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Berry's phase in quantum optics

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It is pointed out that quantum optics provides examples where the origin of geometrical phase factors can be investigated in two different ways. The first possibility relies on a line bundle in which the fibers over each base point in parameter space consist of Stark states, whereas fibers of Floquet states yield a second possibility. Both constructions are compared in some detail, and the Floquet bundle is found to offer distinct advantages.

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Immediately after Berry [1] had pointed out the appearance of a "geometrical phase factor" in the wave function of a quantum system with adiabatically varying parameters, Simon [2] explained this phenomenon as the holonomy in a certain Hermitian line bundle. Since then, Berry's phase has become an intensely studied object which has led to considerable physical insight into a number of different topics [3].

An interesting class of related problems arises in quantum optics: When an atom or a molecule interacts with a laser field that can be described classically, one deals with a periodically-time-dependent quantum system. If, in addition, some parameters such as the laser field strength or the polarization vary on a time scale that is long compared to the period T of the individual laser oscillations, one has a quantum system with a "fast," periodic and an additional "slow," nonperiodic time dependence. Such a situation emerges quite naturally, e.g., if an atom is exposed to a laser pulse with an amplitude that has a smooth shape.

It has been shown in Refs. 4–6 that a consistent use of Floquet states yields a general and particularly simple method to investigate the origin of geometrical phases in such cases, as well as computationally efficient formulas. Recently, the approach developed there has also been employed by Moore and Stedman [7] to calculate Berry phases for "two-level atoms."

As is well known, Berry's phase arises as the integrated curvature of the adiabatic connection in a line bundle which is constructed from the eigenvector space of the family of instantaneous Hamiltonians [2]. Whereas, in general, this bundle is unique, this is no longer the case in quantum optics: As we will discuss in this Brief Report, the twofold time dependence mentioned above leads to two different possibilities. Hence, labeling quantum phases as "dynamical" or "nonadiabatic geometrical" becomes ambiguous without a proper specification of the underlying bundle and a use of the "wrong" frame of reference might lead to unnecessary complications. We will also demonstrate that the previously constructed Floquet bundle [4] has the merit of great conceptual simplicity and clarify some of the details in the work of Moore and Stedman [7].

To be definite, let us consider the Hamiltonian

$$H^{\mathbf{R}}(t)=H_0+\lambda\mathbf{e}\cdot\mathbf{x}\sin\omega t\ , \tag{1}$$

with $T=2\pi/\omega$, where H_0 describes the unperturbed atom or molecule, ω is the frequency of an external laser field, λ denotes the amplitude of the electrical field, and $\mathbf{e}$ is a polarization vector. We arrange all these parameters, as well as possible additional parameters contained in H_0, but with the exception of the frequency ω, in a formal vector $\mathbf{R}$ and indicate the dependence of the Hamiltonian on the latter by a superscript. As long as none of these parameters is varied, the Hamiltonian (1) is merely periodically time dependent.

Now there are two rather different types [8] of "instantaneous eigenstates": On the one hand, one can simply consider the eigenstates $\varphi_n^{\mathbf{R}}(\mathbf{x})$ of the time-independent Hamiltonian

$$\tilde{H}\equiv H_0+\tilde{\lambda}\mathbf{e}\cdot\mathbf{x}\ , \tag{2}$$

which we shall refer to as "Stark states" in analogy to the case where H_0 describes the hydrogen atom; on the other hand, there are Floquet states, i.e., the time-periodic eigenstates $u_n^{\mathbf{R}}(\mathbf{x},t)$ of the operator

$$\mathcal{H}\equiv H^{\mathbf{R}}(t)-i\partial_t\ . \tag{3}$$

Correspondingly, for a given curve $\mathcal{C}$ connecting points $\mathbf{R}_1$ and $\mathbf{R}_2$ in the space of physical parameters, we have to distinguish two different cases (for simplicity, we do no

longer indicate the spatial variable $\mathbf{x}$ explicitly).

(i) If we fix the phase of an initial Stark state $\varphi_0^{\mathbf{R}_1}$, the adiabatic theorem [9] yields a way of transporting this state along a curve $\mathcal{C}$ [2]. More precisely, for every $\mathbf{R}$ on a $\mathcal{C}$, let $\mathbb{H}_S^{\mathbf{R}}$ be the eigenvector space corresponding to the energy $E_0(\mathbf{R})$ of the instantaneous Stark state $\varphi_0^{\mathbf{R}}$. We thus obtain a line bundle over the parameter space, which we shall call the "Stark bundle" in the following, and the adiabatic theorem yields a connection in this bundle in the usual way.

(ii) In a similar manner, we can also set up a "Floquet bundle" to transport a Floquet state $u_0^{\mathbf{R}_1}$. The line bundle is now fixed by associating with every parameter $\mathbf{R}$ on a curve $\mathcal{C}$ the eigenvector space $\mathbb{H}_F^{\mathbf{R}}$ corresponding to the quasienergy $\varepsilon_0(\mathbf{R})$ of the instantaneous Floquet state $u_0^{\mathbf{R}}$. To bestow this bundle with a connection, we proceed as follows. First, we exploit the physically given separation of time scales by introducing two different time variables: t for the "fast," periodic time dependence and τ for the "slow" time dependence of the parameters $\mathbf{R}$. We thus obtain the evolution equation [10]

$$(H^{\mathbf{R}(\tau)}(t)-i\partial_t)\Phi(\tau,t)=i\partial_\tau\Phi(\tau,t) , \tag{4}$$

and from the solutions of this equation, the Schrödinger wave functions ψ can be recovered by setting t equal to τ:

$$\psi(t)=\Phi(\tau,t)|_{\tau=t} . \tag{5}$$

When τ is kept fixed, the Floquet states $u_0^{\mathbf{R}(\tau)}(\mathbf{x},t)$ are eigenvectors of the operator on the left-hand side of Eq. (4). Therefore, we can now apply the adiabatic theorem to the slow evolution of $\mathbf{R}(\tau)$: The initial value

$$\Phi(\tau=0,t)=u_0^{\mathbf{R}(0)}(t) \tag{6}$$

evolves in time as

$$\Phi_0(\tau,t)=\exp\left[-i\int_0^\tau d\tau'\varepsilon_0(\mathbf{R}(\tau'))\right]u_0^{\mathbf{R}(\tau)}(t) , \tag{7}$$

where $\varepsilon_0(\mathbf{R})$ are the instantaneous quasienergies; therefore, the Schrödinger wave function is given by

$$\psi(t)=\exp\left[-i\int_0^t dt'\varepsilon_0(\mathbf{R}(t'))\right]u_0^{\mathbf{R}(t)}(t) . \tag{8}$$

We remark in passing that the present application of the adiabatic principle is not trivial. Even in simple situations, the quasienergy spectrum is a dense point spectrum [11,12], and the usual gap condition in the standard adiabatic theorem has to be replaced by a condition on the ineffectiveness of resonances [13,14]. The point now is that Eqs. (7) and (8) already require a connection to fix the phases of the instantaneous Floquet states $u_0^{\mathbf{R}}(t)$. This observation leads to the geometrical phase: If we denote the scalar product in the space of square-integrable, T-periodic wave functions [15] by

$$\langle\langle\ |\ \rangle\rangle=\frac{1}{T}\int_0^T dt\langle\ |\ \rangle , \tag{9}$$

the obvious identity

$$\langle\langle\Phi_0^{\mathbf{R}(\tau)}|H^{\mathbf{R}(\tau)}-i\partial_t-i\partial_\tau|\Phi_0^{\mathbf{R}(\tau)}\rangle\rangle=0 \tag{10}$$

leads to the transport law

$$\langle\langle u_0^{\mathbf{R}(\tau)}|\partial_\tau u_0^{\mathbf{R}(\tau)}\rangle\rangle=0 . \tag{11}$$

This is the crucial phase-fixing condition [16] for the adiabatic transport of Floquet states along a path $\mathcal{C}$: If we start with an arbitrary *single-valued* choice $\mathbf{R}\to v_0^{\mathbf{R}}$ of Floquet states with quasienergy $\varepsilon_0(\mathbf{R})$, the ansatz

$$u_0^{\mathbf{R}(\tau)}(t)=e^{i\gamma(\tau)}v_0^{\mathbf{R}(\tau)}(t) \tag{12}$$

finally yields

$$\gamma(\tau)=-\mathrm{Im}\int_0^\tau\langle\langle v_0^{\mathbf{R}(\tau')}|\partial_{\mathbf{R}}v_0^{\mathbf{R}(\tau')}\rangle\rangle\dot{\mathbf{R}}(\tau')d\tau' , \tag{13}$$

the geometrical phase for the Floquet bundle.

The difference between both mathematical constructions, i.e., the Stark bundle and the Floquet bundle, becomes most obvious if we consider simply the time evolution generated by the periodic Hamiltonian (1) without varying any parameter. Any solution $\psi(t)$ of the Schrödinger equation can then be expanded as

$$\psi(t)=\sum_n a_n u_n^{\mathbf{R}}(t)\exp(-i\varepsilon_n(\mathbf{R})t) , \tag{14}$$

with time-independent coefficients a_n.

In the context of the Floquet bundle, a description of this situation is fairly simple. The periodic time dependence has already been accounted for in the construction of the bundle, and, therefore, we need no path in parameter space, but only a single point $\mathbf{R}$. Hence, there is no geometry involved, and, of course, no geometrical phase: The phase factors $\exp(-i\varepsilon_n t)$ which the individual Floquet states acquire are of purely dynamical origin.

The very same physical situation appears much more involved when working with the Stark bundle. Since the periodic time dependence is not contained in the fibers, we now need a periodic path, i.e., we set

$$\tilde{\lambda}=\lambda\sin\omega t \tag{15}$$

[for the definition of $\tilde{\lambda}$, see Eq. (2)] and keep all other parameters fixed. To make contact with the Floquet bundle, let us first assume that the frequency ω is so low that the evolution in the Stark bundle is essentially adiabatic, i.e., an initial Stark state

$$\psi(t=0)=\varphi_0^{\tilde{\lambda}=0} \tag{16}$$

evolves in time as

$$\psi(t)=\exp\left[-i\int_0^t dt'E_0(\tilde{\lambda}(t'))\right]\psi_0^{\tilde{\lambda}(t)} , \tag{17}$$

where $E_0(\tilde{\lambda})$ are the Stark energies. [Note that here we have absorbed the geometrical phase in the definition of the instantaneous Stark states. This is possible because the path (15) does not enclose a finite area.] Rewriting (17) as

$$\psi(t)=\left[\varphi_0^{\tilde{\lambda}(t)}\exp\left[-i\int_0^t dt'E_0(\tilde{\lambda}(t'))+i\frac{t}{T}\int_0^T dt'E_0(\tilde{\lambda}(t'))\right]\right]\times\exp\left[-i\frac{t}{T}\int_0^T dt'E_0(\tilde{\lambda}(t'))\right] , \tag{18}$$

we see that the first factor in (18) is a periodic function of time, that is, a low-frequency Floquet state. Hence, the second factor gives the quasienergy: In the low-frequency regime, the quasienergy is equal to the one-cycle average over the Stark energies,

$$\varepsilon_0(\lambda)=\frac{1}{T}\int_0^T dt\, E_0(\tilde{\lambda}(t)) \ . \tag{19}$$

This observation clearly shows that a quasienergy, although it carries no geometrical information about the Floquet bundle, is associated with the path (15) in the context of the Stark bundle and does carry information about the latter.

If we now drop the restriction to low frequencies, the situation remains the same in the Floquet bundle, but the adiabatic approximation (17) in the Stark bundle is no longer valid. In fact, for high frequencies the quasienergy is no longer equal to the mean energy [17]. Now both approaches yield drastically different pictures: What is simply a stationary system from the Floquet point of view appears as a nonadiabatic problem in the Stark context. Correspondingly, the interpretation of the emerging phase factors $\exp(-i\varepsilon_n t)$ differs: Whereas $\varepsilon_n t$ is a dynamical phase for the evolution in the Floquet bundle, one is forced to introduce a "nonadiabatic Berry phase" [7] when working with the Stark bundle.

The same sort of difference remains if we finally allow the parameters $\{\mathbf{R}\}$ to vary adiabatically: Purely adiabatic evolution in the Floquet bundle [4–6] becomes nonadiabatically periodic motion with superimposed adiabatic variation [7] in the Stark bundle, and labeling phases as "dynamical" or "nonadiabatic geometrical" requires a specification of the reference bundle. In addition, an interpretation of phase factors in terms of geometric concepts also requires a differential geometric connection in this bundle, and the choice of such a connection must be based on physical principles.

It is known that the time evolution of the Schrödinger wave function can be considered as an adiabatic motion on quasienergy surfaces when the parameters of a periodically driven quantum system are changing slowly [18–20]. Therefore, from a physical view-point it is natural to choose the Floquet bundle and the connection derived from this adiabatic evolution.

These remarks apply, in particular, to the recent work of Moore and Stedman [7]: Although these authors employ the formalism developed in Refs. [4–6], they do not use the corresponding Floquet bundle. Hence, their conclusions concerning the "easily discriminated adiabatic and nonadiabatic components" of the Berry phase have to be taken with some caution; they are incorrect from the Floquet point of view.

A simple but important example of a quantum system of the type (1) is a periodically forced two-level system:

$$H(t)=(\omega_0/2)\sigma_z+\sigma_x\lambda\sin\omega t \ , \tag{20}$$

where σ_x and σ_z are the usual Pauli matrices and ω_0 denotes the level separation of the undriven system. If the linearly polarized field is decomposed into a superposition of two oppositely circularly polarized fields,

$$H(t)=\frac{\omega_0}{2}\sigma_z+\frac{\lambda}{2}\{[\sigma_x\sin\omega t+\sigma_y\cos\omega t] +[\sigma_x\sin\omega t-\sigma_y\cos\omega t]\} \ , \tag{21}$$

and if one of those fields is neglected, then a transformation to a rotating frame [21] reduces the other field to a static one. Within this rotating-wave approximation (RWA), the quasienergies $\varepsilon_\pm$ are found to be

$$\varepsilon_\pm=\frac{\omega}{2}\pm\frac{\Omega}{2}\bmod\omega \ , \tag{22}$$

with

$$\Omega=[(\omega_0-\omega)^2+\lambda^2]^{1/2} \ , \tag{23}$$

and the use of the Floquet bundle allows a very transparent computation of geometrical phases for two-level systems with slowly changing parameters (see, in particular, the appendix of Ref. [4]).

Although the RWA leads to a time-independent field in the rotating frame, this approach has nothing to do with the simple Stark bundle: The periodic time dependence is hidden in the transformation to that frame.

It should be emphasized, however, that a discussion of geometrical phases within the framework of the Floquet bundle neither requires a two-level approximation nor the use of the RWA. In fact, the formalism outlined in this Brief Report can be employed to study effects which are far beyond the scope of the RWA. The neglected "counterrotating field" introduces avoided crossings into the quasienergy spectrum. These are related to diabolical points, which, in turn, act as sources of nontrivial Berry phases [1]. If, instead of invoking the RWA, one works with the exact Floquet states, such phenomena can be studied in systematic detail.

In conclusion, we have discussed two possible mathematical approaches to describe the quantum mechanics of a system given by a Hamiltonian such as (1) with both a "fast," periodic and a "slow," parametric time dependence. The first approach is based on a bundle in which the fibers over each point in the space of physical parameters consist of Stark states; the second uses a bundle of Floquet states. Both constructions differ crucially: Whereas the Floquet bundle explicitly incorporates the periodic time dependence into the fibers, the Stark bundle does not. Therefore, in the context of the Floquet bundle, a path in the parameter space describes only the slowly changing parameters, whereas the Stark bundle requires that the path contain both the fast and the slow time dependence.

Of course, the actual computation of Stark states is more simple than a determination of Floquet states. But this apparent simplicity is bought at a high price. The time evolution generated by (1) now poses a nonadiabatic problem, and nonadiabatic Berry phases have to be introduced even if not a single parameter is varied.

It is comforting to know that this somewhat paradoxical situation can be avoided by using the proper bundle. In the Floquet bundle, Floquet states play the role of stationary states. If none of the parameters $\mathbf{R}$ is varied, the evolution of a Floquet state is described by

$$\psi_n(\mathbf{x},t)=u_n^{\mathbf{R}}(\mathbf{x},t)e^{-i\varepsilon_n t}, \tag{24}$$

with a purely dynamical phase $\varepsilon_n t$, in complete analogy to the evolution of stationary quantum systems. We point out that the interpretation of Floquet states as stationary states can be strengthened further by observing that they can be calculated by generalized Bohr-Sommerfeld rules [22].

Whereas the Stark bundle is not specifically adapted to a periodic time dependence—it could, in fact, be used to describe *any* variation of the parameters—it is precisely the periodic time dependence which brings the Floquet bundle into being. Equipped with a connection that, physically speaking, stems from the separation of time scales, this bundle becomes an object of its own mathematical interest. But it should be obvious by now that the Floquet point of view is distinguished by its greater conceptual simplicity.

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[1] M. V. Berry, Proc. R. Soc. London Ser. A **392**, 45 (1984).
[2] B. Simon, Phys. Rev. Lett. **51**, 2167 (1983).
[3] See, e.g., *Geometric Phases in Physics,* edited by A. Shapere and F. Wilczek (World Scientific, Singapore, 1989).
[4] H. P. Breuer, K. Dietz, and M. Holthaus, J. Phys. (Paris) **51**, 709 (1990).
[5] H. P. Breuer, K. Dietz, and M. Holthaus, in *Proceedings of the International Conference on Coherent Radiation Processes in Strong Fields,* edited by V. L. Jacobs (Gordon and Breach, New York, 1992).
[6] H. P. Breuer and M. Holthaus, Phys. Lett. A **140**, 507 (1989).
[7] D. J. Moore and G. E. Stedman, Phys. Rev. A **45**, 513 (1992).
[8] Since questions concerning the nature of both Stark states and Floquet states are of no concern in our context, we simply assume spatial boundary conditions which guarantee that both types of states exist and are square integrable, e.g., by confining our system to a large box.
[9] M. Born and V. Fock, Z. Phys. **51**, 165 (1928).
[10] H. P. Breuer and M. Holthaus, Z. Phys. D **11**, 1 (1989).
[11] J. S. Howland, Ann. Inst. Henri Poincaré **49**, 309 (1989).
[12] J. S. Howland, Ann. Inst. Henri Poincaré **49**, 325 (1989).
[13] H. P. Breuer, K. Dietz, and M. Holthaus, Nuovo Cimento B **105**, 53 (1990).
[14] J. E. Avron, J. S. Howland, and B. Simon, Commun. Math. Phys. **128**, 497 (1990).
[15] H. Sambé, Phys. Rev. A **7**, 2203 (1973).
[16] It is worthwhile to point out that the analog of (11) for stationary states is already contained in the original paper by Born and Fock, Ref. [9].
[17] A. G. Fainshtein, N. L. Manakov, and L. P. Rapoport, J. Phys. B **11**, 2561 (1978).
[18] M. V. Kuz'min and V. N. Sazonov, Zh. Eksp. Teor. Fiz. **79**, 1759 (1980) [Sov. Phys. JETP **52**, 889 (1981)].
[19] T. S. Ho and S. I. Chu, Chem. Phys. Lett. **141**, 315 (1987).
[20] H. P. Breuer, K. Dietz, and M. Holthaus, Z. Phys. D **10**, 13 (1988).
[21] I. I. Rabi, N. F. Ramsey, and J. Schwinger, Rev. Mod. Phys. **26**, 167 (1954).
[22] H. P. Breuer and M. Holthaus, Ann. Phys. (N.Y.) **211**, 249 (1991).