periodic Jahn–Teller Hamiltonian

$$H = \begin{pmatrix} B_a & B_b\,\mathrm{e}^{-\mathrm{i}\omega t} \\ B_b\,\mathrm{e}^{\mathrm{i}\omega t} & -B_a \end{pmatrix} \tag{16}$$

discussed in Moore and Stedman (1990a), where we have taken their parameter E to be zero for convenience. Upon writing the Floquet basis $\{|\alpha n\rangle\}$ with $\alpha \in \{+,-\}$ in the order $(\ldots, |+,1\rangle, |-,1\rangle, |+,0\rangle, |-,0\rangle, \ldots)$ we can show that the infinite-dimensional Floquet Hamiltonian is block diagonal with typical block

$$H_n = \begin{pmatrix} -B_a + (n+1)\omega & B_b \\ B_b & B_a + n\omega \end{pmatrix} \tag{17}$$

in the basis $\{|-,(n+1)\rangle, |+,n\rangle\}$. H_n has eigenvalues

$$\varepsilon_{\pm,n}=(n+\tfrac{1}{2})\omega\mp\theta \tag{18}$$

where $\theta^2=B_a^2+B_b^2+\frac{1}{4}\omega^2-\omega B_a$, and corresponding eigenvectors

$$|\varepsilon_{\pm,n}\rangle=x_\pm|-,n+1\rangle+y_\pm|+,n\rangle \tag{19}$$

where $B_b y_\pm=(-\frac{1}{2}\omega+B_a\mp\theta)x_\pm$, $x_\pm^2+y_\pm^2=1$ and we have chosen $x_\pm$ and $y_\pm$ to be real. Using equations (7) and (8) we then find that

$$Q=\begin{pmatrix}-\frac{1}{2}\omega+\theta & 0\\ 0 & -\frac{1}{2}\omega-\theta\end{pmatrix} \tag{20}$$

$$P=\begin{pmatrix}y_+ & y_-\\ x_+\,\mathrm{e}^{\mathrm{i}\omega t} & x_-\,\mathrm{e}^{\mathrm{i}\omega t}\end{pmatrix} \tag{21}$$

and substituting into equations (11) and (12) we find that the cyclic initial states are given by $\phi_\pm(0)=(y_\pm,x_\pm)^T$ and that they have Berry phases $\gamma_\pm=2\pi x_\pm^2$, in agreement with Moore and Stedman. Thus we can use our formalism to calculate Berry phases for simple systems with great ease.

In the preceding discussion we have shown how to use the work of Shirley to make the formalism in Moore and Stedman (1990b) into an efficient computational algorithm for calculating the cyclic initial states and their Berry phases for any $\tilde{t}$-periodic matrix Hamiltonian. We have also given an example of relevance to Jahn–Teller physics where the formalism can be used to derive explicit formulae for the Berry phases of a simple two-dimensional matrix Hamiltonian.

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