Nonequilibrium Approach to Bloch-Peierls-Berry Dynamics

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We examine the Bloch-Peierls-Berry dynamics under a classical nonequilibrium dynamical formulation. In this formulation all coordinates in phase space formed by the position and crystal momentum space are treated on equal footing. Explicitly demonstrations of the no (naive) Liouville theorem and of the validity of Darboux theorem are given. The explicit equilibrium distribution function is obtained. The similarities and differences to previous approaches are discussed. Our results confirm the richness of the Bloch-Peierls-Berry dynamics.

1 Introduction

One of the fundamental dynamical equations in condensed matter physics is the so-called Bloch equation, describing one electron moving in a periodic potential in position and crystal momentum space [1]:

\[ \dot{r} = \frac{1}{\hbar} \nabla_k \epsilon(k), \quad \hbar \dot{k} = -e \nabla_r \phi(r) \]

Here \( r \in \mathbb{R}^3 \) is position, \( k \in \mathbb{R}^3 \) crystal momentum, \( \epsilon(k) \in \mathbb{R}^1 \) kinetic energy, \( \phi(r) \in \mathbb{R}^1 \) the electric potential, \( e \) the electric charge of an electron, and \( \hbar \) the Planck constant. The index \( l \) in the gradient operation, \( \nabla_l \equiv \partial/\partial l \) indicates the corresponding space coordinate. A scalar function \( \mathcal{H}(r,k) \), termed the Bloch Hamiltonian, can be defined as

\[ \mathcal{H}(r,k) = \frac{1}{\hbar} [\epsilon(k) + e\phi(r)] \]  

In this case, the Bloch dynamics can be rewritten in the canonical Hamiltonian form: \( \dot{r} = \nabla_k \mathcal{H} \) and \( \dot{k} = -\nabla_r \mathcal{H} \). The usual incompressible condition, the Liouville theorem, in the six dimensional \( x^T \equiv (r,k) \) phase space follows,

\[ \nabla_x \cdot \dot{x} = \nabla_r \cdot \dot{r} + \nabla_k \cdot \dot{k} = \nabla_r \cdot \nabla_k \mathcal{H} - \nabla_k \cdot \nabla_r \mathcal{H} = 0 \]  

R. Peierls successfully extended the Bloch equations to the case with a weak magnetic field \( \mathbf{B}(r) \) [1]:

\[ \dot{r} = \frac{1}{\hbar} \nabla_k \epsilon(k), \quad \hbar \dot{k} = -e \nabla_r \phi(r) - e \dot{r} \times \mathbf{B}(r) \]

The Hamiltonian in the form of Eq. [1] remains the same for this extended dynamics, and the Liouville theorem of Eq. [2] still holds. Everything appears as expected.

However, the Bloch equations of electron dynamics have been recently modified to include both magnetic field \( \mathbf{B}(r) \) and Berry curvature \( \Omega(k) \) in crystal momentum space [2]. The following extended dynamical
equations in the semiclassical limit were obtained, termed Bloch-Peierls-Berry equations in the present paper:

\[
\begin{align*}
\dot{r} &= \frac{1}{\hbar} \nabla_k \epsilon(k) - \dot{k} \times \Omega(k) \\
\hbar \dot{k} &= -e \nabla_r \phi(r) - e \dot{r} \times B(r)
\end{align*}
\] (3a)

Interesting, unexpected, and rich behaviors occur in the context of this novel dynamics [2, 3]. For example, it has been found that in six dimensional phase space the current flow becomes compressible, that is, the Liouville theorem does not hold [3]:

\[\nabla_x \cdot \dot{x} \neq 0.\] (4)

Thus the straight-forward conventional means to Hamiltonian analysis does not appear available. Such a situation has been called non-Hamiltonian dynamics [3].

To remedy this problem of non-Hamiltonian dynamics, Xiao et al. [3] introduced a density correction factor, denoted \(J(r, k) = 1 + \frac{\hbar}{e} B \cdot \Omega\) in the present paper, to force the divergence in phase space to zero:

\[\nabla_r \cdot (J(r, k) \dot{r}) + \nabla_k \cdot (J(r, k) \dot{k}) = 0\] (5)

Disagreement on the treatment in Ref.[3] exist in literature [4, 5, 6, 7]. For example, in a comment from Duval et al., [5], an alternate approach was pointed out such that a local canonical form, and likewise a Hamiltonian description, is achievable. In addition to the question of mathematical formulation, there is a real issue of possibly different physical consequences in different approaches [8].

In the present paper we study the problem from a completely different point of view to see how the Hamiltonian like structure and the equilibrium distribution function emerge from a nonequilibrium process: the Darwinian dynamics [9]. We will show that a Hamiltonian, or energy function, naturally emerges. In our demonstration it is clear that the Berry phases due to the magnetic field and the Berry curvature of the momentum space appears in equal footing. Furthermore, such a procedure provides a straightforward discussion on the equilibrium distribution: a nonequilibrium setting provides a natural way to select the steady state distribution. Not all of our results are new. Nevertheless, our demonstration appears to provide a clear, consistent, but completely classical starting point to detail the system characteristics as previously described while possessing no proclivity toward an incompressible or canonical phase. For example, a direct solution to the Fokker-Planck equation has been detailed. This solution is found independent of the Liouville theorem and may offer a unique insight into a probability distribution.

We begin the remainder of the paper in section 2 by first describing the generic decomposition of Darwinian dynamics and arranging the Berry modified Bloch equations, Eq. (3), to this form. In section 3
we will present the divergence analytically to show that the system is compressible. In section 4 we evaluate the Jacobi identity to show that a local canonical form exists and in section 5 we reveal the evolution of a probability distribution developed directly from the general form of Darwinian dynamics. Section 6 is a summary and discussion.

2 Evolutionary Decomposition and Conservation of “Energy”

2.1 Darwinian dynamics

The Darwinian dynamics arises from a generic nonequilibrium process common in biological, physical, and social sciences [9]. One of it’s main features is to treat all dynamical variables on an equal footing. This is typically achieved through expression of the dynamics in a set of first order stochastic differential equations.

Given a generic first order dynamic system of states, x, separated into the deterministic, f(x), and stochastic, ζ(x,t), components:

\[ \dot{x} = f(x) + \zeta(x,t) \]  

The noise is typically approximated as Gaussian and white with zero mean, \( \langle \zeta(x,t) \rangle = 0 \), and variance as

\[ \langle \zeta(x,t)\zeta^\tau(x,t') \rangle = 2 \omega D(x) \delta(t-t') . \]  

Here the nonnegative constant \( \omega \) plays the role of temperature in physics. Further characterization of the noise comes from the diffusion matrix \( D \).

There then exists a unique decomposition as follows [9, 10, 11, 12]:

\[ [S(x) + T(x)]\dot{x} = -\nabla_x \Phi(x) + \xi(x,t) \]  

Here \( S \) is a symmetric and positive definite friction matrix, related to the zero-mean Gaussian and white noise as follows

\[ \langle \xi(x,t)\xi^\tau(x,t') \rangle = 2 \omega D(x) \delta(t-t') . \]  

\( T(x) \) is an antisymmetric matrix, \( \Phi(x) \) a scalar potential function and \( S \) a symmetric matrix. By definition \( S \) is positive semi-definite, \( \dot{x}^\tau S \dot{x} \geq 0 \), and will have a dissipative effect on the potential function, showing a tendency to approach the potential minima. The \( T \) matrix describes a non-dissipative part of the dynamics, \( \dot{x}^\tau T \dot{x} = 0 \), and tends to conserve the potential function.

2.2 Reformulation of Bloch-Peierls-Berry equations

Now we reformulate the Bloch-Peierls-Berry equations from the point of view of Darwinian dynamics, treating position and momentum coordinates in equal footing. We begin the decomposition of these equations [9] by arranging them in terms of the complete state vector \( x \) in the form of Darwinian dynamics, Eq.(8). The friction matrix \( S \) may not be known. We assume its existence and may take it to be zero at the end of calculation whenever needed. The existence of electron-phonon interaction and other dissipative
processes and their small possible effect in a solid justifies such a procedure. Beginning from this formation of our descriptive matrices a potential function will then become apparent.

We rewrite the Bloch-Peierls-Berry equations, Eq. (3):

\[ \dot{x} = \left( \begin{array}{c} \dot{\mathbf{r}} \\ \mathbf{k} \end{array} \right) = \left( \begin{array}{c} \frac{1}{\hbar} \nabla_{\mathbf{k}} \epsilon(\mathbf{k}) \\ -\frac{e}{\hbar} \nabla_{\mathbf{r}} \phi(\mathbf{r}) \end{array} \right) - M(x) \dot{x} \]  

(10)

Here the matrix \( M \in \mathbb{R}^{6 \times 6} \) contains the effects of both magnetic field \( B \) in position space and Berry curvature \( \Omega \) in momentum space.

\[
M(x) = \begin{pmatrix}
0 & 0 & 0 & 0 & \Omega_3 & -\Omega_2 \\
0 & 0 & 0 & -\Omega_3 & 0 & \Omega_1 \\
0 & 0 & 0 & \Omega_2 & -\Omega_1 & 0 \\
0 & \frac{e}{\hbar} B_3 & -\frac{e}{\hbar} B_2 & 0 & 0 & 0 \\
-\frac{e}{\hbar} B_3 & 0 & \frac{e}{\hbar} B_1 & 0 & 0 & 0 \\
\frac{e}{\hbar} B_2 & -\frac{e}{\hbar} B_1 & 0 & 0 & 0 & 0 \\
\end{pmatrix}
\]

(11)

With \( I \) as an identity matrix, Eq. (10) becomes:

\[
(I + M(x)) \dot{x} = \left( \begin{array}{c} \frac{1}{\hbar} \nabla_{\mathbf{k}} \epsilon(\mathbf{k}) \\ -\frac{e}{\hbar} \nabla_{\mathbf{r}} \phi(\mathbf{r}) \end{array} \right)
\]

(12)

This is almost in the form of Eq. (3) of Darwinian dynamics and the right hand side appears similar to the gradient of the Bloch Hamiltonian \( \mathcal{H} \), Eq. (1). Suggesting that the Hamiltonian or energy function in the Bloch-Peierls-Berry dynamics may indeed be the original Hamiltonian of Eqs. (3). This makes a notable potential function because it is a straightforward representation of the total energy in the system, we neglect the constants \( e \) and \( \hbar \) when speaking of total energy because they can simply be absorbed into \( x \).

We also must mind the order and sign of the state vector \( x \) compared to the right side of Eq. (12). To be consistent an orthogonal transformation matrix \( R \) is applied to both sides of the equation (12).

\[
R = \begin{pmatrix}
0 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 \\
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
\end{pmatrix}
\]

(13)

The right side of Eq. (12) becomes

\[
R \left( \begin{array}{c} \frac{1}{\hbar} \nabla_{\mathbf{k}} \epsilon(\mathbf{k}) \\ -\frac{e}{\hbar} \nabla_{\mathbf{r}} \phi(\mathbf{r}) \end{array} \right) = \left( \begin{array}{c} \frac{e}{\hbar} \nabla_{\mathbf{r}} \phi(\mathbf{r}) \\ \frac{1}{\hbar} \nabla_{\mathbf{k}} \epsilon(\mathbf{k}) \end{array} \right) = \nabla_{\mathbf{x}} \mathcal{H}(\mathbf{x})
\]

(14)
and the left side contains an antisymmetric matrix $T$:

$$ R[I + M(x)]\dot{x} = T(x)\dot{x} \tag{15} $$

where

$$ T(x) = \begin{pmatrix}
0 & -\frac{e}{\hbar} B_3 & \frac{e}{\hbar} B_2 & -1 & 0 & 0 \\
\frac{e}{\hbar} B_3 & 0 & -\frac{e}{\hbar} B_1 & 0 & -1 & 0 \\
-\frac{e}{\hbar} B_2 & \frac{e}{\hbar} B_1 & 0 & 0 & 0 & -1 \\
1 & 0 & 0 & 0 & \Omega_3 & -\Omega_2 \\
0 & 1 & 0 & -\Omega_3 & 0 & \Omega_1 \\
0 & 0 & 1 & \Omega_2 & -\Omega_1 & 0 \\
\end{pmatrix} \tag{16} $$

Collecting all terms the Bloch-Peierls-Berry equation, Eq. (3), is then transformed into the form of Darwinian dynamics, Eq. (8):

$$ T(x) \dot{x} = -\nabla_x H(x) \tag{17} $$

The $S$ matrix, as well as the diffusion matrix $D$, is null in this case, which may be thought as the zero electron-phonon interaction limit. The equivalent form to Eq. (10) of the Darwinian dynamics is

$$ \dot{x} = -Q(x) \nabla_x H(x), \tag{18} $$

with $Q(x) = T^{-1}(x)$. A Poisson bracket can be easily defined as

$$ [f(x), g(x)] \equiv \sum_{i,j=1}^6 Q_{ij}(x) \frac{\partial f}{\partial x_i} \frac{\partial g}{\partial x_j}. \tag{19} $$

Here $f$ and $g$ are two arbitrary functions of the phase space $x$. The Poisson bracket is anti-symmetric because $Q$ is. With this Poisson bracket, the Bloch-Peierls-Berry equations are now

$$ \dot{x} = [H(x), x], \tag{20} $$

the familiar form in Hamiltonian dynamics.

### 2.3 Conservation of energy

The potential function of Bloch-Peierls-Berry dynamics in the form of Darwinian dynamics may be clearly identified as the Bloch Hamiltonian:

$$ \Phi(x) = H(x) = \frac{1}{\hbar}[\epsilon(k) + e\phi(r)]. \tag{21} $$

It is straightforward to verify that such an “energy” given by the Bloch Hamiltonian is conserved in the Bloch-Peierls-Berry dynamics, as expected:

$$ \frac{d}{dt} H(x) = \frac{\partial x}{\partial t} \frac{\partial H(x)}{\partial x} = \dot{x}^T \nabla_x H(x) = \dot{x}^T T(x) \dot{x} = 0 \tag{22} $$
Thus, we may indeed identify the Bloch Hamiltonian given in Eq.(2) as the candidate for the Hamiltonian for the Bloch-Peierls-Berry dynamics of Eq.(3), upon the clarification of two questions raised in the literature, the validity of the Liouville theorem, and the validity of the Darboux theorem, to be discussed in the next two sections.

3 Compressibility and No Liouville Theorem

Here we will determine an analytical result for the divergence of the Bloch-Peierls-Berry equations (3) from the Darwinian dynamics given by Eq. (17), and show that it is indeed non-zero and thus compressible. This compressibility feature is pronounced and surprising, as pointed out in Ref.[3]. An explicit demonstration is given in light of the present Darwinian dynamics formulation.

The equation in question is, following Eq.(8):

\[ \nabla \cdot \dot{x} = -\nabla \cdot (T^{-1}(x)\nabla H(x)) \quad (23) \]

We first note that because \( T^{-1} \) is antisymmetric only the divergence of the \( T^{-1} \) matrix on the right hand side of the equation need be considered:

\[ \nabla \cdot \dot{x} = (\nabla \cdot T^{-1}) \nabla H(x) \quad (24) \]

Next, we note a useful identity expressing the divergence of \( T^{-1} \) as a function of the divergence of \( T \), because \( T \) is easier to operate on. This identity is found as follows, where \( I \) is the identity matrix:

\[ \nabla \cdot I = \nabla \cdot (T^{-1}T) \]
\[ = (\nabla \cdot T^{-1})T + \sum_{i=1}^{6} T^{-1}(i,:) \frac{\partial T}{\partial x_i} \]
\[ = 0 \quad (25) \]

The \( T^{-1}(i,:) \) denotes the \( i \)th row in the \( T^{-1} \) matrix.

Solving for \( \nabla \cdot T^{-1} \) in Eq. (25) we obtain:

\[ \nabla \cdot T^{-1} = -\left( \sum_{i=1}^{6} T^{-1}(i,:) \frac{\partial T}{\partial x_i} \right) T^{-1} \quad (26) \]

This simplification has also allowed us to express the divergence independent of \( H \) once combined with Eq. (24) as follows (this will prove to be useful later.)

\[ \nabla \cdot \dot{x} = -\left( \sum_{i=1}^{6} T^{-1}(i,:) \frac{\partial T}{\partial x_i} \right) T^{-1} \nabla \cdot H(x) \]
\[ = -\left( \sum_{i=1}^{6} T^{-1}(i,:) \frac{\partial T}{\partial x_i} \right) \dot{x} \quad (27) \]
After fully expanding and condensing the operations in parentheses above we obtain a useful and simplified expression:

$$\sum_{i=1}^{6} T^{-1}(i, \cdot) \frac{\partial T}{\partial x_i} = \frac{\tau}{(1 + \frac{e}{\hbar} \mathbf{B} \cdot \Omega)}$$

(28a)

$$= \nabla_x (1 + \frac{e}{\hbar} \mathbf{B} \cdot \Omega)$$

(28b)

Eq. (28a) is revealed from the fact that the divergence of the Berry curvature, $\Omega$, as well as the magnetic field, $\mathbf{B}$, are equal to zero. Both are defined as the curl of a vector function and the divergence of a curl must be zero, $\nabla \cdot \nabla \times \mathbf{f} = 0$:

$$\nabla_r \cdot \mathbf{B} = \frac{\partial B_1}{\partial r_1} + \frac{\partial B_2}{\partial r_2} + \frac{\partial B_3}{\partial r_3} = 0$$

(29a)

$$\nabla_k \cdot \Omega = \frac{\partial \Omega_1}{\partial k_1} + \frac{\partial \Omega_2}{\partial k_2} + \frac{\partial \Omega_3}{\partial k_3} = 0$$

(29b)

In the first row of (28a), for example, $-\frac{\partial B_2}{\partial r_2} \Omega_1 - \frac{\partial B_3}{\partial r_3} \Omega_1$ is equal to simply $\frac{\partial B_1}{\partial r_1} \Omega_1$. Using the solution in (28b) our phase divergence, Eq. (27), reduces to a final condensed form as follows. Here $J(\mathbf{x}) = 1 + \frac{e}{\hbar} \mathbf{B} \cdot \Omega$.

$$\nabla_x \cdot \dot{\mathbf{x}} = -\nabla_x J(\mathbf{x}) \frac{\dot{\mathbf{x}}}{J(\mathbf{x})}$$

(30a)

$$= -\frac{d}{dt} \ln J(\mathbf{x})$$

(30b)

$$= -\frac{d}{dt} \ln \left(1 + \frac{e}{\hbar} \mathbf{B} \cdot \Omega \right)$$

(30c)

We see that the divergence is time-varying given that both $\mathbf{B}$ and $\Omega$ are non-zero and non-orthogonal. Thus our system phase space is, in general, compressible, that is the Liouville theorem does not hold. This feature was used in Ref. [3] as the indication that the dynamics were non-Hamiltonian. However, different opinions have been voiced [4] [5] [6] [7]. A related point will be explicitly exposed in the next section.

4 Jacobi Identity

In this section we follow a standard procedure in mathematical physics [13, 14] to determine when a system can be (locally) regarded as a Hamiltonian system. In this regard, there are two important conditions the system has to satisfy. The first is the existence of a Poisson bracket which must be explicitly antisymmetric. The second is on the validity of the Darboux theorem. The incompressible condition, or the Liouville theorem, does not appear to be essential in this regard.

The existence of an antisymmetric Poisson bracket has already been defined in the previous section, Eq. (19), which endows the system with a specific dynamical structure which may not be a (local) canonical
Hamiltonian system. For the Darboux theorem, which guarantees that a non-degenerate system can be expressed in local canonical coordinates, the crucial condition to its validation is the presence of the Jacobi identity.

We express the Jacobi identity as the sum of the cyclic permutations of the double Poisson bracket. Here \( f(\eta), g(\eta), \) and \( h(\eta) \) are any functions with continuous second derivatives and \( \eta \) is the system space in consideration. The Jacobi identity is:

\[
[f, [g, h]] + [h, [f, g]] + [g, [h, f]] = 0
\]

(31)

Direct evaluation to verify the Jacobi identity would involve a great deal of algebra. By computing the Poisson bracket as a summation over each vector field we notice most of the terms cancel out.

\[
[f, g] = \sum_{i,j=0}^{n} \frac{\partial f}{\partial x_i} T^{-1}(i,j) \frac{\partial g}{\partial x_j}.
\]

(32)

Here \( T^{-1}(i,j) = Q_{ij}(x) \) is the \( ij \)th element of the \( T^{-1} \) matrix. Also to more easily display derivatives a notation will be used in which \( \frac{\partial f}{\partial x_i} \) is simply \( f_i \). Evaluating the first double Poisson bracket produces,

\[
[f, [g, h]] = \sum_{i,j,k,l=0}^{n} f_i T^{-1}(i,j) \left( g_k T^{-1}(k,l) h_l \right)_j
\]

\[
= \sum_{i,j,k,l=0}^{n} f_i T^{-1}(i,j) \left( g_k T^{-1}(k,l) h_l + g_k T^{-1}(k,l) h_{l,j} + g_k T^{-1}(k,l) h_l \right)
\]

(33)

The next two double Poisson brackets give similar results and because \( T^{-1} \) is antisymmetric the first 2 terms in the parentheses of each will cancel out \[15\]. In the simple case in which the transformation matrix is antisymmetric and independent of \( x \) this will alone satisfy the identity. However, difficulty arises because \( dT^{-1}/dx_i \neq 0 \) and we are left with the third term of each permutation containing the derivative of the \( T^{-1} \) matrix as follows:

\[
[f, [g, h]] + [h, [f, g]] + [g, [h, f]] = \sum_{i,j,k,l=0}^{n} f_i g_k h_l \left( T^{-1}(i,j) T^{-1}(k,l) + T^{-1}(l,j) T^{-1}(i,k) + T^{-1}(k,j) T^{-1}(l,i) \right)
\]

(34)

Eq. (35) is arranged to collect the arbitrary \( f, g, h \) functions. Because each \( f_i g_k h_l \) is unique the expression in parentheses must equal zero for every combination of \( i, k, l \) in order to satisfy the identity.

\[
\sum_{j=0}^{6} T^{-1}(i,j) T^{-1}(k,l) + T^{-1}(l,j) T^{-1}(i,k) + T^{-1}(k,j) T^{-1}(l,i) = 0 \quad \text{for all } i, k, l
\]

(35)

Because \( i, k, l = 1, 2, ..., 6 \) there are \( 6^3 \) equations that we must prove are equal to zero. However, we have been able to express all of them in four general forms through index notation. To show how this is possible it is helpful to first state the \( T^{-1} \) matrix in index notation. Here each quadrant is a 3 × 3 matrix with \( a \) denoting row and \( b \) column

\[
T^{-1}(x) = \frac{1}{\sqrt{\det(T)}} \begin{pmatrix}
\varepsilon_{abc} \Omega_c & \delta_{ab} + \frac{e}{\hbar} B_a \Omega_b \\
-\delta_{ab} - \frac{e}{\hbar} \Omega_a B_b & -\varepsilon_{abc} \frac{e}{\hbar} B_c
\end{pmatrix},
\]

(36)
with the determinant
\[ \det(T(x)) = \left( 1 + \frac{e}{\hbar} B \cdot \Omega \right)^2. \tag{37} \]

When solving Eq. (35) with the index notation given in (36) a distinct difference in solutions is noticed when \( i, k, l \) have values of 1, 2, or 3 and when they have values of 4, 5, or 6. To take advantage of this we will now improve our notation of each subset of \( i, k, l \). A value between 1 and 3 will be denoted by \( r \) and between 4 and 6 by \( k \). Particular values in \( r \) and \( k \) can now be described by integers between 1 and 3 for the sake of index notation. In the following solutions these integers are given, again, by \( a, b, \) and \( c \) which are unrelated to those in (36). The specific process to arrive at each solution is straightforward but lengthy and is excluded here. The final simplified solution for each subset is as follows.

\( (r, r, r) = \varepsilon_{abc} \det(T) (\nabla_k \cdot \Omega) \tag{38a} \)

\( (r, k, k) = \frac{\varepsilon_{bcd} (\frac{e}{\hbar})^2 B_a B_d}{\det(T)} (\nabla_k \cdot \Omega) + \frac{\varepsilon_{bcd} B_a}{\det(T)} \frac{\varepsilon_{c} \Omega_{c}}{\Omega} (\nabla_r \cdot B) - \frac{\varepsilon_{abc}}{\det(T)} \frac{\varepsilon_{b} \Omega_{b}}{\Omega} (\nabla_r \cdot B) \tag{38b} \)

\( (k, k, k) = \frac{\varepsilon_{abc} \frac{e}{\hbar}}{\det(T)} (\nabla_r \cdot B) \tag{38c} \)

\( (k, r, r) = \frac{\varepsilon_{bcd} \frac{e}{\hbar} \frac{\Omega_{c} \Omega_{d}}{\det(T)}}{\det(T)} (\nabla_r \cdot B) + \frac{\varepsilon_{abc} \frac{B_c}{\det(T)}}{\det(T)} (\nabla_k \cdot \Omega) - \frac{\varepsilon_{abc} \frac{B_b}{\det(T)}}{\det(T)} (\nabla_k \cdot \Omega) \tag{38d} \)

As previously mentioned in Eq. (29) the divergence of both Berry curvature in momentum space and the magnetic field in position are zero and each subset above will also be zero. It should also be noticed that the above equations only accommodate one half of the \( 6^3 \) total equations. The rest come from permutations in \( (r, k, k) \) and \( (k, r, r) \) and are similar expressions.

Thus the Jacobi identity is satisfied for the Bloch-Peierls-Berry dynamics. Hence the Darboux theorem holds. Therefore, these dynamics can be locally mapped into a canonical form of Hamiltonian dynamics, and may be named Hamiltonian dynamics. In fact a global transformation has even been suggested [4]. The reformulation of Bloch-Peierls-Berry dynamics into Darwinian dynamics makes this point evident from a completely different perspective.

### 5 Fokker-Planck Equation and Equilibrium Distribution

The general form of the present Darwinian dynamics described by Eq. (5) has been shown to correspond to a Fokker-Planck equation describing probability evolution in phase space [9][11][12]:
\[ \frac{\partial \rho(x, t)}{\partial t} = \nabla_x \cdot \left[ (D(x) + Q(x)) \left[ \omega \nabla_x + \nabla_x \Phi(x) \right] \right] \rho(x, t) \tag{39} \]

Here \( \omega \) is a non-negative constant equivalent to temperature. \( D \) is a symmetric matrix and \( Q \) is an antisymmetric matrix so that
\[ (D + Q) = (S + T)^{-1}. \]

Applying Eq. (39) to the Bloch-Peierls-Berry equation as given in Eq. (17) we find that \( D = 0 \) and \( Q = T^{-1} \), thus there is only an anti-symmetric part and the diffusion matrix \( D \) is in the zero limit:
\[ \frac{\partial \rho(x, t)}{\partial t} = \nabla_x \cdot \left[ Q(x) \left[ \omega \nabla_x + \nabla_x \Phi(x) \right] \right] \rho(x, t) \tag{40} \]
The term on the far right side of the equation can be seen to represent the probability flow divergence, \( \nabla_x \cdot (T^{-1} \nabla_x \Phi \rho) \Rightarrow \nabla_x \cdot (\dot{x} \rho) \), by substituting Eq. (17). Thus in the trivial case where \( \omega = 0 \) Eq. (40) becomes the standard form of the continuity equation. The term \( \nabla_x \cdot (\omega \nabla_x \cdot T^{-1}) \rho \) in Eq. (40) represents the additional effect on distribution at non-zero temperatures.

We now provide a plausible argument for another choice of equilibrium distribution other than that in Ref. [3]. First, we note that in the anti-symmetric matrix \( T \) in Eq. (17), the geometric phases due to the magnetic field \( B \) [16, 17] and the novel Berry curvature \( \Omega \) are in equal footing. They all contribute in the same manner to the geometric phase for a possible close trajectory in the phase space. A unifying description of the dynamics is hence achieved in this Darwinian dynamics formulation.

Second, in the case that dynamics are dissipative in phase space, for example if there are indeed electron-phonon and electron-impurity interactions, then the friction or resistance matrix \( S \), and hence the diffusion matrix \( D \), is not zero. Such a dissipative dynamics is very likely to be described by Eq. (8). Further, such a dissipative dynamics in the presence of Berry phase has been well characterized in condensed matter physics, such as the dynamics of topological singularities in superconductors and superfluids [18]. Thus, extending Bloch-Peierls-Berry dynamics to include dissipation as in the form of Eq. (17) or (8) indeed appears to be a natural choice.

Based on the above considerations we may adopt Eq. (39) as the equation for dynamics of non-interacting electrons in the presence of dissipation. The equilibrium distribution for such dynamics immediately reads:

\[
\rho_{eq}(x) = \frac{1}{Z} \exp \left\{ -\frac{\Phi(x)}{\omega} \right\}. \tag{41}
\]

The partition function summing up all probability in phase space may be defined as

\[
Z = \int d^6x \exp \left\{ -\frac{\Phi(x)}{\omega} \right\}. \tag{42}
\]

The time dependent free energy for such an open system may be defined as

\[
F(t) = -\omega \int d^6x \rho(x, t) \ln \left( \frac{\rho(x, t)}{\rho_{eq}(x)} \right) + F_{eq}, \tag{43}
\]

which always decreases towards the equilibrium value \( F_{eq} = -\omega \ln Z \).

We note that if treating the equilibrium distribution \( \rho_{eq} \) as a single particle distribution, one immediately notices a difference between the present result and the one obtained in Ref. [3] (c.f. their reference [21]) in the same limit.

6 Discussions

We have investigated the Bloch-Peierls-Berry dynamics from a nonequilibrium dynamical point of view. The Bloch-Peierls-Berry equations can be reformulated into a simple and generic form. Using this reformulation we have explicitly demonstrated the compressibility of Bloch-Peierls-Berry dynamics and the embedded Jacobi identity, both were pointed out previously in literature. From the point of view of Hamiltonian dynamics, we explicitly showed that the violation of the “naive” Liouville theorem is not essential. At the same time we reached a distribution function similar to what is implied in Ref. [3].
There are two new features in our study that we would like to point out. The first one is that our study is in the classical domain, and is for one electron. No many-body effect, as strongly suggested in Ref. [3], has been considered here. Hence, from the condensed matter physics point of view, our work may be relevant in the dilute and non-interacting limit, with a relatively high temperature. In this sense, it would be further interesting theoretically to see how the Boltzmann equation implicitly discussed in Ref. [3] would relate to the present Fokker-Planck equation. In particular, how the electron-phonon type interaction with explicit energy dissipation would be incorporated into formulation in Ref. [3].

The second feature is that due to the open system nature our probability dynamics formulation is necessarily in the domain of the canonical ensemble, where the Boltzmann-Gibbs distribution is emphasized. This also implies that there is a preferred and natural choice of phase space. Instead, the discussion of Hamiltonian flow in Ref.’s [4, 5] appears within the micro-canonical ensemble. It is well known that the transition from micro-ensemble to canonical ensemble is not unique. This may be the reason that within the present nonequilibrium formulation there is no compelling reason to emphasize the Liouville theorem, even though the Hamiltonian structure is evident in both approaches.

In conclusion, the present exploration from the Darwinian dynamics perspective has further revealed the richness of Bloch-Peierls-Berry dynamics.

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