Vector $k \cdot p$ approach for photonic band structures

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We point out that $k \cdot p$ treatments of photonic band gap materials based on the usual master equation must employ not only the physical photonic band solutions of that equation, but also unphysical solutions, in order to form a complete set. Nonetheless, it is possible to construct correct $k \cdot p$ expressions for the group velocity and its dispersion in terms of matrix elements involving only the photonic band solutions.

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I. INTRODUCTION

The usefulness of the $k \cdot p$ formalism in describing the motion of electrons in semiconductors has led to its extension to treat light in photonic band gap materials [1–3]. Yet a new subtlety arises in this application in which vector fields are involved. It appears not to have been generally realized, but can easily be described.

For a material with a periodic dielectric constant $\epsilon(\mathbf{r}) = \epsilon(\mathbf{r}+\mathbf{R})$, where $\mathbf{R}$ is any lattice vector, the photonic band structure is often calculated [4] by finding the eigenvalues λ and vector eigenfunctions $\mathbf{H}(\mathbf{r})$ that solve the so-called "master equation,"

$$\mathbf{\Theta}\mathbf{H}(\mathbf{r}) = \lambda \mathbf{H}(\mathbf{r}), \tag{1}$$

where the vector operator

$$\mathbf{\Theta} \equiv \boldsymbol{\nabla} \times \left(\frac{1}{n^2(\mathbf{r})} \nabla \times \right)$$

is Hermitian; we have put $\epsilon(\mathbf{r}) = \epsilon_0 n^2(\mathbf{r})$, and neglected any magnetic effects. According to Bloch's theorem, solutions of Eq. (1) can be found of the form $\mathbf{H}_{m\mathbf{k}}(\mathbf{r}) = N^{-1/2}\mathbf{h}_{m\mathbf{k}}(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})$, with $\mathbf{h}_{m\mathbf{k}}(\mathbf{r}) = \mathbf{h}_{m\mathbf{k}}(\mathbf{r}+\mathbf{R})$, where N is the number of unit cells in the normalization volume; here m labels the band, and $\mathbf{k}$ is the crystal wave vector. Those solutions with nonzero eigenvalue $\lambda = \lambda_{m\mathbf{k}}$ are guaranteed to be divergenceless, $\boldsymbol{\nabla}\cdot\mathbf{H}_{m\mathbf{k}}(\mathbf{r}) = 0$, and can be identified as the magnetic field amplitude of stationary solutions of the Maxwell equations at frequency $\omega_{m\mathbf{k}} = \pm c\sqrt{\lambda_{m\mathbf{k}}}$. The associated electric field follows immediately from the Maxwell equation $\epsilon\dot{\mathbf{E}} = \boldsymbol{\nabla}\times\mathbf{H}$. We refer to these fields and their frequencies as the *photonic bands*.

Proceeding in analogy with the electron problem, from Eq. (1) an eigenvalue equation for $\mathbf{h}_{m\mathbf{k}}(\mathbf{r})$ is derived,

$$\mathcal{H}_{\mathbf{k}}\mathbf{h}_{m\mathbf{k}}(\mathbf{r}) = \lambda_{m\mathbf{k}}\mathbf{h}_{m\mathbf{k}}(\mathbf{r}), \tag{2}$$

where $\mathcal{H}_{\mathbf{k}} = \mathbf{\Theta} + \theta_{\mathbf{k}}$, and the Hermitian operator $\theta_{\mathbf{k}}$ acts on a vector function $\mathbf{g}(\mathbf{r})$ according to

$$\theta_{\mathbf{k}}\mathbf{g}(\mathbf{r}) \equiv \boldsymbol{\nabla}\times\left(\frac{i\mathbf{k}\times\mathbf{g}(\mathbf{r})}{n^2(\mathbf{r})}\right) + \frac{i\mathbf{k}\times[\boldsymbol{\nabla}\times\mathbf{g}(\mathbf{r}) + i\mathbf{k}\times\mathbf{g}(\mathbf{r})]}{n^2(\mathbf{r})}. \tag{3}$$

The $k \cdot p$ formalism involves writing Eq. (2) at $\mathbf{k}+\boldsymbol{\kappa}$ as well, putting $\mathcal{H}_{\mathbf{k}+\boldsymbol{\kappa}} = \mathcal{H}_{\mathbf{k}} + \mathcal{V}_{\mathbf{k},\boldsymbol{\kappa}}$, where $\mathcal{V}_{\mathbf{k},\boldsymbol{\kappa}} = \theta_{\mathbf{k}+\boldsymbol{\kappa}} - \theta_{\mathbf{k}}$, and writing an eigenfunction $\mathbf{h}_{m(\mathbf{k}+\boldsymbol{\kappa})}(\mathbf{r})$ of the "perturbed" $\mathcal{H}_{\mathbf{k}+\boldsymbol{\kappa}}$ in terms of all of the eigenfunctions $\mathbf{h}_{p\mathbf{k}}(\mathbf{r})$ of the "unperturbed" $\mathcal{H}_{\mathbf{k}}$.

If we restrict ourselves to photonic bands, one can see that this strategy fails, even if $\boldsymbol{\kappa}$ is an arbitrarily small wave vector. In that limit we would write

$$\mathbf{h}_{m(\mathbf{k}+\boldsymbol{\kappa})}(\mathbf{r}) = \mathbf{h}_{m\mathbf{k}}(\mathbf{r}) + \sum_{p,a}\gamma_{pa}^{(1)}\kappa^a\mathbf{h}_{p\mathbf{k}}(\mathbf{r}) + \mathcal{O}(\kappa^2), \tag{4}$$

where the $\gamma_{pa}^{(1)}$ are first order expansion coefficients and the a are Cartesian components. The difficulty is that, since both $\mathbf{H}_{m(\mathbf{k}+\boldsymbol{\kappa})}(\mathbf{r})$ and $\mathbf{H}_{m\mathbf{k}}(\mathbf{r})$ are divergenceless we must have

$$\boldsymbol{\nabla}\cdot\mathbf{h}_{m(\mathbf{k}+\boldsymbol{\kappa})}(\mathbf{r}) + i(\mathbf{k}+\boldsymbol{\kappa})\cdot\mathbf{h}_{m(\mathbf{k}+\boldsymbol{\kappa})}(\mathbf{r}) = 0, \tag{5}$$

and the corresponding equation with $\mathbf{k}+\boldsymbol{\kappa}$ replaced everywhere by $\mathbf{k}$. Taking the divergence of Eq. (4) and using these conditions, we find

$$i\boldsymbol{\kappa}\cdot\mathbf{h}_{m\mathbf{k}}(\mathbf{r}) + \mathcal{O}(\kappa^2) = 0. \tag{6}$$

But for this to hold for any $\boldsymbol{\kappa}$ it must be true that $\mathbf{h}_{m\mathbf{k}}(\mathbf{r}) = \mathbf{0}$, which is nonsense. So an expansion of the form (4) cannot be possible.

In the next section we identify the source of this difficulty and correct it, and in Sec. III we develop the $k \cdot p$ expansion. In Sec. IV we compare our results with earlier work and discuss the consequences. Some of the details are presented in an Appendix.

II. THE BASIS SET

The difficulty highlighted above arises because the fields $\mathbf{h}_{p\mathbf{k}}(\mathbf{r})$ associated with photonic bands do not constitute a complete set of functions periodic over the unit cell. To establish such a set it is easiest to return to the master equation (1) and consider not only the physical solutions, but *all* the solutions. These may be taken as a complete set, from which a corresponding complete set of eigenfunctions of $\mathcal{H}_{\mathbf{k}}$ can then be extracted.

We begin by considering three types of solutions of Eq. (1). Besides satisfying Eq. (1), type τ_1 also satisfy $\boldsymbol{\nabla}\cdot\mathbf{H}(\mathbf{r}) = 0$ and have $\lambda \neq 0$, type τ_2 satisfy $\boldsymbol{\nabla}\cdot\mathbf{H}(\mathbf{r}) = 0$ and have $\lambda = 0$, and types τ_3 satisfy $\boldsymbol{\nabla}\times\mathbf{H}(\mathbf{r}) = 0$ and have $\lambda = 0$. Uniform solutions satisfy the conditions for both types τ_2 and τ_3; for definiteness we include them in type τ_3. All three types are also required to satisfy periodic boundary conditions over a normalization volume.

Our categorization clearly exhausts the solutions with either $\boldsymbol{\nabla}\cdot\mathbf{H}(\mathbf{r})=\mathbf{0}$ or $\boldsymbol{\nabla}\times\mathbf{H}(\mathbf{r})=\mathbf{0}$, as can be seen by inspecting Eq. (1) and its divergence. If both $\nabla\cdot\mathbf{H}(\mathbf{r})=\mathbf{0}$ *and* $\boldsymbol{\nabla}\times\mathbf{H}(\mathbf{r})=\mathbf{0}$, the only solution consistent with periodic boundary conditions over a normalization volume is the uniform solution, which is included in type τ_3. More general solutions $\mathbf{H}_G(\mathbf{r})$ of Eq. (1), with $\boldsymbol{\nabla}\cdot\mathbf{H}_G(\mathbf{r})\neq\mathbf{0}$ and $\boldsymbol{\nabla}\times\mathbf{H}_G(\mathbf{r})\neq\mathbf{0}$, can always be written as the sum of a transverse field and a longitudinal field, $\mathbf{H}_G(\mathbf{r})=\mathbf{H}_{GT}(\mathbf{r})+\mathbf{H}_{GL}(\mathbf{r})$, where $\boldsymbol{\nabla}\cdot\mathbf{H}_{GT}(\mathbf{r})=\mathbf{0}$ and $\boldsymbol{\nabla}\times\mathbf{H}_{GL}(\mathbf{r})=0$; we include a possible uniform component in the longitudinal field $\mathbf{H}_{GL}(\mathbf{r})$ for definiteness. Such solutions $\mathbf{H}_G(\mathbf{r})$ must have $\lambda=0$, as can be seen by taking the divergence of Eq. (1). But then since both $\mathbf{H}_G(\mathbf{r})$ and $\mathbf{H}_{GL}(\mathbf{r})$ are solutions of Eq. (1) with eigenvalue zero, $\mathbf{H}_{GT}(\mathbf{r})$ must be also. Thus such an $\mathbf{H}_G(\mathbf{r})$ is the sum of a type τ_2 and a type τ_3 solution. Hence a complete set of types τ_1, τ_2, and τ_3 suffices to identify a basis set of eigenfunctions of Eq. (1). We now examine their nature.

Type τ_1 solutions identify the photonic bands, and correspond to the magnetic fields of stationary solutions of Maxwell equations with nonzero frequency $\omega_{m\mathbf{k}}$, $\lambda_{m\mathbf{k}}=\omega_{m\mathbf{k}}^2/c^2$.

Type τ_2 solutions, if they exist, are unphysical, in the sense that a solution $\mathbf{H}(\mathbf{r})$ of type τ_2 cannot be identified with the magnetic field of a stationary solution of the Maxwell equations. For suppose that it could, with frequency $\omega=0$. Then from the Maxwell equations we must have $\boldsymbol{\nabla}\times\mathbf{H}(\mathrm{r})=\mathbf{0}$, and both the divergence and curl of $\mathbf{H}(\mathbf{r})$ would vanish. But there is no nontrivial solution of the Maxwell equations, periodic over a normalization volume, satisfying this condition other than a uniform solution, which by our convention is considered to be type τ_3. Suppose then that a solution $\mathbf{H}(\mathbf{r})$ of type τ_2 could be identified with the magnetic field of a stationary solution of the Maxwell equations with a frequency $\omega\neq 0$. From the Maxwell equations one can then immediately derive that such an $\mathbf{H}(\mathbf{r})$ should satisfy Eq. (1) with $\lambda=\omega^2/c^2$, contradicting our assumption that it is of type τ_2.

Type τ_3 are longitudinal fields, and we can easily construct a full set of such solutions. Putting $\boldsymbol{v}(\mathbf{V})\equiv\mathbf{V}/|\mathbf{V}|$ for any nonvanishing vector $\mathbf{V}$, we construct a set of type τ_3 solutions according to

$$\mathbf{H}_{mL\mathbf{k}}(\mathbf{r})\equiv\frac{\boldsymbol{v}(\mathbf{k}+\mathbf{G}_m)e^{i(\mathbf{k}+\mathbf{G}_m)\cdot\mathbf{r}}}{\sqrt{\Omega}}=\frac{\mathbf{h}_{mL\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{N}},$$

where

$$\mathbf{h}_{mL\mathbf{k}}(\mathbf{r})\equiv\frac{\boldsymbol{v}(\mathbf{k}+\mathbf{G}_m)e^{i\mathbf{G}_m\cdot\mathbf{r}}}{\sqrt{\Omega_c}};\tag{7}$$

here Ω is the normalization volume, Ω_c is the volume of a unit cell, and the $\mathbf{G}_m$ label the reciprocal lattice vectors. Clearly $\mathbf{h}_{mL\mathbf{k}}(\mathbf{r})=\mathbf{h}_{mL\mathbf{k}}(\mathbf{r}+\mathbf{R})$. As $\mathbf{k}$ ranges over the first Brillouin zone and the $\mathbf{G}_m$ vary over all the reciprocal lattice vectors, $\mathbf{k}+\mathbf{G}_m$ ranges over all of reciprocal space. By construction the fields $\mathbf{H}_{mL\mathbf{k}}(\mathbf{r})$ are all longitudinal, and they form a basis for describing any longitudinal field. Uniform solutions, characterized by $\mathbf{k}=\mathbf{G}_m=\mathbf{0}$, are a special case. A uniform field is both longitudinal and transverse, and instead of one function $\mathbf{h}_{mL\mathbf{0}}(\mathbf{r})$ we have three, which we can take as $\mathbf{h}_{(x)L0}(\mathbf{r})=\hat{\mathbf{x}}/\sqrt{\Omega_c}$, $\mathbf{h}_{(y)L0}(\mathbf{r})=\hat{\mathbf{y}}/\sqrt{\Omega_c}$, and $\mathbf{h}_{(z)L0}(\mathbf{r})=\hat{\mathbf{z}}/\sqrt{\Omega_c}$. In sums and relations involving $\mathbf{H}_{mL\mathbf{k}}(\mathbf{r})$ we understand there to be these three terms in the special case $\mathbf{k}=\mathbf{G}_m=\mathbf{0}$. Except for these uniform solutions, type τ_3 solutions have $\boldsymbol{\nabla}\cdot\mathbf{H}_{mL\mathbf{k}}(\mathbf{r})\neq 0$, and hence they are unphysical in that they do not correspond to the magnetic field of any stationary solution of the Maxwell equations. We label the eigenvalues of type τ_3 solutions, which all vanish, as $\lambda_{mL\mathbf{k}}=0$.

To simplify the notation, we combine type τ_1 and any type τ_2 solutions in the notation $\mathbf{H}_{mT\mathbf{k}}(\mathbf{r})=N^{-1/2}\mathbf{h}_{mT\mathbf{k}}(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})$, since they are both transverse; we denote their eigenvalues by $\lambda_{mT\mathbf{k}}$. For the physical type τ_1 solutions these eigenvalues are $\omega_{m\mathbf{k}}^2/c^2$; for type τ_2 solutions the eigenvalues are zero. We will, however, continue to use $\mathbf{H}_{m\mathbf{k}}(\mathbf{r})$ and $\mathbf{h}_{m\mathbf{k}}(\mathbf{r})$ when we want to refer specifically to a type τ_1 solution. With a choice of overall normalization factors in the eigenfunctions, it is easy to see that

$$\int\mathbf{H}_{pS\mathbf{k}}^{*}(\mathbf{r})\cdot\mathbf{H}_{p'S'\mathbf{k}'}(\mathbf{r})d\mathbf{r}=\delta_{pp'}\delta_{SS'}\delta_{\mathbf{k}\mathbf{k}'},\tag{8}$$

where S and S' can be either T or L: The photonic band type τ_1 solutions are orthogonal among themselves, with a proper choice of any degenerate states at a given $\mathbf{k}$, and any type τ_2 solutions can be similarly chosen to be orthogonal among themselves; type τ_3 are orthogonal among themselves because two wave vectors $(\mathbf{k}+\mathbf{G}_p,\mathbf{k}'+\mathbf{G}_{p'})$ in the allowed set cannot be equal unless $\mathbf{k}=\mathbf{k}'$ and $\mathbf{G}_p=\mathbf{G}_{p'}$; type τ_2 and type τ_3 solutions are orthogonal to type τ_1 solutions because of different eigenvalues; type τ_2 solutions are orthogonal to type τ_3 solutions because of the orthogonality of transverse and longitudinal functions. For a given $\mathbf{k}$, it then follows from the definition of the $\mathbf{h}_{pS\mathbf{k}}(\mathbf{r})$ and Eq. (8) that

$$\int_{unit}\mathbf{h}_{pS\mathbf{k}}^{*}(\mathbf{r})\cdot\mathbf{h}_{p'S'\mathbf{k}}(\mathbf{r})d\mathbf{r}=\delta_{pp'}\delta_{SS'},\tag{9}$$

where the integration ranges over a unit cell. All the functions $\mathbf{h}_{pS\mathbf{k}}(\mathbf{r})$ satisfy

$$\mathcal{H}_{\mathbf{k}}\mathbf{h}_{pS\mathbf{k}}(\mathbf{r})=\lambda_{pS\mathbf{k}}\mathbf{h}_{pS\mathbf{k}}(\mathbf{r}).\tag{10}$$

III. $k\cdot p$ THEORY

By identifying *all* the eigenfunctions of the Hermitian operator $\boldsymbol{\Theta}$, whether they correspond to physical magnetic fields or not, we have been led to a set of functions $\mathbf{h}_{pS\mathbf{k}}(\mathbf{r})$ that can thus be taken as a complete set of functions periodic over the unit cell. When this larger set, instead of just the $\mathbf{h}_{p\mathbf{k}}(\mathbf{r})$ corresponding to the photonic bands, is used to expand $\mathbf{h}_{m(\mathbf{k}+\boldsymbol{\kappa})}(\mathbf{r})$ we expect that the correct divergence condition (5) should indeed be satisfied. We confirm this in the Appendix. In this section we find the expressions for $\partial\omega_{m\mathbf{k}}/\partial k^a$ and $\partial^2\omega_{m\mathbf{k}}/\partial k^a\partial k^b$ for a photonic band m that is nondegenerate at $\mathbf{k}$; the extension to degenerate points follows in the usual way. The expression for $\partial^2\omega_{m\mathbf{k}}/\partial k^a\partial k^b$ leads to a kind of effective mass sum rule that initially involves matrix elements connecting the photonic band state $\mathbf{h}_{m\mathbf{k}}(\mathbf{r})$ to *all* functions $\mathbf{h}_{pS\mathbf{k}}(\mathbf{r})$, but it can be reduced to one involving only matrix elements between photonic band states.

We begin with Eq. (10), which we write in shorthand as

$$(\mathcal{H}_{\mathbf{k}}-\lambda_{\sigma\mathbf{k}})\mathbf{h}_{\sigma\mathbf{k}}, \tag{11}$$

using a single Greek subscript to denote (pS) where convenient. We take all the states at $\mathbf{k}$ to be normalized,

$$\langle\mathbf{h}_{\sigma\mathbf{k}}|\mathbf{h}_{\sigma'\mathbf{k}}\rangle=\delta_{\sigma\sigma'},$$

where in general

$$\langle\mathbf{a}|\mathbf{b}\rangle\equiv\int_{unit}\mathbf{a}^*(\mathbf{r})\cdot\mathbf{b}(\mathbf{r})d\mathbf{r}.$$

Now at $\mathbf{k}$ we choose a type τ_1 band that is nondegenerate; we denote the particular state by $\mathbf{h}_{m\mathbf{k}}$. We now imagine allowing $\mathbf{k}$ to move to neighboring points $\mathbf{k}+\boldsymbol{\kappa}$ in the Brillouin zone, in the course of which $\mathbf{h}_{m\mathbf{k}}$ evolves; we forego normalization at $\boldsymbol{\kappa}\neq\mathbf{0}$ by insisting that $\mathbf{h}_{m(\mathbf{k}+\boldsymbol{\kappa})}-\mathbf{h}_{m\mathbf{k}}$ is orthogonal to $\mathbf{h}_{m\mathbf{k}}$. Hence

$$\left\langle\mathbf{h}_{m\mathbf{k}}\middle|\frac{\partial\mathbf{h}_{m\mathbf{k}}}{\partial k^a}\right\rangle=0,$$

$$\left\langle\mathbf{h}_{m\mathbf{k}}\middle|\frac{\partial^2\mathbf{h}_{m\mathbf{k}}}{\partial k^a\partial k^b}\right\rangle=0, \tag{12}$$

etc., where the superscript on k^a indicates a Cartesian component. Normalization could always be imposed at the end of the calculation if desired. Taking the derivative of Eq. (11) yields

$$\left(\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^a}-\frac{\partial\lambda_{m\mathbf{k}}}{\partial k^a}\right)\mathbf{h}_{m\mathbf{k}}+(\mathcal{H}_{\mathbf{k}}-\lambda_{m\mathbf{k}})\frac{\partial\mathbf{h}_{m\mathbf{k}}}{\partial k^a}=0. \tag{13}$$

Dotting into $\mathbf{h}^*_{m\mathbf{k}}$ and integrating over a unit cell, and using Eq. (11), we find

$$\frac{\partial\lambda_{m\mathbf{k}}}{\partial k^a}=\left\langle\mathbf{h}_{m\mathbf{k}}\middle|\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^a}\mathbf{h}_{m\mathbf{k}}\right\rangle. \tag{14}$$

Since $\lambda_{m\mathbf{k}}=\omega^2_{m\mathbf{k}}/c^2$, this immediately yields

$$\frac{\partial\omega_{m\mathbf{k}}}{\partial k^a}=\frac{c^2}{2\omega_{m\mathbf{k}}}\left\langle\mathbf{h}_{m\mathbf{k}}\middle|\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^a}\mathbf{h}_{m\mathbf{k}}\right\rangle, \tag{15}$$

an expression for the group velocity associated with band m at point $\mathbf{k}$ in the Brillouin zone.

Next, dotting Eq. (13) into $\mathbf{h}^*_{\sigma\mathbf{k}}$, for σ not equal to our state of interest, and integrating over a unit cell, gives

$$\left\langle\mathbf{h}_{\sigma\mathbf{k}}\middle|\frac{\partial\mathbf{h}_{m\mathbf{k}}}{\partial k^a}\right\rangle=-\frac{\langle\mathbf{h}_{\sigma\mathbf{k}}|(\partial\mathcal{H}_{\mathbf{k}}/\partial k^a)\mathbf{h}_{m\mathbf{k}}\rangle}{(\lambda_{\sigma\mathbf{k}}-\lambda_{m\mathbf{k}})}. \tag{16}$$

Proceeding, we take $\partial/\partial k^b$ of Eq. (13) and, dotting the result into $\mathbf{h}^*_{m\mathbf{k}}$ and integrating over a unit cell, using Eq. (12) and the expansion

$$\begin{aligned}\frac{\partial\mathbf{h}_{m\mathbf{k}}}{\partial k^a}&=\sum_\sigma{}'\ \mathbf{h}_{\sigma\mathbf{k}}\left\langle\mathbf{h}_{\sigma\mathbf{k}}\middle|\frac{\partial\mathbf{h}_{m\mathbf{k}}}{\partial k^a}\right\rangle\\&=-\sum_\sigma{}'\ \mathbf{h}_{\sigma\mathbf{k}}\frac{\langle\mathbf{h}_{\sigma\mathbf{k}}|(\partial\mathcal{H}_{\mathbf{k}}/\partial k^a)\mathbf{h}_{m\mathbf{k}}\rangle}{(\lambda_{\sigma\mathbf{k}}-\lambda_{m\mathbf{k}})},\end{aligned} \tag{17}$$

where the prime indicates that σ is not to be equal to our state of interest, we find that

$$\begin{aligned}\frac{\partial^2\lambda_{m\mathbf{k}}}{\partial k^a\partial k^b}=&\left\langle\mathbf{h}_{m\mathbf{k}}\middle|\frac{\partial^2\mathcal{H}_{\mathbf{k}}}{\partial k^a\partial k^b}\mathbf{h}_{m\mathbf{k}}\right\rangle\\&-\sum_\sigma{}'\ \frac{\langle\mathbf{h}_{m\mathbf{k}}|(\partial\mathcal{H}_{\mathbf{k}}/\partial k^a)\mathbf{h}_{\sigma\mathbf{k}}\rangle\langle\mathbf{h}_{\sigma\mathbf{k}}|(\partial\mathcal{H}_{\mathbf{k}}/\partial k^b)\mathbf{h}_{m\mathbf{k}}\rangle}{(\lambda_{\sigma\mathbf{k}}-\lambda_{m\mathbf{k}})}\\&-\sum_\sigma{}'\ \frac{\langle\mathbf{h}_{m\mathbf{k}}|(\partial\mathcal{H}_{\mathbf{k}}/\partial k^b)\mathbf{h}_{\sigma\mathbf{k}}\rangle\langle\mathbf{h}_{\sigma\mathbf{k}}|(\partial\mathcal{H}_{\mathbf{k}}/\partial k^a)\mathbf{h}_{m\mathbf{k}}\rangle}{(\lambda_{\sigma\mathbf{k}}-\lambda_{m\mathbf{k}})}.\end{aligned} \tag{18}$$

We can write this as the sum of two terms,

$$\frac{\partial^2\lambda_{m\mathbf{k}}}{\partial k^a\partial k^b}=\left(\frac{\partial^2\lambda_{m\mathbf{k}}}{\partial k^a\partial k^b}\right)_{pb}+\left(\frac{\partial^2\lambda_{m\mathbf{k}}}{\partial k^a\partial k^b}\right)_0,$$

where the term labeled with the subscript pb contains the first term in Eq. (18) and the terms in the summations involving photonic bands (type τ_1 solutions); the second term involves terms in the summations in Eq. (18) involving type τ_2 and type τ_3 solutions (with eigenvalue $\lambda_{\sigma\mathbf{k}}=0$). Then using $\lambda_{m\mathbf{k}}=\omega^2_{m\mathbf{k}}/c^2$, we write

$$\frac{\partial^2\omega_{m\mathbf{k}}}{\partial k^a\partial k^b}=\left(\frac{\partial^2\omega_{m\mathbf{k}}}{\partial k^a\partial k^b}\right)_{pb}+\left(\frac{\partial^2\omega_{m\mathbf{k}}}{\partial k^a\partial k^b}\right)_0, \tag{19}$$

where

$$\left(\frac{\partial^2\omega_{m\mathbf{k}}}{\partial k^a\partial k^b}\right)_{pb}\equiv\frac{c^2}{2\omega_{m\mathbf{k}}}\left(\frac{\partial^2\lambda_{m\mathbf{k}}}{\partial k^a\partial k^b}\right)_{pb}-\frac{1}{\omega_{m\mathbf{k}}}\frac{\partial\omega_{m\mathbf{k}}}{\partial k^a}\frac{\partial\omega_{m\mathbf{k}}}{\partial k^b}$$

and

$$\left(\frac{\partial^2\omega_{m\mathbf{k}}}{\partial k^a\partial k^b}\right)_0\equiv\frac{c^2}{2\omega_{m\mathbf{k}}}\left(\frac{\partial^2\lambda_{m\mathbf{k}}}{\partial k^a\partial k^b}\right)_0.$$

We include the group velocity terms in the photonic band (pb) component of the group velocity dispersion because the group velocity (15) involves only the photonic band of interest. From the expressions above we find

$$\left(\frac{\partial^2\omega_{m\mathbf{k}}}{\partial k^a\partial k^b}\right)_{pb}=\frac{c^2}{2\omega_{m\mathbf{k}}}\left\langle \mathbf{h}_{m\mathbf{k}}\left|\frac{\partial^2\mathcal{H}_{\mathbf{k}}}{\partial k^a\partial k^b}\mathbf{h}_{m\mathbf{k}}\right.\right\rangle-\frac{c^4}{2\omega_{m\mathbf{k}}}\sum_p{}'\frac{\langle\mathbf{h}_{m\mathbf{k}}|(\partial\mathcal{H}_{\mathbf{k}}/\partial k^a)\mathbf{h}_{p\mathbf{k}}\rangle\langle\mathbf{h}_{p\mathbf{k}}|(\partial\mathcal{H}_{\mathbf{k}}/\partial k^b)\mathbf{h}_{m\mathbf{k}}\rangle}{(\omega_{p\mathbf{k}}^2-\omega_{m\mathbf{k}}^2)}$$
$$-\frac{c^4}{2\omega_{m\mathbf{k}}}\sum_p{}'\frac{\langle\mathbf{h}_{m\mathbf{k}}|(\partial\mathcal{H}_{\mathbf{k}}/\partial k^b)\mathbf{h}_{p\mathbf{k}}\rangle\langle\mathbf{h}_{p\mathbf{k}}|(\partial\mathcal{H}_{\mathbf{k}}/\partial k^a)\mathbf{h}_{m\mathbf{k}}\rangle}{(\omega_{p\mathbf{k}}^2-\omega_{m\mathbf{k}}^2)}-\frac{c^4}{4\omega_{m\mathbf{k}}^3}\left\langle \mathbf{h}_{m\mathbf{k}}\left|\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^a}\mathbf{h}_{m\mathbf{k}}\right.\right\rangle\left\langle \mathbf{h}_{m\mathbf{k}}\left|\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^b}\mathbf{h}_{m\mathbf{k}}\right.\right\rangle, \tag{20}$$

where the sum over p is over photonic bands other than our band of interest, and

$$\left(\frac{\partial^2\omega_{m\mathbf{k}}}{\partial k^a\partial k^b}\right)_0=\frac{c^4}{2\omega_{m\mathbf{k}}^3}\sum_{\sigma\notin\tau_1}\left\langle \mathbf{h}_{m\mathbf{k}}\left|\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^a}\mathbf{h}_{\sigma\mathbf{k}}\right.\right\rangle\left\langle \mathbf{h}_{\sigma\mathbf{k}}\left|\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^b}\mathbf{h}_{m\mathbf{k}}\right.\right\rangle+\frac{c^4}{2\omega_{m\mathbf{k}}^3}\sum_{\sigma\notin\tau_1}\left\langle \mathbf{h}_{m\mathbf{k}}\left|\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^b}\mathbf{h}_{\sigma\mathbf{k}}\right.\right\rangle\left\langle \mathbf{h}_{\sigma\mathbf{k}}\left|\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^a}\mathbf{h}_{m\mathbf{k}}\right.\right\rangle. \tag{21}$$

The sum over σ in Eq. (21) ranges over only the type τ_2 and type τ_3 solutions for which $\lambda_{\sigma\mathbf{k}}=0$. Yet it is possible to write this contribution to $\partial^2\omega_{m\mathbf{k}}/\partial k^a\partial k^b$ in terms of the matrix elements involving only the photonic bands (type τ_1 solutions), because the sum over type τ_2 and τ_3 solutions in Eq. (21) appears only in the form

$$\sum_{\sigma\notin\tau_1}|\mathbf{h}_{\sigma\mathbf{k}}\rangle\langle\mathbf{h}_{\sigma\mathbf{k}}|. \tag{22}$$

Using the resolution of unity $\mathcal{I}$ in the usual obvious schematic notation,

$$\mathcal{I}=|\mathbf{h}_{m\mathbf{k}}\rangle\langle\mathbf{h}_{m\mathbf{k}}|+\sum_{\sigma\in\tau_1}{}'|\mathbf{h}_{\sigma\mathbf{k}}\rangle\langle\mathbf{h}_{\sigma\mathbf{k}}|+\sum_{\sigma\notin\tau_1}|\mathbf{h}_{\sigma\mathbf{k}}\rangle\langle\mathbf{h}_{\sigma\mathbf{k}}|,$$

to solve for the sum (22), we can then write Eq. (21) as

$$\left(\frac{\partial^2\omega_{m\mathbf{k}}}{\partial k^a\partial k^b}\right)_0=\frac{c^4}{2\omega_{m\mathbf{k}}^3}\left\langle \mathbf{h}_{m\mathbf{k}}\left|\left(\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^a}\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^b}+\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^b}\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^a}\right)\mathbf{h}_{m\mathbf{k}}\right.\right\rangle-\frac{c^4}{\omega_{m\mathbf{k}}^3}\left\langle \mathbf{h}_{m\mathbf{k}}\left|\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^a}\mathbf{h}_{m\mathbf{k}}\right.\right\rangle\left\langle \mathbf{h}_{m\mathbf{k}}\left|\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^b}\mathbf{h}_{m\mathbf{k}}\right.\right\rangle-\frac{c^4}{2\omega_{m\mathbf{k}}^3}\sum_p{}'\left\langle \mathbf{h}_{m\mathbf{k}}\left|\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^a}\mathbf{h}_{p\mathbf{k}}\right.\right\rangle\times\left\langle \mathbf{h}_{p\mathbf{k}}\left|\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^b}\mathbf{h}_{m\mathbf{k}}\right.\right\rangle-\frac{c^4}{2\omega_{m\mathbf{k}}^3}\sum_p{}'\left\langle \mathbf{h}_{m\mathbf{k}}\left|\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^b}\mathbf{h}_{p\mathbf{k}}\right.\right\rangle\times\left\langle \mathbf{h}_{p\mathbf{k}}\left|\frac{\partial\mathcal{H}_{\mathbf{k}}}{\partial k^a}\mathbf{h}_{m\mathbf{k}}\right.\right\rangle. \tag{23}$$

Equation (15) for the group velocity and Eq. (19) for the group velocity dispersion are the main results of this section. The first contribution to Eq. (19), that of Eq. (20), is directly associated with the photonic bands. The other contribution, Eq. (21), is associated with solutions of type τ_2 and τ_3, which are unphysical except in the case of a uniform solution $\mathbf{H}$. But since type τ_2 and τ_3 solutions of Eq. (1) all have the same eigenvalue of zero, in the end that contribution can be written in terms of matrix elements involving photonic bands as well [Eq. (23)].

IV. DISCUSSION

Applications of the $k\cdot p$ theory in electron physics begin, depending on the problem at hand, with eigenstates of the Schrödinger, Pauli, or Dirac Hamiltonian. Since the corresponding time-dependent equation is the fundamental equation of the theory being employed, the eigenstates of the Hamiltonian are therefore all physical solutions. Hence, in expanding the periodic part of a Bloch function at $\mathbf{k}+\boldsymbol{\kappa}$ in terms of those at $\mathbf{k}$ it naturally suffices to consider the physical solutions, since they exhaust the mathematical ones.

The situation is qualitatively different in the study of photonic band gap materials. There the eigenfunctions of interest are those of the master equation (1), but the Hamiltonian-like operator $\boldsymbol{\Theta}$ of that equation is *not* directly associated with the fundamental theory at hand. Rather, it is the Maxwell equations that define the fundamental theory. And there are many solutions of the master equation, with eigenvalue $\lambda=0$, that *do not* correspond to the physical solutions, i.e., solutions of the Maxwell equations. Hence the physical solutions of the master equation—the photonic bands—do not exhaust the mathematical solutions.

Now both a photonic band function at $\mathbf{k}$, $\mathbf{H}_{m\mathbf{k}}(\mathbf{r})$, and a neighboring one at $\mathbf{k}+\boldsymbol{\kappa}$, $\mathbf{H}_{m(\mathbf{k}+\boldsymbol{\kappa})}(\mathbf{r})$, are physical solutions, and are therefore transverse vector fields. But in general neither of the periodic parts $\mathbf{h}_{m\mathbf{k}}(\mathbf{r})$ and $\mathbf{h}_{m(\mathbf{k}+\boldsymbol{\kappa})}(\mathbf{r})$ are transverse, and indeed they differ from transversality by different amounts [see Eq. (5)]. The result is that $\mathbf{h}_{m(\mathbf{k}+\boldsymbol{\kappa})}(\mathbf{r})$ cannot be expanded in terms of periodic functions $\mathbf{h}_{p\mathbf{k}}(\mathbf{r})$ corresponding only to physical solutions; the periodic parts of unphysical solutions at $\mathbf{k}$ must be employed as well.

To our knowledge this has not been pointed out in the literature. Yet if the sums appearing in previous calculations (see, e.g., Johnson *et al.* [3]), essentially corresponding to those appearing in Eq. (18), are taken to range over *all* the $\mathbf{h}_{\sigma\mathbf{k}}(\mathbf{r})$, both the physical *and* unphysical solutions, those results are correct. That is, if one works with the *full* set of eigenfunctions of the master equation, including the unphysical solutions with $\boldsymbol{\nabla}\cdot\mathbf{H}(\mathbf{r})\neq 0$, one will not go astray. Of course in practical applications, where it suffices to approximate the sums by contributions from only a few neighboring bands, the neglect of the unphysical solutions at zero frequency should lead to no significant error; both the unphysical solutions and the physical ''remote bands'' have a negligible effect on $\partial^2\omega_{m\mathbf{k}}/\partial k^a\partial k^b$.

Nonetheless, since in formal developments it can be crucially important to include all terms in a sum rule [5], the appearance of these unphysical solutions in the expression for $\partial^2\omega_{m\mathbf{k}}/\partial k^a\partial k^b$ [the contribution $(\partial^2\omega_{m\mathbf{k}}/\partial k^a\partial k^b)_0$ of Eq. (21)] is worthy of note. Further, we have shown that, using closure, it is in fact possible to write the contribution of these unphysical solutions to $\partial^2\omega_{m\mathbf{k}}/\partial k^a\partial k^b$ in terms of matrix elements involving only physical solutions [Eq. (23)], hence in the end producing a correct sum rule (i.e., a correct expression for $\partial^2\omega_{m\mathbf{k}}/\partial k^a\partial k^b$) involving *only the photonic bands*. We stress that if the sums in previous expressions for $\partial^2\omega_{m\mathbf{k}}/\partial k^a\partial k^b$ in the literature [3] are taken to involve *only* the photonic bands, they are incorrect.

Finally, we note that it is straightforward to work out the expression for $\partial\mathcal{H}_{\mathbf{k}}/\partial k^a$ $[=\partial\theta_{\mathbf{k}}/\partial k^a$; see Eqs. (2) and (3)] and hence the matrix elements involve in the expressions (15) and (19) for the group velocity and the group velocity dispersion. Yet the complicated form of Eqs. (20) and (23) suggests that there may be a route, different from that based on the master equation (1), which might lead to a simpler expression for terms such as $\partial^2\omega_{m\mathbf{k}}/\partial k^a\partial k^b$. We plan to address this issue in a future publication.

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APPENDIX

In this Appendix we confirm that, if we use our full basis set and perform a $k\cdot p$ expansion to move from $\mathbf{k}$ to $\mathbf{k}+\boldsymbol{\kappa}$, then we do indeed recover Eq. (5). We use the fact that this equation is satisfied at the $\mathbf{k}$ at which we begin the expansion,

$$\nabla\cdot\mathbf{h}_{m\mathbf{k}}(\mathbf{r})+i\mathbf{k}\cdot\mathbf{h}_{m\mathbf{k}}(\mathbf{r})=0, \tag{A1}$$

where $\mathbf{h}_{m\mathbf{k}}$ corresponds to a type τ_1 solution of the master equation (1). It will suffice to restrict ourselves to small $\boldsymbol{\kappa}$; we use Eq. (17) for $\partial\mathbf{h}_{m\mathbf{k}}/\partial k^a$ to write

$$\begin{aligned}\mathbf{h}_{m(\mathbf{k}+\boldsymbol{\kappa})}(\mathbf{r})&=\mathbf{h}_{m\mathbf{k}}(\mathbf{r})+\kappa^a\frac{\partial\mathbf{h}_{m\mathbf{k}}(\mathbf{r})}{\partial k^a}+\mathcal{O}(\kappa^2)\\&=\mathbf{h}_{m\mathbf{k}}(\mathbf{r})+\kappa^a{\sum_\sigma}'\ \mathbf{h}_{\sigma\mathbf{k}}(\mathbf{r})\left\langle\mathbf{h}_{\sigma\mathbf{k}}\left|\frac{\partial\mathbf{h}_{m\mathbf{k}}}{\partial k^a}\right.\right\rangle\\&\quad+\mathcal{O}(\kappa^2),\end{aligned}$$

where repeated Cartesian components are to be summed over, or

$$\mathbf{h}_{m(\mathbf{k}+\boldsymbol{\kappa})}(\mathbf{r})=\mathbf{h}_{m\mathbf{k}}(\mathbf{r})-\kappa^a{\sum_\sigma}'\ \mathbf{h}_{\sigma\mathbf{k}}(\mathbf{r})\frac{\langle\mathbf{h}_{\sigma\mathbf{k}}|(\partial\mathcal{H}_{\mathbf{k}}/\partial k^a)\mathbf{h}_{m\mathbf{k}}\rangle}{(\lambda_{\sigma\mathbf{k}}-\lambda_{m\mathbf{k}})}+\mathcal{O}(\kappa^2).$$

Breaking the sum into $\sigma\in\tau_1,\tau_2$ (meaning σ is either a type τ_1 or a type τ_2 solution) and $\sigma\in\tau_3$, we can write

$$\mathbf{h}_{m(\mathbf{k}+\boldsymbol{\kappa})}(\mathbf{r})=\mathbf{h}_{m\mathbf{k}}(\mathbf{r})+\tilde{\mathbf{h}}_{mT\mathbf{k}}(\mathbf{r})+\tilde{\mathbf{h}}_{mL\mathbf{k}}(\mathbf{r})+\mathcal{O}(\kappa^2), \tag{A2}$$

where

$$\tilde{\mathbf{h}}_{mT\mathbf{k}}(\mathbf{r})=-\kappa^a{\sum_{\sigma\in\tau_1,\tau_2}}'\ \mathbf{h}_{\sigma\mathbf{k}}(\mathbf{r})\frac{\langle\mathbf{h}_{\sigma\mathbf{k}}|(\partial\mathcal{H}_{\mathbf{k}}/\partial k^a)\mathbf{h}_{m\mathbf{k}}\rangle}{(\lambda_{\sigma\mathbf{k}}-\lambda_{m\mathbf{k}})}, \tag{A3}$$

and

$$\begin{aligned}\tilde{\mathbf{h}}_{mL\mathbf{k}}(\mathbf{r})&=-\kappa^a\sum_{\sigma\in\tau_3}\mathbf{h}_{\sigma\mathbf{k}}(\mathbf{r})\frac{\langle\mathbf{h}_{\sigma\mathbf{k}}|(\partial\mathcal{H}_{\mathbf{k}}/\partial k^a)\mathbf{h}_{m\mathbf{k}}\rangle}{(\lambda_{\sigma\mathbf{k}}-\lambda_{m\mathbf{k}})}\\&=\kappa^a\sum_{\sigma\in\tau_3}\mathbf{h}_{\sigma\mathbf{k}}(\mathbf{r})\frac{\langle\mathbf{h}_{\sigma\mathbf{k}}|(\partial\mathcal{H}_{\mathbf{k}}/\partial k^a)\mathbf{h}_{mT\mathbf{k}}\rangle}{\lambda_{m\mathbf{k}}}.\end{aligned} \tag{A4}$$

Now using Eq. (A2) we have

$$\begin{aligned}\nabla\cdot\mathbf{h}_{m(\mathbf{k}+\boldsymbol{\kappa})}(\mathbf{r})&=\nabla\cdot\mathbf{h}_{m\mathbf{k}}(\mathbf{r})+\nabla\cdot\tilde{\mathbf{h}}_{mT\mathbf{k}}(\mathbf{r})+\nabla\cdot\tilde{\mathbf{h}}_{mL\mathbf{k}}(\mathbf{r})\\&\quad+\mathcal{O}(\kappa^2),\end{aligned}$$

while

$$\begin{aligned}i(\mathbf{k}+\boldsymbol{\kappa})\cdot\mathbf{h}_{m(\mathbf{k}+\boldsymbol{\kappa})}(\mathbf{r})&=i(\mathbf{k}+\boldsymbol{\kappa})\cdot\mathbf{h}_{m\mathbf{k}}(\mathbf{r})+i\mathbf{k}\cdot\tilde{\mathbf{h}}_{mT\mathbf{k}}(\mathbf{r})\\&\quad+i\mathbf{k}\cdot\tilde{\mathbf{h}}_{mL\mathbf{k}}(\mathbf{r})+\mathcal{O}(\kappa^2),\end{aligned}$$

where we have used the fact that $\tilde{\mathbf{h}}_{m(T,L)\mathbf{k}}(\mathbf{r})$ are already first order in $\boldsymbol{\kappa}$. Then, using Eq. (A1), which holds for functions of both types τ_1 and τ_2, we find that for Eq. (5) to be satisfied we require

$$i\boldsymbol{\kappa}\cdot\mathbf{h}_{m\mathbf{k}}(\mathbf{r})+\nabla\cdot\tilde{\mathbf{h}}_{mL\mathbf{k}}(\mathbf{r})+i\mathbf{k}\cdot\tilde{\mathbf{h}}_{mL\mathbf{k}}(\mathbf{r})=0 \tag{A5}$$

[cf. Eq. (6)].

Now in the special case that $\mathbf{k}=\mathbf{0}$ there will be three functions $\mathbf{h}_{\sigma\mathbf{k}}(\mathbf{r})$ in the sum in Eq. (A4) for which $\mathbf{G}_m=\mathbf{0}$. But these functions are uniform, so their divergence is clearly zero. Thus, to satisfy Eq. (A5) it is sufficient to require

$$i\boldsymbol{\kappa}\cdot\mathbf{h}_{m\mathbf{k}}(\mathbf{r})+\nabla\cdot\overline{\mathbf{h}}_{mL\mathbf{k}}(\mathbf{r})+i\mathbf{k}\cdot\overline{\mathbf{h}}_{mL\mathbf{k}}(\mathbf{r})=0,$$

where

$$\overline{\mathbf{h}}_{m\mathbf{k}L}(\mathbf{r})=\kappa^a\sum_{\sigma\in\overline{\tau}_3}\mathbf{h}_{\sigma\mathbf{k}}(\mathbf{r})\frac{\langle\mathbf{h}_{\sigma\mathbf{k}}|(\partial\mathcal{H}_{\mathbf{k}}/\partial k^a)\mathbf{h}_{mT\mathbf{k}}\rangle}{\lambda_{mT\mathbf{k}}}, \tag{A6}$$

where the overbar on $\overline{\tau}_3$ indicates that all terms of type τ_3 are to be included if $\mathbf{k}\neq\mathbf{0}$, while only the $\mathbf{G}_m\neq\mathbf{0}$ terms are to be included if $\mathbf{k}=\mathbf{0}$. To proceed we need to work out the expression (A6) for $\overline{\mathbf{h}}_{mL\mathbf{k}}(\mathbf{r})$. The overlap integral involved is complicated to work out directly, but a simple expression for it can be derived using the fact that

$$\langle\mathbf{h}_{\sigma\mathbf{k}}|\mathcal{H}_{\mathbf{k}}\mathbf{h}_{m\mathbf{k}}\rangle=0$$

for $\sigma\in\overline{\tau}_3$, since the $\mathbf{h}_{\sigma\mathbf{k}}(\mathbf{r})$ are eigenfunctions of the Hermitian operator $\mathcal{H}_{\mathbf{k}}$ with eigenvalue zero. Hence

$$\frac{\partial}{\partial k^a}\langle \mathbf{h}_{\sigma\mathbf{k}}|\mathcal{H}_{\mathbf{k}}\mathbf{h}_{mT\mathbf{k}}\rangle = \left\langle \frac{\partial \mathbf{h}_{\sigma\mathbf{k}}}{\partial k^a}\middle| \mathcal{H}_{\mathbf{k}}\mathbf{h}_{m\mathbf{k}}\right\rangle + \left\langle \mathbf{h}_{\sigma\mathbf{k}}\middle| \frac{\partial \mathcal{H}_{\mathbf{k}}}{\partial k^a}\mathbf{h}_{m\mathbf{k}}\right\rangle + \left\langle \mathbf{h}_{\sigma\mathbf{k}}\middle| \mathcal{H}_{\mathbf{k}}\frac{\partial \mathbf{h}_{m\mathbf{k}}}{\partial k^a}\right\rangle = 0.$$

Now the last of the three terms here is itself zero, again since the $\mathbf{h}_{\sigma\mathbf{k}}(\mathbf{r})$ of interest are eigenfunctions of $\mathcal{H}_{\mathbf{k}}$ with eigenvalue zero. Thus we find

$$\left\langle \mathbf{h}_{\sigma\mathbf{k}}\middle| \frac{\partial \mathcal{H}_{\mathbf{k}}}{\partial k^a}\mathbf{h}_{m\mathbf{k}}\right\rangle = -\left\langle \frac{\partial \mathbf{h}_{\sigma\mathbf{k}}}{\partial k^a}\middle| \mathcal{H}_{\mathbf{k}}\mathbf{h}_{m\mathbf{k}}\right\rangle = -\lambda_{m\mathbf{k}}\left\langle \frac{\partial \mathbf{h}_{\sigma\mathbf{k}}}{\partial k^a}\middle| \mathbf{h}_{m\mathbf{k}}\right\rangle,$$

and the expression (A6) becomes

$$\overline{\mathbf{h}}_{mL\mathbf{k}}(\mathbf{r}) = -\kappa^a \sum_{\sigma\in\tau_3} \mathbf{h}_{\sigma\mathbf{k}}(\mathbf{r})\left\langle \frac{\partial \mathbf{h}_{\sigma\mathbf{k}}}{\partial k^a}\middle| \mathbf{h}_{m\mathbf{k}}\right\rangle. \tag{A7}$$

To evaluate this expression we need $\partial \mathbf{h}^*_{\sigma\mathbf{k}}(\mathbf{r})/\partial k^a$.

Consider first the case where $\mathbf{k}\neq\mathbf{0}$. We recall the expression (7) for a general $\mathbf{h}_{nL\mathbf{k}}(\mathbf{r})$ and, since $v(\mathbf{k}+\mathbf{G}_n)=(\mathbf{k}+\mathbf{G}_n)/|\mathbf{k}+\mathbf{G}_n|$, we find immediately

$$\frac{\partial v(\mathbf{k}+\mathbf{G}_n)}{\partial k^a} = \frac{\hat{\mathbf{a}}}{|\mathbf{k}+\mathbf{G}_n|} - \frac{[\hat{\mathbf{a}}\cdot(\mathbf{k}+\mathbf{G}_n)]v(\mathbf{k}+\mathbf{G}_n)}{|\mathbf{k}+\mathbf{G}_n|^2}.$$

Thus for $\sigma=(nL)$ we have

$$\kappa^a \frac{\partial \mathbf{h}^*_{nL\mathbf{k}}(\mathbf{r})}{\partial k^a} = \frac{1}{\sqrt{\Omega_c}}\left(\frac{\boldsymbol{\kappa}}{|\mathbf{k}+\mathbf{G}_n|} - \frac{[\boldsymbol{\kappa}\cdot(\mathbf{k}+\mathbf{G}_n)]v(\mathbf{k}+\mathbf{G}_n)}{|\mathbf{k}+\mathbf{G}_n|^2}\right)e^{-i\mathbf{G}_n\cdot\mathbf{r}}.$$

Next, using the Fourier expansion of the periodic function $\mathbf{h}_{m\mathbf{k}}(\mathbf{r})$,

$$\mathbf{h}_{m\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{\Omega_c}}\sum_p \mathbf{h}^p_{m\mathbf{k}} e^{i\mathbf{G}_p\cdot\mathbf{r}},$$

we find

$$\kappa^a\left\langle \frac{\partial \mathbf{h}_{nL\mathbf{k}}}{\partial k^a}\middle| \mathbf{h}_{m\mathbf{k}}\right\rangle = \frac{\boldsymbol{\kappa}\cdot\mathbf{h}^n_{m\mathbf{k}}}{|\mathbf{k}+\mathbf{G}_n|} - \frac{[\boldsymbol{\kappa}\cdot(\mathbf{k}+\mathbf{G}_n)]v(\mathbf{k}+\mathbf{G}_n)\cdot\mathbf{h}^n_{m\mathbf{k}}}{|\mathbf{k}+\mathbf{G}_n|^2} = \frac{\boldsymbol{\kappa}\cdot\mathbf{h}^n_{m\mathbf{k}}}{|\mathbf{k}+\mathbf{G}_n|},$$

where in the last line we have used the fact that, since $\mathbf{H}_{m\mathbf{k}}(\mathbf{r})$ is transverse, the components $\mathbf{h}^n_{m\mathbf{k}}$ must be perpendicular to $\mathbf{k}+\mathbf{G}_n$. Hence Eq. (A7) yields

$$\overline{\mathbf{h}}_{mL\mathbf{k}}(\mathbf{r}) = -\sum_n \mathbf{h}_{nL\mathbf{k}}(\mathbf{r})\frac{\boldsymbol{\kappa}\cdot\mathbf{h}^n_{m\mathbf{k}}}{|\mathbf{k}+\mathbf{G}_n|} = -\frac{1}{\sqrt{\Omega_c}}\sum_n v(\mathbf{k}+\mathbf{G}_n)\frac{\boldsymbol{\kappa}\cdot\mathbf{h}^n_{m\mathbf{k}}}{|\mathbf{k}+\mathbf{G}_n|}e^{i\mathbf{G}_n\cdot\mathbf{r}}, \tag{A8}$$

and finally

$$\begin{aligned}\nabla\cdot\overline{\mathbf{h}}_{mL\mathbf{k}}(\mathbf{r}) + i\mathbf{k}\cdot\overline{\mathbf{h}}_{mL\mathbf{k}}(\mathbf{r}) &= -\frac{1}{\sqrt{\Omega_c}}\sum_n i(\mathbf{k}+\mathbf{G}_n)\cdot v(\mathbf{k}+\mathbf{G}_n)\frac{\boldsymbol{\kappa}\cdot\mathbf{h}^n_{m\mathbf{k}}}{|\mathbf{k}+\mathbf{G}_n|}e^{i\mathbf{G}_n\cdot\mathbf{r}}\\ &= -\frac{i}{\sqrt{\Omega_c}}\sum_n \boldsymbol{\kappa}\cdot\mathbf{h}^n_{m\mathbf{k}}e^{i\mathbf{G}_n\cdot\mathbf{r}}\\ &= -i\boldsymbol{\kappa}\cdot\mathbf{h}_{m\mathbf{k}}(\mathbf{r}),\end{aligned} \tag{A9}$$

so we find that Eq. (A5) is indeed satisfied.

In the case that $\mathbf{k}=\mathbf{0}$, the reduction proceeds in the same way except that, instead of Eq. (A8), we find

$$\overline{\mathbf{h}}_{mL0}(\mathbf{r}) = -\sum_{n,\mathbf{G}_n\neq\mathbf{0}} \mathbf{h}_{nL0}(\mathbf{r})\frac{\boldsymbol{\kappa}\cdot\mathbf{h}^n_{m0}}{|\mathbf{G}_n|},$$

so instead of Eq. (A9) we find

$$\nabla\cdot\overline{h}_{mL0}(\mathbf{r}) = -\frac{1}{\sqrt{\Omega_c}}\sum_{n,\mathbf{G}_n\neq\mathbf{0}} i\mathbf{G}_n\cdot v(\mathbf{G}_n)\frac{\boldsymbol{\kappa}\cdot\mathbf{h}^n_{m0}}{|\mathbf{G}_n|}e^{i\mathbf{G}_n\cdot\mathbf{r}} = -\frac{i}{\sqrt{\Omega_c}}\sum_{n,\mathbf{G}_n\neq\mathbf{0}} \boldsymbol{\kappa}\cdot\mathbf{h}^n_{m0}e^{i\mathbf{G}_n\cdot\mathbf{r}}.$$

But any $\mathbf{H}_{m0}(\mathbf{r})$ of type $\tau_1$must be orthogonal to $\mathbf{H}_{(x)L0}(\mathbf{r})$, $\mathbf{H}_{(y)L0}(\mathbf{r})$, and $\mathbf{H}_{(z)L0}(\mathbf{r})$, since the latter three functions have eigenvalue zero, so it must be that $\mathbf{h}^n_{m0}=\mathbf{0}$ for $\mathbf{G}_n=\mathbf{0}$. Hence we can write

$$\nabla\cdot\overline{\mathbf{h}}_{mL0}(\mathbf{r}) = -\frac{i}{\sqrt{\Omega_c}}\sum_n \boldsymbol{\kappa}\cdot\mathbf{h}^n_{m0}e^{i\mathbf{G}_n\cdot\mathbf{r}} = -i\boldsymbol{\kappa}\cdot\mathbf{h}_{m0}(\mathbf{r}),$$

and again we satisfy Eq. (A5).

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