Topological effects in the magnetoresistance of Au and Ag.

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We present the results of our numerical exploration of the asymptotic properties of quasi-electron orbits in Au and Ag under a strong magnetic field. Our analysis represents the first quantitative comparison between the magnetorestance maps obtained from experimental data in early Sixties and the Lifshitz model for the transverse magnetoresistance behaviour in metals with a topologically non-trivial Fermi Surface.

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The relevance of the geometry and topology of the Fermi Surface (FS) in physical phenomena is well known since Thirties, when Justi and Scheffers showed evidences that the FS of Gold is open [1]. One of the most striking examples of such phenomena is the behaviour of magnetoresistance in monocrystals at low temperatures in high magnetic fields [2].

It was Lifshitz *et al.* [3] the first to notice that, under the conditions stated above, the magnetoresistance behaviour is dictated only by the topological properties of orbits of quasi-momenta: as the magnetic field $H \to \infty$ the magnetoresistance saturates isotropically to an asymptotic value if the orbits are all closed, while it grows quadratically with H if there are open orbits (Fig. 1). Stereographic Maps (SM) showing the set of $\boldsymbol{H}$ directions for which the magnetoresistance does not saturate were experimentally obtained in the following years for about thirty metals [9], initially by Gaidukov *et al.* (e.g. [4, 5]) and later by several other groups.

Such SM were, in those years, one of the main tools to study electron energy spectra; nowadays such use is out of fashion, since many different and more precise methods are available, but nevertheless SM constitute a highly non-trivial experimental data in themselves and no verification of them from first principles was provided till now in literature, except for qualitative sketches like those published by Lifshitz (see Fig. 4b).

Several papers (e.g. [6–10]), mainly published in Fifties and Sixties, testify a large efforts of the Physics community to understand the relation between the direction of $\boldsymbol{H}$ and the topology of the orbits of quasi-momenta for a generic FS but the problem turned out to be too difficult was eventually abandoned. The method we introduce in this letter, suggested by I. Dynnikov and implemented by the author, allows for the first time not only to verify the SM available in literature but also to predict extremely accurate SM for new FS. In this work we focus our attention to Au and Ag, whose SM were measured by Gaidukov and Alexeevskii in early Sixties [4, 5].

In order to make fully understandable the nature of our results we will summarize below the results [11–13] on the subject obtained recently by Mathematicians.

The extremely rich topological structure underlying this phenomenon was discovered indeed only in Eighties and Nineties by former S.P. Novikov's students A. Zorich and I. Dynnikov after that Novikov [14] recognized the purely topological character of the problem. Their results lead to the following picture: once a FS is given, if open orbits arise for electrons quasi-momenta for some direction of the magnetic field, then such directions are sorted in some finite number of "islands" called Stability Zones (SZ) (e.g see Fig. 4c); each SZ is labeled by a Miller index $\boldsymbol{L}$ in such a way that each open orbit generated by any $\boldsymbol{H}$ belonging to a SZ with label $\boldsymbol{L}$ is a finite deformation of a straight line whose direction is given by $\boldsymbol{H} \times \boldsymbol{L}$; all directions that do not belong to these SZ give rise only to closed orbits, except for a negligible set of exceptional directions that can be safely disregarded in this Letter.

The Miller index $\boldsymbol{L}$ is a new quantum first integral whose existance was totally unexpected before the analysis by Novikov and his pupils and we will show below that it constitutes the key to build an algorithm able to evaluate the topology of quasi-electrons momenta.

As it is well known, under the appropriate conditions, namely a $\boldsymbol{H}$ so strong to make electrons' mean path big enough to feel the FS topology (i.e. $\omega_c \tau \gg 1$) but not strong enough to destroy the FS by magnetic breakdown (that sets the range of $\boldsymbol{H}$ ranges roughly between $10T$ and $10^3 T$), quasi-electrons orbits are given by

$$\dot{\boldsymbol{p}} = \boldsymbol{H} \times \partial \mathcal{E}_n(\boldsymbol{p}) / \partial \boldsymbol{p} = \{\boldsymbol{p}, \mathcal{E}_n(\boldsymbol{p})\}_H \qquad (1)$$

where $\mathcal{E}_n(\boldsymbol{p})$ is the energy function for the electrons occupying the n-th band and $\{,\}_H$ is the so-called "magnetic bracket": $\{p_\alpha, p_\beta\}_H = \epsilon_{\alpha\beta\gamma} H^\gamma$.

This dynamical system looks at first sight like a standard classical mechanics system but at a more accurate look it reveals to be of a rather different nature. In classical mechanics indeed momenta belong necessarily to a linear space while in these case the Bloch theorem dictates that they belong to the first Brillouin zone, topolog-

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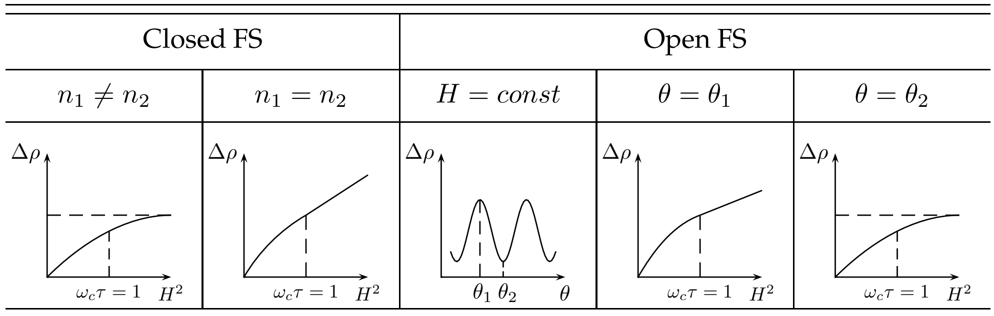

FIG. 1: [15] Behaviour of $\boldsymbol{\rho}$ in metals with closed and open FS. (Closed) $\boldsymbol{\rho}$ is isotropic and saturates unless the density of electrons and holes coincide, in which case $\boldsymbol{\rho} \sim H^2$. (Open) $\boldsymbol{\rho}$ is highly anisotropic and it shows qualitatively different behaviour in min and max: in max $\boldsymbol{\rho} \sim H^2$ while in min it saturates (θ is the angle between H and the crystallographic axis).

ically equivalent to a three-torus $\mathbb{T}^3$ and therefore carrying a non-trivial topology. It is noteworthy to point out that not even the most trivial of such systems were studied till now by the dynamical systems community, probably because such problems only originate from quantum mechanical systems, and it was a striking surprise to discover a rich structure even in the most simple cases.

The non-trivial topology of $\mathbb{T}^3$ has strong consequences on eq. 1: indeed the second of its two first integrals $\mathcal{E}_n$ and $\boldsymbol{p} \cdot \boldsymbol{H}$ is not a well-defined function but rather a *multi*-valued function, since it depends linearly by the "angular" variables p_i. It is exactly this fact that allows the existence of open orbits, since in the three-space any dynamical system with a closed energy surface and a *single*-valued second integral of motions can give rise only to closed orbits.

The origin of the quantum first integral $\boldsymbol{L}$ is easily seen by looking at what happens for any *rational* $\boldsymbol{H}_0$, i.e. any magnetic field pointing at some lattice direction, giving rise to open orbits. In that case indeed we can indeed assume with no loss of generality that $\boldsymbol{H}_0 = (0, 0, 1)$ and in the generic case all sections of the FS $\mathcal{E}(\boldsymbol{p}) = E_F$ by the planes $\boldsymbol{p} \cdot \boldsymbol{H}_0 = c$ are a finite set of disjoint closed and/or open orbits except for some finite number of critical levels where pairs of orbits meet. The cases shown in Fig. 2a,b represent the only critical levels that involve open orbits: the first one represents the meeting of two open orbits that annihilate to give rise to a closed orbit, or equivalently an open orbit that meets a closed orbit and bounces back; the second one the merging of a closed orbit in an open one. In each case it turns out that a single open orbit will never disappear but rather will either bounce or merge with closed orbits till it will come back to itself by periodicity, describing so either a warped cylinder or a warped plane with some finite number of holes corresponding to closed orbits. The critical observation is that closed orbits are stable by small perturbations of $\boldsymbol{H}_0$ and therefore open orbits will be *confined* to the warped planes and cylinders above for any $\boldsymbol{H}$ close enough to $\boldsymbol{H}_0$. Since a generic $\boldsymbol{H}$ gives rise only to closed orbits on any warped cylinder, we are finally

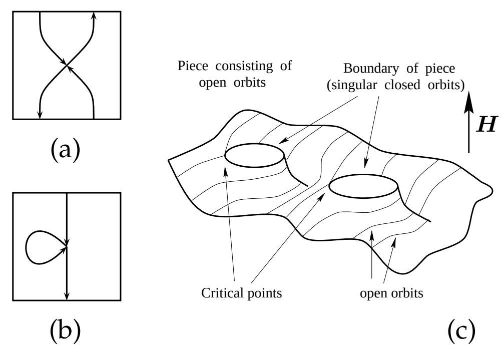

FIG. 2: Possible kind of open saddles for rational H: (a) Fully open saddle. (b) Half-open saddle. (c) Warped plane covered by open orbits [13].

led to the conclusion that open orbits for a generic $\boldsymbol{H}$ are confined to warped planes separated from each other by cylinders of closed orbits (see Fig 2c).

Such warped planes are made by components of the FS plus some number of flat discs covering their holes and they are therefore periodic and can be sandwiched between a pair of parallel lattice plane with some Miller index $\boldsymbol{L}$. Small perturbations in $\boldsymbol{H}$ direction cannot destroy but only slightly modify warped planes so that, since the Miller indices depend continously on the warped planes and are a discrete set, it turns out that $\boldsymbol{L}$ is a locally constant function of the direction of $\boldsymbol{H}$.

This quantum first integral was unknown to Physicist that worked on the problem in Fifties and Sixties and was first discovered by Zorich [16] in Eighties. Its knowledge is enough on one hand to grant that no two SZ overlap, since all warped planes appearing for some $\boldsymbol{H}$ must have the same Miller index, and on the other hand to determine completely the asymptotic behaviour of open orbits, since they clearly are asymptotic to a straight line with direction $\boldsymbol{H} \times \boldsymbol{L}$. In particular this shifts the numerical problem from determining the asymptotic behaviour of open orbits, clearly impossible to be carried out exactly in the generic case, to evaluate the Miller index. We leave

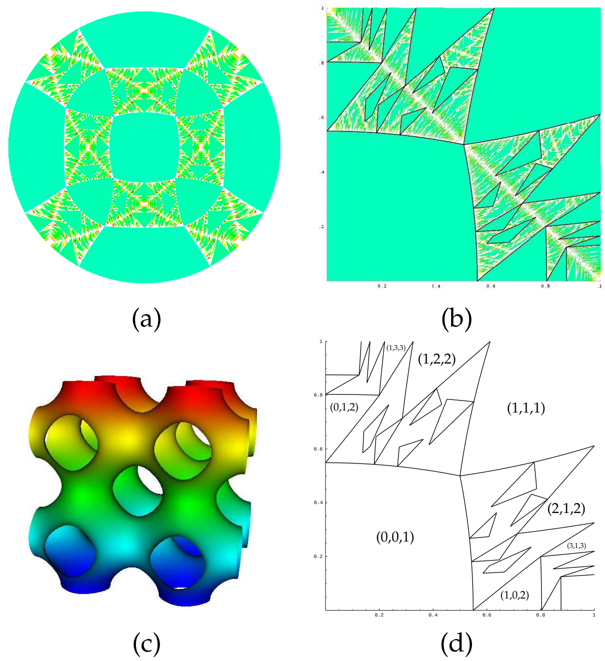

FIG. 3: [17] (a) SM relative to $\sum \cos(x^i) = 0$. Infinitely many SZ appear because the symmetry of the FF makes all SZ appear at the level 0. (b) Detail of the unitary square at $H_z = 1$. (c) The FS $\sum \cos(x^i) = 0$. (d) Boundaries of the larger SZ above found analytically.

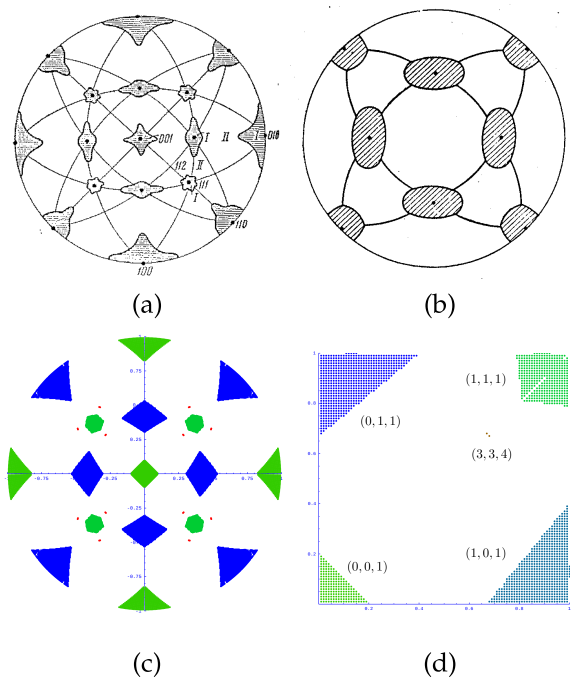

FIG. 4: (a) Experimental SM of magnetic field directions for Gold [4] (b) Qualitative sketch of it got by Lifshitz from his topological analysis [7] (c) Map obtained numerically (d) SZ in the unitary square at $H_z = 1$ and their Miller indices for $\boldsymbol{H} = (m/100, n/100, 1)$, $1 \leq m, n \leq 100$.

to a longer article the detailed description of how to get the Miller index components and we just point out that, since $\boldsymbol{L}$ is locally constant, we can determine each SZ with any desired degree of accuracy just sampling magnetic fields with rational direction, that incidentally are the only ones we can "exactly" treat from the numerical point of view.

We performed accurate numerical tests on simple "toy" Fermi Functions (FF) for which it is possible to obtain an analytical expressions of the SZ boundaries and verified that there is an excellent agreement between the analytical boundaries and the numerical data obtained evaluating the label for all magnetic fields in a squared grid (e.g. see Fig. 3 [17]). Note that in this case the SZ structure is fractal-like just because the toy FF used has a particular symmetry such that there is an energy level E_0 for which all magnetic fields giving rise at open orbits at some level do so also at E_0. More in general, since maps relative to different energy levels of the same FF are always compatible [11] (i.e. the same $\boldsymbol{L}$ corresponds to the same $\boldsymbol{H}$ at all levels where open orbits arise), it makes sense to build "all energies" SMs labeling each $\boldsymbol{H}$ by a label $\boldsymbol{L}$ if that label corresponds to that magnetic field at some energy. For a generic FF *all* rational directions give rise to open orbits at some energy level [12] and boundaries of SZ are always transversal it so that, when at least two different Miller indices $\boldsymbol{L}$ appear for two magnetic fields directions, then *infinitely* many SZ appear in the "all energies" SM, distributed in a fractal-like way.

SMs have been produced, mainly in Sixties and Seventies, for many metals and first of all for noble metals, whose FS is a sphere with four handles oriented like the diagonals of a cube (see Fig. 5b). We chose Au and Ag for our first numerical exploration with real FSs because in the literature are available analytical expressions for their FF and Fermi Energies [18] Much more precise FS approximations can be currently obtained e.g. using the Slater-Kostner tight-binding method [19], and we surely plan to make use of such tools in the future, but we opted for using the analytical approximation for two main reasons: on one hand, dealing with an analytical expression makes the numerical exploration much faster; on the other hand, Gaidukov experimental data have been taken with a magnetic field intensity of the order of $\simeq 10T$, barely at the boundary of the range for which the phenomenon manifests. We expect that the boundaries of the SZ will slightly but noticeably change after increasing the intensity by an order of magnitude, bringing it well inside the validity range of the semiclassical approximation, so we felt allowed to give more importance to calculations speed than to FS accuracy for this first numerical runs.

The SMs are obtained by evaluating the label (if any) associated to every magnetic field in a $10^2 \times 10^2$ grid in the unitary square, representing magnetic fields with di-

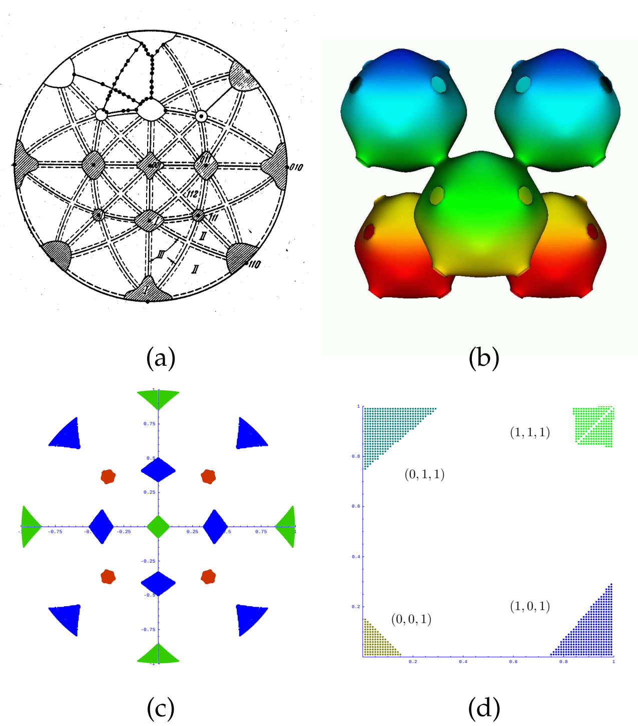

FIG. 5: (a) SM of magnetic field directions for Silver [5] (b) Fermi Surface of Silver (c) SM obtained numerically (d) SZ in the unitary square at $H_z = 1$ and their Miller indices for $\boldsymbol{H} = (m/100, n/100, 1)$, $1 \le m, n \le 100$.

rection $(m, n, 100)$, $1 \le m, n \le 100$ (Figs. 4d and 5d), and then by applying the stereographic projection and extending the regions above by symmetry (Figs. 4c and 5c). Even with a non-optimal approximation for FSs and experimental data taken just at the threshold, the correspondence between the numerical and experimental SMs turns out to be excellent for both Ag and Au (Figs. 4a,c and 5a,c). In both cases we find three big regions centered around the lattice directions $(0, 0, 1)$, $(1, 0, 1)$ and $(1, 1, 1)$ that, once symmetrized, reproduce in number, shape and size the seventeen SZ detected by Gaidukov. Miller indices associated to each those regions coincide with the lattice direction at their center, as it is supposed to happen for SZ around axis of symmetry for the FS [11]. We point out once again that the knowledge of the Miller index enables us to predict the current direction for all magnetic fields whose direction falls inside the SZ, except for the direction parallel to the SZ label. In the Au case we also found a fourth small region not detected experimentally with Miller index $(3, 3, 4)$ centered around the direction $(.67, .68, 1)$. Only two points belong to the SZ at the resolution used to generate Fig. 4c but further tests carried out at higher resolutions confirm that the SZ exists and has a triangular shape.

In summary, our numerical investigations allowed for the first time to compare the SMs found experimentally for Ag and Au by Gaidukov in Sixties and the corresponding ones built numerically from semiclassical considerations based on the galvanometric theory of Lifschitz. When open orbits occur, and therefore the conducibility tensor has a null eigenvalue, we are also able to predict the directions of the current. Our results indicate a striking agreement between experiment and theory but also indicate small discrepancies that may be due to the fact that the magnetic field used for the experiments was barely enough to let the phenomenon take place. New experiments performed with magnetic fields of order $10^2 T$ would give a final answer on the degree of accuracy of the Lifschitz model. Our next steps will be to start working with more accurate approximation of the FSs, e.g. using the Slater-Kostner tight-binding approach, and to produce numeric maps for the other metals for which a SM has been published.

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