Modifying Velocity and Force Vectors to Accommodate Berry Phases

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Introduction

We will examine two modified equations (velocity and force) which is attributed to the addition of a Berry phase. We will then make these equations linearly independent from each other.

Calculations

We begin by the original, unadulterated equations:

$$\partial_t \vec{r} = \nabla_{\vec{k}} \varepsilon$$

$$\partial_t \vec{k} = q\vec{E} + q(\frac{\partial \vec{r}}{\partial t} \times \vec{B})$$

However, when we consider a Berry phase in momentum, the velocity equation must be adjusted accordingly to properly account for motion properly. We thence have...

$$\partial_t \vec{r} = \nabla_{\vec{k}} \varepsilon + \frac{\partial \vec{k}}{\partial t} \times \vec{\Omega} \tag{1}$$

$$\partial_t \vec{k} = -q\nabla_{\vec{r}} \phi + q(\frac{\partial \vec{r}}{\partial t} \times \vec{B}) \tag{2}$$

We will now make equations (1) and (2) linearly independent from each other. We start by taking the cross product of $\vec{\Omega}$ on both sides of (2).

$$\partial_t \vec{k} \times \vec{\Omega} = -q(\nabla_{\vec{r}} \phi) \times \vec{\Omega} + q(\frac{\partial \vec{r}}{\partial t} \times \vec{B}) \times \vec{\Omega}$$

We will proceed by using the vectorial property which states $(\vec{a} \times \vec{b}) \times \vec{c} = -\vec{a}(\vec{c} \cdot \vec{b}) + \vec{b}(\vec{c} \cdot \vec{a})$. We now get:

$$\partial_t \vec{k} \times \vec{\Omega} = -q(\nabla_{\vec{r}} \phi) \times \vec{\Omega} - q\frac{\partial \vec{r}}{\partial t}(\vec{\Omega} \cdot \vec{B}) + q\vec{B}(\vec{\Omega} \cdot \frac{\partial \vec{r}}{\partial t}) \tag{3}$$

We will now try to simplify $\vec{\Omega} \cdot \frac{\partial \vec{r}}{\partial t}$. To do so, we recognize the property that $\vec{A} \cdot (\vec{A} \times \vec{B}) = 0$. Taking advantage of this vector identity, we take the dot product of $\vec{\Omega}$ on both sides of Equation (1).

$$\vec{\Omega} \cdot \frac{\partial \vec{r}}{\partial t} = \vec{\Omega} \cdot (\nabla_{\vec{k}} \varepsilon) + \vec{\Omega} \cdot (\frac{\partial \vec{k}}{\partial t} \times \vec{\Omega})$$

$$\Rightarrow$$

$$\vec{\Omega} \cdot \frac{\partial \vec{r}}{\partial t} = \vec{\Omega} \cdot (\nabla_{\vec{k}} \varepsilon) \tag{4}$$

We now plug in Equation (4) into Equation (3) for $\vec{\Omega} \cdot \frac{\partial \vec{r}}{\partial t}$. The results is:

$$\partial_t \vec{k} \times \vec{\Omega} = -q(\nabla_{\vec{r}} \phi) \times \vec{\Omega} - q\frac{\partial \vec{r}}{\partial t}(\vec{\Omega} \cdot \vec{B}) + q\vec{B}(\vec{\Omega} \cdot (\nabla_{\vec{k}} \varepsilon))$$

We now plug in this result to Equation (1) and rearrange to solve for $\frac{\partial \vec{r}}{\partial t}$:

$$\frac{\partial \vec{r}}{\partial t} = \nabla_{\vec{k}} \varepsilon - q(\nabla_{\vec{r}} \phi) \times \vec{\Omega} - q\frac{\partial \vec{r}}{\partial t}(\vec{\Omega} \cdot \vec{B}) + q\vec{B}(\vec{\Omega} \cdot (\nabla_{\vec{k}} \varepsilon))$$

$$\Rightarrow$$

$$\frac{\partial \vec{r}}{\partial t} + q\frac{\partial \vec{r}}{\partial t}(\vec{\Omega} \cdot \vec{B}) = \nabla_{\vec{k}} \varepsilon - q(\nabla_{\vec{r}} \phi) \times \vec{\Omega} + q\vec{B}(\vec{\Omega} \cdot (\nabla_{\vec{k}} \varepsilon))$$

$$\Rightarrow$$

$$\frac{\partial \vec{r}}{\partial t}(1 + q(\vec{\Omega} \cdot \vec{B})) = \nabla_{\vec{k}} \varepsilon - q(\nabla_{\vec{r}} \phi) \times \vec{\Omega} + q\vec{B}(\vec{\Omega} \cdot (\nabla_{\vec{k}} \varepsilon))$$

$$\Rightarrow$$

$$\frac{\partial \vec{r}}{\partial t} = \frac{\nabla_{\vec{k}} \varepsilon - q(\nabla_{\vec{r}} \phi) \times \vec{\Omega} + q\vec{B}(\vec{\Omega} \cdot (\nabla_{\vec{k}} \varepsilon))}{1 + q(\vec{\Omega} \cdot \vec{B})} \tag{5}$$

This finally provides to us the uncoupled solution (Equation (5)) to the velocity vector. As a check, we see we retain the unmodified version from the beginning, if we let $\vec{\Omega} = 0$. We now proceed to uncoupling Equation (2). With a definitive expression for $\frac{\partial \vec{r}}{\partial t}$, we can directly plug this into (2). We get:

$$\partial_t \vec{k} = q\vec{E} + q(\frac{\nabla_{\vec{k}} \varepsilon - q(\nabla_{\vec{r}} \phi) \times \vec{\Omega} + q\vec{B}(\vec{\Omega} \cdot (\nabla_{\vec{k}} \varepsilon))}{1 + q(\vec{\Omega} \cdot \vec{B})} \times \vec{B})$$

$$\frac{\partial \vec{k}}{\partial t} = -q\nabla_{\vec{r}} \phi + q(\frac{(\nabla_{\vec{k}} \varepsilon) \times \vec{B} - q((\nabla_{\vec{r}} \phi) \times \vec{\Omega}) \times \vec{B}}{1 + q(\vec{\Omega} \cdot \vec{B})})$$

We again utilize the vectorial properties of the triple product.

$$\frac{\partial \vec{k}}{\partial t} = -q\nabla_{\vec{r}} \phi + q(\frac{(\nabla_{\vec{k}} \varepsilon) \times \vec{B} + q(\nabla_{\vec{r}} \phi)(\vec{B} \cdot \vec{\Omega}) - q\vec{\Omega}((\nabla_{\vec{r}} \phi) \cdot \vec{B})}{1 + q(\vec{\Omega} \cdot \vec{B})})$$

$$\frac{\partial \vec{k}}{\partial t} = \frac{-q\nabla_{\vec{r}}\phi - q^2\nabla_{\vec{r}}\phi(\vec{\Omega}\cdot\vec{B}) + (q\nabla_{\vec{k}}\varepsilon)\times\vec{B} + q^2(\nabla_{\vec{r}}\phi)(\vec{B}\cdot\vec{\Omega}) - q^2\vec{\Omega}((\nabla_{\vec{r}}\phi)\cdot\vec{B})}{1+q(\vec{\Omega}\cdot\vec{B})}$$

$$\frac{\partial \vec{k}}{\partial t} = \frac{-q\nabla_{\vec{r}}\phi + q(\nabla_{\vec{k}}\varepsilon)\times\vec{B} - q^2\vec{\Omega}((\nabla_{\vec{r}}\phi)\cdot\vec{B})}{1+q(\vec{\Omega}\cdot\vec{B})} \tag{6}$$

As a final check, if we let $\vec{\Omega} = 0$, we get back the same result as the original force vector, as expected.