How to Measure the Quantum Geometry of Bloch Bands

Titus Neupert,1 Claudio Chamon,2 and Christopher Mudry1

1 Condensed Matter Theory Group, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland
2 Physics Department, Boston University, Boston, Massachusetts 02215, USA

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Single-particle states in electronic Bloch bands form a Riemannian manifold whose geometric properties are described by two gauge invariant tensors, one being symmetric the other being antisymmetric, that can be combined into the so-called Fubini-Study metric tensor of the projective Hilbert space. The latter directly controls the Hall conductivity. Here we show that the symmetric part of the Fubini-Study metric tensor also has measurable consequences by demonstrating that it enters the current noise spectrum. In particular, we show that a non-vanishing equilibrium current noise spectrum at zero temperature is unavoidable whenever Wannier states have non-zero overlap with any of the bands above the gap.

We illustrate our results by three examples: (1) atomic layers of hexagonal boron nitride, (2) graphene, and (3) the surface states of three-dimensional topological insulators when gaped by magnetic dopants.

The connection between geometry and quantum mechanics was explored systematically during the 80’s when it was realized that the projective space of normalized quantum states can be equipped with a distance, making it a Riemannian manifold [1]. A symplectic form, making it a Kählerian manifold [1][2]. Berry famously showed that a quantum state acquires a measurable phase factor of purely geometric origin during a cyclic adiabatic evolution [3], i.e., he showed that the symplectic form (the Berry curvature) on the projective space of normalized quantum states is proportional to the phase acquired by a state under an infinitesimal adiabatic cycle. As this description applies to any subspace of the projective Hilbert space that smoothly depends on a set of external parameters, it is also of relevance to non-interacting Bloch bands [2][8][12], where the crystal momentum parametrizes the manifold of quantum states.

Most known measurable consequences of the quantum geometry of band insulators are limited to the Berry curvature. For example, the integral over the Brillouin zone (BZ) of the Berry curvature is quantized and proportional to the Hall conductivity of a band insulator [2]. It also enters the semiclassical equations of motion and semiclassically equations of motion of electronic wavepackets [13]. Here, we show that the quantum geometric tensor, also known as the Fubini-Study metric tensor of complex projective spaces in the mathematical literature [14], is an observable that can be measured via the current noise spectrum of a band insulator.

We consider the family of single-particle Bloch Hamiltonians

$$\mathcal{H}(k) := \sum_{a=1}^{N} \varepsilon_a(k) |u_a(k)\rangle \langle u_a(k)|$$

labeled by the momentum $k$ from the $d$-dimensional BZ of volume $\Omega_{\text{BZ}}$ acting on the Hilbert space $\mathbb{C}^N$. For any momentum $k \in \text{BZ}$, the single-particle Bloch eigenstates $|u_a(k)\rangle$ labeled by the band index $a = 1, \ldots, N$ are orthonormal $N$-dimensional complex-valued vectors that span the Hilbert space $\mathbb{C}^N$. The projective Hilbert space $\mathbb{CP}^{N-1}$ is obtained from $\mathbb{C}^N$ by identifying any two vectors $v$ and $w$ from $\mathbb{C}^N$ related to each other by the multiplication of a non-vanishing complex number.

We first review how the Fubini-Study metric tensor on the projective Hilbert space $\mathbb{CP}^{N-1}$ arises. To this end, we define the normalized single-particle state

$$|\Psi(k)\rangle := \sum_{a=1}^{\tilde{N}} c_a(k) |u_a(k)\rangle, \quad \sum_{a=1}^{\tilde{N}} |c_a(k)|^2 = 1, \quad (2)$$

whereby we assume that the first $\tilde{N}$ bands are separated from the remaining $N - \tilde{N}$ bands by a spectral gap. We want to compute the infinitesimal increment

$$(ds)^2 := \sum_{\mu,\nu=1}^{d} \langle \partial_{\nu} \Psi(k) | \partial_{\nu} \Psi(k) \rangle \, dk^{\mu} \, dk^{\nu} \quad (3)$$

under the (adiabatic) assumption that the state $|\Psi(k+dk)\rangle$ has no overlap with any of the bands above the gap [geometrically, we parallel transport the state $|\Psi(k)\rangle$ to the state $|\Psi(k+dk)\rangle$]. One finds that [10]

$$(ds)^2 = \sum_{\mu,\nu=1}^{d} \left( \sum_{a,b=1}^{\tilde{N}} c_{a}^{*}(k) Q_{\mu
u}^{ab}(k) c_{b}(k) \right) \, dk^{\mu} \, dk^{\nu}. \quad (4a)$$

For any pair $\mu, \nu = 1, \ldots, \tilde{N}$, the non-Abelian Fubini-Study metric tensor $Q_{\mu\nu}(k)$ on the complex projective space $\mathbb{CP}^{N-1}$ is here the $\tilde{N} \times \tilde{N}$ Hermitean matrix

$$Q_{\mu\nu}(k) := g_{\mu\nu}(k) + i \omega_{\mu\nu}(k). \quad (4b)$$

It can be decomposed additively in a unique way into the Hermitean $\tilde{N} \times \tilde{N}$ matrix $g_{\mu\nu}(k)$ with the components

$$g_{\mu\nu}(k) := \frac{1}{2} \left[ (\partial_{\mu} u_{\tilde{a}}(k) | \partial_{\nu} u_{\tilde{b}}(k) \rangle - \sum_{\tilde{c}=1}^{\tilde{N}} A_{\mu\nu}^{\tilde{a}\tilde{b}}(k) A_{\nu\mu}^{\tilde{b}\tilde{a}}(k) \right. \right.$$}

$$+ (\mu \leftrightarrow \nu) \right] \right.$$}

$$+ (\mu \leftrightarrow \nu) \right] \right.$$}
and the Hermitian $\tilde{N} \times \tilde{N}$ matrix $\omega_{\mu\nu}(k)$ with the components
\[
\omega^{\tilde{a}\tilde{b}}(k) := \frac{1}{2} F^{\tilde{a}\tilde{b}}_{\mu\nu}.
\]
We have made use of the non-Abelian Berry connection
\[
A^{ab}_{\mu}(k) := -i \langle u_a| \partial_{\mu} u_b(k) \rangle
\]
(4e)

for any pair $a,b = 1,\cdots,N$ that we have projected onto the $\tilde{N}$ lower bands by restricting the band labels to $\tilde{a}, \tilde{b} = 1,\cdots,\tilde{N}$. In the following, we shall consider the case of a band insulator with $\tilde{N} = 1$, i.e., with a single band $a = 1$ filled and all other bands $a = 2,\cdots,N$ empty and separated by an energy gap from the lowest band [15]. The current noise spectrum is the Fourier transform of the current-current correlation function [16,19]
\[
S_{\mu\nu}(\omega) := \int dt e^{-i\omega t} \langle 0| J_\mu(t) J_\nu(0) |0\rangle
\]
for any pair $\mu, \nu = 1,\cdots,d$. The insulating non-interacting many-body ground state is here denoted $|0\rangle$. It has the lowest band $a \equiv 1$ filled and all other bands $a = 2,\cdots,N$ empty. The time-dependence of the current operator is
\[
J(t) := e^{iHt} J e^{-iHt}.
\]
(5b)
The initial value of the current operator
\[
J \equiv J(0) := i[H, X]
\]
is proportional to the commutator between the non-interacting Hamiltonian $H$ with the single-particle representation $[\ ]$ and the position operator $X$ with the single-particle representation
\[
X = \int \frac{d^d k}{\Omega_{\text{BZ}}} |u_a(k)\rangle \left(-i \delta^{ab} \partial + A^{ab}(k)\right) |u_b(k)\rangle
\]
(5d)
(the sum over the repeated band labels $a,b = 1,\cdots, N$ is implicit and $\Omega_{\text{BZ}}$ denotes the volume of the BZ). To proceed with the derivation of our main result, we assume that the current in the ground state vanishes,
\[
\langle 0|J(t)|0\rangle = 0.
\]
(6)
With the help of the resolution of the identity
\[
\mathbb{1} = \sum_{n=0}^{\infty} |n\rangle \langle n| + \sum_{m=1}^{\infty} |m\rangle \langle m|,
\]
(7)
where $|m\rangle$ denotes any one of the many-body eigenstates except for the ground state with the many-body eigenenergy $E_m$, measured relative to the ground state eigenenergy, we can rewrite Eq. (5a) using Eqs. (5b), (5c), and (6) as
\[
S_{\mu\nu}(\omega) = \sum_m \int dt e^{-i(\omega - E_m)t} \langle 0| J_\mu |m\rangle \langle m| J_\nu |0\rangle.
\]
(8)
As $J$ is a single-particle operator, it can only create particle-hole excitations above the ground state with energy $E_m = \varepsilon_m(k) - \varepsilon_1(k')$, where $m= (a,k,k')$, $a > 1$, $k,k' \in \text{BZ}$. Thus,
\[
S_{\mu\nu}(\omega) = \int \frac{d^d k}{\Omega_{\text{BZ}}} \int \frac{d^d k'}{\Omega_{\text{BZ}}} \sum_{a>1} \int dt e^{-i(\omega - \epsilon_a(k) + \epsilon_1(k'))t} \times [\epsilon_a(k) - \epsilon_1(k')]^2 \langle 0| X_\mu |m\rangle \langle m| X_\nu |0\rangle
\]
\[
= 2\pi \omega^2 \int \frac{d^d k}{\Omega_{\text{BZ}}} \int \frac{d^d k'}{\Omega_{\text{BZ}}} \sum_{a>1} \times \delta(\omega - \epsilon_a(k) + \epsilon_1(k')) \langle 0| X_\mu |m\rangle \langle m| X_\nu |0\rangle.
\]
(9)
By inspection of Eq. (5d), we observe that the position operator decomposes additively into a band-diagonal but momentum-off-diagonal part (the derivative in momentum space) and a band-non-diagonal but momentum-diagonal part (the non-Abelian Berry connection). Only the latter contributes to the matrix elements $\langle 0| X_\mu |m\rangle$, since the electron has to be excited to an upper band $a > 1$. Hence,
\[
S_{\mu\nu}(\omega) = 2\pi \omega^2 \int \frac{d^d k}{\Omega_{\text{BZ}}} \sum_{a>1} \delta(\omega - \epsilon_a(k) + \epsilon_1(k)) \times A^{1a}_\mu(k) A^{1a}_\nu(k).
\]
(10)
To relate Eq. (10) to the quantum geometric tensor $Q_{\mu\nu}$, we would like to resort to the following manipulation (we need the single-particle resolution of the identity to establish the first equality)
\[
\sum_{a>1} A^{1a}_\mu(k) A^{1a}_\nu(k) = A^{11}_\mu(k) A^{11}_\nu(k) - \langle \partial_\mu u_1(k) \partial_\nu u_1(k) \rangle = -Q^{11}_{\mu\nu}(k).
\]
(11)
However, in general we cannot perform the summation over $a > 1$ in Eq. (10), for the energies $\varepsilon_a(k)$ also depend on $a = 1,\cdots,N$, so that energetics and quantum geometry combine in $S_{\mu\nu}(\omega)$. We will now discuss two ways to distill the contribution from the quantum geometry. On the one hand, we have the sum rule
\[
S_{\mu\nu} := \int \frac{d\omega}{2\pi} S_{\mu\nu}(\omega) = - \int \frac{d^d k}{\Omega_{\text{BZ}}} Q^{11}_{\mu\nu}(k)
\]
(12)
that relates the frequency integral of the current noise spectrum divided by $\omega^2$ to the integral of the quantum geometric tensor over the BZ. On the other hand, when $N=2$, i.e., for exactly two bands,

$$S_{\mu\nu}(\omega) = -2\pi\omega^2 \int_{BZ} \frac{d^d k}{\Omega_{BZ}} \delta[\omega - \varepsilon_2(k) + \varepsilon_1(k)] Q^I_{\mu\nu}(k),$$

(13)

so that $S_{\mu\nu}(\omega)/\omega^2$ equals the integral of the quantum geometric tensor over the region in momentum space where the direct band gap equals $\omega$. The reduction to a two-band model with $a = 1,2$ is justified when the orbital character of the bands $a \geq 3$ is sufficiently different from the band $a = 1$, such that

$$|P_1, P_a| \approx 0, \quad a \geq 3,$$

(14)

holds, where $P_a := \int d^d k \Omega_{BZ}^{-1} |u_a(k)\rangle \langle u_a(k)|$ is the projector on the single-particle states of the band $a = 1,2, \cdots$. In this case $A^I_{\mu\nu}(k)$ is negligible for $a \geq 3$ and so do its contributions to Eq. (10).

Equations (12) and (13) establish a connection between the quantum geometry of the Bloch states and the physically measurable current noise spectrum. On the one hand, the frequency dependence of the noise can reveal information on the Fubini-Study metric tensor. On the other hand, in multi-orbital systems or materials with spin-orbit interactions (in which the quantum metric tensor is generically non-trivial), there are interesting structures in the noise spectra even at equilibrium. To illustrate the latter case, we consider three examples that can be realized experimentally.

**Example 1** — We consider atomic layers of hexagonal boron nitride. In the tight-binding approximation, the electronic structure is described by the gapped Hamiltonian

$$\mathcal{H}^\text{BN}(k) := \begin{pmatrix} -\mu_s & -t \gamma(k) \\ -t \gamma^*(k) & -\mu_s \end{pmatrix},$$

(15)

where $\gamma(k) = 1 + e^{-i a_1 \cdot k} + e^{-i a_2 \cdot k}$, $t = 2.92$ eV is the nearest neighbor hopping, $\mu_s = 9.0$ eV is the difference in chemical potential between boron and nitrogen sites, and $a_1 = (\sqrt{3}, 3)^T/2$, $a_2 = (-\sqrt{3}, 3)^T/2$ are the primitive lattice vectors (in units of the atomic spacing). Hamiltonian (15) has two bands separated by the band gap $2\mu_s$. While neither of these bands has a nontrivial topological attribute, they still represent a nontrivial quantum geometry. The off-diagonal components of the quantum geometric tensor are nonzero, but average to zero along equal energy contours in momentum space, so that $S_{12}(\omega) = 0$ according to Eq. (13). As far as the Berry curvature is concerned, this averaging is a consequence of time-reversal symmetry. On the other hand, $S_{\mu\nu}(\omega), \mu = 1,2$, is nonzero and shown in Fig. 1. Finally, $S_{\mu\nu}, \mu = 1,2$, defined in Eq. (12), are given by

$$S_{11} = -1.54 a^2$$

and $S_{22} = -3.56 a^2$, where the lattice spacing $a$ has been reinstated.

**Example 2** — The limit $\mu_s \rightarrow 0$ in Eq. (15) delivers a tight-binding two-band approximation to the bands of graphene. When the chemical potential is tuned to the charge-neutral point, graphene realizes a quantum critical point characterized by a density of states that scales linearly with the deviation in energy away from the charge-neutral point. Correspondingly, the diagonal entries $S_{\mu\mu}(\omega)$ with $\mu = 1,2$ scale linearly with $\omega$ as $\omega \rightarrow 0$. It follows that $S_{\mu\mu}$ with $\mu = 1,2$ are logarithmically divergent due to the critical nature of the Bloch states at the charge-neutral point.

**Example 3** — We consider a single species of massive Dirac elections in $d=2$ dimensions, as a model for the surface states of the three-dimensional topological insulator Bi$_2$Se$_3$ [21], when doped with ferromagnetically ordered ions. The Hamiltonian is given by

$$\mathcal{H}^\text{TI}(k) := \begin{pmatrix} m & v(k_2 + i k_1) \\ v(k_2 - i k_1) & -m \end{pmatrix},$$

(16)

where $v$ is the Fermi velocity and $m$ is the magnetization out of the plane of the surface. Hamiltonian (16) has two bands with energies $\pm \varepsilon(k)$, $\varepsilon(k) := \sqrt{v^2 k^2 + m^2}$, separated by the band gap $2m$. We regulate the theory with a high-energy cut-off $\Lambda \gg m$ such that $\Omega_{BZ} = \pi (\Lambda/v)^2$. The quantum geometric tensor reads

$$Q^{11} = \frac{v^2}{4\varepsilon(k)^2} \begin{pmatrix} 2k^2 \sin^2 \varphi + 2m^2 & \im \varepsilon(k) - k^2 \sin 2\varphi \\ -\im \varepsilon(k) - k^2 \sin 2\varphi & 2k^2 \cos^2 \varphi + 2m^2 \end{pmatrix},$$

(17)
Here, we used the parametrization \( v \mathbf{k} = k (\cos \varphi, \sin \varphi)^T \). For the current noise spectrum, we obtain (\( \mu = 1, 2 \))

\[
S_{\mu\mu}(\omega) = -\frac{\pi v^2}{A^2} \left( \omega + \frac{4m^2}{\omega} \right) \Theta \left( \frac{\omega}{2m} - 1 \right), \tag{18a}
\]

\[
S_{12}(\omega) = -i \frac{2\pi v^2 m}{A^2} \Theta \left( \frac{\omega}{2m} - 1 \right), \tag{18b}
\]

while

\[
S_{12} = -i \frac{2\pi}{\Omega_{\text{BZ}}} \left[ \frac{1}{2} + \mathcal{O} \left( \frac{M}{A} \right) \right], \tag{19}
\]

reveals that the Chern number of a single species of Dirac fermions is 1/2. In contrast, \( \Omega_{\text{BZ}} \times S_{\mu\mu}, \mu = 1, 2 \), is logarithmically divergent for \( \Lambda \to \infty \). One might wonder whether bulk states, that have not been considered here, will spoil these results. If fact, the results are valid as long as \( \omega \) in Eq. (18) and \( \Lambda \) in Eq. (19) are much smaller than the bulk energy gap.

The results for \( S_{\mu\mu}(\omega) \) and \( S_{\mu\nu} \) obtained in these three examples illustrate how the quantum geometry is manifest in the noise. Notice that in example 2 there is no current noise at equilibrium conditions, while in examples 1 and 3 there is necessarily noise even at equilibrium.

We have shown that the tensor \( S \) defined by the first equality of Eq. (12) is connected to the current noise spectrum by the second equality of Eq. (12). We are going to provide yet two complementary interpretations for this tensor.

Two physical quantities that are revealed in \( S \) are the minimum spread of Wannier states and the Hall conductivity of a Bloch band. As shown by Marzari and Vanderbilt [8], the spread of the Wannier states can be broken into two positive definite contributions \( \Omega_{\mu}, \Omega_{\nu} \), one of which (\( \Omega_{\mu} \)) is gauge invariant and is tied to the trace of the quantum geometric tensor. It turns out that

\[
\Omega_{\mu} = \int_{\text{BZ}} \frac{d^2k}{\Omega_{\text{BZ}}} \text{tr} g^{11}(k) = -\text{tr} S. \tag{20}
\]

Remarkably, current noise is present even at equilibrium for any band insulator in which either multi-orbital or spin-orbit coupling causes the Wannier states to spread. Furthermore, the imaginary part of \( S \) is proportional to the Hall conductivity \( \sigma_{\mu\nu}^H \) with \( \mu \neq \nu = 1, 2 \) of the lower band \( a = 1 \)

\[
\sigma_{\mu\nu}^H = 2\pi e^2 \hbar \int_{\text{BZ}} \frac{d^2k}{\Omega_{\text{BZ}}} F_{\mu\nu}(k) = \frac{2\pi e^2}{\hbar} \text{Im} S_{\mu\nu}. \tag{21}
\]

The fluctuation-dissipation theorem relates \( S_{\mu\nu}(\omega) \) to the frequency-resolved inter-band Kubo conductivity \( \sigma_{\mu\nu}(\omega) \) per unit volume \( V \). At zero temperature,

\[
\sigma_{\mu\nu}(\omega) = \frac{i}{2\pi V} \int d\omega' \frac{S_{\mu\nu}(\omega + \omega') - S_{\mu\nu}(\omega')}{\omega - \omega' + i0^+}. \tag{22}
\]

This implies sum rules relating the Fubini-Study metric \( Q_{\mu\nu}(k) \) and \( \sigma_{\mu\nu}(\omega) \) [22].

The integrated noise spectrum \( S \) can also be interpreted as the action of the \( \mathbb{C}P^{N-1} \) nonlinear sigma model (NL\( \sigma \)M) [23]. To this end, we note that the orthonormal eigenstates of the \( N \times N \) Bloch Hamiltonian [11] can be represented as points \( z(k) \) on the surface of the unit sphere \( S^{2N-1} \). Any two pair of points \( z(k) \) and \( z(k') \) from \( S^{2N-1} \) differing by a phase are not distinct, i.e., it is the projective space \( \mathbb{C}P^{N-1} \) that realizes physical states. We can interpret \( \mathbb{C}P^{N-1} \) as a \((2N-2)\)-dimensional real Riemannian manifold, with the “angular” coordinates \( \phi_a(k), \ a = 1, \cdots, 2N-2 \). In this parametrization, the Fubini-Study metric tensor decomposes into the symmetric

\[
g_{\mu\nu}^{11} = \partial_\mu \phi_a G^{ab}(\phi) \partial_\nu \phi_b = +g_{\nu\mu}^{11} \tag{23}
\]

and antisymmetric

\[
F_{\mu\nu}^{11} = \partial_\nu \phi_a F^{ab}(\phi) \partial_\mu \phi_b = -F_{\nu\mu}^{11} \tag{24}
\]
tensors, respectively (summation over repeated \( a, b = 1, \cdots, 2N-2 \) is implied). In \( d = 2 \) dimensions, given the flat Euclidean metric tensor \( \delta^{\mu\nu} = +\delta^{\nu\mu} \) and the Levi-Civita antisymmetric tensor \( \epsilon^{\mu\nu} = -\epsilon^{\nu\mu} \), we can write (summation over repeated indices implied)

\[
\delta^{\mu\nu} S_{\mu\nu}[\phi] = -\int_{\text{BZ}} \frac{d^2k}{\Omega_{\text{BZ}}} \partial_\mu \phi_a G^{ab}(\phi) \partial_\nu \phi_b, \tag{25a}
\]

and

\[
\epsilon^{\mu\nu} S_{\mu\nu}[\phi] = -\frac{i}{2} \int_{\text{BZ}} \frac{d^2k}{\Omega_{\text{BZ}}} \epsilon^{\mu\nu} \partial_\mu \phi_a G^{ab}(\phi) \partial_\nu \phi_b. \tag{25b}
\]

Equation (25a) is the kinetic term in the action of the \( \mathbb{C}P^{N-1} \) NL\( \sigma \)M in two-dimensional Euclidean space. Equation (25b) is the Wess-Zumino term of the \( \mathbb{C}P^{N-1} \) NL\( \sigma \)M [24]. The quantization and with it the topological character of the Wess-Zumino term is guaranteed by the quantization of the first Chern number. Measuring all the components of the tensor \( S_{\mu\nu} \) can thus be viewed as measuring the action of the \( \mathbb{C}P^{N-1} \) NL\( \sigma \)M augmented by a topological term with the field configuration \( \phi(k) \) that is dictated by the Bloch Hamiltonian.

Finally, we point out that the Fubini-Study metric tensor enters the algebra obeyed by the single-particle position operator [5d], which we denote by \( \mathbf{X} \) after projection onto the \( N \) lower bands, according to

\[
\left< u_\tilde{\alpha}(k) \left| \mathbf{X}_\mu \mathbf{X}_\nu \right| u_\tilde{b}(k) \right> = Q_{\mu\nu}^{\tilde{\alpha}\tilde{b}}(k) \tag{26}
\]

for any pair \( \mu, \nu = 1, \cdots, d \) and for any pair \( \tilde{\alpha}, \tilde{b} = 1, \cdots, N \) from the lower bands. Furthermore, the Fubini-Study metric tensor determines the algebra obeyed by the
Fourier components of projected density operators

\[ \tilde{\rho}(q) := \int \frac{d^d k}{\Omega_{\text{BZ}}} |u_\alpha(k)\rangle\langle u_\alpha(k)| u_\beta(k + q)\rangle\langle u_\beta(k + q)|, \]

(27)

that reads in the limit of long wavelength, i.e., to second order in the momenta \( q, q' \in \text{BZ}, \)

\[ \tilde{\rho}(q)\tilde{\rho}(q') - \tilde{\rho}(q + q') = g_{\mu\nu} q_{\mu}' \int \frac{d^d k}{\Omega_{\text{BZ}}} |u_\alpha(k)\rangle Q_{\mu\nu}^\dagger(k) |u_\beta(k)\rangle. \]

(28)

In conclusion, we showed that the quantum geometric tensor of band insulators is related to a measurable quantity, the current noise spectrum. We also introduced a frequency-weighted integral of the noise spectrum that can be physically interpreted as the minimal spread of Wannier orbitals and takes the form of the action of the \( \mathbb{CP}^{N-1} \) \( N\sigma \)M augmented by a topological term.

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