Asymptotic analysis of Berry phase governed by the scalar wave equation

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Abstract

We deploy an asymptotic model for the interaction between nearby dispersion surfaces and respective eigenstates toward explicit evaluation of the Berry phase governed by the scalar wave equation in 2D periodic continua. The model, featuring a pair of coupled Dirac equations, endows the interacting Bloch eigenstates with an explicit gauge that caters for analytical integration in the wavenumber domain. Among the featured parameters, the one ($\mathfrak{s} \in [0, \frac{1}{2}]$) that synthesizes the phase information on the coupling term is shown to decide whether the Berry connection round the loop is singular ($\mathfrak{s} = 0$) or analytic ($\mathfrak{s} > 0$). We show that the Berry phase is π-quantal and topological when $\mathfrak{s} = 0$, equalling π when the contour encloses the apex of a Dirac cone and zero otherwise. The analogous result is obtained when $\mathfrak{s} \simeq 0$ and similarly for $\mathfrak{s} \simeq \frac{1}{2}$. In the interior of the $\mathfrak{s}$-domain, we find that the Berry phase either equals π or is not quantal.

Keywords: Berry phase, scalar wave equation, periodic continua

1 Introduction

In 1984, Michael Berry discovered [1] that when an eigenstate of quantum system is cycled "slowly" (i.e. adiabatically) in the parametric space, it acquires a geometrical phase factor, the so-called Berry phase Υ, that is not removable under a gauge transformation. This finding has permeated all branches of physics and bears analogues in gauge theory and differential geometry [2]. In the original paper [1] it is shown, under a particular restriction on the parametric space, that $\Upsilon = \pi$ (modulo 2π) when the closed contour encloses the apex of a Dirac cone and $\Upsilon = 0$ otherwise. Even though originally derived within the framework of quantum mechanics, this concept is readily applicable throughout wave physics, see e.g. [3] in the context of classical electromagnetism and Bloch waves – which allow for system cycling in the physical, i.e. wavenumber (as opposed to parametric) space [4]. In principle, evaluation of the Berry phase is inherently numerical and entails quadrature of the phase increment, the co-called Berry connection, over a loop in the wavenumber space enclosing the suspect degeneracy. For 2D systems, Υ is known to be "generally" $0/\pi$ quantal and possibly topological [3,4]. In the absence of analytical results, however, it is difficult to draw definitive conclusions.

2 Berry phase

Consider the wave equation in an unbounded periodic medium $S \subseteq \mathbb{R}^2$ at frequency ω, namely

$$\nabla\cdot\big(G(\boldsymbol{x})\nabla u\big) \,+\, \omega^2\rho(\boldsymbol{x})u \;=\; 0 \quad \text{in } S, \qquad (1)$$

where $0 < G < \infty$ and $0 < \rho < \infty$ are Y-periodic and bounded away from zero. We next seek the Bloch-wave solutions of (1) as

$$u(\boldsymbol{x}) \;=\; \tilde{u}(\boldsymbol{x})e^{i\boldsymbol{k}\cdot\boldsymbol{x}}, \quad \tilde{u} : Y\text{-periodic} \qquad (2)$$

where $\tilde{u}$ depends implicitly on $\boldsymbol{k}\in\mathcal{B}$ and $\omega\in\mathbb{R}^+$ ($\mathcal{B}$ denotes the first Brillouin zone). With such premise, (1) reduces to

$$\nabla_{\boldsymbol{k}}\cdot\big(G(\boldsymbol{x})\nabla_{\boldsymbol{k}}\tilde{u}\big) \,+\, \omega^2\rho(\boldsymbol{x})\tilde{u} \;=\; 0 \quad \text{in } Y \qquad (3)$$

subject to the usual quasi-periodic boundary conditions, where $\nabla_{\boldsymbol{k}} = \nabla + i\boldsymbol{k}$.

As demonstrated in [5], for given $\boldsymbol{k}\in\mathcal{B}$ the field equation (3) (with relevant boundary conditions) is affiliated with the eigensystem $\{\tilde{\lambda}_n(\boldsymbol{k}) \in\mathbb{R},\ \tilde{\phi}_n(\boldsymbol{k})\in H^1_{\rho p}(Y),\ \|\tilde{\phi}_n\| = 1\}$ that satisfies

$$\rho(\boldsymbol{x})^{-1}\nabla_{\boldsymbol{k}}\cdot\big(G(\boldsymbol{x})\nabla_{\boldsymbol{k}}\,\tilde{\phi}_n\big) + \tilde{\lambda}_n\tilde{\phi}_n \;=\; 0 \quad \text{in } Y, \qquad (4)$$

where $H^1_{\rho p}(Y) = \{\tilde{g}\in L^2_{\rho p(Y)} : \nabla\tilde{g}|_Y \in (L^2_{\rho p}(Y))^2\}$, and $L^2_{\rho p}(Y) = \{\tilde{g} : Y\text{-periodic}, \int_Y \rho g\bar{g}\,\mathrm{d}\boldsymbol{x} < \infty\}$.

On denoting by $C \subset \mathbb{R}^2$ be a closed path enclosing some $\boldsymbol{k}_s \in \mathcal{B}$, we consider the Berry phase characterizing the nth dispersion branch at $\boldsymbol{k} = \boldsymbol{k}_s$ as a closed line integral

$$\Upsilon_n(\boldsymbol{k}_s) \;=\; \oint_C \mathrm{d}\Upsilon_n(\boldsymbol{k}), \qquad (5)$$

where $\mathrm{d}\Upsilon_n$ is an infinitesimal phase difference between neighboring eigenstates [6] given by

$$\mathrm{d}\Upsilon_n(\boldsymbol{k}) \;=\; -i\,\mathrm{d}\boldsymbol{k}\cdot\big(\rho\tilde{\phi}_{n,\boldsymbol{k}}(\boldsymbol{k}),\tilde{\phi}_n(\boldsymbol{k})\big); \tag{6}$$

$\tilde{\phi}_{n,\boldsymbol{k}} = \partial\tilde{\phi}_n/\partial\boldsymbol{k}$; $(\cdot,\cdot)$ is the usual inner product over Y, and the quantity contracted with $\mathrm{d}\boldsymbol{k}$ is referred to as the *Berry connection.* We aim to evaluate (5) in instances where branches n and $n+1$ are close to each other at $\boldsymbol{k}_s$.

3 Asymptotic model

Let the eigenvalue problem due to (4) yield a pair of nearby eigenvalues $\lambda_n := \omega_n^2$ and $\lambda_{n+1} := \omega_{n+1}^2$ for some $\boldsymbol{k}_s \in \mathcal{B}$, and consider the affiliated dispersion map over a small neighborhood

$$\boldsymbol{k} \;=\; \boldsymbol{k}_s + \epsilon\hat{\boldsymbol{k}}, \qquad \epsilon = o(1). \tag{7}$$

Writing $\omega_{nj}^2(\boldsymbol{k}) := \omega_{n+j-1}^2(\boldsymbol{k})$ $(j=\overline{1,2})$, we assume "tight" eigenvalue separation in that

$$\omega_{n2}^2(\boldsymbol{k}_s) \;=\; \omega_{n1}^2(\boldsymbol{k}_s) \,+\, \epsilon\gamma, \qquad \gamma = o(1).$$

As shown in [5], eigenfunctions $\tilde{\phi}_{n_j}$ within spectral neighborhood (7) can be expanded as

$$\tilde{\phi}_{n_j}(\boldsymbol{k}_s+\epsilon\hat{\boldsymbol{k}}) = \boldsymbol{u}^{[j]}(\hat{\boldsymbol{k}})\cdot\begin{bmatrix}\tilde{\phi}_{n_1}(\boldsymbol{k}_s)\\ \tilde{\phi}_{n_2}(\boldsymbol{k}_s)\end{bmatrix} + O(\epsilon), \tag{8}$$

where $\boldsymbol{u}^{[j]} \in \mathbb{C}^2$ solve the eigenvalue problem

$$\big(\boldsymbol{A}^{\gamma} + \hat{\lambda}_j\boldsymbol{I}\big)\,\boldsymbol{u}^{[j]} = \boldsymbol{0}, \tag{9}$$

$$\boldsymbol{A}^{\gamma} = \begin{bmatrix}\boldsymbol{\theta}_{11}\cdot i\hat{\boldsymbol{k}} & \boldsymbol{\theta}_{12}\cdot i\hat{\boldsymbol{k}}\\ -\overline{\boldsymbol{\theta}_{12}}\cdot i\hat{\boldsymbol{k}} & \boldsymbol{\theta}_{22}\cdot i\hat{\boldsymbol{k}}-\gamma\end{bmatrix}. \tag{10}$$

Here $\boldsymbol{I}$ is the 2×2 identity matrix, and

$$\boldsymbol{\theta}_{pq} = (G\nabla_{\boldsymbol{k}}\tilde{\phi}_{n_q},\tilde{\phi}_{n_p}) - \overline{(G\nabla_{\boldsymbol{k}}\tilde{\phi}_{n_p},\tilde{\phi}_{n_q})} \;\in \mathbb{C}^2$$

are evaluated at $\boldsymbol{k}_s$. Note that the coefficient matrix $\boldsymbol{A}^{\gamma}$ is Hermitian [5]; specifically, we have $\boldsymbol{\theta}_{qq} \in i\mathbb{R}^2$ thanks to the fact that $\boldsymbol{\theta}_{pq} = -\overline{\boldsymbol{\theta}_{qp}}$. In the sequel, we write $\boldsymbol{\theta}_{12} := (t_1,t_2)$. Note that (8) resembles the tight binding model in the condensed matter physics literature.

4 Results

Assuming the circular path of integration in (5) by letting $\hat{\boldsymbol{k}} = \epsilon\varrho\boldsymbol{e}$ where $\boldsymbol{e}\in\mathbb{R}^2$ is a unit vector and $\varrho = O(1)$, from (5)–(6) and (8)–(11) one finds that the Berry phase can be recast in a 4-dimensional parametric space as

$$\Upsilon_{n_j}(\boldsymbol{k}_s) \;=\; F(\mathfrak{s}, \|\widetilde{\Delta\boldsymbol{\theta}}\|, \widetilde{\gamma}_{\varrho}, \beta_j),$$

where

$$\mathfrak{s} \;=\; \|\boldsymbol{\theta}_{12}\|^{-2}|\Im(\overline{t_1}t_2)| \;\in\; [0,\tfrac{1}{2}]; \tag{11}$$

$\|\widetilde{\Delta\boldsymbol{\theta}}\| = \Delta\boldsymbol{\theta}/\|\boldsymbol{\theta}_{12}\|$; $\Delta\boldsymbol{\theta} = \Im(\boldsymbol{\theta}_{11}-\boldsymbol{\theta}_{22})$; $\widetilde{\gamma}_{\varrho} = \gamma/(\varrho\|\boldsymbol{\theta}_{12}\|)$; $\beta_2 = \beta_1+\pi$, and β_1 is the angle between the directions where $|\overline{\boldsymbol{\theta}_{12}}\cdot\boldsymbol{e}|$ and $|\Delta\boldsymbol{\theta}\cdot\boldsymbol{e}|$ are respectively minimized.

In this setting, $\mathfrak{s}$ is shown to decide whether the Berry connection round the loop is singular ($\mathfrak{s}=0$) or analytic ($\mathfrak{s}>0$). The analysis demonstrates that the Berry phase for 2D lattices is π-quantal and topological when $\mathfrak{s}=0$, equalling π (modulo 2π) when the contour encloses a Dirac i.e. diabolical point and zero in all other situations (avoided crossings or line crossings). The analogous result is obtained, up to an $O(\mathfrak{s})$ residual, when $\mathfrak{s}\simeq 0$ and similarly for $\mathfrak{s}\simeq\frac{1}{2}$. In the interior of the $\mathfrak{s}$-domain, on the other hand, we find that the Berry phase either approximately equals π (for sufficiently small $\widetilde{\gamma}_{\varrho}$) or is not quantal. Beyond shedding light on the anatomy of the Berry phase for 2D periodic continua, the featured analysis carries a practical benefit for it permits single-wavenumber evaluation of this geometrical phase quantity.

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