Gauge Fields, Geometric Phases, and Quantum Adiabatic Pumps

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Quantum adiabatic pumping of charge and spin between two reservoirs (leads) has recently been demonstrated in nanoscale electronic devices. Pumping occurs when system parameters are varied in a cyclic manner and sufficiently slowly that the quantum system always remains in its ground state. We show that quantum pumping has a natural geometric representation in terms of gauge fields (both Abelian and non-Abelian) defined on the space of system parameters. Tunneling from a scanning tunneling microscope tip through a magnetic atom could be used to demonstrate the non-Abelian character of the gauge field.

Normally transport of electrical charge is dissipative (i.e., it produces heat). However, quantum adiabatic pumping [1] provides a means in nanoscale electronic devices to use novel quantum effects to transport single electrons with minimal dissipation [2]. Furthermore, it is also possible to pump electron spin without pumping charge [3,4]. Both charge [5] and spin [6] pumping have been recently achieved experimentally, by cyclic variation of the gate voltages that control the shape of an open quantum dot. This motivated extensive theoretical research in this topic [7,8]. Quantum spin pumping opens the way for applications in spintronics. It is sometimes suggested, but not explicitly shown, that quantum pumping is related to Berry's phase. As first emphasized by Berry [9], discrete quantum systems have the counterintuitive property that when some of the parameters controlling the system are slowly varied and brought back to their initial values the quantum state of the system is different to the initial state. That is, a quantum state may acquire a geometric phase in addition to the normal dynamic phase factor. Subsequent work showed that non-Abelian gauge potentials can arise as a result of degeneracies of energy levels of the system [10–12]. However, it is unlikely that adiabatic pumping, characteristic of quantum *open* systems considered in this Letter, results from Berry's phase for *closed discrete* systems [13].

We present a systematic treatment of quantum adiabatic pumping in open systems in terms of parallel transport and gauge fields(both Abelian and non-Abelian) defined on the system parameter space, which reveals a unifying concept of geometric phases underlying scattering states. We make explicit the similarities and differences with Berry's phase associated with cyclic variations of closed quantum systems(both degenerate and nondegenerate) (see Table I). In the scattering approach developed by Brouwer [14], based on earlier work of Büttiker, Thomas, and Prêtre [15], a compact formula was presented for the pumped charge (current) in terms of the parametric derivatives of the time-dependent scattering matrix subjected to the modulating potential. We show that the pumped charge, given by Brouwer's formula [14], is essentially the geometric phase associated with the U(1) subgroup of the gauge group U(M) (M is the number of channels in a certain lead), whereas the non-Abelian sector SU(M) describes the adiabatic pumping associated with the internal degrees of freedom such as spin. Expressions are given for the gauge potentials associated with tunneling from an STM (scanning tunneling microscope) through a magnetic atom. We suggest an experiment which can be used to illustrate the non-Abelian character of the gauge field.

The quantum system.—Consider a mesoscopic system with N leads, and for the nth lead there are M_n channels.

TABLE I. Comparison of Berry's phase and the quantum scattering (pumping) geometric phase.

Berry's phase	Scattering (pumping) geometric phase
Closed systems	Open systems
Wave functions $|\psi_\alpha\rangle$	Row (column) vectors $\mathbf{n}_\alpha$ ($\hat{\mathbf{n}}_\alpha$) of the S matrix
nth energy level with M_n degeneracies	nth lead with M_n channels
Discrete spectrum (bound states)	Continuous spectrum (scattering states)
Parallel transport due to adiabatic theorem	Parallel transport due to adiabatic scattering (pumping)
Gauge potential $A_{\alpha\beta\nu} = \langle\psi_\beta^*|\partial_\nu|\psi_\alpha\rangle$	Gauge potentials $A_{\alpha\beta\nu} = \mathbf{n}_\beta^* \cdot \partial_\nu \mathbf{n}_\alpha$ and $\hat{A}_{\alpha\beta\nu} = \hat{\mathbf{n}}_\beta^* \cdot \partial_\nu \hat{\mathbf{n}}_\alpha$
Gauge group U(M) arising from different choices of bases	Gauge group U(M) arising from redistribution of the scattering particles among different channels

Our aim is to study quantum pumping by periodically varying a set of the independent external parameters $X \equiv (X^1, \ldots, X^\nu, \ldots, X^p)$ slowly as a function of time t. In the scattering approach, the S matrix is an $\mathcal{N} \times \mathcal{N}$ matrix with $\mathcal{N}$ the total number of channels, $\mathcal{N} = \sum_{n=1}^{N} M_n$. We define vectors $\mathbf{n}_\alpha \equiv (S_{\alpha 1}, \ldots, S_{\alpha \mathcal{N}})$ in terms of the rows of the scattering matrix $S[X(t)]$ associated with the nth lead. The unitarity of the scattering matrix implies that these vectors are orthonormal $\mathbf{n}_\alpha^* \cdot \mathbf{n}_\beta = \delta_{\alpha\beta}$, $\alpha, \beta = 1, \ldots, M_n$. That is, this provides us with a smooth set of (local frame) bases $\mathbf{n}_\alpha(t)$.

The gauge potential.—Assume that the parallel transport law

$$\Psi_\alpha^* \cdot d\Psi_\beta = 0 \qquad (1)$$

holds for (fiber) vectors Ψ_α, where $d\Psi_\alpha$ is the variation in Ψ_α resulting from a variation dX in the external parameters. If $\Psi_\alpha(0) = \mathbf{n}_\alpha(0)$, i.e., the initial vector describing the scattering process in which the incident particle comes from the αth channel in the nth lead, then the degeneracy of the channels implies that the transported vector $\Psi_\alpha(t)$ *must be a linear combination of all* $\mathbf{n}_\alpha(t)$, $\Psi_\alpha(t) = \sum_\beta U_{\alpha\beta}(t)\mathbf{n}_\beta(t)$. Expressed another way, the transported vector describes a combined scattering process in which particles come from all channels in the nth lead. Obviously, $U(t)$ is unitary, i.e., $U(t) \in U(M_n)$. Physically, this means certain information about where the incident particles come from is lost during parallel transport, and is encoded in the unitary matrix $U(t)$. Inserting into the parallel transport law in Eq. (1), we have

$$(U^{-1}dU)_{\alpha\beta} = -\mathbf{n}_\beta^* \cdot d\mathbf{n}_\alpha. \qquad (2)$$

Since $\mathbf{n}_\alpha$ varies as the parameters X^ν vary with time, we can thus define the gauge potential $A_{\alpha\beta\nu} \equiv \mathbf{n}_\beta^* \cdot \partial_\nu \mathbf{n}_\alpha$, where $\partial_\nu \equiv \partial/\partial X^\nu$ so that $(U^{-1}dU)_{\alpha\beta} = -\sum_\nu A_{\alpha\beta\nu} dX^\nu$. This can be integrated in terms of exponential integrals. For the period τ of an adiabatic cycle, we have

$$U(\tau) = \mathrm{P}\exp\left(-\oint \sum_\nu A_\nu dX^\nu\right), \qquad (3)$$

where P denotes path ordering. Defining $A \equiv \sum_\nu A_\nu dX^\nu$, one can see it is Lie algebra $u(M_n)$ valued and thus anti-Hermitian. A plays the role of a gauge potential, as in the case of Berry's phase [10] for closed (discrete) quantum systems.

Gauge transformation.—The gauge group $U(M_n)$ originates from the unitary freedom in choosing local bases $\mathbf{n}_\alpha(\alpha = 1, \ldots, M_n)$, $\mathbf{n}'_\alpha(t) = \sum_\beta \omega_{\alpha\beta}(t)\mathbf{n}_\beta(t)$. This amounts to different choices of the scattering matrix: $S'(t) = \Omega(t)S(t)$ with $\Omega(t)$ a diagonal block matrix, the nth block of which is an $M_n \times M_n$ unitary matrix $\omega(t)$. Physically speaking, left multiplication of the scattering matrix $S(t)$ by $\Omega(t)$ just redistributes the scattering particles among different incoming channels associated with a certain lead, which does not affect correlations at the

scatterer and so the physics remains the same. The gauge potential $A(t)$ transforms as

$$A'(t) = d\omega \omega^{-1} + \omega A \omega^{-1}. \qquad (4)$$

The gauge field strength defined by $F \equiv dA - A \wedge A$ transforms covariantly $F' = \omega F \omega^{-1}$. Therefore, a $U(M_n) \equiv U(1) \times SU(M_n)$ gauge field is defined on a p-dimensional parameter space.

Justification of parallel transport.—Physically, by "adiabatic" we mean that the dwell time τ_p during which particles scatter off the scatterer is much shorter than the time period $\tau = 2\pi/\omega_a$ during which the system completes the adiabatic cycle. Here ω_a is a slow frequency characterizing the adiabaticity and τ_p is related to (but not determined alone by) Wigner time delay matrix $\tau_w(s, E) \equiv -iS^\dagger(s, E)\partial S(s, E)/\partial E$ with E being the energy of scattering particles and s being the so-called *epoch* defined as $s = \omega_a t$ [16]. Then the response to the variation of the particle distribution in a certain channel *is only limited to* channels associated with the same lead. That means we ignore any responses which involve channels in different leads. Such a response can be treated as dissipation, a correction to the adiabatic limit. Then, the parallel transport law in Eq. (1) follows from the parallel transport law for the wave function. The latter is a solution of the time-dependent Schrödinger equation $i\hbar\partial_t|\Phi(t)\rangle = H(t)|\Phi(t)\rangle$. As is well known, the Schrödinger equation induces a parallel transport law $\mathrm{Im}\langle\phi(t)|\partial_t\phi(t)\rangle = 0$ [17], with $|\phi(t)\rangle \equiv \exp[i\int h(t)dt] \times |\Phi(t)\rangle$, where $h(t) = \langle\Phi|H|\Phi\rangle/\langle\Phi|\Phi\rangle$. We can write the wave function $|\phi(t)\rangle$ as a linear combination of *all* scattering states associated with a certain lead in the adiabatic case. Formally, $|\phi(t)\rangle = \sum_\alpha c_\alpha|\psi_\alpha(t)\rangle$, with $|\psi_\alpha(t)\rangle$ denoting the scattering states in which the scattered particles come from channels associated with the nth lead, and c_α being arbitrary constants. Then we have $\langle\psi_\alpha(t)|\partial_t\psi_\beta(t)\rangle = 0$. The adiabatic assumption implies that $|\psi_\alpha(t)\rangle$ may be expanded in terms of instantaneous asymptotic scattering states, $|\psi_\alpha(t)\rangle = \sum_\beta U_{\alpha\beta}(t)|\psi_\beta^S(t)\rangle$, with $|\psi_\alpha^S(t)\rangle = |\alpha\rangle_{\mathrm{in}} + \sum_{\beta=1}^{\mathcal{N}} S_{\alpha\beta}(t)|\beta\rangle_{\mathrm{out}}$, $\alpha = 1, \ldots, M_n$. Here, $|\alpha\rangle_{\mathrm{in}}$ and $|\beta\rangle_{\mathrm{out}}$ denote, respectively, the incoming and outgoing scattering states, which are normalized such that they carry a unit flux. Substituting into the parallel transport law for $|\psi_\alpha\rangle$, one gets Eq. (2) which is equivalent to the parallel transport law for row vectors of the scattering matrix.

Quantum adiabatic pumping.—To establish the connection between the geometric phase above and the quantum pumping charge, we need to consider the time-reversed scattering states $|\hat\psi_\alpha^S(t)\rangle = |\hat\alpha\rangle_{\mathrm{in}} + \sum_{\beta=1}^{\mathcal{N}} S_{\beta\alpha}(t)|\hat\beta\rangle_{\mathrm{out}}$ with $\hat{}$ denoting the counterparts under time reversal operation [18], which constitute a solution of the Schrödinger equation for the time-reversed Hamiltonian $\hat{H}$ at any given (frozen) time *at the epoch scale* [16]. This gives rise to another gauge potential $\hat{A}_{\alpha\beta\nu} \equiv \hat{\mathbf{n}}_\beta^* \cdot \partial_\nu \hat{\mathbf{n}}_\alpha$ with $\hat{\mathbf{n}}_\alpha \equiv (S_{1\alpha}, \ldots, S_{\mathcal{N}\alpha})$, i.e., the column

vectors of the scattering matrix $S(t)$. In this case, the gauge group arises from redistribution of scattering particles among different outgoing channels. If $\hat{\mathbf{n}}'_\alpha(t) = \sum_\beta \hat{\omega}_{\alpha\beta}\hat{\mathbf{n}}_\beta(t)$, then the gauge transformation takes $\hat{A}'(t) = d\hat{\omega}\hat{\omega}^{-1} + \hat{\omega}\hat{A}\hat{\omega}^{-1}$. The gauge fields A and $\hat{A}$ are connected via time reversal operation. If we identify the emissivity into the αth channel in the nth lead as $\text{Im}[\hat{A}_{\alpha\alpha}/2\pi]$ [15], then we immediately reproduce Brouwer's formula [14] describing charge pumping, which turns out to be associated with the Abelian subgroup U(1),

$$Q = \frac{e}{2\pi}\text{Im}\oint\text{Tr}\hat{A}, \tag{5}$$

with Q being the charge transferred into the nth lead during one cycle. That is, the charge transferred during adiabatic pumping is essentially the geometric phase associated with the charge sector U(1). This also explains why Planck's constant $\hbar$ does not occur in the adiabatic quantum pumped charge (current), a peculiar feature different from the Landauer-Büttiker conductance. However, as is well known, the geometric phase is determined only up to a multiple of 2π. This concerns global geometric properties, i.e., the winding number of the overall phase of the gauge transformation in Eq. (4), $N \equiv (1/2\pi i)\oint\text{Tr}(d\hat{\omega}\hat{\omega}^{-1})$. The requirement that all physical observables be invariant under the gauge transformation leads us to the conclusion that $O(Q) = O(Q - eN)$, with O denoting any observable. This result has been noticed by Makhlin and Mirlin [8], without proper justification, for the counting statistics in quantum charge pumps (see also, Ref. [7]).

To see the effects caused by non-Abelian gauge potentials, we need to consider gauge invariant quantities. Besides $\text{Tr}\hat{U}(\tau)$, we see that both the determinant and eigenvalues of $\hat{U}(\tau)$ are gauge invariant. Actually, there are M_n independent gauge invariant quantities such as the eigenvalues $\exp[i\gamma_\alpha]$. On the other hand, there are M_n independent simultaneous observables such as the pumping currents I_α flowing into the αth channel, which must be gauge invariant. Therefore, one may expect that the pumping currents I_α are some functions of $\gamma_1, \ldots, \gamma_{M_n}$. Because our argument relies only on gauge invariance and does not depend on any details of the system, such functions must be model independent. Guided by the results for the so-called "Abelianized" non-Abelian gauge potentials, i.e., the gauge potentials which turn out to be diagonal in a certain gauge, we have

$$I_\alpha = -\frac{1}{2\pi\tau}\gamma_\alpha. \tag{6}$$

Especially, the charge pumping current I_c corresponding to the Abelian sector U(1) is $I_c \equiv \sum_\alpha I_\alpha = -(1/2\pi\tau)\times\sum_\alpha\gamma_\alpha$. One may verify that this is consistent with Eq. (5) since $\dot{Q}(t) = eI_c$ and $d\det\hat{U}(t) = -\text{Tr}\hat{A}(t)\det\hat{U}(t)$. Alternatively, $Q = -(e/2\pi)\text{Im}\ln\det\hat{U}(\tau)$. Similarly, we

may define generalized "spin" pumping currents associated with the Cartan subalgebra of the non-Abelian sector SU(M_n). The simplest non-Abelian case U(2) is relevant to the charge and spin pumping.

Tunneling through a single magnetic spin.—Consider the Hamiltonian describing two leads coupled to a single site, the spin of which has an exchange interaction J with a magnetic spin [19],

$$H = \sum_{k\in L,R,\sigma}\epsilon_{k\sigma}c^\dagger_{k\sigma}c_{k\sigma} + J\sum_{\sigma,\sigma'}d^\dagger_\sigma\Omega_{\sigma\sigma'}d_{\sigma'}$$
$$+ \sum_{k\in L,R,\sigma;\sigma'}(V_{k\sigma,\sigma'}c^\dagger_{k\sigma}d_{\sigma'} + \text{H.c.}). \tag{7}$$

Here $c^\dagger_{k\sigma}$ and $c_{k\sigma}$ are, respectively, the creation and destruction operators of an electron with momentum k and spin σ in either the left (L) or the right (R) lead, and $d^\dagger_\sigma$ and d_σ are the counterparts of the single electron with spin σ at the spin site. The quantity $\epsilon_{k\sigma}$ are the single particle energies of conduction electrons in the two leads, which we will assume $\epsilon_{k\sigma} = v_F(|k| - k_F)$ with the convention that $v_F = 1$, and the momentum is measured from the Fermi surface for electrons in leads. The electrons on the spin site are connected to those in the two leads with the tunneling matrix elements $V_{k\sigma,\sigma'}$. For simplicity, we assume symmetric tunneling barriers between the local spin and the leads, and keep only the spin-conserved coupling; viz. $V_{k\sigma\sigma'} = V$ for $\sigma = \sigma'$ and 0 for $\sigma \neq \sigma'$. The entries of the coupling matrix Ω take the form $\Omega_{++} = -\Omega_{--} = \cos\theta$ and $\Omega_{+-} = \Omega^*_{-+} = \sin\theta\exp(-i\phi)$. For this model, in each lead, there are two channels corresponding to up and down spin.

The model is exactly soluble as far as the scattering matrix is concerned. Our general formalism leads us to the non-Abelian gauge potential,

$$\hat{A} = \hat{A}_\theta d\theta + \hat{A}_\phi d\phi, \tag{8}$$

where $\hat{A}_{\theta(\phi)} \equiv \sum_{j=1}^3\hat{A}^j_{\theta(\phi)}\sigma^j/4$ with $\hat{A}^1_\theta = i(a\cos\theta\cos\phi + b\sin\phi)$, $\hat{A}^2_\theta = i(a\cos\theta\sin\phi - b\cos\phi)$, $\hat{A}^3_\theta = -ia\sin\theta$, and $\hat{A}^1_\phi = -i(a\sin\theta\sin\phi - b\sin\theta\cos\theta\cos\phi)$, $\hat{A}^2_\phi = i(a\sin\theta\cos\phi + b\sin\theta\cos\theta\sin\phi)$, $\hat{A}^3_\phi = -ib\sin^2\theta$. Here $a = \sin(\delta_+ - \delta_-)$, $b = 1 - \cos(\delta_+ - \delta_-)$, and the phase shifts are $\delta_\pm = -2\tan^{-1}[\Gamma/(k \mp J)]$ with the tunneling rate $\Gamma \equiv V^2$.

The gauge field strength $\hat{F}$ then takes the form $\hat{F} = -i[1 - \cos(\delta_+ - \delta_-)]\vec{n}\cdot\vec{\sigma}d\Omega/4$. Here $d\Omega = \sin\theta d\theta \wedge d\phi$ is the invariant area element and $\vec{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ is the direction of the magnetic spin. Obviously, this is just a simple rotation of the standard form $\hat{F} = -i(\alpha^2 - 1)\sigma^3d\Omega/2$. Up to a gauge transformation, this is the same non-Abelian gauge potential, found by Moody *et al.* [11] for a diatomic molecule. This is consistent with a theorem, proved in [20], stating that the rotationally invariant connection on the sphere is essentially unique. To establish the relation between α and $\cos(\delta_+ - \delta_-)$, we need to calculate the gauge invariant
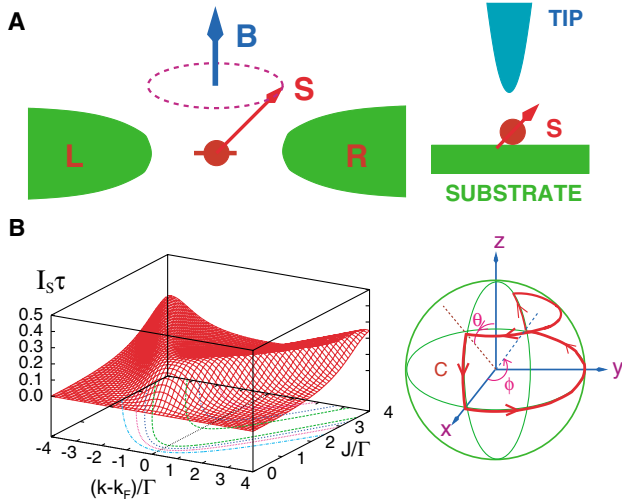
FIG. 1 (color). The dependence of the spin pumping current I_s (times τ, the period of cyclic variation) on system parameters for two leads connected to a single magnetic spin whose direction is slowly varied around the path shown on the right. (a) Left: Schematic of the magnetic spin coupled to left (L) and right (R) leads. The magnetic spin **S** precesses around the direction of the magnetic field **B**. Right: An equivalent scanning tunneling microscope experimental setup. (b) The pumping cycle on the parameter (θ, ϕ)-sphere is taken to be $C(\theta_1, \phi_1, \theta_2, \phi_2) = (\pi/8, 0, \pi/2, \pi)$.

quantity $\mathrm{Tr}\hat{F} \wedge *\hat{F}$, with $*\hat{F}$ being the dual of $\hat{F}$. Then we have $\alpha^2 = [3 - \cos(\delta_+ - \delta_-)]/2$. When $J = 0$, i.e., in the absence of the direct exchange interaction between electrons and the local spin, the gauge field is a pure gauge because $\hat{F} = 0$. Since the Pauli matrices are traceless, we have $\mathrm{Tr}\hat{A} = 0$, meaning that charge pumping is absent in the model under consideration. That implies $\gamma_+ = -\gamma_-$. Therefore, the spin pumping current defined by $I_s = I_+ - I_-$ becomes $I_s = -\gamma_+/(\pi\tau)$.

One can compute a phase factor $\hat{U}_{SR}$ which is obtained from the time-reversed counterpart of Eq. (3) for a "spherical rectangle (SR)." From $\frac{1}{2}\mathrm{Tr}\hat{U}_{SR} = \cos[\pi\tau I_s]$, the spin pumping current I_s may be extracted and is shown in Fig. 1 as a function of system parameters for a path C. The spin pumping current takes its maximum value around the resonant scattering lines $k = \pm J$.

Possible experiments.—A scanning tunneling microscope (STM) has been used to detect a quantum mirage around a single magnetic cobalt atom placed on a nonmagnetic metallic copper surface [21]. Electron spin resonance (ESR)-STM experiments [22] have advanced to the point that they have spatial resolution at the level of a few spins [23]. The STM setup as shown in Fig. 1(a) should make it possible to observe gauge invariant spin pumping via a single magnetic atom on the surface of the substrate. To measure the spin pumping current I_s, one could replace one of the leads by a ferromagnetic one. The spin pumping current can then be measured via the charge pumping currents.

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