Adiabatic Response of Quantum Systems Pinching a Gap Closure

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Abstract

A vanishing cause can lead to a large response in quantum systems which undergo cyclic deformations that pinch a point of level crossing. We call such behavior homeopathic. We illustrate this behavior by studying charge circulation in quantum models of necklaces of atoms driven by a running wave of small amplitude.

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Consider a molecular ring, such as a benzene ring or a triangular molecule of, say, H_3 [1]. Suppose that the molecule is taken through a cycle of adiabatic deformations where each atom is displaced only slightly from its initial position, and eventually returns to it. What is the elecronic charge transported around the molecule in one such cycle? As we shall explain below, there are two cases: If the cycle of atomic deformations can be shrunk to zero without trapping a point of level crossing (of the electronic energy levels) then one gets normal behavior in the sense that the weaker the deformation, the less the charge transported in one cycle. If, however, the cycle of atomic deformations pinches a point of level crossing, then the smaller the cycle, the *larger* the transported charge. We dub such anomalous behavior, where the weaker the cause the larger the effect, *homeopathic.* We shall illustrate this for tight binding models of molecular rings.

Homeopathic behavior in adiabatic transport has been shown to occur in certain Harper like models [2]. The models described here are simpler, and belong to a different symmetry class with respect to time reversal. This suggests that homeopathic behavior is prevalent.

Consider, for simplicity, the tight-binding (Hückel) model Hamiltonian for non interacting electrons in a general triangular molecule of three identical atoms. The Hamiltonian is the 3×3 Hermitian matrix

$$H(a,b,c,\phi) = \begin{pmatrix} 0 & a & \bar{\xi} c \\ a & 0 & b \\ \xi c & b & 0 \end{pmatrix}, \tag{1}$$

where a, b, c are the (real) hopping amplitudes associated to the three bonds of the triangle. (The triangle is not necessarily equilateral.) We assume that a, b, c are all positive. $\xi = \exp i\phi$, with ϕ an auxiliary phase variable associated with a *fictitious* Aharonov-Bohm flux tube which carries flux ϕ and threads the molecule. The explicit form of Eq. (1) involves a choice of gauge for the flux tube. (We shall consider observables that are independent of this choice.) The role of ϕ will become clear below. Deformations of the molecule change the hopping amplitudes, and a closed cycle of deformations is a closed path in the three dimensional space whose points are the hopping amplitudes $(a, b, c) \in \mathbb{R}^3_+$. Such a closed path is shown in Fig. 1. For notational convenience we denote by X the triplet (a, b, c).

The reason for introducing the fictitious flux tube ϕ is to define the current operator which circulates in such a ring. For the choice of gauge we have made for the Aharonov-Bohm flux, the current is associated with a single bond, the c bond, and is

$$(\partial_\phi H)(X,\phi) = c \begin{pmatrix} 0 & 0 & -i\,\bar{\xi} \\ 0 & 0 & 0 \\ i\,\xi & 0 & 0 \end{pmatrix}. \tag{2}$$

This is the sole role of ϕ and in all our calculations we shall eventually set $\phi = 0$, which is the case with no flux at all. In this case the Hamiltonian $H(X, 0)$ is real and therefore time reversal invariant. The observable associated to the circulating current, Eq. (2) is pure imaginary when $\phi = 0$ and so odd under time reversal. Because the model for $\phi = 0$ is time reversal invariant, there are no persistent currents in any eigenstate. Let $P(X, \phi)$ be a spectral projection for $H(X, \phi)$, i.e. $H(X, \phi)P(X, \phi) = E(X, \phi)P(X, \phi)$ with $E(X, \phi) \in \mathbb{R}$ an eigenvalue. The vanishing of the persistent currents is the statement $Tr\,(P\partial_\phi H)|_{\phi=0} = 0$ for all X.

We are interested in the current that flows around the molecule when it is slowly driven so that X traces a closed path in parameter space, as e.g. in Fig. 1. In the theory of adiabatic transport [3]– [12] this current is related to the adiabatic curvature. The basic equation reads:

$$Tr\,(P_t\,\partial_\phi H)\Big|_{\phi=0} = Tr\,\Big(\Omega_{\phi X}(P)\Big)\,\dot{X}\Big|_{\phi=0} + O(1/\tau^2). \tag{3}$$

X stands for the triplet a, b and c and the dot denotes time derivative. P_t is a solution of the quantum evolution equation, with the (adiabatic) time dependent Hamiltonian $H(X, \phi)$ and with initial condition that $P_{t=0}$ is an eigenstate. $P(X, \phi)$ is an instanteneous spectral projection for the instanteneous $H(X, \phi)$. $\Omega_{\phi X}(P) = -i\,P\,[\partial_\phi P, \partial_x P]\,P$ is the ϕX component of the adiabatic curvature [13]. $\tau \to \infty$ is the adiabatic time scale. The charge transported around the ring in one cycle is

$$Q = \int dt\,Tr\,(P_t\,\partial_\phi H) = \oint Tr\,\Big(\Omega_{\phi X}(P)\Big)\,dX + O(1/\tau). \tag{4}$$

Analysis of the characteristic equation of Eq. (1) shows that level crossing can occur only if $a = b = c$ and $\xi = \pm 1$. For $\xi = 1$, the case we consider here, the simple eigenvalue is $2a$ (the top state since a is positive) and the corresponding eigenvector is $|0\rangle = \frac{1}{\sqrt{3}}(1,1,1)$. The two fold degenerate eigenvalue is $-a$ and the projection to its subspace is $1 - |0\rangle\langle 0|$. For $\phi = 0$, level crossings occur on a ray in X space.

The essence of homeopathic behavior is the following. Suppose first that the cycle of deformation does not pinch level crossing. (For the top state this holds for any closed cycle in the positive quadrant.) The adiabatic curvature is smooth and bounded along the path and the right hand side of Eq. (4) is of order of the length of the cycle of deformations. Q goes to zero when the cycle shrinks to zero. Now suppose that the cycle of deformation pinches the ray of level crossing. A cycle of deformations which pinches the line of level crossing is, e.g.

$$a(x) = 1 + \omega\bar{x} + \bar{\omega}x; \quad b(x) = 1 + \bar{x} + x; \quad c(x) = 1 + \overline{\omega x} + \omega x, \tag{5}$$

where ω is here a (complex) cube root of unity and $x \in \mathbb{C}$ runs on a small circle in the complex plane surrounding the origin, see Fig. 1. As the cycle shrinks, the adiabatic curvature in Eq. (4) diverges quadratically, like a monopole [13,14], while the length of the cycle shrinks only linearly. It follows that now Q *diverges* as the cycle shrinks to zero, i.e. $Q = O\left(\frac{1}{|x|}\right)$.

In the simple case at hand the homeopathic behavior can be calculated explicitly. The degeneracy splits in first order of perturbation theory, both in ϕ and in x, and the local behavior near crossing of the two bottom states is given by the 2×2 matrix

$$\frac{1}{3}\begin{pmatrix} -\sqrt{3}\phi & 6\omega\bar{x} \\ 6\bar{\omega}x & \sqrt{3}\phi \end{pmatrix}. \tag{6}$$

This matrix has the form of Berry spin 1/2 model and the adiabatic curvature of its two states is explicitly computable. So, to leading order, the equation for the charge Q, Eq. (4), reduces to

$$Q = \pm\frac{\sqrt{3}}{12}\oint \frac{1}{|x|}\, d\ Angle \tag{7}$$

where *Angle* is the angle swept by x as it moves around the origin in the complex plane. The $\pm$ signs refer to the ground and first state respectively. A simple formula is obtained for a circular orbit, $|x| = const$, where $Q = \frac{\sqrt{3}\pi}{6|x|}$. Evidently, the smaller the cycle that pinches the degeneracy, the more charge it transports and $Q \to \pm\infty$ as $|x| \to 0$.

It should be stressed that this result *does not* imply that the current is large. In Eq. (3) only the ratio of the current to the rate of driving is large. The current is not large because, as the circle is shrunk, the rate of driving must also decrease in order for the adiabatic theory to apply.

The homeopathic behavior of charge transport is closely related to an observation of Longuet-Higgins [1], who showed that a cycle of deformation (of a time reversal invariant system) is reflected in the sign of the electronic wave function when the cycle encloses a point of level crossing.

Similar analysis can be made for a necklace of p equivalent atoms with p an arbitrary integer larger than 2. (For benzene $p = 6$.) The tight binding Hamiltonian is a $p \times p$ Hermitian matrix with nearest neighbors hoppings only. Now suppose that such a ring is deformed by means of a running sinusoidal wave of commensurate wavelength, i.e. the hopping amplitude between the k-th and $(k+1)$-th atom is time dependent and is given by $1 + 2\kappa\cos[2\pi(jk/p - t/\tau)]$, where κ (which is held fixed) stands for the amplitude of the distortion and j is a natural number smaller than p. (This is an analog of Eq. (5)). When $\phi = \kappa = 0$, there are twofold degeneracies at energies $2\cos(2m\pi/p)$ for $m = \pm 1, \ldots, \pm[p/2]$. The new feature of this model is that the the order of perturbation theory that splits the degeneracies depends on $|m|$, p and j, and can be large if p is large. As a consequence, the singularity of the adiabatic curvature near crossing can be quite strong. The charge transported can be calculated here as well, but the details will be described elsewhere. The result is that the charge trasported in the pair of nearly crossing states near energy $2\cos(2m\pi/p)$ is:

$$Q = \pm \frac{\pi q \sin m\theta}{p\kappa^q \cos(m - j/2)\theta} \left(\prod_{k=1}^{q-1} \frac{\cos(m - jk)\theta - \cos m\theta}{\cos(m + j/2 - kj)\theta} \right). \tag{8}$$

$q \geq 1$ is the order of perturbation theory that splits the degeneracy. The numerator and the denominator never vanish under the conditions that lead to Eq. (8). (This includes, for instance, the case that p is odd and $j = 1$.) The value of q and the sign of m in Eq. (8) depend on $|m|$, p and j. θ is shorthand for $2\pi/p$. We see that the amplitude of the perturbation κ enters this expression with a negative exponent. This is the homeopathic effect. The sign of Q reflects the fact that each member of the pair of nearly crossing states transports charge in opposite sense.

We finally comment on the Jahn Teller [15] instability. If the ground state of the undeformed molecule in the tight-binding model is degenerate, the total energy may be decreased by deforming the molecule. This is the case if the elastic energy is proportional to the square of the amplitude of the deformation (i.e. is harmonic) and if the degeneracy lifts to first order in the deformation. An example is the triangle we treated above. In this case a cycle of deformations around the ground state has to be sufficiently large in order to also include the point of degeneracy. In other words, the Jahn Teller instability censors homeopathic behavior and there is no true divergence of the charge transport in the limit of an infinitesimal cycle of deformation of the ground state around its equilibrium configuration. In contrast, for crossings where the splitting in the tight-binding model is cubic or higher, the equilibrium configuration coincides with the configuration where there is level crossing and in this case the homeopathic behavior holds for deformations of the equilibrium configuration.

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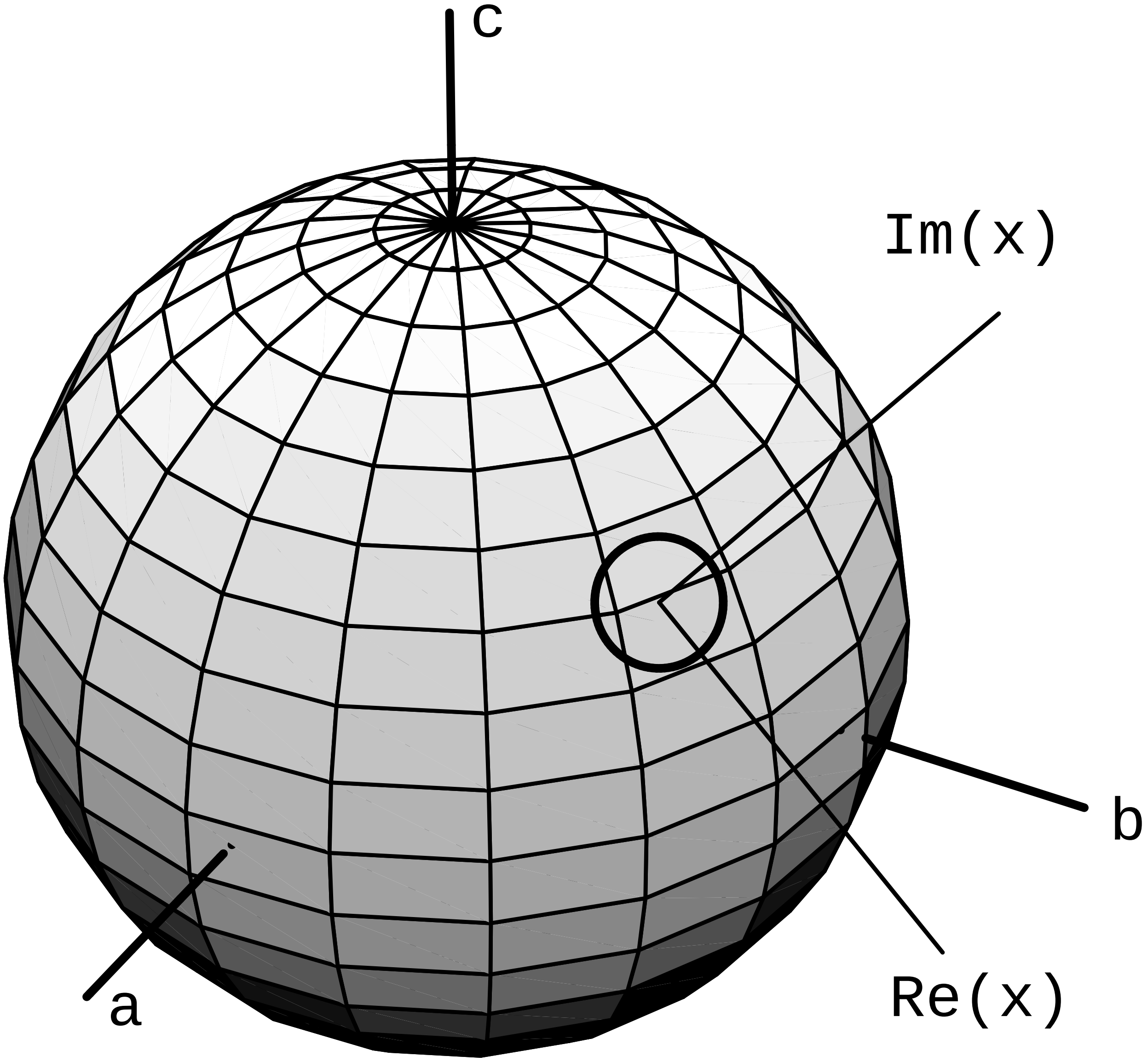

FIG. 1. A cycle of deformation for a molecule with three atoms.