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.

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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 Piétre [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.

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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 $X \equiv (X^1, \ldots, X^r, \ldots, X^p)$ 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 $\mathbf{n}_n = (S_{1n}, \ldots, S_{2\mathcal{N}})$ in terms of the rows of the scattering matrix $S[X(t)]$ associated with the $n$th 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 $\mathbf{n}_n(t)$.

The gauge potential.—Assume that the parallel transport law

$$\Psi^*_\alpha \cdot d\Psi_\beta = 0 \quad (1)$$

holds for (fiber) vectors $\Psi_\alpha$, where $d\Psi_\alpha$ is the variation in $\Psi_\alpha$ 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 $\alpha$th channel in the $b$th 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 $b$th 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

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

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

$$U(\tau) = \text{P exp} \left( -i \sum_{\nu} A_{\nu} dX^\nu \right). \quad (3)$$

where P denotes path ordering. Defining $A = \sum_{\nu} A_{\nu} dX^\nu$, one can see that $A$ is a 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 $\mathbf{n}_\alpha$, $\alpha = 1, \ldots, M_n$, $\mathbf{n}_\alpha'(t) = \sum_\beta \omega_{\alpha\beta}(t) \mathbf{n}_\beta'(t)$, without affecting the scattering matrix and so the physics remains the same. The gauge potential $A(t)$ transforms as

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

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

Justification of parallel transport.—Physically, by “adiabatic” we mean that the dwell time $\tau_p$ 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 $\omega_a$ is a slow frequency characterizing the adiabaticity and $\tau_p$ is related to (but not determined alone by) Wigner time delay matrix $\tau_w(s,E) = -iS^\dagger(s,E)\partial S(s,E)/\partial E$ with $E$ being the energy of scattering particles and $s$ being the so-called epoch defined as $s = \omega_a \tau$ [16]. Then 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 $i\hbar \partial_t |\Psi(t)\rangle = H(t)|\Psi(t)\rangle$. As is well known, the Schrödinger equation induces a parallel transport law $\text{Im} \langle \phi(t) |\partial_t \phi(t) = 0$ [17], with $|\phi(t)\rangle = \exp[i \int H(t)dt] |\Psi(t)\rangle$, where $H(t) = (\Phi |H| \Phi)$. 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, $|\phi(t)\rangle = \sum_c c_{\alpha} |\psi_{\alpha}(t)\rangle$, with $|\psi_{\alpha}(t)\rangle$ denoting the scattering states in which the scattered particles come from channels associated with the $\alpha$th lead, and $c_{\alpha}$ being arbitrary constants. Then we have $\langle \psi_{\alpha}(t) |(\partial_t - \partial_\beta) \psi_{\beta}(t) = 0$. The adiabatic assumption implies that $|\psi_{\alpha}(t)\rangle$ may be expanded in terms of instantaneous asymptotic scattering states $|\psi_{\alpha}(t)\rangle = \sum_\beta U_{\alpha\beta}(t) |\phi_{\beta}^S(t)\rangle$, with $|\phi_{\alpha}^S(t)\rangle = |\alpha\rangle_{\text{in}} + \sum_{\beta=1}^N S_{\alpha\beta}(t) |\beta\rangle_{\text{out}}$, $\alpha = 1, \ldots, M_n$. Here, $|\alpha\rangle_{\text{in}}$ and $|\beta\rangle_{\text{out}}$ 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 $|\psi_{\alpha}(t)\rangle$, 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 $|\psi_{\alpha}^S(t)\rangle = |\alpha\rangle_{\text{in}} + \sum_{\beta=1}^N S_{\alpha\beta}(t) |\beta\rangle_{\text{out}}$ with $\beta$ denoting the counterparts under time reversal operation [18], which constitute a solution of the Schrödinger equation for the time-reversed Hamiltonian $\widetilde{H}$ at any given (frozen) time at the epoch scale $t$ [16]. This gives rise to another gauge potential $\tilde{A}_{\alpha\beta}(t) = \tilde{\mathbf{n}}_\beta^* \cdot \partial_t \tilde{\mathbf{n}}_\alpha$ with $\tilde{\mathbf{n}}_\alpha = (S_{1\alpha}, \ldots, S_{N\alpha})$, 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 $\mathbf{n}_{\alpha}(t) = \sum_{\alpha} \mathbf{A}_{\alpha}(t)$, then the gauge transformation takes $\tilde{A}(t) = d\omega \tilde{A}^{-1} + \tilde{A} \omega \tilde{A}^{-1}$. The gauge fields $A$ and $\tilde{A}$ are connected via time reversal operation. If we identify the emittance into the $\alpha$th channel in the $n$th lead as $\text{Im}[\tilde{A}_{\alpha \alpha}/2\pi]$ [15], then we immediately reproduce Brouwer’s formula [14] describing charge pumping, which turns out to be associated with the Abelian subgroup $U(1)$,

$$Q = \frac{e}{2\pi} \text{Im} \int \text{Tr} \tilde{A},$$  

with $Q$ being the charge transferred into the $n$th 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 $2\pi$. This concerns global geometric properties, i.e., the winding number of the overall phase of the gauge transformation in Eq. (4), $N = (1/2\pi) \int \text{Tr} (d\omega \tilde{A}^{-1})$. 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 $\text{Tr} \tilde{U}(\tau)$, we see that both the determinant and eigenvalues of $\tilde{U}(\tau)$ 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 $I_{\alpha}$ flowing into the $\alpha$th channel, which must be gauge invariant. Therefore, one may expect that the pumping currents $I_{\alpha}$ 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 $I_e$ corresponding to the Abelian sector $U(1)$ is $I_e = \sum_{\alpha} I_{\alpha} = -(1/2\pi \tau) \times \sum_{\alpha} \gamma_{\alpha}$. One may verify that this is consistent with Eq. (5) since $Q(t) = eI_e$ and $d\text{det} \tilde{U}(t) = -\text{Tr} \tilde{A}(t) \text{det} \tilde{U}(t)$. Alternatively, $Q = -(e/2\pi) \text{Im} \text{det} \tilde{U}(\tau)$. 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],

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

Here $c_{k\sigma}^\dagger$ and $c_{k\sigma}$ are, respectively, the creation and destruction operators of an electron with momentum $k$ and spin $\sigma$ in either the left (L) or the right (R) lead, and $d_{\sigma}$ and $d_{\sigma'}$ are the counterparts of the single electron with spin $\sigma$ 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 $\Omega$ take the form $\Omega_{\sigma,\sigma'} = -\Omega_{\sigma',\sigma} = \cos \theta$ and $\Omega_{\sigma,\sigma'} = \Omega_{\sigma',\sigma} = \sin \theta \exp(-i\phi)$. 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,

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

where $\tilde{A}_{\phi,\phi} = \sum_{n=1}^{3} \tilde{A}_{\phi,\phi}^{n}/4$ with $\tilde{A}_{\phi} = (a \cos \theta \cos \phi + b \sin \phi)$, $\tilde{A}_{\phi}^{2} = (a \cos \theta \sin \phi - b \cos \phi)$, $\tilde{A}_{\phi}^{3} = -ia \sin \theta$, and $\tilde{A}_{\phi}^{4} = (a \sin \theta \cos \phi + b \sin \phi \cos \theta)$. Here $a = \sin(\delta_{\alpha} - \delta_{\beta})$, $b = 1 - \cos(\delta_{\alpha} - \delta_{\beta})$, and the phase shifts are $\delta_{\pm} = -2\tan^{-1}[G/(k \mp J)]$ with the tunneling rate $G = V_{\phi}^2$.

The gauge field strength $\tilde{F}$ then takes the form $\tilde{F} = -i[1 - \cos(\delta_{+} - \delta_{-})] \tilde{n} \delta d\Omega/4$. Here $d\Omega = \sin \theta d\theta \wedge d\phi$ is the invariant area element and $\tilde{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ is the direction of the magnetic spin. Obviously, this is just a simple rotation of the standard form $\tilde{F} = -i(a^2 - 1) \sigma^2 d\Omega/2$. 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 $\alpha$ and $\cos(\delta_{+} - \delta_{-})$, we need to calculate the gauge invariant...
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[18] The time reversal operation here is carried out for the Hamiltonian at the frozen time, which may be or may not be broken, depending on the Hamiltonian concerned. However, there is another time reversal operation at large time scale, which is always broken during pumping.