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Topological Order, Mixed States and Open Systems

Manuel Asorey[1], Paolo Facchi[2], and Giuseppe Marmo[3]

[1] *Centro de Astropartículas y Física de Altas Energías*
Departamento de Física Teórica
Universidad de Zaragoza, E-50009 Zaragoza, Spain

e-mail: asorey@unizar.es

[2] *Dipartimento di Fisica and MECENAS*
Università di Bari, I-70126 Bari, Italy
and
INFN, Sezione di Bari, I-70126 Bari, Italy

e-mail: paolo.facchi@ba.infn.it

[3] *Dipartimento di Fisica, Università di Napoli Federico II, I-80126 Napoli, Italy*

e-mail: marmo@na.infn.it

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Abstract. The role of mixed states in topological quantum matter is less known than that of pure quantum states. Generalisations of topological phases appearing in pure states have received attention in the literature only quite recently. In particular, it is still unclear whether the generalisation of the Aharonov–Anandan phase for mixed states due to Uhlmann plays any physical role in the behaviour of the quantum systems. We analyse, from a general viewpoint, topological phases of mixed states and the robustness of their invariance. In particular, we analyse the role of these phases in the behaviour of systems with periodic symmetry and their evolution under the influence of an environment preserving its crystalline symmetries.

Keywords: Topological phases, open systems, mixed states.

We dedicate this paper to the memory of George Sudarshan, with gratitude for the many years of friendship and for sharing with us his great insights in physics.

1. Introduction

Although the existence of topological phases of quantum theories is known since a long time (see, e.g., [1] for a review and references therein), topological aspects of quantum matter have been intensively exploited only in recent years. Topological phases are characterised in terms of topological invariants and some discrete symmetries such as time reversal invariance. The robustness of the corresponding effects under perturbations follows from the topological nature of the phenomena, especially under two kinds of disorder perturbations: either generated by impurities or by small deformations of the material. Most of the studies where formulated in terms of pure quantum states. In this paper we analyse the relevance of such topological invariants for mixed states of closed and open quantum systems, corresponding for example to electrons in crystalline solids, either in isolated conditions or under the effects of interaction with the environment.

2. Quantum States, Principal Fibre Bundles and Geometrical Phases

According to Dirac, the simplest way to take into account interference phenomena is to associate with every quantum system a Hilbert space $\mathcal{H}$. The evolution is ruled by the linear Schrödinger equation and solutions may be "superposed". Then the evolution of a quantum system can be considered as a parallel transport of unitary operators acting on a bundle of Hilbert spaces along the time axis with respect to a generalised connection associated with the Hamiltonian operator [2]. If the Hamiltonian has a smooth dependence on a family of parameters with a cyclic symmetry, an adiabatic evolution of the system can develop a cyclic evolution of quantum states. Moreover, the final state can have a phase different from that of the initial state. The difference between these phases is known as Berry phase [3]. Such a phase difference has one component which is dynamical, depending on the Hamiltonian, and another one which has a purely geometric origin. This component goes often under the name of Aharonov–Anandan phase [4].

2.1. A fibre bundle description of the Aharonov–Anandan phase

To avoid technicalities we shall restrict our considerations to finite dimensional quantum systems. The Hilbert space is then $\mathcal{H} = \mathbb{C}^N$, and we shall denote by $\mathcal{H}_0 = \mathbb{C}_0^N = \mathbb{C}^N \setminus \{0\}$ the space deprived of the zero vector. The probabilistic interpretation of quantum mechanics requires that pure states are rays of $\mathbb{C}_0^N$; the space of rays is a differential manifold called the complex projective space, and is denoted by $\mathbb{C}\mathrm{P}^{N-1}$. As a matter of fact, $\mathbb{C}_0^N$ is a $\mathbb{C}_0$ principal fibre bundle whose action

$$\boldsymbol{z}^\lambda = \lambda \boldsymbol{z}\,, \quad \boldsymbol{z} \in \mathbb{C}_0^N \text{ and } \lambda \in \mathbb{C}_0\,, \tag{1}$$

provides a *space of orbits*, the base of the bundle given by $\mathbb{C}\mathrm{P}^{N-1}$. We shall denote the bundle by

$$\mathbb{C}_0^N\big(\mathbb{C}\mathrm{P}^{N-1}, \mathbb{C}_0\big)\,, \tag{2}$$

where the base space $\mathbb{C}\mathrm{P}^{N-1}$ and the Lie group $\mathbb{C}_0$ are specifically indicated.

The Hermitian scalar product

$$\langle \boldsymbol{z}|\boldsymbol{w}\rangle \;=\; \sum_{i=1}^{N} \overline{z}_i w_i \tag{3}$$

among vectors of the Hilbert space $\mathbb{C}^N$ allows to define a Hermitian tensor which coincides with the Hermitian product on $T\mathbb{C}^N$. In this manner we consider the Hilbert space as a Hilbert manifold so that $\mathbb{C}^N$, $\mathbb{C}_0^N$ and $\mathbb{C}\mathrm{P}^{N-1}$ are all Hilbert manifolds. This twist from vector spaces to manifolds is the content of the manifold (or geometrical) approach to quantum mechanics [5, 6, 7].

From this geometric point of view, $\mathbb{C}_0^N$ becomes a Riemann manifold carrying a symplectic structure and a related complex structure.

They may be simply described in coordinates, with $\mathbb{C}_0^N$ thought of as a real differential manifold. The Hermitian tensor will be, for any $\boldsymbol{z} \in \mathbb{C}^N$,

$$h \;=\; \langle \mathrm{d}\boldsymbol{z}|\mathrm{d}\boldsymbol{z}\rangle \,. \tag{4}$$

If we use an orthonormal basis $|e_1\rangle, \ldots, |e_N\rangle$, we have

$$\begin{aligned} |\boldsymbol{z}\rangle \;&=\; z^j|e_j\rangle \;=\; (x^j + iy^j)|e_j\rangle \\ |\mathrm{d}\boldsymbol{z}\rangle \;&=\; \mathrm{d}z^j|e_j\rangle \;=\; (\mathrm{d}x^j + i\mathrm{d}y^j)|e_j\rangle \,, \end{aligned} \tag{5}$$

where we use Einstein notation for vector index contractions. By spelling out (4) we find

$$h \;=\; (\mathrm{d}x^j \otimes \mathrm{d}x^j + \mathrm{d}y^j \otimes \mathrm{d}y^j) + i(\mathrm{d}x^j \wedge \mathrm{d}y^j) \,, \tag{6}$$

the real part is a Riemannian structure, the imaginary part is a symplectic structure. The two structures define a complex structure

$$J \;=\; \mathrm{d}x^j \otimes \frac{\partial}{\partial y^j} - \mathrm{d}y^j \otimes \frac{\partial}{\partial x^j} \,. \tag{7}$$

The infinitesimal generators of the $\mathbb{C}_0$ action, the fundamental vector fields, are

$$\Delta \;=\; x^j \frac{\partial}{\partial x^j} + y^j \frac{\partial}{\partial y^j} \,, \qquad \Gamma \;=\; x^j \frac{\partial}{\partial y^j} - y^j \frac{\partial}{\partial x^j} \,. \tag{8}$$

If, according to the probabilistic interpretation, we had to consider only quantities which are "gauge invariant", they should be invariant under the joint action of Δ and Γ. Clearly, for this to be the case, we should modify h by means of a conformal factor, namely

$$\tilde{h} = \frac{1}{\langle \boldsymbol{z}|\boldsymbol{z}\rangle} \langle \mathrm{d}\boldsymbol{z}|\mathrm{d}\boldsymbol{z}\rangle. \tag{9}$$

The connection form of the principal bundle is easily seen to be

$$\mathcal{A} \;=\; \Delta \otimes \frac{1}{2}\frac{\mathrm{d}\langle \boldsymbol{z}|\boldsymbol{z}\rangle}{\langle \boldsymbol{z}|\boldsymbol{z}\rangle} + \Gamma \otimes \frac{1}{2} J\Big(\frac{\mathrm{d}\langle \boldsymbol{z}|\boldsymbol{z}\rangle}{\langle \boldsymbol{z}|\boldsymbol{z}\rangle}\Big)\,, \tag{10}$$

indeed

$$\mathcal{A}(\Delta) \;=\; \Delta\,, \qquad \mathcal{A}(\Gamma) \;=\; \Gamma\,. \tag{11}$$

In coordinates we have

$$\frac{1}{2}\frac{\mathrm{d}\langle \boldsymbol{z}|\boldsymbol{z}\rangle}{\langle \boldsymbol{z}|\boldsymbol{z}\rangle} \;=\; \frac{1}{2}\frac{\mathrm{d}(\|\boldsymbol{x}\|^2+\|\boldsymbol{y}\|^2)}{\|\boldsymbol{x}\|^2+\|\boldsymbol{y}\|^2} \;=\; \frac{\boldsymbol{x}\cdot\mathrm{d}\boldsymbol{x}+\boldsymbol{y}\cdot\mathrm{d}\boldsymbol{y}}{\|\boldsymbol{x}\|^2+\|\boldsymbol{y}\|^2} \;=\; \vartheta\,, \tag{12}$$

$$\frac{1}{2}J\Big(\frac{\mathrm{d}\langle \boldsymbol{z}|\boldsymbol{z}\rangle}{\langle \boldsymbol{z}|\boldsymbol{z}\rangle}\Big) \;=\; \frac{\boldsymbol{y}\cdot\mathrm{d}\boldsymbol{x}-\boldsymbol{x}\cdot\mathrm{d}\boldsymbol{y}}{\|\boldsymbol{x}\|^2+\|\boldsymbol{y}\|^2} \;=\; J(\vartheta)\,. \tag{13}$$

We find that $\mathrm{d}\vartheta = 0$,

$$\mathrm{d}J(\vartheta) \;=\; 2\frac{\mathrm{d}\boldsymbol{y}\wedge\mathrm{d}\boldsymbol{x}}{\|\boldsymbol{x}\|^2+\|\boldsymbol{y}\|^2} - 2\frac{(\boldsymbol{x}\cdot\mathrm{d}\boldsymbol{x}+\boldsymbol{y}\cdot\mathrm{d}\boldsymbol{y})\wedge(\boldsymbol{y}\cdot\mathrm{d}\boldsymbol{x}-\boldsymbol{x}\cdot\mathrm{d}\boldsymbol{y})}{(\|\boldsymbol{x}\|^2+\|\boldsymbol{y}\|^2)^2}\,, \tag{14}$$

which gives the curvature.

If we think of $\tilde{h}$ in the spirit of the Kaluza–Klein theory, it is clear that the pull-back of the metric tensor on $\mathbb{C}\mathrm{P}^{N-1}$ should be

$$\frac{1}{\langle \boldsymbol{z}|\boldsymbol{z}\rangle}\langle \mathrm{d}\boldsymbol{z}|\mathrm{d}\boldsymbol{z}\rangle - \frac{\langle \mathrm{d}\boldsymbol{z}|\boldsymbol{z}\rangle\langle \boldsymbol{z}|\mathrm{d}\boldsymbol{z}\rangle}{\langle \boldsymbol{z}|\boldsymbol{z}\rangle^2}\,, \tag{15}$$

the second term being associated with the connection form, i.e.,

$$\frac{\langle \mathrm{d}\boldsymbol{z}|\boldsymbol{z}\rangle\otimes\langle \boldsymbol{z}|\mathrm{d}\boldsymbol{z}\rangle}{\langle \boldsymbol{z}|\boldsymbol{z}\rangle^2} \;=\; \vartheta\otimes\vartheta + J(\vartheta)\otimes J(\vartheta) + i\vartheta\wedge J(\vartheta)\,. \tag{16}$$

This can be easily computed in coordinates, or in intrinsic terms by using the properties of J, $J^2 = -\mathbb{I}$.

It is also possible to consider the action of Δ and Γ separately so that we identify the quotient of $\mathbb{C}_0^N$ under dilations to be represented by the unit sphere

$$S^{2N-1} \;=\; \{\boldsymbol{z}\in\mathbb{C}^N \,:\, \|\boldsymbol{z}\| = 1\} \tag{17}$$

and Γ acts on the unit sphere S^{2N-1} to define a U(1)-principal bundle

$$S^{2N-1}\big(\mathbb{C}\mathrm{P}^{N-1}, \mathrm{U}(1)\big)\,. \tag{18}$$

Now the connection one-form will simply be

$$\mathcal{A} \;=\; -(\boldsymbol{x}\cdot\mathrm{d}\boldsymbol{y} - \boldsymbol{y}\cdot\mathrm{d}\boldsymbol{x})\,, \qquad \|\boldsymbol{x}\|^2+\|\boldsymbol{y}\|^2 = 1\,. \tag{19}$$

The symplectic structure on $\mathbb{C}\mathrm{P}^{N-1}$ represents the curvature of our connection. The second homotopy group of the projective space $\mathbb{C}\mathrm{P}^{N-1}$ is $\mathbb{Z}$, i.e., $\pi_2(\mathbb{C}\mathrm{P}^{N-1}) = \mathbb{Z}$. The first Chern number of the bundle (2) restricted to any noncontractible compact submanifold $\Sigma_2 \subset \mathbb{C}\mathrm{P}^{N-1}$ is nontrivial, i.e.,

$$c_1 \;=\; \frac{1}{2\pi}\int_{\Sigma_2} F \;\neq\; 0\,. \tag{20}$$

Moreover,

$$\frac{1}{(2\pi)^N}\int_{\mathbb{C}\mathrm{P}^{N-1}} F^{\wedge N} \;\neq\; 0\,, \tag{21}$$

also showing that the bundle (18) is nontrivial.

2.2. Uhlmann phase

If we consider the projection from the unit sphere $S^{2N-1} = \{\boldsymbol{z} \in \mathbb{C}^N : \|\boldsymbol{z}\| = 1\}$ to the complex projective space, it is possible to define

$$\begin{aligned} \pi : \mathbb{C}_0^N \;&\longrightarrow\; \mathbb{C}\mathrm{P}^{N-1} \\ |\boldsymbol{z}\rangle \;&\longmapsto\; \frac{|\boldsymbol{z}\rangle\langle\boldsymbol{z}|}{\langle\boldsymbol{z}|\boldsymbol{z}\rangle} \;=\; \rho_{\boldsymbol{z}}\,, \end{aligned} \tag{22}$$

i.e., pure states are represented by rank-one projectors.

This representation is an embedding of the complex projective space in the real vector space of Hermitian operators. This point of view is quite convenient because Hermitian matrices are isomorphic to the vector space of the Lie algebra $\mathfrak{u}(N)$ of the unitary group $\mathrm{U}(N)$.

We can briefly review the previous arguments by means of this identification. Remember that $\mathbb{C}\mathrm{P}^{N-1}$ is the manifold of rays of $\mathbb{C}^N$. At each point $\rho_{\boldsymbol{z}} \in \mathbb{C}\mathrm{P}^{N-1}$, the vectors in the tangent space $T_{\rho_{\boldsymbol{z}}}\mathbb{C}\mathrm{P}^{N-1}$ arise from

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{U(t)|\boldsymbol{z}\rangle\langle\boldsymbol{z}|U(t)^\dagger}{\langle\boldsymbol{z}|\boldsymbol{z}\rangle}\Big|_{t=0} \;=\; -i[K,\rho_{\boldsymbol{z}}] \;=\; X\,, \quad K = K^\dagger, \quad X \in T_{\rho_{\boldsymbol{z}}}\mathbb{C}\mathrm{P}^{N-1}\,, \tag{23}$$

where $U(t) = \exp(-itK)$ is the unitary group generated by K. Thus K is determined by X up to a matrix commuting with $\rho_{\boldsymbol{z}}$. However, this ambiguity will not affect the definition of the symplectic structure we are going to give.

If $\rho_{\boldsymbol{z}} = |\boldsymbol{z}\rangle\langle\boldsymbol{z}|$ and $\boldsymbol{w}$ is a vector orthogonal to $\boldsymbol{z}$, $\langle\boldsymbol{z}|\boldsymbol{w}\rangle = 0$, we may write

$$\begin{aligned} K \;&=\; i(|\boldsymbol{w}\rangle\langle\boldsymbol{z}| - |\boldsymbol{z}\rangle\langle\boldsymbol{w}|)\,, \\ X \;&=\; |\boldsymbol{w}\rangle\langle\boldsymbol{z}| + |\boldsymbol{z}\rangle\langle\boldsymbol{w}|. \end{aligned} \tag{24}$$

The connection one-form $\mathcal{A}$ may be used to define horizontal lifts of smooth curves in $\mathbb{C}\mathrm{P}^{N-1}$. If $\gamma = \{\rho(s) \in \mathbb{C}\mathrm{P}^{N-1} : s \in [s_1, s_2], \rho(s_1) = \rho(s_2)\} \subset$

$\mathbb{C}\mathrm{P}^{N-1}$ is a smooth parametrised closed curve in $\mathbb{C}\mathrm{P}^{N-1}$, and $\gamma_h = \{\boldsymbol{z}(s) \in S^{2N-1} : s \in [s_1, s_2]\} \subset S^{2N-1}$ is a horizontal lift of γ to S^{2N-1}, then at each point of γ_h we have

$$\mathcal{A}_{\boldsymbol{z}(s)}(\dot{\boldsymbol{z}}(s)) \;=\; -i\langle \boldsymbol{z}(s)|\dot{\boldsymbol{z}}(s)\rangle \;=\; 2\,\mathrm{Im}\langle \boldsymbol{z}(s)|\dot{\boldsymbol{z}}(s)\rangle \;=\; 0\,. \tag{25}$$

This lift γ_h of γ is not closed in general, as $\boldsymbol{z}(s_1)$ and $\boldsymbol{z}(s_2)$ may differ by an element in U(1). This is the U(1) holonomy group element and gives the geometric phase associated with γ:

$$\arg\langle \boldsymbol{z}(s_1)|\boldsymbol{z}(s_2)\rangle \;=\; -\int_\Sigma \mathrm{d}\mathcal{A}\,, \quad \partial\Sigma = \gamma\,, \tag{26}$$

where $\Sigma \subset \mathbb{C}\mathrm{P}^{N-1}$ is any smooth two-dimensional surface with boundary γ. This geometric phase is the Aharonov–Anandan phase of pure quantum states.

The bundle picture emerges very simply if we notice that given a fiducial normalised vector $\boldsymbol{z}$, such that $|\boldsymbol{z}\rangle\langle\boldsymbol{z}| = \rho_{\boldsymbol{z}}$, then S^{2N-1} can be identified with $\mathrm{U}(N)/\mathrm{U}(N-1)$, as $\mathrm{U}(N)$ acts transitively on all normalised vectors and $\mathrm{U}(N-1)$ is the isotropy group of $\boldsymbol{z}$. By further modding out by U(1), to go from $\boldsymbol{z}$ to $\rho_{\boldsymbol{z}} = |\boldsymbol{z}\rangle\langle\boldsymbol{z}|$, we get the U(1)-bundle

$$\mathrm{U}(1) \;\longrightarrow\; \frac{\mathrm{U}(N)}{\mathrm{U}(N-1)} \;\longrightarrow\; \frac{\mathrm{U}(N)}{\mathrm{U}(N-1)\times\mathrm{U}(1)}\,. \tag{27}$$

What is remarkable is that not only $\mathrm{U}(N)$ acts on rank-one projections but also its complexification $\mathrm{GL}(N,\mathbb{C})$. Indeed, for any vector $\boldsymbol{z} \in \mathbb{C}^N_0$, we have $T : \boldsymbol{z} \mapsto T\boldsymbol{z}$. To obtain a normalised vector we have to modify the action into a nonlinear one

$$T : \boldsymbol{z} \;\longmapsto\; \frac{T\boldsymbol{z}}{\sqrt{\langle T\boldsymbol{z}|T\boldsymbol{z}\rangle}}\,, \tag{28}$$

however, this action passes to the complex projective space according to

$$\frac{T|\boldsymbol{z}\rangle\langle\boldsymbol{z}|T^\dagger}{\langle T\boldsymbol{z}|T\boldsymbol{z}\rangle} \;=\; \frac{T\rho T^\dagger}{\mathrm{tr}(T\rho T^\dagger)}\,. \tag{29}$$

Thus the complex projective space is also an orbit of $\mathrm{SL}(N,\mathbb{C})$. These remarks are useful when dealing with generic mixed states, not only pure states.

2.3. A bundle picture for the Uhlmann phase of mixed states

In finite dimensions there are a few remarkable "coincidences". Given the complex Hilbert space $\mathbb{C}^N$, the space $B(\mathbb{C}^N)$ of linear operators is isomorphic to $\mathbb{C}^N \otimes \mathbb{C}^{N*}$ and may be considered itself a Hilbert space. $B(\mathbb{C}^N)$ is a C^*-algebra, it carries a $*$-involution $A \mapsto A^\dagger$. Every element $M \in B(\mathbb{C}^N)$ may be written uniquely as $M = A + iB$, where $A = A^\dagger$ and $B = B^\dagger$ are Hermitian operators. $B(\mathbb{C}^N)$ has a Lie algebra structure and corresponds to the Lie algebra $\mathfrak{gl}(N, \mathbb{C})$ of $\mathrm{GL}(N, \mathbb{C})$, the complexification of $\mathrm{U}(N)$. The Hermitian scalar product on $B(\mathbb{C}^N)$ given by the Hilbert–Schmidt product

$$\langle M_1 | M_2 \rangle \; = \; \mathrm{tr}(M_1^\dagger M_2) \tag{30}$$

may be split into its real and imaginary part: $\mathrm{tr}(M_1^\dagger M_2 + M_2^\dagger M_1)/2$ and $-i\,\mathrm{tr}(M_1^\dagger M_2 - M_2^\dagger M_1)/2$. It turns out that $\mathfrak{gl}(N, \mathbb{C})$ as a Lie algebra is symplectomorphic to $T^*(\mathfrak{u}(N))$, i.e., $\mathrm{GL}(N, \mathbb{C})$ is symplectomorphic to $T^*(\mathrm{U}(N))$.

These various "coincidences" have been exploited to consider $B(\mathbb{C}^N)$ as a bundle space whose group is the unitary group and the base manifold is the space of mixed states. The construction goes along the following lines. We consider the projection

$$\begin{aligned} \pi : B(\mathbb{C}^N) \;&\longrightarrow\; H_+ \\ M \;&\longmapsto\; MM^\dagger\,, \end{aligned} \tag{31}$$

where H_+ is the space of Hermitian positive operators. Each fibre is diffeomorphic to $\mathrm{U}(N)$, indeed MU and M give rise to the same positive operator

$$MU(MU)^\dagger = MM^\dagger \quad \text{for all} \quad U \in \mathrm{U}(N)\,. \tag{32}$$

It may be convenient to consider also the projection $M \mapsto M^\dagger M$, where the fibre will be generated by the left action of the unitary group $M \mapsto UM$, so that $M \mapsto M^\dagger M = (UM)^\dagger UM$.

If we "normalise" our projection, say

$$\tilde{\pi} : M \longmapsto \frac{MM^\dagger}{\mathrm{tr}(MM^\dagger)}\,, \tag{33}$$

the image of this projection does coincide with the space of all mixed states. Having defined the normalised projection by means of the right action, it follows that the left action of $\mathrm{GL}(N, \mathbb{C})$ passes to the quotient. We have

$$T \longmapsto TM\,, \qquad \tilde{\pi} : TM \longmapsto \frac{TMM^\dagger T^\dagger}{\mathrm{tr}(TMM^\dagger T^\dagger)}\,. \tag{34}$$

By introducing the polar decomposition $M = \sqrt{\rho}U$ we find

$$MM^\dagger \; = \; \sqrt{\rho}UU^\dagger\sqrt{\rho} \; = \; \rho\,. \tag{35}$$

The orbits generated by the action of $\mathrm{GL}(N, \mathbb{C})$, say

$$\frac{T\rho T^\dagger}{\mathrm{tr}(T\rho T^\dagger)}\,, \tag{36}$$

decompose the space of mixed states into strata, according to the rank of ρ. Therefore, the total space is partitioned into N-strata of orbits, the one corresponding to rank-one operators M will give the complex-projective space of pure states we have considered earlier. Except for the rank-one orbit, the other orbits are not symplectic manifolds and turn out to be the union of symplectic orbits with changing dimensions. This fact is related to the circumstance that symplectic orbits are associated with the spectrum of the mixed state, while the orbits of $\mathrm{GL}(N, \mathbb{C})$ are associated with the rank of the state.

Taking into account the normalisation, it is immediate to notice that the central subgroup of $\mathrm{GL}(N, \mathbb{C})$, generated by $\lambda\mathbb{I}$, with $\lambda \in \mathbb{C}_0$, acts trivially, therefore the orbits are actually orbits of $\mathrm{SL}(N, \mathbb{C})$.

Let us now restrict ourselves to mixed states of maximal rank. They span the main stratum, a dense subset, $\mathcal{D}_0 \in \mathcal{D}$ of the space of all mixed states $\mathcal{D}$. In order to define a connection which generalizes the Aharonov–Anandan connections we need to consider a principal $U(N)$-bundle structure over $\mathcal{D}_0$ [9 − 12].

Let us consider the submanifold $\mathrm{GL}_0(N, \mathbb{C})$ of $\mathrm{GL}(N, \mathbb{C})$ given by the matrices of unit Hilbert–Schmidt norm, i.e., $\mathrm{GL}_0(N, \mathbb{C}) = \{M \in \mathrm{GL}(N, \mathbb{C}) : \langle M|M\rangle = 1\}$.

The right action of $U(N)$ on $\mathrm{GL}_0(N, \mathbb{C})$: $A \mapsto AU$ defines a principal fibre bundle over the space of mixed states of maximal rank $\mathcal{D}_0$,

$$\mathrm{GL}_0(N, \mathbb{C})(\mathcal{D}_0, \mathrm{U}(N))\,. \tag{37}$$

Following the definition of the metric in the case of pure states we can define a metric in $\mathrm{GL}_0(N, \mathbb{C})$ by

$$g(M_1, M_2) \;=\; \mathrm{Re}\langle M_1|M_2\rangle\,, \tag{38}$$

associated with the Hilbert–Schmidt inner product (30). This metric can be related to the Bures metric defined on the same space [13, 17].

As in the case of pure states, the Riemannian metric structure (38) of $\mathrm{GL}_0(N, \mathbb{C})$ induces a connection on the bundle (37) given by the distribution of horizontal spaces of $T_M\mathrm{GL}_0(N, \mathbb{C})$ which are orthogonal to the $\mathrm{U}(N)$ fibres. This connection is the Uhlmann connection [9 − 12]. The connection is defined by the one-form $\mathcal{A}_U$ with values on the Lie algebra $\mathfrak{u}(N)$ of $\mathrm{U}(N)$ which vanish on the horizontal subspaces of $T_M\mathrm{GL}_0(N, \mathbb{C})$. The explicit form of the connection is more involved than that of the Aharonov–Anandan connection for pure states, although can be derived from a quite simple analysis.

The space of horizontal vectors $T_M\mathrm{GL}_0(N, \mathbb{C})$ is given by all vectors X which satisfy

$$X^\dagger M - M^\dagger X \;=\; 0\,. \tag{39}$$

This is so, because any vector tangent to the fibres is of the form $iM\phi$, where ϕ is any $N \times N$ Hermitian matrix, and since $g(X, iM\phi) = 0$, it follows that $\mathrm{Re}\,\mathrm{tr}(iX^\dagger M\phi) = 0$. Since the equation holds for any Hermitian matrix ϕ, $X^\dagger M$ must be Hermitian, which implies (39).

In the same way it can be shown that the vertical vectors of $T_M \mathrm{GL}_0(N, \mathbb{C})$ which are tangent to the gauge fibres are of the form $Y_\phi = iM\phi$ and can be identified with the solutions of

$$Y_\phi^\dagger M + M^\dagger Y_\phi \; = \; 0 \,. \tag{40}$$

Therefore, the one form $\mathcal{A}_U$ characterising Uhlmann connection has to satisfy the two conditions

$$\mathcal{A}_U(X) \; = \; 0 \quad \text{and} \quad \mathcal{A}_U(Y_\phi) \; = \; i\phi \,. \tag{41}$$

This implies that

$$\mathcal{A}_U M^\dagger M + M^\dagger M \mathcal{A}_U \; = \; M^\dagger \mathrm{d}M - (\mathrm{d}M^\dagger)M \,. \tag{42}$$

Notice that from this relation it follows that $\mathcal{A}_U$ take values in $\mathfrak{u}(N)$ and vanish for horizontal tangent vectors.

This implicit formula can be made more explicit if we consider an orthonormal basis $\{|e_j\rangle,\, j = 1, 2, \ldots, N\}$ of $\mathbb{C}^N$ which diagonalises the positive definite matrix $M^\dagger M$,

$$M^\dagger M|e_j\rangle \; = \; c_j|e_j\rangle \,. \tag{43}$$

In such a case

$$\langle e_j|\mathcal{A}_U M^\dagger M|e_k\rangle + \langle e_j|M^\dagger M \mathcal{A}_U|e_k\rangle = \langle e_j|M^\dagger \mathrm{d}M|e_k\rangle - \langle e_j|(\mathrm{d}M^\dagger)M|e_k\rangle \tag{44}$$

which implies, by setting $M = U\sqrt{M^\dagger M}$,

$$\begin{aligned}(c_k + c_j)\langle e_j|\mathcal{A}_U|e_k\rangle \; &= \; \langle e_j|M^\dagger \mathrm{d}M|e_k\rangle - \langle e_j|(\mathrm{d}M^\dagger)M|e_k\rangle \qquad (45)\\ &= \; \langle e_j|[\,\sqrt{M^\dagger M}, \mathrm{d}\sqrt{M^\dagger M}\,]|e_k\rangle + 2\sqrt{c_j c_k}\langle e_j|U^\dagger \mathrm{d}U|e_k\rangle \,,\end{aligned}$$

whence

$$\langle e_j|\mathcal{A}_U|e_k\rangle \; = \; \frac{\langle e_j|[\,\sqrt{M^\dagger M}, \mathrm{d}\sqrt{M^\dagger M}\,]|e_k\rangle}{c_k + c_j} \,. \tag{46}$$

The holonomy of this connection is the Uhlmann phase [9, 10].

2.4. Remark

The bundle (37) which we have constructed over the space of maximal rank mixed states is trivial, unlike the one we have constructed for pure states.

Indeed the base manifold is contractible being diffeomorphic to a vector space (this may be seen from the diffeomorphism $\mathrm{GL}(N,\mathbb{C}) \simeq T^*\mathrm{U}(N)$). A direct proof follows from the polar decomposition $M = \sqrt{\rho}U = \sqrt{MM^\dagger}U$, which allows to define a global section $\sigma : \mathcal{D}_0 \to S^{2N-1} \subset \mathrm{GL}_0(N,\mathbb{C})$ given by $\sigma(\rho) = M_\rho = \sqrt{\rho}$ [18].

Thus, all the characteristic classes of the bundle vanish. In particular, for any $n = 1, 2, \ldots, \left[(N^2-1)/2\right]$, where the bracket denotes the integer part, one gets

$$c_n(\mathcal{A}_U) = \frac{1}{(2\pi)^{2n}} \int_{\Sigma^{2n}} \mathrm{tr}\left\{F(\mathcal{A}_U)^{\wedge 2n}\right\} = 0\,, \tag{47}$$

for any closed $2n$-dimensional submanifold Σ^{2n} of $\mathcal{D}_0$.

This result is quite remarkable because it is in contrast with what happens for pure states, where the connection that generates the Aharanov–Ananadan phase is topologically nontrivial, and the corresponding Chern class does not vanish, whereas for mixed states the connection which generates the Uhlmann phase has vanishing Chern classes.

Among the states which are of maximal rank there are *thermal states*:

$$\rho_T = \frac{e^{-H/T}}{\mathrm{tr}(e^{-H/T})}\,. \tag{48}$$

Now, thermal states converge in the zero temperature limit to a pure state, provided that the Hamiltonian $H = H^\dagger$ has a non-degenerated ground state $|0\rangle$, i.e.,

$$\lim_{T\to 0} \rho_T = |0\rangle\langle 0|\,. \tag{49}$$

This leads to a surprising phenomenon: the emergence of topological order in the zero temperature limit of thermal states. How the triviality of the Uhlmann phase topology for any finite temperature can lead to the non-trivial Aharonov–Anandan topology in the zero temperature limit [19–23]? This is a well posed problem which deserves to be understood.

In order to find a framework, where the nontrivial topology can play a role in the dynamics of mixed states it is convenient to exclude from the space of mixed states the state of maximal entropy which corresponds to maximal disorder

$$\rho_* = \frac{1}{N}\mathbb{I}\,. \tag{50}$$

This extra requirement might be physically motivated by the fact that Gibbs thermal states ρ_T (48) of nondegenerated Hamiltonians are only maximally disordered at infinite temperature, i.e., ρ_T (48) belongs to the main strata of mixed states $\mathcal{D}_0$ for any finite temperature T. Therefore, excluding such singular states will be natural for generic thermal systems.

In such case it is trivial to see that the corresponding space of physical states $\mathcal{D}_* = \mathcal{D}_0 \backslash \{\rho_*\}$ acquires a nontrivial topology. In fact $\mathcal{D}_*$ becomes homeomorphic to $S^{N^2-2} \times (0,1)$ which inherits the nontrivial topology of the sphere S^{2N-1}. However, the restriction of the bundle (37) to $\mathcal{D}_*$

$$\mathrm{GL}_*(N,\mathbb{C})(\mathcal{D}_*, \mathrm{U}(N))\,, \tag{51}$$

where $\mathrm{GL}_*(N,\mathbb{C}) = \{M \in \mathrm{GL}_0(N,\mathbb{C}) : \det M = 1/\sqrt{N}\}$ is again a trivial bundle because the section $\sigma : \mathcal{D}_* \to \mathrm{GL}_*(N,\mathbb{C})$ given by $\sigma(\rho) = \sqrt{\rho}$ is a global section in the new framework too.

For such a reason there have been many attempts to define new topological invariants which extend the topological order to thermal states at finite temperatures [19 − 29]. For instance, one proposal is to define the modified Chern classes by weighting them with the density matrix, e.g.,

$$c_n(\mathcal{A}_U) \;=\; \frac{1}{(2\pi)^{2n}} \int_{\Sigma^{2n}} \mathrm{tr}\Big\{ M M^\dagger F(\mathcal{A}_U)^{\wedge 2n} \Big\}\,. \tag{52}$$

Unfortunately this approach is not stable under small perturbations.

If we have a family of nonmaximally-disordered mixed states periodically depending on N^2-2 parameters $\rho(\epsilon_1, \epsilon_2, \ldots, \epsilon_{N^2-2})$, there is a new possibility for the introduction of new topological invariants by means of the winding number

$$\nu \;=\; \frac{1}{(2\pi)^{N^2-2}} \int_{\mathbb{T}^{N^2-2}} \mathrm{tr}\Big\{ (\rho^{-1}\mathrm{d}\rho)^{\wedge N^2-2} \Big\} \tag{53}$$

of the map $\rho : \mathbb{T}^{N^2-2} \to \mathcal{D}_0$. The winding number of the map ρ is a topological invariant which is stable under smooth perturbations. In particular, it might survive in the zero temperature limit. This opens a new perspective in the analysis of topological matter at finite temperature, extending the standard theory which has been formulated at zero temperature.

3. Topology and Floquet–Bloch Theorems

In order to analyse the extension of recent analyses of topological matter to finite temperature and open dynamics let us consider the example of an electron in a perfect crystal.

Electrons moving in the periodic potential of a perfect crystal split their Hilbert space of quantum states on a bundle of Floquet–Bloch states over a d-dimensional torus $\mathbb{T}^d$. If we assume a cubic symmetry, the translation symmetry group $\mathbb{Z}^d$ is generated by the lattice of space translations $T_j = \mathrm{e}^{iap_j}$, $j = 1, 2, \ldots, d$, where a is the crystal cell period and $p_j = -i\partial_j$ the momentum operator.

The symmetry of the crystal implies that the Hamiltonian is invariant under lattice translations

$$T_j H = H T_j \quad \text{or} \quad T_j H T_j^\dagger = H \,. \tag{54}$$

The Hilbert space can be decomposed as a direct sum (in fact, a direct integral) of irreducible representations of $\mathbb{Z}^d$

$$\mathcal{H} \;=\; \bigoplus_{\epsilon\in\mathbb{T}^d} \mathcal{H}_\epsilon \,, \tag{55}$$

where $\epsilon \in \mathbb{T}^d$ is the label of the irreducible representation of $\mathbb{Z}^d$, i.e.,

$$T_j \boldsymbol{z}_\epsilon(x) \;=\; \mathrm{e}^{ia\epsilon_j} \boldsymbol{z}_\epsilon(x) \,, \quad 0 \le \epsilon_j \le \frac{2\pi}{a} \,, \tag{56}$$

which defines the Brillouin zone of the crystal. Now, since the periodic Hamiltonian H of the system commutes with the symmetry group, it can be decomposed into diagonal blocks labeled by the irreducible representations of $\mathbb{Z}^d$,

$$H \;=\; \bigoplus_{\epsilon\in\mathbb{T}^d} H_\epsilon \,. \tag{57}$$

More precisely, the Floquet–Bloch decomposition defines a bundle over $\mathbb{T}^d$ whose fibres are the Hilbert spaces $\mathcal{H}_\epsilon$ defined by the states satisfying the conditions (56), i.e.,

$$\boldsymbol{z}_\epsilon(x + a e_j) \;=\; \mathrm{e}^{ia\epsilon_j} \boldsymbol{z}_\epsilon(x) \,, \tag{58}$$

where e_j is the j-th vector of the canonical basis of $\mathbb{R}^d$. If there are N bands, the Hilbert spaces $\mathcal{H}_\epsilon$ are N-dimensional $\mathcal{H}_\epsilon \simeq \mathbb{C}^N$, and the bundle is a rank-N bundle $E(\mathbb{T}^d, \mathbb{C}^N)$. Pure states of the solid bands are sections of such a bundle.

Now, if the bundle is nontrivial as in the two-dimensional ($d = 2$) integer Hall effect, its nontrivial topology gives rise to interesting conducting/insulating properties characterised by topological invariants [30, 31]. These phenomena can be associated with the appearance of nontrivial phases in periodic cycles of pure band states. The phases are not pure Aharanov–Anandan phases because they are twisted by the dynamics induced by the connection $\mathcal{A}$ of the bundle E. Using the Fourier–Mukai transform [32, 33] we can associate with $\mathcal{A}$ another connection $\hat{\mathcal{A}}$ in the dual bundle $\hat{E}(\hat{\mathbb{T}}^2, \mathbb{C}^k)$ with rank k, the first Chern number $k = c_1(E)$ of E, and with $c_1(\hat{E}) = N$ [32, 33, 31]. This duality transformation is the source of quantisation of the Hall conductivity [30].

However, these topological arguments cannot be extended to the case of mixed systems because if we consider mixed states which are invariant under the $\mathbb{Z}^2$ lattice symmetry,

$$T_j \rho \;=\; \rho T_j \,, \tag{59}$$

they can be decomposed as a sum of mixed states on the first Brillouin zone $\mathbb{T}^2$

$$\rho \;=\; \bigoplus_{\epsilon\in\mathbb{T}^2} \rho_\epsilon\,, \tag{60}$$

or in other terms as a section in the bundle of $\mathcal{E}(\mathbb{T}^2, H_+)$ associated with E by the adjoint representation of $\mathrm{U}(N)$, where H_+ denotes the space of nonnegative Hermitian operators in $\mathbb{C}^N$. In such a case there is no phase associated with ρ in periodic cycles of $\mathbb{T}^2$. However, the global map given by the section ρ can have a nontrivial winding number given by

$$\nu_2 \;=\; \frac{1}{2\pi}\int_{\mathbb{T}^2} \mathrm{tr}\{\rho_\epsilon^{-1}\mathrm{d}\rho_\epsilon \wedge \rho_\epsilon^{-1}\mathrm{d}\rho_\epsilon\}\,, \tag{61}$$

where we assumed that ρ_ϵ is neither pure for any ϵ nor maximally disordered, i.e., $\det\rho_\epsilon \neq 0$ and $\rho_\epsilon \neq \alpha\,\mathbb{I}$.

In such a case we can associate a nontrivial topology with the mixed states with $\nu_2 \neq 0$, but the physical effects of such a property are unclear because they cannot be related to the quantisation of Hall conductivity. In fact, there exist topologically nontrivial mixed states even in the absence of magnetic fields, i.e., when the bundle E is trivial.

4. Open Systems

The dynamics of open systems is governed by the GKLS equation [34, 35, 36]

$$\dot\rho \;=\; -i[H,\rho] + \sum_{i=1}^{N^2-1}\Big(K_i\rho K_i^\dagger - \frac{1}{2}\{K_i^\dagger K_i,\rho\}\Big)\,, \tag{62}$$

where $H = H^\dagger$ is the generator of the unitary part of the evolution, while the jump operators K_i yield decoherence and dissipation.

In the case of a particle in a periodic lattice one can generalise the analysis of the previous section, provided that, together with the Hamiltonian invariance (54), one also has

$$T_j K_i T_j^\dagger \;=\; K_i\,. \tag{63}$$

In such a case, all jump operators have a direct sum decomposition on the first Brillouin zone, $\epsilon \in \mathbb{T}^2$,

$$H \;=\; \bigoplus_{\epsilon\in\mathbb{T}^d} H_\epsilon\,, \qquad K_i \;=\; \bigoplus_{\epsilon\in\mathbb{T}^d} K_{\epsilon,i}\,. \tag{64}$$

Moreover, since

$$T_j\dot\rho T_j^\dagger \;=\; \dot\rho\,, \tag{65}$$

one gets that the block decomposition (60) is preserved and the evolution of each block is decoupled from the others, namely

$$\dot{\rho}_\epsilon \;=\; -i[H_\epsilon, \rho_\epsilon] + \sum_{i=1}^{N^2-1} \left(K_{\epsilon,i}\rho_\epsilon K_{\epsilon,i}^\dagger - \frac{1}{2}\{K_{\epsilon,i}^\dagger K_{\epsilon,i}, \rho_\epsilon\} \right), \tag{66}$$

for all $\epsilon \in \mathbb{T}^2$.

Now, one can show that the winding number (61) is invariant under the evolution of the open system, because

$$\nu_2(\dot{\rho}_\epsilon) \;=\; 0\,, \tag{67}$$

whenever for any value of ϵ the time evolution does not drive the system into the maximally disorder state ρ_* or into lower rank states.

The topological stability of an open system is essentially due to the continuity of dynamical evolution driven by the GKLS equation [37]. The analysis and classification of topological transitions, where the winding number jumps is an open interesting problem which deserves further study.

From the topological viewpoint the behaviour of the dynamics of open systems is richer than that driven by the adiabatic evolution of thermal systems, where such a transition only occurs in the extreme limits of zero and infinite temperature.

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