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Spectral properties of $\mathbf{k} \cdot \mathbf{p}$ Schrödinger operators in one space dimension

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Dedicated to Günter Albinus on the occasion of his 60^{th} *birthday.*

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Abstract

In the physics of layered semiconductor devices the $\mathbf{k} \cdot \mathbf{p}$ method in combination with the envelope–function approach is a well established tool for band structure calculations. We perform a rigorous mathematical analysis of spectral properties for the corresponding spatially one dimensional $\mathbf{k} \cdot \mathbf{p}$ Schrödinger operators; thereby regarding a wide class of such operators. This class covers many of the $\mathbf{k} \cdot \mathbf{p}$ operators prevalent in solid state physics. It includes $\mathbf{k} \cdot \mathbf{p}$ Schrödinger operators with piecewise constant coefficients which is a prerequisite for dealing with the important case of semiconductor heterostructures. We also introduce a regularization of the problem which gives rise to a consistent discretization of $\mathbf{k} \cdot \mathbf{p}$ operators with jumping coefficients and describe our toolbox KPLIB for the numerical treatment of $\mathbf{k} \cdot \mathbf{p}$ operators. In particular we address the question of persistence of a spectral gap over the wave vector range.

Contents

Introduction

Many properties of semiconductor devices depend on the electronic band structure of the device material. This applies to electronic circuits as well as to optoelectronic and other internally coupled devices. For semiconductor lasers the band structure within the optical active zone of the laser is an important design parameter [8].

The $\mathbf{k} \cdot \mathbf{p}$ method in combination with the envelope function approximation (see e.g. [4, 19, 7, 8, 9, 6]) is frequently used to calculate the near bandedge electronic band structure of semiconductor heterostructures, such as quantum wells. This approach requires only measurable properties of the bulk materials and provides the band structure in a small range of the Brillouin zone.

In a homogeneous material there is translational symmetry, hence, the (quasi) wave vector $\mathbf{k}$ is a good quantum number. The $\mathbf{k} \cdot \mathbf{p}$ approach to the problem in bulk material (see e.g. [2, 8]) uses a perturbation theory description of band dispersion within a certain set of near bandedge Bloch waves $u_{\iota,\mathbf{k}_0}(\mathbf{r})\exp(i\mathbf{k}_0\mathbf{r})$. Thereby one has to deal with an eigenvalue problem for matrix Schrödinger operators, which parametrically depends on $\mathbf{k} - \mathbf{k}_0$, $\mathbf{k}_0$ being a wave vector at the bandedge under consideration.

In stratified semiconductor heterostructures, such as quantum wells, where translational symmetry is broken in one, say the z–direction, the respective component k_z of the wave vector $\mathbf{k}$ is no longer a good quantum number, while the reduced wave vector $\mathbf{k}_{||} = (k_x, k_y, 0)$ remains a good quantum number. In such cases the wave functions are

$$\Psi_{l,\mathbf{k}_{||}}(\mathbf{r}) = \exp(i\mathbf{k}_{||}\mathbf{r}_{||}) \sum_{\iota} F_{\iota l}(z, \mathbf{k}_{||} - \mathbf{k}_0) u_{\iota,\mathbf{k}_0}(\mathbf{r}),$$

with envelope functions $F_{\iota l}(z, \mathbf{k}_{||} - \mathbf{k}_0)$ which vary in space on a larger scale than the lattice constant, approximately 5 Å, of the material. For the different materials one still uses the $\mathbf{k} \cdot \mathbf{p}$ matrices of the respective bulk material, substituting k_z properly by the derivative $-i\ d/dz$. Thus one ends up with an eigenvalue problem for a hermitian matrix Schrödinger operator in one space dimension, which parametrically depends on the reduced wave vector $\mathbf{k}_{||} - \mathbf{k}_0$. The solutions of this family of eigenvalue problems provides the subband structure $E_l(\mathbf{k}_{||} - \mathbf{k}_0)$ and the corresponding envelope functions $\mathbf{F}_l(z, \mathbf{k}_{||} - \mathbf{k}_0)$.

In direct semiconductors the bandedge usually is the Γ–point $\mathbf{k}_0 = \mathbf{0}$, which we assume in the following for the sake of simplicity of notation.

In this paper we perform a functional analytic investigation of matrix Schrödinger operators in one space dimension which arise from the above outlined $\mathbf{k} \cdot \mathbf{p}$ method for stratified semiconductor heterostructures, in particular quantum wells. We prove certain spectral properties in dependence on the reduced wave vector $\mathbf{k}_{||}$, which are essential for the applicability of the $\mathbf{k}\cdot\mathbf{p}$ approach in band structure calculations for semiconductor heterostructures.

In particular, it turns out that the eigenvalue curves $E_l(\mathbf{k}_{||})$ are analytic with at most algebraic singularities for finite $\mathbf{k}_{||}$. These singularities could be excluded for slightly regularized versions of the problem.

Another important question is the persistence of a spectral gap, the band gap in semiconductors, at $\mathbf{k}_{||} = 0$ for $\mathbf{k}_{||} \neq 0$. We will derive a certain range of $\mathbf{k}_{||} \neq 0$, in dependence on the data of the problem, where the gap persists.

1 Formulation of the problem

As announced in the introduction, we will investigate spectral properties of Schrödinger operators occuring in $\mathbf{k}\cdot\mathbf{p}$ theory for stratified media. We will now write $\mathbf{k} = (k_1, k_2) \in \mathbb{C}^2$ for the reduced wave vector, and x for the direction of quantization. Let us first specify the $\mathbf{k}\cdot\mathbf{p}$ Schrödinger operators. If $\varphi = (\varphi_1, ..., \varphi_d)$ denotes a suitable $\mathbb{C}^d$–valued function on the space interval $[0, T]$, then the j–th component of the image of φ under the Schrödinger operator is given by

$$\begin{aligned} -\frac{d}{dx}\Big(m_j\,\frac{d\varphi_j}{dx}\Big) &+ \sum_{l=1}^{d}\Big(M_{0\,j\,l}\frac{d\varphi_l}{dx} - \frac{d}{dx}\Big(\overline{M}_{0\,l\,j}\,\varphi_l\Big)\Big) \\ &+ \sum_{\alpha=1,2} k_\alpha \sum_{l=1}^{d}\Big(M_{\alpha\,j\,l}\frac{d\varphi_l}{dx} - \frac{d}{dx}\Big(\overline{M}_{\alpha\,l\,j}\,\varphi_l\Big)\Big) \\ &+ \sum_{\alpha=1,2} k_\alpha \sum_{l=1}^{d} U_{\alpha\,j\,l}\,\varphi_l + \sum_{\alpha,\beta=1,2} k_\alpha k_\beta \sum_{l=1}^{d} U_{\alpha\,\beta\,j\,l}\,\varphi_l \\ &+ \sum_{l=1}^{d} v_{j\,l}\,\varphi_l + e_j\varphi_j, \end{aligned} \tag{1.1}$$

where m_j, $M_{0\,j\,l}$, $M_{\alpha\,j\,l}$, $U_{\alpha\,j\,l}$, $U_{\alpha\,\beta\,j\,l}$, $v_{j\,l}$ and e_j are essentially bounded functions on the space interval $[0, T]$ with additional properties, due to the underlying physics, which we will specify later. Our first aim is to give (1.1) a precise meaning between adequate function spaces; we will do this separately for the several parts because the resulting operators are to be investigated in their relation to each other.

By $W^{1,2}$ we denote the space of $\mathbb{C}^d$–valued functions having a square integrable (generalized) derivative on the interval $[0, T]$ and satisfying homogeneous Dirichlet boundary conditions on both interval ends. We will regard $W^{1,2}$ equipped with the norm

$$\|\psi\|_{W^{1,2}} = \sqrt{\int_0^T \left\| \frac{d\psi}{dx}(x) \right\|_{\mathbb{C}^d}^2 dx}, \tag{1.2}$$

where $\langle \cdot, \cdot \rangle_{\mathbb{C}^d}$ is the canonic bilinear form on $\mathbb{C}^d$ and $\| \cdot \|_{\mathbb{C}^d}$ the corresponding norm. By L^2 we denote the space of C^d–valued, square integrable functions on the interval $[0, T]$ with its usual norm. $W^{-1,2}$ shall be the space of antilinear forms on $W^{1,2}$, while $\langle \cdot, \cdot \rangle$ denotes the dual pairing between both spaces, which extends the scalar product on L^2, see e.g. [5]. (1.2) together with the induced norm on $W^{-1,2}$ implies the following interpolation inequality

$$\|\psi\|_{L^2} \leq \|\psi\|_{W^{1,2}}^{\frac{1}{2}} \|\psi\|_{W^{-1,2}}^{\frac{1}{2}}. \tag{1.3}$$

$\mathcal{B}$ denotes spaces of bounded linear operators.

1.1. Assumption. Let

$$m_j \in L^\infty([0,T], \mathbb{R}), \quad e_j \in L^\infty([0,T], \mathbb{R}), \quad j = 1, \dots, d,$$

$$\begin{aligned}
M_\alpha &\in L^\infty([0,T]; \mathcal{B}(\mathbb{C}^d)), & \alpha &\in \{0,1,2\}, \\
U_\alpha &\in L^\infty([0,T]; \mathcal{B}(\mathbb{C}^d)), & \alpha &\in \{1,2\}, \\
U_{\alpha\beta} &\in L^\infty([0,T]; \mathcal{B}(\mathbb{C}^d)), & \alpha, \beta &\in \{1,2\}, \\
v &\in L^\infty([0,T]; \mathcal{B}(\mathbb{C}^d)),
\end{aligned}$$

be the coefficients of Schrödinger's operator with the following properties:

i) There is a (possibly empty) subset $D \subset \{1, \dots, d\}$ such that

$$\min_{j \in \{1,\dots,d\} \setminus D} \operatorname*{vraimin}_{x \in [0,T]} m_j(x) > 0, \qquad \max_{j \in D} \operatorname*{vraimax}_{x \in [0,T]} m_j(x) < 0,$$

$$\min_{j \in \{1,\dots,d\} \setminus D} \operatorname*{vraimin}_{x \in [0,T]} e_j(x) > 0, \qquad \max_{j \in D} \operatorname*{vraimax}_{x \in [0,T]} e_j(x) < 0.$$

ii) For almost all $x \in [0, T]$ and all $\alpha, \beta \in \{1, 2\}$ the operators $U_\alpha(x)$, $U_{\alpha\beta}(x)$, and $v(x)$ are selfadjoint over $\mathbb{C}^d$.

iii) There is a finite, disjoint partition

$$0 = t_0 < t_1 < \ldots < t_L < t_{L+1} = T \tag{1.4}$$

of the interval $[0, T[$ such that the functions m_j, $j = 1, \dots, d$ take exactly one value $\widehat{m}_{j,l}$ on each of the subintervals $[t_l, t_{l+1}[$.

iv) If the opposite is not explicitly stated, then we assume that the matrix valued functions M_α, $\alpha = 0, 1, 2$ take the constant values $\widehat{M_{\alpha,l}}$ on the subintervals $[t_l, t_{l+1}[$, $l = 0, \ldots, L$.

1.2. Definition. We define the several parts of the $\mathbf{k}\cdot\mathbf{p}$ Schrödinger operator as operators acting on $W^{1,2}$ into $W^{-1,2}$, i.e. in the sense of forms. We start with the second order differential operator

$$\langle H\varphi, \psi\rangle = \sum_{j=1}^{d} \int_0^T m_j \, \frac{d\varphi_j}{dx} \, \frac{d\overline{\psi}_j}{dx} \, dx. \tag{1.5}$$

continue with the first order differential operators

$$\begin{aligned}\langle A_\alpha\varphi, \psi\rangle = \int_0^T & \Big\langle M_\alpha(x) \, \frac{d\varphi}{dx}(x), \psi(x)\Big\rangle_{\mathbb{C}^d} \\ & + \Big\langle M_\alpha^*(x) \, \varphi(x), \frac{d\psi}{dx}(x)\Big\rangle_{\mathbb{C}^d} \, dx, \quad \alpha = 0, 1, 2,\end{aligned} \tag{1.6}$$

and finish with the zero order differential operators

$$\langle B_\alpha \, \varphi, \psi\rangle = \int_0^T \big\langle U_\alpha(x) \, \varphi(x), \psi(x)\big\rangle_{\mathbb{C}^d} \, dx, \qquad \alpha = 1, 2, \tag{1.7}$$

$$\langle B_{\alpha\beta} \, \varphi, \psi\rangle = \int_0^T \big\langle U_{\alpha\beta}(x) \, \varphi(x), \psi(x)\big\rangle_{\mathbb{C}^d} \, dx, \qquad \alpha, \beta = 1, 2, \tag{1.8}$$

$$\langle V\varphi, \psi\rangle = \sum_{j=1}^{d} \int_0^T \big\langle v(x) \, \varphi(x), \psi(x)\big\rangle_{\mathbb{C}^d} \, dx, \tag{1.9}$$

$$\langle E\varphi, \psi\rangle = \sum_{j=1}^{d} \int_0^T e_j \, \varphi_j(x) \, \overline{\psi}_j(x) \, dx, \tag{1.10}$$

where the functions φ and ψ are from $W^{1,2}$. The formal $\mathbf{k}\cdot\mathbf{p}$ Schrödinger operator (1.1) is precisely defined by

$$H_{\mathbf{k}} = H + T_{\mathbf{k}} \tag{1.11a}$$

$$T_{\mathbf{k}} = A_0 + \sum_{\alpha=1,2} k_\alpha A_\alpha + \sum_{\alpha=1,2} k_\alpha B_\alpha + \sum_{\alpha,\beta=1,2} k_\alpha \, k_\beta \, B_{\alpha\beta} + V + E, \tag{1.11b}$$

where $\mathbf{k} = (k_1, k_2) \in \mathbb{C}^2$ is the reduced wave vector.

The questions which are of interest concerning the operator family $\{H_{\mathbf{k}}\}_{\mathbf{k}\in\mathbb{C}^2}$ are the following ones:

1.3. Problem. What is the domain of $H_{\mathbf{k}}$, and is it independent of $\mathbf{k}$?

1.4. Problem. Are the operators $H_{\mathbf{k}}$ closable on an adequate domain?

1.5. Problem. If ψ is any element from $W^{1,2}$, then what can be said about the quality of the functions

$$\mathbf{k} \longmapsto H_{\mathbf{k}}\psi$$

depending on $\mathbf{k} \in \mathbb{C}^2$?

1.6. Problem. How do spectral properties of the $H_{\mathbf{k}}$ depend on $\mathbf{k}$?

1.7. Problem. What is the relationship between the operator $H_{\mathbf{k}}$ and its restriction to L^2, especially concerning their spectral behaviour?

1.8. Problem. What about selfadjointness of $H_{\mathbf{k}}|_{L^2}$, if $\mathbf{k} \in \mathbb{R}^2$?

1.9. Problem. May the problem be suitably regularized?

The answers to these questions will be given in the subsequent sections.

2 General properties of $\mathbf{k} \cdot \mathbf{p}$ operators

In general we will regard the $\mathbf{k} \cdot \mathbf{p}$ Schrödinger operators and its parts in the Hilbert space $W^{-1,2}$.

We introduce a conjugation operator $\tilde{\Theta}$ on $\mathbb{C}^d$ by

$$\tilde{\Theta}(c_1, \dots, c_d) = (r_1 c_1, \dots, r_d c_d), \quad r_j = \begin{cases} 1 & \text{if } j \in \{1, \dots, d\} \setminus D, \\ -1 & \text{if } j \in D, \end{cases} \tag{2.1}$$

which induces an conjugation operator $\Theta : W^{-1,2} \longmapsto W^{-1,2}$. The restrictions of Θ to L^2 and $W^{1,2}$ we denote also by Θ and notice some properties of Θ, which are straight forward to verify:

i) Θ is an idempotent isometry on each of the spaces $W^{1,2}$, L^2 and $W^{-1,2}$.

ii) There is

$$\langle \Theta\psi, \varphi \rangle \;=\; \langle \psi, \Theta\varphi \rangle,$$

for all $\psi \in W^{-1,2}$ and $\varphi \in W^{1,2}$. In particular, Θ is on L^2 the difference of two orthoprojections and hence selfadjoint.

iii) Θ commutes with the operators H and E from Definition 1.2.

If $D = \emptyset$, then $\tilde{\Theta}$ is the identical operator on $\mathbb{C}^d$, and the induced operators Θ are the identical operators on $W^{-1,2}$, L^2, and $W^{1,2}$. We do not specially denote these identical operators, but represent them by the scalar factors attached to them.

Next we state and prove two lemmata by means of which many of our results on the $\mathbf{k}\cdot\mathbf{p}$ Schrödinger operators may be derived.

2.1. Lemma. *For any $\xi \in \mathbb{R}$ the operator $H + i\xi$ provides a topological isomorphism between $W^{1,2}$ and $W^{-1,2}$, or, in other words, $W^{1,2}$ is the domain for $H+i\xi$. H has a compact resolvent in $\mathcal{B}(W^{-1,2}, W^{-1,2})$, hence a pure point spectrum, cf. Kato [16, III.6.29]. Moreover, one may estimate*

$$\sup_{\xi\in\mathbb{R}} \|H(H+i\xi)^{-1}\|_{\mathcal{B}(W^{-1,2},W^{-1,2})} \le \frac{\max\limits_{j=1,\dots,d}\ \operatorname*{vraimax}\limits_{x\in[0,T]} |m_j(x)|}{\min\limits_{j=1,\dots,d}\ \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|} < \infty, \tag{2.2}$$

and

$$\|(H+i\xi)^{-1}\|_{\mathcal{B}(W^{-1,2},W^{-1,2})} \le \frac{1}{|\xi|}\left(1 + \frac{\max\limits_{j=1,\dots,d}\ \operatorname*{vraimax}\limits_{x\in[0,T]} |m_j(x)|}{\min\limits_{j=1,\dots,d}\ \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|}\right), \qquad 0 \ne \xi \in \mathbb{R}^d. \tag{2.3}$$

Proof. We regard the quadratic form

$$\psi \longmapsto \langle \Theta(H+i\xi)\psi, \psi\rangle = \sum_{j=1}^{d} \int_0^T |m_j| \left|\frac{d\psi_j}{dx}\right|^2 dx \; + \; i\xi\langle\Theta\psi,\psi\rangle_{L^2}, \tag{2.4}$$

corresponding to the operator $\Theta(H+i\xi)$. One estimates this form from below:

$$|\langle \Theta(H+i\xi)\psi, \psi\rangle| \ \ge\ \|\psi\|^2_{W^{1,2}} \min_{j=1,\dots,d}\ \operatorname*{vraimin}_{x\in[0,T]} |m_j(x)|.$$

This implies that the form is $W^{1,2}$–elliptic and its ellipticity constant is not smaller than $\min\limits_{j=1,\dots,d}\ \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|$. Hence, by the Lax–Milgram lemma $\Theta(H+i\xi)$ is surjective and the following estimate is valid:

$$\|(H+i\xi)^{-1}\|_{\mathcal{B}(W^{-1,2},W^{1,2})} \ =\ \|\Theta(H+i\xi)^{-1}\|_{\mathcal{B}(W^{-1,2},W^{1,2})} \le \frac{1}{\min\limits_{j=1,\dots,d}\ \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|}. \tag{2.5}$$

This proves that $(H + i\xi) : W^{1,2} \to W^{-1,2}$ is a topological isomorphism.

The embedding $W^{1,2} \hookrightarrow W^{-1,2}$ — defined by the duality $\langle \cdot, \cdot \rangle$, which extends the scalar product in L^2 — is compact. This implies the compactness of the resolvent of H in $\mathcal{B}(W^{-1,2}, W^{-1,2})$.

In order to show (2.2) one has only to combine (2.5) and the trivial inequality

$$\|H\|_{\mathcal{B}(W^{1,2},W^{-1,2})} \le \max_{j=1,\dots,d} \operatorname*{vraimax}_{x\in[0,T]} |m_j(x)|. \tag{2.6}$$

(2.3) is obtained from (2.2) and the estimate

$$\begin{aligned}\|(H+i\xi)^{-1}\|_{\mathcal{B}(W^{-1,2},W^{-1,2})} &= \frac{1}{|\xi|}\|i\xi(H+i\xi)^{-1}\|_{\mathcal{B}(W^{-1,2},W^{-1,2})} \\ &\le \frac{1}{|\xi|}\Big(1 + \|H(H+i\xi)^{-1}\|_{\mathcal{B}(W^{-1,2},W^{-1,2})}\Big).\end{aligned}$$

□

2.2. Lemma. *The operators A_α, $\alpha \in \{0,1,2\}$, B_α, $B_{\alpha\beta}$, $\alpha,\beta \in \{1,2\}$, V and E (cf. Definition 1.2) acting in the Hilbert space $W^{-1,2}$, are relatively bounded with respect to H and their relative bounds are zero.*

Proof. We begin with the first order operators. Let φ be an arbitrary element from $W^{1,2}$, the domain of H:

$$\begin{aligned}\|A_\alpha\varphi\|_{W^{-1,2}} &= \sup_{\|\psi\|_{W^{1,2}}=1} |\langle A_\alpha\varphi, \psi\rangle| \\ &= \sup_{\|\psi\|_{W^{1,2}}=1} \Bigg| \int_0^T \Big\langle M_\alpha(x)\,\frac{d\varphi}{dx}(x)\,,\psi(x)\Big\rangle_{\mathbb{C}^d} dx \\ &\qquad + \int_0^T \Big\langle M_\alpha^*(x)\,\varphi(x), \frac{d\psi}{dx}(x)\Big\rangle_{\mathbb{C}^d} dx \Bigg|. \end{aligned} \tag{2.7}$$

If $\widehat{M}_{\alpha,l}$ denotes the constant value of the function M_α on the interval $[t_l, t_{l+1}[$ (cf. Assumption 1.1), then we may rewrite the first integral, integrating by parts:

$$\begin{aligned}&\int_0^T \Big\langle M_\alpha(x)\,\frac{d\varphi}{dx}(x)\,,\psi(x)\Big\rangle_{\mathbb{C}^d} dx \\ &\qquad = -\int_0^T \Big\langle M_\alpha(x)\,\varphi(x), \frac{d\psi}{dx}(x)\Big\rangle_{\mathbb{C}^d} dx \\ &\qquad\qquad + \sum_{l=1}^{L} \Big\langle \big(\widehat{M}_{\alpha,l-1} - \widehat{M}_{\alpha,l}\big)\,\varphi(t_l)\,,\psi(t_l)\Big\rangle_{\mathbb{C}^d}.\end{aligned}$$

Hence, the right hand side of (2.7) is not greater than

$$\sup_{\|\psi\|_{W^{1,2}}=1} \left| \int_0^T \left\langle \big(M_\alpha^*(x) - M_\alpha(x)\big)\varphi(x)\,, \frac{d\psi}{dx}(x) \right\rangle_{\mathbb{C}^d} dx \right| \\ + \sup_{\|\psi\|_{W^{1,2}}=1} \left| \sum_{l=1}^{L} \left\langle \big(\widehat{M}_{\alpha,l-1} - \widehat{M}_{\alpha,l}\big)\varphi(t_l)\,, \psi(t_l) \right\rangle_{\mathbb{C}^d} \right|. \tag{2.8}$$

The first term may be estimated as follows:

$$\sup_{\|\psi\|_{W^{1,2}}=1} \left| \int_0^T \left\langle \big(M_\alpha^*(x) - M_\alpha(x)\big)\varphi(x)\,, \frac{d\psi}{dx}(x) \right\rangle_{\mathbb{C}^d} dx \right| \\ \leq 2\|M_\alpha\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}\ \|\varphi\|_{L^2} \\ \leq 2\|M_\alpha\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}\ \|\varphi\|_{W^{1,2}}^{\frac{1}{2}}\ \|\varphi\|_{W^{-1,2}}^{\frac{1}{2}}. \tag{2.9}$$

Using (2.5), one may estimate

$$\|\varphi\|_{W^{1,2}}^{\frac{1}{2}} \leq \sqrt{\frac{1}{\min\limits_{j=1,\dots,d}\ \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|}}\ \|H\varphi\|_{W^{-1,2}}^{\frac{1}{2}}. \tag{2.10}$$

Thus we may estimate the right hand side of (2.9) from above — using Young's inequality — by

$$\delta\ \|H\varphi\|_{W^{-1,2}}\ +\ \frac{1}{\delta}\ \frac{\|M_\alpha\|^2_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}}{\min\limits_{j=1,\dots,d}\ \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|}\ \|\varphi\|_{W^{-1,2}}$$

for all $\delta > 0$.

Let $C([0,T];\mathbb{C}^d)$ denote the space of $\mathbb{C}^d$–valued, continuous functions over $[0,T]$. Elementary calculations show that the embedding constant from $W^{1,2}$ into $C([0,T];\mathbb{C}^d)$ does not exceed $\sqrt{\frac{T}{2}}$. Using this, it is easy to see that the second term of (2.8) is not greater than

$$\sum_{l=1}^{L} \|\widehat{M}_{\alpha,l-1} - \widehat{M}_{\alpha,l}\|_{\mathcal{B}(\mathbb{C}^d)}\ \|\varphi\|_{C([0,T];\mathbb{C}^d)} \sup_{\|\psi\|_{W^{1,2}}=1} \|\psi\|_{C([0,T];\mathbb{C}^d)} \\ \leq \sqrt{\frac{T}{2}}\ \|\varphi\|_{C([0,T];\mathbb{C}^d)} \sum_{l=1}^{L} \|\widehat{M}_{\alpha,l-1} - \widehat{M}_{\alpha,l}\|_{\mathcal{B}(\mathbb{C}^d)}.$$

We continue by applying the estimate

$$\|\varphi\|_{C([0,T];\mathbb{C}^d)}\ \leq\ \sqrt{2}\,\|\varphi\|_{W^{1,2}}^{\frac{1}{2}}\,\|\varphi\|_{L^2}^{\frac{1}{2}}$$

and then use the interpolation inequality (1.3); thus we obtain that the second term of (2.8) is not greater than

$$
\begin{aligned}
&T^{\frac{1}{2}}\, \|\varphi\|_{W^{1,2}}^{\frac{3}{4}}\, \|\varphi\|_{W^{-1,2}}^{\frac{1}{4}} \sum_{l=1}^{L} \|\widehat{M}_{\alpha,l-1} - \widehat{M}_{\alpha,l}\|_{\mathcal{B}(\mathbb{C}^d)} \\
&\le T^{\frac{1}{2}} \min_{j=1,\dots,d} \operatorname*{vraimin}_{x\in[0,T]} |m_j(x)|^{-\frac{3}{4}}\, \|H\varphi\|_{W^{-1,2}}^{\frac{3}{4}}\, \|\varphi\|_{W^{-1,2}}^{\frac{1}{4}} \sum_{l=1}^{L} \|\widehat{M}_{\alpha,l-1} - \widehat{M}_{\alpha,l}\|_{\mathcal{B}(\mathbb{C}^d)} \\
&\le \frac{3}{4}\,\delta\, \|H\varphi\|_{W^{-1,2}} + \frac{T^2}{4\,\delta^3} \frac{\left(\sum_{l=1}^{L} \|\widehat{M}_{\alpha,l-1} - \widehat{M}_{\alpha,l})\|_{\mathcal{B}(\mathbb{C}^d)}\right)^4}{\left(\min\limits_{j=1,\dots,d} \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|\right)^3} \|\varphi\|_{W^{-1,2}},
\end{aligned}
$$

for all $\delta > 0$, (Young's inequality). Thus we have proved that the first order parts A_α of $H_{\mathbf{k}}$ are relatively bounded with respect to the second order part H and that the corresponding constants may be chosen arbitrarily small. Now we will show the same for the zero order parts of $H_{\mathbf{k}}$:

$$
\begin{aligned}
\|B_\alpha\varphi\|_{W^{-1,2}} &= \sup_{\|\psi\|_{W^{1,2}}=1} |\langle B_\alpha\varphi, \psi\rangle| \\
&= \sup_{\|\psi\|_{W^{1,2}}=1} \left| \int_0^T \langle U_\alpha(x)\,\varphi(x)\,,\psi(x)\rangle_{\mathbb{C}^d}\, dx \right| \\
&\le \|U_\alpha\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}\, \|\varphi\|_{L^2} \sup_{\|\psi\|_{W^{1,2}}=1} \|\psi\|_{L^2} \qquad (2.11)
\end{aligned}
$$

Noticing that the embedding constant from from $W^{1,2}$ into L^2 is equal to T/π and thus estimating the last factor by this number, (2.11) can be further estimated by means of (1.3) and Young's inequality:

$$
\begin{aligned}
&\le \frac{T}{\pi}\, \|U_\alpha\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}\, \|\varphi\|_{W^{1,2}}^{\frac{1}{2}}\, \|\varphi\|_{W^{-1,2}}^{\frac{1}{2}} \\
&\le \frac{T}{\pi}\, \|U_\alpha\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))} \sqrt{\frac{1}{\min\limits_{j=1,\dots,d} \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|}}\, \|H\varphi\|_{W^{-1,2}}^{\frac{1}{2}}\, \|\varphi\|_{W^{-1,2}}^{\frac{1}{2}} \\
&\le \frac{\delta}{2}\, \|H\varphi\|_{W^{-1,2}} + \frac{T^2}{2\pi^2\delta} \frac{\|U_\alpha\|^2_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}}{\min\limits_{j=1,\dots,d} \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|} \|\varphi\|_{W^{-1,2}},
\end{aligned}
$$

where δ is an arbitrary positive number. Similarly, one shows

$$
\|B_{\alpha\beta}\,\varphi\|_{W^{-1,2}} \le \frac{\delta}{2} \|H\varphi\|_{W^{-1,2}} + \frac{T^2}{2\pi^2\delta} \frac{\|U_{\alpha\beta}\|^2_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}}{\min\limits_{j=1,\dots,d} \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|} \|\varphi\|_{W^{-1,2}}
$$

$$\|V\varphi\|_{W^{-1,2}} \leq \frac{\delta}{2}\|H\varphi\|_{W^{-1,2}} + \frac{T^2}{2\pi^2\delta}\frac{\|v\|^2_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}}{\min_{j=1,\dots,d}\ \operatorname{vraimin}_{x\in[0,T]}|m_j(x)|}\|\varphi\|_{W^{-1,2}}$$

and

$$\|E\varphi\|_{W^{-1,2}} \leq \frac{\delta}{2}\|H\varphi\|_{W^{-1,2}} + \frac{T^2}{2\pi^2\delta}\frac{\left(\max_{j=1,\dots,d}\ \operatorname{vraimax}_{x\in[0,T]}|e_j|\right)^2}{\min_{j=1,\dots,d}\ \operatorname{vraimin}_{x\in[0,T]}|m_j(x)|}\|\varphi\|_{W^{-1,2}}.$$

□

2.3. Remark. It is easy to see that Lemma 2.2 can be extended to the case of coefficient functions M_α with bounded total variation. If M_α is from the space BV (cf. [11]), then in the estimates the term $\sum_{l=1}^{L}\|\widehat{M}_{\alpha,l-1}-\widehat{M}_{\alpha,l}\|_{\mathcal{B}(\mathbb{C}^d)}$ has to be replaced by the total variation of the $\mathcal{B}(\mathbb{C}^d)$–valued measure which is the distributional derivative of the function M_α. Because there is up to now no physical necessity to regard such coefficients we did not expatiate these things.

Now we can prove several results on the Schrödinger operator (1.11a) from Definition 1.2:

2.4. Theorem. i) *For any $\mathbf{k}\in\mathbb{C}^2$ the operator $H_\mathbf{k}$ from Definition 1.2 has the same domain as H, namely $W^{1,2}$, and all these operators are closed.*

ii) *For all $\psi\in W^{1,2}$ the mapping*

$$\mathbb{C}^2 \ni \mathbf{k} \longmapsto H_\mathbf{k}\psi$$

is analytic. Hence, for any one dimensional complex analytic submanifold $\mathcal{S}$ of $\mathbb{C}^2$ the operator family $\{H_\mathbf{k}\}_{\{\mathbf{k}\in\mathcal{S}\}}$ is a holomorphic operator family of type (A), cf. Kato [16, VII.2].

iii) *Let for fixed $\mathbf{k}\in\mathbb{C}^2$ and*

$$b < \frac{\min_{j=1,\dots,d}\ \operatorname{vraimin}_{x\in[0,T]}|m_j(x)|}{\max_{j=1,\dots,d}\ \operatorname{vraimax}_{x\in[0,T]}|m_j(x)|}$$

$a = a(\mathbf{k}, b)$ be a constant such that for all $\psi\in W^{1,2} = \mathrm{dom}(H)$

$$\|T_\mathbf{k}\psi\|_{W^{-1,2}} \leq a\,\|\psi\|_{W^{-1,2}} + b\,\|H\psi\|_{W^{-1,2}}$$

holds. (According to Lemma 2.2 there is such an a for every positive b.) If $\xi \in \mathbb{R}$ satisfies

$$|\xi| > \frac{a\left(1 + \dfrac{\max\limits_{j=1,\dots,d} \operatorname*{vraimax}\limits_{x\in[0,T]} |m_j(x)|}{\min\limits_{j=1,\dots,d} \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|}\right)}{1 - b\,\dfrac{\max\limits_{j=1,\dots,d} \operatorname*{vraimax}\limits_{x\in[0,T]} |m_j(x)|}{\min\limits_{j=1,\dots,d} \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|}}, \tag{2.12}$$

then $i\xi$ belongs to the resolvent set of $H_{\mathbf{k}}$.

Additionally, the resolvent of $H_{\mathbf{k}}$ is compact. Consequently (cf. Kato [16, III.6.29], the spectrum of $H_{\mathbf{k}}$ only consists of at most countably many eigenvalues with finite multiplicity, which do not accumulate in the finite.

In Theorem 2.5 we will give more spectral properties of $H_{\mathbf{k}}$.

Proof. Ad i. The first statement follows from Lemma 2.2 and a well known perturbation theorem for relatively bounded operators, cf. Kato [16, IV.1.1].

Ad ii. It suffices to prove that for all $k_\alpha \in \mathbb{C}$ both the mappings

$$\mathbb{C} \ni k_\beta \longmapsto H_{(k_\alpha,k_\beta)}\psi \qquad \text{and} \qquad \mathbb{C} \ni k_\beta \longmapsto H_{(k_\beta,k_\alpha)}\psi, \tag{2.13}$$

where $\psi \in W^{1,2}$, are weakly analytic in $W^{-1,2}$. This implies according to Kato [16, III.1.37] that the mappings (2.13) are even strongly analytic. Now Hartog's theorem [14, 2.2.8] provides the analyticity of the mappings $\mathbf{k} \mapsto H_{\mathbf{k}}\psi$.

The weak analyticity of the mappings introduced in (2.13) follows directly from the Definition 1.2 of the operator family $H_{\mathbf{k}}$.

Ad iii. (2.12) is equivalent to the inequality

$$\frac{a}{|\xi|}\left(1 + \frac{\max\limits_{j=1,\dots,d} \operatorname*{vraimax}\limits_{x\in[0,T]} |m_j(x)|}{\min\limits_{j=1,\dots,d} \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|}\right) + b\,\frac{\max\limits_{j=1,\dots,d} \operatorname*{vraimax}\limits_{x\in[0,T]} |m_j(x)|}{\min\limits_{j=1,\dots,d} \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|} < 1.$$

From (2.2) and (2.3) thus follows

$$a\,\|(H - i\xi)^{-1}\|_{\mathcal{B}(W^{-1,2},W^{-1,2})} + b\,\|H(H - i\xi)^{-1}\|_{\mathcal{B}(W^{-1,2},W^{-1,2})} < 1$$

for all $\xi \in \mathbb{R}$ satisfying (2.12). Now the assertions follow from a well known stability theorem, cf. Kato [16, IV.3.17]. $\square$

Theorem 2.4 enables us to give a first answer to Problem 1.6: The spectral properties of the operator $H_{\mathbf{k}}$ do indeed depend analytically on $\mathbf{k}$, or, in other words, the Theorems 1.7, 1.8, 1.9 from [16, VII.1] apply to our situation.

We will now pass to the consideration of the restriction of the operator $H_{\mathbf{k}}$ to the space L^2.

2.5. Theorem. i) *For any vector* $\mathbf{k} = (k_1, k_2) \in \mathbb{R}^2$ *the operator* $H_{\mathbf{k}}|_{L^2}$ *is selfadjoint and has a compact resolvent. Hence, there is an orthonormal basis of eigenfunctions in* L^2.

ii) *Using the notations* $\widehat{m}_l$ *and* $\widehat{M}_{\alpha,l}$ *as in Assumption 1.1 the domain of* $H_{\mathbf{k}}|_{L^2}$ *can be characterized as follows:*

$$\begin{aligned} \operatorname{dom}(H_{\mathbf{k}}|_{L^2}) = W^{1,2} \cap \Bigg\{ \varphi \;\Bigg|\; & \varphi|_{]t_l,t_{l+1}[} \in W^{2,2}(]t_l, t_{l+1}[), \\ & \widehat{m}_l \lim_{\substack{t\to t_l \\ t>t_l}} \frac{d\varphi}{dx}(t) - \widehat{m}_{l-1} \lim_{\substack{t\to t_l \\ t<t_l}} \frac{d\varphi}{dx}(t) + \big(\widehat{M}^*_{0,l+1} - \widehat{M}^*_{0,l}\big)\varphi(t_l) \\ & + \sum_{\alpha=1,2} k_\alpha \big(\widehat{M}^*_{\alpha,l+1} - \widehat{M}^*_{\alpha,l}\big)\varphi(t_l) = 0,\ l = 0, \dots, L \Bigg\}. \end{aligned} \tag{2.14}$$

iii) *The spectrum of* $H_{\mathbf{k}}|_{L^2}$ *is the same as for* $H_{\mathbf{k}}$ *and, consequently, depends locally analytically on* $\mathbf{k}$ *as stated in Theorem 2.4.*

iv) *The resolvent of* $H_{\mathbf{k}}|_{L^2}$ *is nuclear.*

v) *For any* $\mathbf{k} \in \mathbb{C}^2$ *the geometric spectral multiplicity is at most* d. *If* $\mathbf{k}$ *is from* $\mathbb{R}^2$, *then the same is true for the algebraic multiplicity.*

Proof. Ad i. From item iii) of Theorem 2.4 follows the existence of a real number $\delta = \delta(\mathbf{k})$ such that

$$(H_{\mathbf{k}} + \delta) : W^{1,2} \longmapsto W^{-1,2} \tag{2.15}$$

is a topological isomorphism. Obviously, the restriction of $H_{\mathbf{k}} + \delta$ to L^2 remains a surjection. This, together with the symmetry of $H_{\mathbf{k}}|_{L^2}$ in the case of $\mathbf{k} \in \mathbb{R}^2$ implies the asserted selfadjointness of $H_{\mathbf{k}}|_{L^2}$, cf. [1, VI.46 Satz 2]. The compactness of the resolvent easily follows from the isomorphism property of the mapping (2.15) and the compactness of the embedding $W^{1,2} \hookrightarrow L^2$. The next statement is implied by a classical structure theorem for compact, selfadjoint operators [1, V.61].

Ad ii. $\varphi \in W^{2,2}(]t_l, t_{l+1}[)$ implies $\frac{d\varphi}{dx} \in C^\gamma([t_l, t_{l+1}])$. Thus, the limits occuring in (2.14) exist. The assertion follows by partial integration in the sense of distributions.

Ad iii. Spectral points of $H_{\mathbf{k}}$ and $H_{\mathbf{k}}|_{L^2}$ needs must be eigenvalues. Moreover any eigenfunction of $H_{\mathbf{k}}$ belonging to $W^{-1,2}$, in fact is from the space L^2, and even from $W^{1,2}$.

Ad iv. If λ is from the resolvent set of $H_{\mathbf{k}}|_{L^2}$, then $\|(H_{\mathbf{k}}-\lambda)^{-1}\|_{\mathcal{B}(W^{-1,2},W^{1,2})}$ is finite, cf. Theorem 2.4 and item iii) of the present theorem. Let $\mathbb{1}_{(W^{1,2}\hookrightarrow L^2)}$ and $\mathbb{1}_{(L^2\hookrightarrow W^{-1,2})}$ denote the embedding operators, and $\|\cdot\|_1$ and $\|\cdot\|_2$ the nuclear and Hilbert–Schmidt norm respectively. We can estimate:

$$\begin{aligned}&\|(H_{\mathbf{k}}-\lambda)^{-1}\|_1\\ &\quad\le \|\mathbb{1}_{(W^{1,2}\hookrightarrow L^2)}\|_2\,\|(H_{\mathbf{k}}-\lambda)^{-1}\|_{\mathcal{B}(W^{-1,2},W^{1,2})}\,\|\mathbb{1}_{(L^2\hookrightarrow W^{-1,2})}\|_2<\infty.\end{aligned} \tag{2.16}$$

N.B. $\mathbb{1}_{(W^{1,2}\hookrightarrow L^2)}$ and $\mathbb{1}_{(L^2\hookrightarrow W^{-1,2})}=\mathbb{1}^*_{(W^{1,2}\hookrightarrow L^2)}$ are Hilbert–Schmidt operators, cf. [5, I Th. 3.2].

Ad v. Let λ be any eigenvalue of the operator $H_{\mathbf{k}}|_{L^2}$ and $\psi_1,\dots,\psi_{d+1}$ eigenfunctions corresponding to λ. We will show that these eigenfunctions are linearly dependent. For this purpose we rewrite each of the equations

$$(H_{\mathbf{k}}-\lambda)\psi_j=0,\qquad j=1,\dots,d+1$$

in the usual way as the corresponding first order system. Because the $d+1$ vectors of initial values $\big(0,\frac{d\psi_1}{dx}(0)\big),\dots,\big(0,\frac{d\psi_{d+1}}{dx}(0)\big)$ from $\mathbb{C}^{2d}$ for these systems needs must be linearly dependent, they satisfy a linear relation. It is well known [17, §6.3] that the C^{2d}–valued functions $\big(\psi_1,\frac{d\psi_1}{dx}\big),\dots,\big(\psi_{d+1},\frac{d\psi_{d+1}}{dx}\big)$ satisfy the same linear relation on the whole interval $]t_0,t_1]$ and in particular this relation holds for the vectors

$$\Big(\psi_1(t_1),\lim_{\substack{x\to t_1\\ t<t_1}}\frac{d\psi_1}{dx}(x)\Big),\dots,\Big(\psi_{d+1}(t_1),\lim_{\substack{x\to t_1\\ t<t_1}}\frac{d\psi_{d+1}}{dx}(x)\Big).$$

Now it is easy to see that the conditions in the domain definition (2.14) entail this linear relation to the initial vector for the next interval $[t_1,t_2[$ and the igeargument repeats over all subintervals.

If $\mathbf{k}\in\mathbb{R}^2$, then $H_{\mathbf{k}}|_{L^2}$ is selfadjoint, hence the geometric and algebraic eigenspaces coincide [16, V.3.5]. □

Unfortunately, it turns out that the operators $H_{\mathbf{k}}$ behave in the L^2–context much more irregularly than over $W^{-1,2}$. We collect the properties in the subsequent theorem:

2.6. Theorem. i) *Let us denote*

$$\mathcal{D}_L=\operatorname{dom}(H|_{L^2})\cap\Big\{\psi\;\Big|\;\psi(t_l)=0,\ l=1,\dots,L\Big\}.$$

For all $\mathbf{k} \in \mathbb{C}^2$ there is the following decomposition

$$\mathrm{dom}(H_{\mathbf{k}}|_{L^2}) = \mathcal{D}_L \oplus X_{\mathbf{k}},$$

where $X_{\mathbf{k}} \subset W^{1,2}$ is a vector space, depending on $\mathbf{k}$, of dimension $d\,L$.

ii) *Restricted to the subspace $\mathcal{D}_L$, the operators A_α from Definition 1.2 are relatively bounded with respect to the operator H and the relative bound is zero; more precisely one has for any $\varphi \in \mathcal{D}_L$:*

$$\begin{aligned}\|A_\alpha\varphi\|_{L^2} &\le \frac{\|M_\alpha - M_\alpha^*\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}}{\sqrt{\min\limits_{j=1,\dots,d}\ \operatorname*{vraimin}\limits_{x\in[0,T]}|m_j(x)|}}\,\gamma_H\,\|H\varphi\|_{L^2}^{\frac12}\,\|\varphi\|_{L^2}^{\frac12}\\ &\le \delta\,\|H\varphi\|_{L^2} + \frac{1}{4\delta}\,\frac{\|M_\alpha - M_\alpha^*\|^2_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}}{\min\limits_{j=1,\dots,d}\ \operatorname*{vraimin}\limits_{x\in[0,T]}|m_j(x)|}\,\gamma_H^2\,\|\varphi\|_{L^2},\end{aligned}$$

where δ is any positive number and γ_H is a positive interpolation constant, cf. (2.18).

iii) *On dom$(H|_{L^2})$, however, one cannot find relative L^2–bounds for $A_\alpha|_{L^2}$ with respect to $H|_{L^2}$.*

iv) *Even worse, if there are more than one jumping points t_l for the coefficients, then there is no symmetric extension of $A_\alpha|_{\mathcal{D}_L}$ to dom$(H|_{L^2})$ at all.*

Proof. Ad i. The assertion follows directly from item ii) of Theorem 2.5.

Ad ii. If $\varphi \in \mathcal{D}_L$, then

$$\begin{aligned}\|A_\alpha\varphi\|_{L^2} &= \sup_{\substack{\psi\in W^{1,2}\\ \|\psi\|_{L^2}=1}} |\langle A_\alpha\varphi,\psi\rangle|\\ &= \sup_{\substack{\psi\in W^{1,2}\\ \|\psi\|_{L^2}=1}} \left|\int_0^T \big\langle M_\alpha(x)\,\frac{d\varphi}{dx}(x),\psi(x)\big\rangle_{\mathbb{C}^d} + \big\langle M_\alpha^*(x)\,\varphi(x),\frac{d\psi}{dx}(x)\big\rangle_{\mathbb{C}^d}\,dx\right|\\ &= \sup_{\substack{\psi\in W^{1,2}\\ \|\psi\|_{L^2}=1}} \left|\int_0^T \Big\langle \big(M_\alpha(x) - M_\alpha^*(x)\big)\,\frac{d\varphi}{dx}(x),\psi(x)\Big\rangle_{\mathbb{C}^d}\,dx\right|\\ &= \Big\|\big(M_\alpha(x) - M_\alpha^*(x)\big)\,\frac{d\varphi}{dx}\Big\|_{L^2} \le \|M_\alpha - M_\alpha^*\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}\,\Big\|\frac{d\varphi}{dx}\Big\|_{L^2}\end{aligned}$$

We continue by further estimating

$$\left\|\frac{d\varphi}{dx}\right\|_{L^2} \le \sqrt{\frac{\int_0^T \langle m(x)\frac{d\varphi}{dx}(x), \Theta\frac{d\varphi}{dx}(x)\rangle_{\mathbb{C}^d}\, dx}{\min\limits_{j=1,\dots,d}\ \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|}}$$

$$= \sqrt{\frac{\langle |H|\varphi,\varphi\rangle_{L^2}}{\min\limits_{j=1,\dots,d}\ \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|}} = \frac{\left\||H|^{\frac{1}{2}}\varphi\right\|_{L^2}}{\sqrt{\min\limits_{j=1,\dots,d}\ \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|}}. \qquad (2.17)$$

$|H| = \Theta H$ is a strictly positive, selfadjoint operator, hence by a well known interpolation result [18, §2 Th. 6.10] we may continue as follows:

$$\|(\Theta H)^{\frac{1}{2}}\varphi\|_{L^2} \le \gamma_H\ \|\Theta H\varphi\|_{L^2}^{\frac{1}{2}}\|\varphi\|_{L^2}^{\frac{1}{2}} = \gamma_H\ \|H\varphi\|_{L^2}^{\frac{1}{2}}\|\varphi\|_{L^2}^{\frac{1}{2}}, \qquad (2.18)$$

where γ_H is the corresponding (finite, positive) interpolation constant. Fitting the inequalities together, and finally applying Young's inequality one obtains the assertion.

Ad iii. From the first item of this theorem follows, that there are elements in $\operatorname{dom}(H|_{L^2})$ which do not belong to $\mathcal{D}_L$. Because every $\psi \in \operatorname{dom}(H|_{L^2}) \subset W^{1,2}$ is continuous, the functions $M_\alpha\psi$ are jumping in those jumping points of M_α where ψ does not vanish. Consequently, the distributional derivative of such functions $M_\alpha\psi$ contains Dirac measures in one of the jumping points, what prevents $\frac{d}{dx}(M_\alpha\psi)$ having a finite L^2–norm.

Ad iv. We will not prove this item in detail but give the idea how to do this: One uses the general characterization of symmetric extensions for symmetric operators, cf. e.g. Neumark [17, §14.8] by means of the kernels $\mathcal{K}_+$, $\mathcal{K}_-$ of the adjoint operator, shifted by plus or minus i, respectively. It turns out that the space of the corresponding combinations $\psi^+ - \psi^-$, where

$$\psi^+ \in \mathcal{K}_+, \quad \psi^- \in \mathcal{K}_-, \quad \|\psi^+\|_{L^2} = \|\psi^-\|_{L^2}, \quad \psi^+ - \psi^- \in \operatorname{dom}(H|_{L^2})$$

is at most d dimensional [17, §14.8 Th. 7]. But if there are at least two jumping points for the coefficients, then the defect of $\mathcal{D}_L$ in $\operatorname{dom}(H|_{L^2})$ is at least $2d$ and, hence, cannot be filled up this way. □

Next we consider the operators $H_{\mathbf{k}}$ on L^2 in their dependence on $\mathbf{k} \in \mathbb{C}^2$. As we have shown in Theorem 2.5, and in contrast to the situation on $W^{-1,2}$, cf. Theorem 2.4, the concept of holomorphic families of type (A) is <u>not</u> adequate for the family $\{H_{\mathbf{k}}|_{L^2}\}_{\mathbf{k}\in\mathbb{C}^2}$ because $\operatorname{dom}(H_{\mathbf{k}}|_{L^2})$ is not independent from $\mathbf{k}$. However, the following is true:

2.7. Theorem. *For any one dimensional complex analytic submanifold $\mathcal{S} \in \mathbb{C}^2$ the family $\{H_{\mathbf{k}}|_{L^2}\}_{\mathbf{k}\in\mathcal{S}}$ is an analytic family of operators in the sense of Kato [16, VII.1.2].*

Proof. It easily follows from the definition that $\{H_{\mathbf{k}}|_{L^2}\}_{\mathbf{k}\in\mathcal{S}}$ is an analytic operator family iff $\{\Theta H_{\mathbf{k}}|_{L^2}\}_{\mathbf{k}\in\mathcal{S}}$ is. We show this by proving that the corresponding forms constitute an (a)–analytic family of forms, cf. [16, VII.4.2]. For this it is sufficient to confirm that the quadratic forms associated to the operators $\Theta H_{\mathbf{k}}$

i) have a domain of definition independent from $\mathbf{k}$, namely $W^{1,2}$,

ii) are sectorial and closed on this domain, and

iii) depend analytically on $\mathbf{k}$ in the following sense: for any ψ from the domain of the form the mapping $\mathbb{C}^2 \ni \mathbf{k} \longmapsto \langle H_{\mathbf{k}}\psi, \psi\rangle$ is holomorphic.

It is easy to see that the domain of the form $\mathfrak{t}$, which corresponds to the operator $\Theta H = |H|$, is $W^{1,2}$ and that this form is closed on that space. It is also sectorial because it is the form of a positive selfadjoint operator. Now according to Kato [16, VII Th.4.8] it is sufficient to know:

2.8. Proposition. *The forms $\langle T_{\mathbf{k}}\cdot,\cdot\rangle$, cf. Definition 1.2, are relatively bounded with respect to the form $\mathfrak{t}$ correspondimg to the operator $\Theta H = |H|$. The $\mathfrak{t}$–bound is equal to zero.*

We show that the forms corresponding to the operators ΘA_α, ΘB_α, and $\Theta B_{\alpha,\beta}$ are relatively bounded with respect to $\mathfrak{t}$ and that the relative bounds may be taken arbitrarily small. For the forms corresponding to ΘB_α, and $\Theta B_{\alpha,\beta}$ this is obvious, because they are even bounded on L^2. It remains to prove the statement for the form $\mathfrak{t}_\alpha$ which corresponds to the operators ΘA_α. For $\psi \in W^{1,2}$ there is

$$\mathfrak{t}_\alpha[\psi] = \int_0^T \big\langle \tilde{\Theta} M_\alpha(x)\,\frac{d\psi}{dx}(x), \psi(x)\big\rangle_{\mathbb{C}^d} \;+\; \big\langle \tilde{\Theta} M_\alpha^*(x)\,\psi(x), \frac{d\psi}{dx}(x)\big\rangle_{\mathbb{C}^d}\, dx,$$

where $\tilde{\Theta} : \mathbb{C}^d \mapsto \mathbb{C}^d$ is the conjugation operator from (2.1). One has

$$\begin{aligned}\|\tilde{\Theta} M_\alpha\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))} &= \|M_\alpha\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}\\ &= \|M_\alpha^*\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))} = \|\tilde{\Theta} M_\alpha^*\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}.\end{aligned}$$

Now we estimate $\mathfrak{t}_\alpha[\psi]$:

$$\begin{aligned}
\big|\mathfrak{t}_\alpha[\psi]\big| &\le \Big(\|\tilde{\Theta} M_\alpha\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))} + \|\tilde{\Theta} M_\alpha^*\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}\Big) \Big\|\frac{d\psi}{dx}\Big\|_{L^2} \|\psi\|_{L^2} \\
&\le 2\|M_\alpha\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))} \sqrt{\frac{\langle \Theta H\varphi, \varphi\rangle_{L^2}}{\min\limits_{j=1,\dots,d} \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|}}\, \|\psi\|_{L^2} \qquad (2.19) \\
&\le \delta\, \mathfrak{t}[\psi] + \frac{1}{\delta}\, \|M_\alpha\|^2_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))} \frac{1}{\min\limits_{j=1,\dots,d} \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|} \|\psi\|^2_{L^2}
\end{aligned}$$

for all $\delta > 0$. The analytical dependence of the forms $\langle T_{\mathbf{k}}\cdot, \cdot\rangle$, on $\mathbf{k}$ now follows immediately, cf. Kato [16, VII.1.1 and VII.3.1] for details. □

Theorem 2.7 has far reaching consequences, namely:

2.9. Corollary. *A closed curve, separating two parts of the spectrum of $H_{\mathbf{k}}$ for $\mathbf{k} = \mathbf{k}_0$, also separates corresponding parts of the spectrum of $H_{\mathbf{k}}$ for $\mathbf{k}$ from a suitable neighbourhood of $\mathbf{k}_0$, cf. Kato [16, Th. VII.1.7].*

2.10. Corollary. *Any finite system of eigenvalues of $H_{\mathbf{k}}$ consists of branches of one or several analytic functions which have at most algebraic singularities. The same is true for the corresponding eigenprojections and eigennilpotents, cf. Kato [16, Th. VII.1.8].*

2.11. Problem. From the physical point of view it is of particular interest for which $\mathbf{k} \in \mathbb{R}^2$ the spectral gap between the positive and negative parts of H can be found in the spectrum of $H_{\mathbf{k}}$, and how one can estimate the size of the gap in terms of $\mathbf{k}$ and the data of the problem.

Proposition 2.8 allows to tackle this problem. To that end, and in compliance with the physical situation, cf. e.g. [2, 9, 10, 3], we make, apart of Assumption 1.1, the following additional assumption on the coefficients of the $\mathbf{k} \cdot \mathbf{p}$ operator which allow to give the cutting edge to our estimates.

2.12. Assumption. For almost all $x \in [0,T]$

$$\begin{aligned}
&M_0(x) &&\text{is skewadjoint,} &&\tilde{\Theta} M_0(x) &&\text{is selfadjoint,} &&(2.20)\\
&\tilde{\Theta} U_\alpha(x) &&\text{are skewadjoint,} &&\alpha \in \{1,2\}, && &&(2.21)\\
&\tilde{\Theta} U_{\alpha\alpha}(x) &&\text{are not negative,} &&\alpha \in \{1,2\}, && &&(2.22)
\end{aligned}$$

over $\mathbb{C}^d$.

2.13. Theorem. *We make the Assumptions 1.1 and 2.12 and regard the operators from Definition 1.2. Let μ be the lowest eigenvalue of $|H|$,*

$$e \stackrel{\text{def}}{=} \min_{j=1,\dots,d} \operatorname*{vraimin}_{x\in[0,T]} |e_j(x)| \geq \|v\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}, \tag{2.23}$$

and let λ be such that

$$0 \leq \lambda \leq e - \|v\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}. \tag{2.24}$$

We abbreviate

$$M \stackrel{\text{def}}{=} \frac{\max_{\alpha=1,2} \|M_\alpha\|^2_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}}{\min\limits_{j=1,\dots,d} \operatorname*{vraimin}\limits_{x\in[0,T]} |m_j(x)|}. \tag{2.25}$$

If $\mathbf{k} = (k_1, k_2) \in \mathbb{R}^2$ satisfies

$$|k_1| + |k_2| \leq \sqrt{\frac{\mu}{M}} \tag{2.26a}$$

and

$$\begin{aligned} 0 < \gamma(\mathbf{k}) \stackrel{\text{def}}{=} &\mu - 2\Big(|k_1| + |k_2|\Big)\sqrt{\mu M} \\ &- |k_1|\,|k_2| \Big(\|U_{12}\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))} + \|U_{21}\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}\Big) \\ &+ k_1^2 \operatorname*{vraimin}_{x\in[0,T]} \inf\operatorname{spec}\big(\tilde{\Theta} U_{11}(x)\big) \\ &+ k_2^2 \operatorname*{vraimin}_{x\in[0,T]} \inf\operatorname{spec}\big(\tilde{\Theta} U_{22}(x)\big) \\ &- \|v\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))} + e - \lambda, \end{aligned} \tag{2.26b}$$

then λ belongs to the resolvent set of $H_\mathbf{k}$ and

$$\big\|(H_\mathbf{k} - \lambda)^{-1}\big\| \leq \frac{1}{\gamma(\mathbf{k})}. \tag{2.27}$$

Proof. First, one easily verifies that $\lambda \in \mathbb{R}$ is from the resolvent set for $H_\mathbf{k}$ iff 0 is from the resolvent set of $\Theta H_\mathbf{k} - \lambda\Theta$. Next, Proposition 2.8 implies: if

$$\xi \in \mathbb{C}, \qquad \Re\xi < 0, \qquad |\xi| \text{ sufficiently large}, \tag{2.28}$$

then ξ is from the resolvent set of $\Theta H_\mathbf{k}$, cf. Kato [16, VI Th.3.4]. Thus, it is sufficient to prove, cf. Kato [16, V Th.3.2], that 0 is not in the closure of the numerical range of $\Theta H_\mathbf{k} - \lambda\Theta$ for $\mathbf{k} \in \mathbb{R}^2$ satisfying the conditions (2.26).

We will show this now by estimating the real part of the numerical range of $\Theta H_{\mathbf{k}} - \lambda\Theta$ from below; one has:

$$\begin{aligned}\big\langle(\Theta H_{\mathbf{k}} - \lambda\Theta)\psi,\psi\big\rangle &= \mathfrak{t}[\psi] + \mathfrak{t}_0[\psi] + \sum_{\alpha=1,2} k_\alpha \mathfrak{t}_\alpha[\psi] \\ &\quad + \sum_{\alpha=1,2} k_\alpha \big\langle \Theta B_\alpha\psi,\psi\big\rangle + \sum_{\alpha,\beta=1,2} k_\alpha\, k_\beta \big\langle\Theta B_{\alpha\beta}\psi,\psi\big\rangle \\ &\quad + \big\langle\Theta V\psi,\psi\big\rangle + \big\langle\Theta E\psi,\psi\big\rangle - \big\langle\lambda\Theta\psi,\psi\big\rangle \end{aligned} \tag{2.29}$$

Due to (2.20) the term $\mathfrak{t}_0[\psi]$ is purely imaginary. Indeed

$$\begin{aligned}\mathfrak{t}_0[\psi] &= \int_0^T \big\langle\tilde\Theta M_0(x)\frac{d\psi}{dx}(x),\psi(x)\big\rangle_{\mathbb{C}^d} + \big\langle\tilde\Theta M_0^*(x)\psi(x),\frac{d\psi}{dx}(x)\big\rangle_{\mathbb{C}^d}\,dx \\ &= \int_0^T \big\langle\tilde\Theta M_0(x)\frac{d\psi}{dx}(x),\psi(x)\big\rangle_{\mathbb{C}^d} - \big\langle\tilde\Theta M_0(x)\psi(x),\frac{d\psi}{dx}(x)\big\rangle_{\mathbb{C}^d}\,dx \\ &= \int_0^T \big\langle\tilde\Theta M_0(x)\frac{d\psi}{dx}(x),\psi(x)\big\rangle_{\mathbb{C}^d} - \big\langle\psi(x),\tilde\Theta M_0(x)\frac{d\psi}{dx}(x)\big\rangle_{\mathbb{C}^d}\,dx \\ &= \int_0^T \big\langle\tilde\Theta M_0(x)\frac{d\psi}{dx}(x),\psi(x)\big\rangle_{\mathbb{C}^d}\,dx - \overline{\int_0^T \big\langle\tilde\Theta M_0(x)\frac{d\psi}{dx}(x),\psi(x)\big\rangle_{\mathbb{C}^d}\,dx}.\end{aligned}$$

Due to (2.21) the terms $\big\langle\Theta B_\alpha\psi,\psi\big\rangle$, $\alpha = 1,2$ are also purely imaginary. Now, taking into account (2.19) and obvious estimates for the operators B_{12}, B_{21}, ΘB_{11}, ΘB_{22}, ΘV, $|E|$ and $\lambda\Theta$, one obtains for any $\psi \in \operatorname{dom}\mathfrak{t} = W^{1,2}$ with $\|\psi\|_{L^2} = 1$:

$$\begin{aligned}&\Re\big\langle(\Theta H_{\mathbf{k}} - \lambda\Theta)\psi,\psi\big\rangle \\ &\geq \mathfrak{t}[\psi] - \delta\big(|k_1| + |k_2|\big)\mathfrak{t}[\psi] - \frac{1}{\delta}\big(|k_1| + |k_2|\big)M \\ &- |k_1|\,|k_2|\,\Big(\|U_{12}\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))} + \|U_{21}\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}\Big) \\ &+ k_1^2 \operatorname*{vraimin}_{x\in[0,T]} \inf\operatorname{spec}(\tilde\Theta U_{11}(x)) \\ &+ k_2^2 \operatorname*{vraimin}_{x\in[0,T]} \inf\operatorname{spec}(\tilde\Theta U_{22}(x)) \\ &- \|v\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))} + e - \lambda,\end{aligned} \tag{2.30}$$

where δ is arbitrary from $]0,\infty[$. Now we specify δ. We want to replace $\mathfrak{t}[\psi]$ in (2.30) by μ, without enlarging the right hand side. Hence, one has to ensure the nonnegativity of $1 - \delta\left(|k_1| + |k_2|\right)$, or, in other words, $|k_1| + |k_2| \leq 1/\delta$. Finally we choose $\delta > 0$ such that the function

$$]0,\infty[\ni \delta \longmapsto -\mu\delta - \frac{M}{\delta},$$

corresponding to the δ–dependent terms in (2.30) takes its maximal possible value; the maximizing δ is

$$\delta_{max} = \sqrt{\frac{M}{\mu}}.$$

Thus we have got

$$\Re\Big(\mathfrak{t}[\psi] + \sum_{\alpha=1,2} k_\alpha \mathfrak{t}_\alpha[\psi]\Big) \geq \mu - 2\left(|k_1| + |k_2|\right)\sqrt{\mu M} \tag{2.31}$$

what implies (cf. (2.30))

$$\Re\big\langle(\Theta H_{\mathbf{k}} - \lambda\Theta)\psi, \psi\big\rangle \geq \gamma(\mathbf{k}) \tag{2.32}$$

provided that $\mathbf{k}$ satisfies $|k_1| + |k_2| \leq 1/\delta_{max}$ i.e. (2.26a).

Thus, (2.26) implies that the closure of the numerical range of $\Theta H_{\mathbf{k}} - \lambda\Theta$ does not contain zero, what we wanted to prove. □

2.14. Remark. Using (2.26a) and the fact that the right hand side of (2.31) is not smaller than $-\mu$, one can simplify the condition (2.26b):

$$\begin{aligned} 0 \;<\; & -\mu + e - \lambda - \|v\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))} \\ & - |k_1|\,|k_2|\left(\|U_{12}\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))} + \|U_{21}\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}\right) \\ & + k_1^2 \operatorname*{vraimin}_{x\in[0,T]} \inf \operatorname{spec}\big(\tilde{\Theta} U_{11}(x)\big) \\ & + k_2^2 \operatorname*{vraimin}_{x\in[0,T]} \inf \operatorname{spec}\big(\tilde{\Theta} U_{22}(x)\big). \end{aligned} \tag{2.33}$$

In many cases of physical interest, cf. e.g. [2, 9, 10, 3] one has

$$e \;>\; \mu + \|v\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))} \tag{2.34}$$

hence,

$$0 \;<\; -\mu + e - \lambda - \|v\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}, \tag{2.35}$$

at least for small λ.

2.15. Remark. The reader will easily notice that the set of $\mathbf{k}$'s defined by the conditions (2.26), or (2.26a) and (2.33), possesses the following properties: If $\mathbf{k} \in \mathbb{R}^2$ satisfies any of the conditions, then $-\mathbf{k}$ also does. The condition (2.26a) defines a convex set, while (2.26b) does not. In general (2.26b) is not even radial in $\mathbf{k}$. However, if (2.35), then the condition (2.33) is radial, but in general not convex.

2.16. Remark. μ, the lowest eigenvalue of $|H|$, can be estimated in terms of the data of the problem:

$$\min_{j=1,\dots,d} \operatorname*{vraimin}_{x\in[0,T]} |m_j(x)| \le \frac{\mu}{\mu_0} \le \max_{j=1,\dots,d} \operatorname*{vraimax}_{x\in[0,T]} |m_j(x)|, \tag{2.36}$$

where $\mu_0 = \pi^2/T^2$ is the lowest eigenvalue of the operator $-d^2/dx^2$ with homogeneous Dirichlet boundary conditions on $[0,T]$.

The assumption (2.22) is solely concerned with the matrices $U_{\alpha\beta}$ related to the coordinate directions in the $\mathbf{k}$–plane. In the following we are looking for results analogous to Theorem 2.13 which are uniform in all $\mathbf{k}$–space directions. To that end we replace the condition (2.22) in Assumption 2.12 and make instead the

2.17. Assumption. In addition to the Assumptions 1.1 and 2.12, for almost all $x \in [0,T]$ holds

$$\frac{1}{2} \operatorname*{vraimin}_{\chi\in[0,2\pi[,x\in[0,T]} \inf \operatorname{spec} \left(\tilde{\Theta} U_\chi(x) + U_\chi(x)\tilde{\Theta}\right) \stackrel{\text{def}}{=} \nu \ge 0, \tag{2.37}$$

where

$$U_\chi(x) \stackrel{\text{def}}{=} \cos^2\chi U_{11}(x) + \sin^2\chi U_{22}(x) + \sin\chi\cos\chi\big(U_{12}(x) + U_{21}(x)\big).$$

Assumption 2.17 is quite reasonable from the physical point of view, cf. e.g. [2, 9, 10, 3].

2.18. Theorem. *We make the Assumptions 1.1 and 2.17. Let μ, e and M be as in Theorem 2.13, and let λ be with (2.24). If*

$$\mathbf{k} = \big(k\cos\chi, k\sin\chi\big), \qquad \chi \in [0,2\pi[, \qquad k \ge 0 \tag{2.38a}$$

satisfies

$$k \le f_1(\delta) \stackrel{\text{def}}{=} \frac{1}{\delta\sqrt{2}} \tag{2.38b}$$

and

$$0 < \gamma_{rad}(k) \stackrel{\text{def}}{=} \mu - k\sqrt{2}\left(\mu\delta + \frac{M}{\delta}\right) + k^2\nu - \|v\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))} + e - \lambda, \tag{2.38c}$$

for some $\delta > 0$, then λ belongs to the resolvent set of $H_\mathbf{k}$ and

$$\left\|(H_\mathbf{k} - \lambda)^{-1}\right\| \le \frac{1}{\gamma_{rad}(k)}. \tag{2.39}$$

Proof. The proof of Theorem 2.18 is analogous to that of Theorem 2.13. N.B.

$$|k_1| + |k_2| = k\big(|\cos\chi| + |\sin\chi|\big) \le k\sqrt{2}$$

and

$$\sum_{\alpha,\beta=1,2} k_\alpha\, k_\beta \Re\big\langle \Theta B_{\alpha\beta}\psi, \psi\big\rangle = \frac{k^2}{2}\int_0^T \Big\langle \big(\tilde{\Theta}U_\chi + U_\chi\tilde{\Theta}\big)\psi(x), \psi(x)\Big\rangle_{\mathbb{C}^d} dx \ge k^2\nu.$$

$\square$

2.19. Remark. The benefit of Theorem 2.18 depends on the proper choice of the variable δ in (2.38). In order to get the maximal k–range one has to solve

$$\max_{\delta>0}\min_{l=1,2} f_l(\delta), \tag{2.40}$$

where f_1 and f_2 are the restrictions on k implied by (2.38b) and (2.38c), respectively. As f_1 is a decreasing function one has to look for the smallest possible value $\delta = \delta_{opt}$ such that

$$f_1(\delta_{opt}) = f_2(\delta_{opt}). \tag{2.41}$$

This can be done by determining and analysing f_2 explicitly. For the case $\nu > 0$, cf. Assumption 2.17, this has been performed in [3]. If one neglects the term $k^2\nu$ in (2.38c) this condition becomes

$$k < f_2(\delta) = \frac{\mu + e - \|v\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}}{\sqrt{2}\big(\delta\mu + \frac{M}{\delta}\big)}. \tag{2.42}$$

For

$$\delta_{opt} = \sqrt{\frac{M}{e - \lambda - \|v\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}}} \tag{2.43}$$

one obtains a single condition on k, which does not depend on μ:

$$0 \le k < \sqrt{\frac{e - \lambda - \|v\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))}}{2\,M}}. \tag{2.44}$$

For some choices of δ one can simplify the conditions (2.38).

2.20. Remark. Proceeding in the same way as in the proof of Theorem 2.13 and in Remark 2.14 one obtains in the situation of Theorem 2.18 for $\delta = \delta_{max} = \sqrt{M/\mu}$ a single condition on k, which does only depend on μ and M:

$$0 \leq k \leq \sqrt{\frac{\mu}{2\,M}}, \tag{2.45}$$

because the second condition

$$0 < k^2 \nu + e - \lambda - \|v\|_{L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))} \tag{2.46}$$

is always fulfilled, cf. (2.24) and (2.37).

We still have to address the question of global existence of the eigenvalue (and eigenfunction) branches. In fact, the authors have been trying hard to prove this, but all attempts have failed. The reasons are the followings:

On $W^{-1,2}$, where the problem was considered first, the operators are not selfadjoint; consequently results on global existence cannot be expected. On L^2 the family of operators $\{H_\mathbf{k}\}_\mathbf{k}$ is neither a holomorphic family of type (A), cf. Kato [16, VII.2], nor a holomorphic family of type (B), cf. Kato [16, VII.4]. The type (B) concept fails because the operators are not semibounded on L^2, hence they cannot be defined via the form calculus. Moreover, if one applies the transformation Θ to $H_\mathbf{k}$, then one obtains a sectorial, but essentially nonselfadjoint operator family.

Another idea was to regard the family $\{P_\mathbf{k} H_\mathbf{k}\}_\mathbf{k}$, $P_\mathbf{k}$ being the spectral projector corresponding to the interval $[0, \infty[$, but we could not prove that the dependence $\mathbf{k} \mapsto P_\mathbf{k}$ is analytic.

So it remains an open question whether or not the eigenvalue branches can explode in the finite. However, in §3 we will show that this is never the case for $\mathbf{k} \cdot \mathbf{p}$ operators with a definite main part. Moreover, in §4 we define approximating problems, for which explosion of eigenvalue branches cannot happen.

3 $\mathbf{k} \cdot \mathbf{p}$ operators with definite main part

The hierarchy of $\mathbf{k} \cdot \mathbf{p}$ Hamiltonians in solid state physics contains with the 4×4 and 6×6 Hamiltonians, cf. e.g. [19, 7, 8, 6], $\mathbf{k} \cdot \mathbf{p}$ operators with positive, or negative, definite main part. With respect to Assumption 1.1 this means $D = \emptyset$ or $D = \{1, \dots, d\}$, respectively. Without loss of generality we assume in this section $D = \emptyset$, i.e.

$$\min_{j \in \{1,\dots,d\}} \operatorname*{vraimin}_{x \in [0,T]} m_j(x) > 0, \qquad \min_{j \in \{1,\dots,d\}} \operatorname*{vraimin}_{x \in [0,T]} e_j(x) > 0. \tag{3.1}$$

The operators Θ and $\tilde{\Theta}$, cf. (2.1), introduced at the beginning of §2 are the identical operators on L^2 and $\mathbb{C}^d$, respectively. If the operator H, cf. Definition 1.2 is definite, then the operators $H_{\mathbf{k}}$ and the corresponding forms are semibounded, and one obtains sharper results about the behaviour of the eigenvalues and eigenvectors in dependence on $\mathbf{k}$. Naturally the fundamental results of §2 still apply, in particular the form estimates (2.19).

3.1. Theorem. *Under the Assumption 1.1 and* (3.1) *the eigenvalue curves and eigenfunction curves exist on all one dimensional analytic submanifold $\mathcal{S}$ of $\mathbb{R}^2$ and they are real holomorphic on $\mathcal{S}$.*

Proof. The form estimate (2.19) teaches that any family $\{H_{\mathbf{k}}\}_{\mathbf{k}\in\mathcal{S}}$ is a holomorphic family of type (B). This implies immediately the assertion, cf. Kato [16, VII.4]. □

4 Regularization of $\mathbf{k}\cdot\mathbf{p}$ operators

In this section we will also regard coefficient functions M_α, $\alpha = 0, 1, 2$ which do not satisfy the fourth assumption in Assumption 1.1. Our aim is to show how one can define 'approximating' $\mathbf{k}\cdot\mathbf{p}$ operators which do not have the unsatisfactory properties stated in Theorem 2.6 and for which the eigenvalue curves globally exist. The idea is to replace the step functions M_α by smoothed ones and then to show, that if a sequence of such smoothed functions converges in $L^p([0,T];\mathcal{B}(\mathbb{C}^d))$ to the original coefficient function, then the sequence of resolvents of the thus regularized operators are converging in the nuclear norm to the resolvent of the original operator. This in particular implies that asymptotically all spectral properties are preserved. We start by proving a preparatory lemma:

4.1. Lemma. *Let $\{M_\alpha^{(n)}\}_{n\in\mathbb{N}}$, $\alpha = 0, 1, 2$, be uniformly bounded sequences of continuously differentiable functions on $[0,T]$ with values in $\mathcal{B}(\mathbb{C}^d)$. If each of these sequences converges pointwise almost everywhere to a $L^\infty([0,T];\mathcal{B}(\mathbb{C}^d))$–function M_α, then it converges by Lebesgue dominance in any $L^p([0,T];\mathcal{B}(\mathbb{C}^d))$ with $p\in[1,\infty[$, and*

i) *The image of the operators $A_\alpha^{(n)}$ defined by the functions $M_\alpha^{(n)}$, cf. Definition 1.2, is contained in L^2.*

ii) *One has $A_\alpha^{(n)} \to A_\alpha$ in $\mathcal{B}(W^{1,2}, W^{-1,2})$ as $n\to\infty$.*

iii) *For any $\mathbf{k}\in\mathbb{C}^2$ and any point λ from the resolvent set of the operator $H_{\mathbf{k}}$ there is an n_0 such that for any $n > n_0$ the point λ also belongs to the* *resolvent set of the operators* $H_{\mathbf{k}}^{(n)}$. *Furthermore,*

$$\big(H_{\mathbf{k}}^{(n)} - \lambda\big)^{-1} \longrightarrow \big(H_{\mathbf{k}} - \lambda\big)^{-1} \qquad \text{in } \mathcal{B}(W^{-1,2}, W^{1,2}). \tag{4.1}$$

iv) *The convergence in* (4.1) *is locally uniform in* $\mathbf{k}$ *and* λ, *more precisely: If* $K \subset \mathbb{C}^2$ *is compact,* $\Lambda \subset \mathbb{C}$ *is compact, and*

$$\Lambda \cap \Big(\bigcup_{\mathbf{k} \in K} \operatorname{spec}(H_{\mathbf{k}}) \Big) = \emptyset, \tag{4.2}$$

then there is an integer $n_0 > 0$ *such that for any* $n > n_0$ *no point* λ *from* Λ *belongs to any of the spectra of the operators* $H_{\mathbf{k}}^{(n)}$, $\mathbf{k} \in K$. *Moreover, the convergence* (4.1) *is uniform for* $\mathbf{k} \in K$ *and* $\lambda \in \Lambda$.

Proof. Ad i. The functions $M_\alpha^{(n)}$ are continuously differentiable, hence, one can partially integrate the second term in the definition (1.6) of the operators $A_\alpha^{(n)}$.

Ad ii. Let φ be from $W^{1,2}$. According to (1.6) there is

$$\begin{aligned} \big\|(A_\alpha^{(n)} - A_\alpha)\varphi\big\|_{W^{-1,2}} &= \sup_{\|\psi\|_{W^{1,2}}=1} \big\langle (A_\alpha^{(n)} - A_\alpha)\varphi, \psi \big\rangle \\ &= \sup_{\|\psi\|_{W^{1,2}}=1} \int_0^T \Big\langle \big(M_\alpha^{(n)}(x) - M_\alpha(x)\big) \frac{d\varphi}{dx}(x), \psi(x) \Big\rangle_{\mathbb{C}^d} \\ &\qquad\qquad + \Big\langle \big(M_\alpha^{(n)}(x) - M_\alpha(x)\big)^* \varphi(x), \frac{d\psi}{dx}(x) \Big\rangle_{\mathbb{C}^d} \, dx. \end{aligned}$$

For $p > 2$ we can estimate this expression by means of Hölder's inequality:

$$\begin{aligned} &\le \big\|M_\alpha^{(n)} - M_\alpha\big\|_{L^p([0,T];\mathcal{B}(\mathbb{C}^d))} \sup_{\|\psi\|_{W^{1,2}}=1} \left(\Big\|\frac{d\varphi}{dx}\Big\|_{L^2} \|\psi\|_{L^{\frac{2p}{p-2}}} + \|\varphi\|_{L^{\frac{2p}{p-2}}} \Big\|\frac{d\psi}{dx}\Big\|_{L^2} \right) \\ &\qquad \le 2\big\|\mathbb{1}\big\|_{\mathcal{B}(W^{1,2}, L^{\frac{2p}{p-2}})} \big\|M_\alpha^{(n)} - M_\alpha\big\|_{L^p([0,T];\mathcal{B}(\mathbb{C}^d))} \|\varphi\|_{W^{1,2}}. \end{aligned}$$

The assertion now follows from the convergence $M_\alpha^{(n)} \to M_\alpha$ in the space $L^p([0,T];\mathcal{B}(\mathbb{C}^d))$.

Ad iii. Let $\mathbf{k}$ be from $\mathbb{C}^2$ and λ from the resolvent set of $H_{\mathbf{k}}$. According to (1.11) there is

$$H_{\mathbf{k}}^{(n)} - \lambda = H_{\mathbf{k}} - \lambda + \sum_{\alpha=1,2} k_\alpha \big(A_\alpha^{(n)} - A_\alpha\big).$$

We already know $(A_\alpha^{(n)} - A_\alpha) \to 0$ in $\mathcal{B}(W^{1,2}, W^{-1,2})$, hence, for all n greater than some n_0 one has

$$\Big\| \sum_{\alpha=1,2} k_\alpha \big(A_\alpha^{(n)} - A_\alpha\big) \Big\|_{\mathcal{B}(W^{1,2},W^{-1,2})} < \frac{1}{\big\|(H_{\mathbf{k}} - \lambda)^{-1}\big\|_{\mathcal{B}(W^{-1,2},W^{1,2})}} \tag{4.3}$$

and

$$(H_{\mathbf{k}}^{(n)} - \lambda)^{-1} = (H_{\mathbf{k}} - \lambda)^{-1} \sum_{j=0}^{\infty} \Big(\sum_{\alpha=1,2} k_\alpha \big(A_\alpha - A_\alpha^{(n)}\big) \big(H_{\mathbf{k}} - \lambda\big)^{-1} \Big)^{j}, \tag{4.4}$$

as the series on the right hand side converges in $\mathcal{B}(W^{-1,2}, W^{1,2})$. The asserted convergence (4.1) follows immediately from the representation (4.4) and item i) of this lemma.

Ad iv. First one proves

$$\sup_{\substack{k\in K\\ \lambda\in\Lambda}} \big\|(H_{\mathbf{k}} - \lambda)^{-1}\big\|_{\mathcal{B}(W^{-1,2},W^{1,2})} < \infty. \tag{4.5}$$

This follows from the fact that the mapping

$$K \times \Lambda \ni (\mathbf{k}, \lambda) \longmapsto (H_{\mathbf{k}} - \lambda) \longmapsto (H_{\mathbf{k}} - \lambda)^{-1} \in \mathcal{B}(W^{-1,2}, W^{1,2})$$

is well defined and continuous. Hence, (4.3) is fulfilled uniformly in $(\mathbf{k}, \lambda) \in K \times \Lambda$ for $n > n_0$. The uniform convergence for (4.1) follows immediately from (4.5) and the representation (4.4) of $(H_{\mathbf{k}}^{(n)} - \lambda)^{-1}$. $\square$

4.2. Theorem. *Let the families of coefficient functions* $\{M_\alpha^{(n)}\}_{n\in\mathbb{N}}$, $\alpha = 0, 1, 2$ *satisfy the assumptions of Lemma 4.1.*

i) *For any* $n \in \mathbb{N}$ *and any* $\mathbf{k} \in \mathbb{C}^2$ *the operator* $H_{\mathbf{k}}^{(n)}|_{L^2}$ *has the same domain as* $H|_{L^2}$*, namely*

$$\operatorname{dom}(H_{\mathbf{k}}^{(n)}|_{L^2}) = \operatorname{dom}(H|_{L^2}) = W^{1,2} \cap \Big\{ \varphi \;\Big|\; \varphi|_{]t_l,t_{l+1}[} \in W^{2,2}(]t_l, t_{l+1}[), \\ \widehat{m}_l \lim_{\substack{t\to t_l\\ t>t_l}} \frac{d\varphi}{dx}(t) = \widehat{m}_{l-1} \lim_{\substack{t\to t_l\\ t<t_l}} \frac{d\varphi}{dx}(t),\ l = 0, \ldots, L \Big\}. \tag{4.6}$$

ii) *For any* $n \in \mathbb{N}$ *and any one dimensional analytic manifold* $\mathcal{S} \subset \mathbb{C}^2$ *the operator family* $\{H_{\mathbf{k}}^{(n)}|_{L^2}\}_{\mathbf{k}\in\mathcal{S}}$ *is a holomorphic family of type (A), cf. Kato [16, VII.2]. In particular, if* $\hat{\mathbf{k}} \in \mathbb{R}^2$*, then the operators* $\{H_{\mathbf{k}}^{(n)}\}_{\{\mathbf{k}=\xi\hat{\mathbf{k}},\,\xi\in\mathbb{C}\}}$ *form a selfadjoint holomorphic family of type (A), and the corresponding results* *from Kato [16, VII.2] apply. In the latter case the eigenvalue curves cannot explode in finite, real* $\mathbf{k}$*–range.*

iii) *For any* $\lambda \notin \operatorname{spec} H_{\mathbf{k}}$ *the operators* $(H_{\mathbf{k}}^{(n)}|_{L^2} - \lambda)^{-1}$ *are converging to* $(H_{\mathbf{k}}|_{L^2} - \lambda)^{-1}$ *with respect to the nuclear norm. Moreover, this convergence is uniform in* $\mathbf{k}$ *and* λ *as described in Lemma 4.1.*

iv) *If* $\mathbf{k} \in \mathbb{R}^2$*, which implies according to item ii) selfadjointness of the operators* $H_{\mathbf{k}}^{(n)}$ *and* $H_{\mathbf{k}}$*, then the spectrum of* $H_{\mathbf{k}}$ *asymptotically appears in the spectra of the operators* $H_{\mathbf{k}}^{(n)}$*; more precisely: If* λ *is an eigenvalue of the operator* $H_{\mathbf{k}}$ *and* $\mathcal{U} \subset \mathbb{C}$ *is an arbitrary neighbourhood of* λ*, then there is a* n_0 *such that for any* $n > n_0$ *the operator* $H_{\mathbf{k}}^{(n)}$ *possesses an eigenvalue within* $\mathcal{U}$*.*

Proof. As far as item i) and item ii) are concerned it is sufficient to prove that the operators $A_\alpha^{(n)}|_{L^2}$ are relatively bounded with respect to $H|_{L^2}$ with relative bound zero. Then the assertions follow by Theorem IV.1.1 and Theorem VII.2.6 from Kato [16].

By partial integration of the second term one derives from (1.6) for any $\varphi \in \operatorname{dom}(H|_{L^2})$:

$$\begin{aligned}
&\left\|A_\alpha^{(n)}\varphi\right\|_{L^2} = \left\|\left(M_\alpha^{(n)} - (M_\alpha^{(n)})^*\right)\frac{d\varphi}{dx} - \varphi\frac{d}{dx}(M_\alpha^{(n)})^*\right\|_{L^2} \\
&\leq \left\|M_\alpha^{(n)} - (M_\alpha^{(n)})^*\right\|_{L^\infty([0,T],\mathcal{B}(\mathbb{C}^d))}\|\varphi\|_{W^{1,2}} + \left\|\frac{d}{dx}M_\alpha^{(n)}\right\|_{L^\infty([0,T],\mathcal{B}(\mathbb{C}^d))}\|\varphi\|_{L^2}.
\end{aligned}$$

Estimating $\|\varphi\|_{W^{1,2}} = \|d\varphi/dx\|_{L^2}$ by means of (2.17) and (2.18) one may continue:

$$\leq \gamma_H\sqrt{\frac{\|H\varphi\|_{L^2}\|\varphi\|_{L^2}}{\min\limits_{j=1,\dots,d}\ \operatorname*{vraimin}\limits_{x\in[0,T]}|m_j(x)|}} \leq \delta\|H\varphi\|_{L^2} + \frac{1}{4\delta}\frac{\gamma_H^2\|\varphi\|_{L^2}}{\min\limits_{j=1,\dots,d}\ \operatorname*{vraimin}\limits_{x\in[0,T]}|m_j(x)|},$$

where δ is an arbitrary positive number and γ_H is the finite and positive interpolation constant from (2.18).

Ad iii. Using item iii) and item iv) of Lemma 4.1 one can estimate the nuclear norm of

$$(H_{\mathbf{k}} - \lambda)^{-1} - (H_{\mathbf{k}}^{(n)} - \lambda)^{-1}$$

in the same way as this was done in the proof of item iv) of Theorem 2.5, cf. (2.16).

Ad iv. Theorem 4.2, item iii) implies that the operators $H_{\mathbf{k}}^{(n)}$ are converging to $H_{\mathbf{k}}$ in the generalized sense of Kato [16]. Thus, the assertion follows from the selfadjointness of $H_{\mathbf{k}}$ and a general perturbation theorem for selfadjoint operators, cf. Kato [16, V.4.3]. □

5 Discretization of $\mathbf{k}\cdot\mathbf{p}$ operators

The numerical solution of the eigenvalue problem for the $\mathbf{k}\cdot\mathbf{p}$ operators requires a suitable finite dimensional approximation of the problem. This can be done by defining the operators in Definition 1.2 in the sense of forms on finite dimensional subspaces of $W^{1,2}([0,T];\mathbb{C}^d)$. We will regard a discretization by piecewise linear finite elements. For the definition of the discrete $\mathbf{k}\cdot\mathbf{p}$ operators we make the Assumption 1.1, but we will also regard coefficient functions M_α, $\alpha = 0,1,2$ which do not satisfy the fourth item in Assumption 1.1. Additionally we make

5.1. Assumption. For almost all $x \in [0,T]$ the matrices $M_\alpha(x)$, $\alpha \in \{0,1,2\}$ are skewadjoint over $\mathbb{C}^d$.

Under these Assumptions the form defining the operator A_α, $\alpha \in \{0,1,2\}$ from Definition 1.2 can be expressed as

$$\begin{aligned}\langle A_\alpha\varphi,\psi\rangle &= \int_0^T \big\langle M_\alpha(x)\frac{d\varphi}{dx}(x),\psi(x)\big\rangle_{\mathbb{C}^d} - \big\langle M_\alpha(x)\varphi,\frac{d\psi}{dx}(x)\big\rangle_{\mathbb{C}^d}\,dx \\ &= \sum_{j,l=1}^d \int_0^T M_{\alpha\,j\,l}(x)\Big(\frac{d\varphi_l}{dx}(x)\overline{\psi}_j(x) - \varphi_l(x)\frac{d\overline{\psi}_j}{dx}(x)\Big)\,dx,\end{aligned} \tag{5.1}$$

for all φ and ψ from $W^{1,2}([0,T];\mathbb{C}^d)$. For the second order differential operators from Definition 1.2 we used the standard finite element discretization, while for the zero order differential operators we used mass lumping. In the following we will regard the discretization of a scalar first order differential operator

$$\begin{aligned}&\big\langle Au,w\big\rangle_{[W^{-1,2}([0,T];\mathbb{C}),W^{1,2}([0,T];\mathbb{C})]} \\ &\qquad = \int_0^T M(x)\Big(\frac{du}{dx}(x)\overline{w}(x) - u(x)\frac{d\overline{w}}{dx}(x)\Big)\,dx,\end{aligned} \tag{5.2}$$

where M is any of the functions $M_{\alpha\,j\,l}$, and u, w are from $W^{1,2}([0,T];\mathbb{C})$.

5.2. Definition. With respect to a finite, disjoint partition (1.4) of the space interval $[0,T]$ we define the finite elements u_l, $l = 1,\dots,L$,

$$u_l(x) \stackrel{\text{def}}{=} \begin{cases} \frac{x-t_{l-1}}{t_l-t_{l-1}} & \text{if } t_{l-1} < x \le t_l, \\ \frac{t_{l+1}-x}{t_{l+1}-t_l} & \text{if } t_l < x \le t_{l+1}, \\ 0 & \text{else,} \end{cases} \tag{5.3}$$

which span a L dimensional subspace of $W^{1,2}([0,T];\mathbb{C})$.

5.3. Remark. The functions u_l are finite and the support of u_l is just $[t_{l-1}, t_{l+1}]$. For almost all $x \in [t_1, t_L]$ the functions u_l satisfy the relations

$$\sum_{l=1}^{L} \frac{du_l}{dx}(x) = 0, \qquad \text{and} \qquad \sum_{l=1}^{L} u_l(x) = 1. \tag{5.4}$$

5.4. Theorem. *The discretization of the operator A from (5.2) with respect to the finite element basis from Definition 5.2 is given by the complex $L \times L$–matrix $\mathcal{T} = \{\mathcal{T}_{l,j}\}_{l,j=1,\dots,L}$,*

$$\mathcal{T}_{l,j} \stackrel{\text{def}}{=} \langle Au_l, u_j \rangle_{[W^{-1,2}([0,T];\mathbb{C}),W^{1,2}([0,T];\mathbb{C})]} = \begin{cases} \frac{\int_{t_{l-1}}^{t_l} M(x)\,dx}{t_l - t_{l-1}} & \text{if } j = l-1, \\ \frac{-\int_{t_l}^{t_{l+1}} M(x)\,dx}{t_{l+1} - t_l} & \text{if } j = l+1, \\ 0 & \text{if } |j-l| \neq 1. \end{cases}$$

Proof. According to (5.2) there is

$$\mathcal{T}_{l,j} = \int_0^T M(x)\Big(\frac{du_l}{dx}(x)u_j(x) - u_l(x)\frac{du_j}{dx}(x)\Big)\,dx = -\mathcal{T}_{j,l}.$$

As the support of u_l is $[t_{l-1}, t_{l+1}]$ now follows immediately

$$\mathcal{T}_{l,j} = 0 \qquad \text{for } |l-j| \neq 1.$$

Further, by means of (5.3) and (5.4), $\mathcal{T}_{l,l+1}$ can be evaluated as

$$\begin{aligned} \mathcal{T}_{l,l+1} &= \int_{t_l}^{t_{l+1}} M(x)\Big(\frac{du_l}{dx}(x)u_{l+1}(x) - u_l(x)\frac{du_{l+1}}{dx}(x)\Big)\,dx \\ &= \int_{t_l}^{t_{l+1}} M(x)\,\frac{du_l}{dx}(x)\Big(u_{l+1}(x) + u_l(x)\Big)\,dx \\ &= \frac{-1}{t_{l+1} - t_l}\int_{t_l}^{t_{l+1}} M(x)\,dx. \end{aligned}$$

□

5.5. Corollary. *Under Assumption 5.1 and the full Assumption 1.1, including that the coefficient functions M take the constant values $\widehat{M_l}$ on the space intervals $[t_l, t_{l+1}]$, there is*

$$\mathcal{T}_{l,j} = \begin{cases} \widehat{M}_{l-1} & \text{if } j = l-1, \\ -\widehat{M_l} & \text{if } j = l+1, \\ 0 & \text{if } |j-l| \neq 1. \end{cases} \tag{5.5}$$

From Theorem 5.4 follows immediately

5.6. Theorem. *Let M^{reg} be a regularization of the coefficient function M in the sense of Lemma 4.1. If*

$$\int_{t_l}^{t_{l+1}} \big(M^{reg}(x) - M(x)\big)\, dx = 0, \qquad \textit{for } l = 1, \dots, L,$$

then the discretizations $\mathcal{T}$, cf. Theorem 5.4, of the operators (5.2) *corresponding to M^{reg} and M are the same.*

5.7. Remark. Theorem 5.6 is the underpinning of the finite element discretization schema. In fact the finite element discretization acts as a regularization of the problem in the sense of §4, thus Theorem 4.2 applies to the spectral behaviour of the discretized problems.

5.8. Remark. Numerical validation of the discretization schema from Theorem 5.4 on several benchmark problems shows a convergence of the eigenvalues of order $h^{2.000\pm0.004}$, where h denotes the maximal mesh size of the space discretization

$$h = \max_{l=0,\dots,L} (t_{l+1} - t_l).$$

A detailed discussion of this validation process has been performed in [3]. Some examples are given in the Appendix.

For the numerical treatment of the eigenvalue problem for $\mathbf{k}\cdot\mathbf{p}$ Schrödinger operators, we developed the toolbox KPLIB, which is based on PDELIB–components [12] of the Weierstrass Institute for Applied Analysis and Stochastics, Berlin. KPLIB is an object oriented code, written in ANSI–C, which makes use of the design patterns proposed in [13].

We regard $\mathbf{k}\cdot\mathbf{p}$ operators as instances of the base class `kpHamiltonOperator`. This approach enables the user to handle various types of $\mathbf{k}\cdot\mathbf{p}$ operators through a unified interface. A `kpHamiltonOperator` possesses methods to set the parameters, to perform the discretization, and to solve the eigenvalue problem.

The objects of the class `kpHamiltonOperator` have a common skeleton, which is fleshed out by a `kpModel`. In KPLIB the skeleton of a specific $\mathbf{k}\cdot\mathbf{p}$ operator will be produced by a factory of class `kpFactory`, while the flesh is added by means of the interface `kpModel`. A `kpModel` is a plug–in and registers dynamically to the system. In the following we describe the data structure of `kpHamiltonOperator` together with the interface `kpModel`.

The skeleton data, common to all $\mathbf{k} \cdot \mathbf{p}$ operators, are the mesh, the boundary conditions, the $\mathbf{k}$–vector, the band edges, the elastic stress tensors, the external potentials and the data needed to perform and to store the discretization. The model data which specify a particular `kpModel` are the effective mass parameters (e.g. the Luttinger parameters), the strain parameters (e.g. the Pikus–Bir deformation potentials) and auxiliary data. The base class `kpHamiltonOperator` possesses methods to set parameters stored in the skeleton data, while the developer of a specific $\mathbf{k} \cdot \mathbf{p}$ model takes care of the access to the model data. To that end the design pattern *Decorator* [13] proved useful. An alternative would be subclassing.

A `kpModel` has to provide methods for the construction and destruction of the $\mathbf{k} \cdot \mathbf{p}$ model data, and methods to perform the discretization of scalar components of the $\mathbf{k} \cdot \mathbf{p}$ operator.

Based upon the extension and scripting language *lua* [15] we implemented an object orientied user interface to KPLIB as an alternative to the application programming interface in C. By means of this user interface we realized a simple band structure simulator, which we used to perform the calculations for the validation of the discretization schema.

Appendix: Examples

In order to validate the proposed discretization schema we investigated the convergence of the eigenvalues for two test problems. The first is the scalar Hamiltonian

$$H_k = -\frac{d^2}{dx^2} + ik\frac{d}{dx}, \qquad k \in \mathbb{R}.$$

defined of $[0, T]$ with homogeneous Drichlet boundary conditions. The eigenfunctions and eigenvalues are given by

$$\psi_n(x) = \sin\big(\frac{n\pi x}{T}\big)\exp\big(i\frac{kx}{2}\big), \qquad E_n = \Big(\frac{n\pi}{T}\Big)^2 - \frac{k^2}{4}.$$

With this simple example we checked the discretization of the momentum like operators A defined by (5.2). Because the solution is known explicitly, we are able to calculate easily the error of the approximated solution. We studied the error reduction through uniform mesh refinements for different values of k, $0 \le k \le 10$ for the four lowest eigenvalues. These numerical experiments showed a convergence of the eigenvalues of order $h^{\approx 2.000 \pm 0.001}$.

As the second test problem we selected a 4×4–Hamiltonian for a layered semiconductor heterostructure from Chuang [8, 4.5.3], given by

$$H_{\mathbf{k}} = -\frac{\hbar^2}{2m_0}\begin{pmatrix} P+Q & -S & R & 0 \\ -S^* & P-Q & 0 & R \\ R^* & 0 & P-Q & S \\ 0 & R^* & S^* & P+Q \end{pmatrix} + E_v \mathbb{1}_{\mathbb{C}^4}$$

with

$$P = \gamma_1(k_x^2 + k_y^2) - \frac{d}{dz}\gamma_1\frac{d}{dz}, \qquad R = \sqrt{3}\big(-\gamma_2(k_x^2 - k_y^2) + 2i\gamma_3 k_x k_y\big),$$
$$Q = \gamma_2(k_x^2 + k_y^2) + 2\frac{d}{dz}\gamma_2\frac{d}{dz}, \quad S = -2\sqrt{3}(k_y + ik_x)\Big(\gamma_3\frac{d}{dz} + \frac{d}{dz}(\gamma_3\ \cdot\ )\Big),$$

where, in compliance with the crystal symmetry, $\mathbf{k} = (k_x, k_y, 0)$ is the reduced wave vector and z is the direction of quantization. This Hamiltonian describes the band mixing of two heavy holes and two light holes for most III–V semiconductors with a decisively separated split–off band. The standard Luttinger parameters γ_1, γ_2, γ_3 are related to the band structure of the bulk materials at the Γ–point, and there is $\gamma_1 > 2\gamma_2$ for all direct zinc–blende semiconductors, i.e. the operator possesses a definite main part. The relative effective masses of the heavy and light holes are given by

$$\frac{m^*_{HH}}{m_0} = \frac{1}{\gamma_1 - 2\gamma_2}, \quad \text{and} \quad \frac{m^*_{LH}}{m_0} = \frac{1}{\gamma_1 + 2\gamma_2},$$

respectively, where m_0 is the free electron mass. E_v is the valence band edge.

As test problem for this Hamiltonian we used a single quantum well structure [8, 4.8.3] given by a three layer stack (barrier, quantum well, barrier) consisting of $Al_xGa_{1-x}As$, $x = 0.315$ barriers and a 51Å thick $GaAs$ quantum well. This leads to a Hamiltonian with jumping coefficents. We calculated the band structure of the two lowest subbands. The results are shown in Figure 1 and coincide with those of Chuang [8, 8.4.3 Fig. 4.19b]. At $\mathbf{k} = 0$ the upper subband belongs to heavy holes and the lower subband belongs to light holes. We can observe the non–parabolicity of bands and the dependence of the energy from the **k**–direction (warping).

As in the first example we investigated the convergence of the eigenvalues through refinement of an equidistant mesh, to check the discretization. The relative error in dependence of the number of nodes in the quantum well is shown in Figure 2 for different eigenvalues and different **k**'s. As for the error the approximations refer to a solution on a very fine grid, in comparison with the grids under consideration in the investigation of convergence. In these numerical experiments we observed a convergence of the eigenvalues of order $h^{\approx 2.000 \pm 0.004}$.

The test problems showed, that the finite element discretization schema is useful for the numerical solution of the eigenvalue problem of $\mathbf{k} \cdot \mathbf{p}$ Hamilton operators with jumping coefficents.

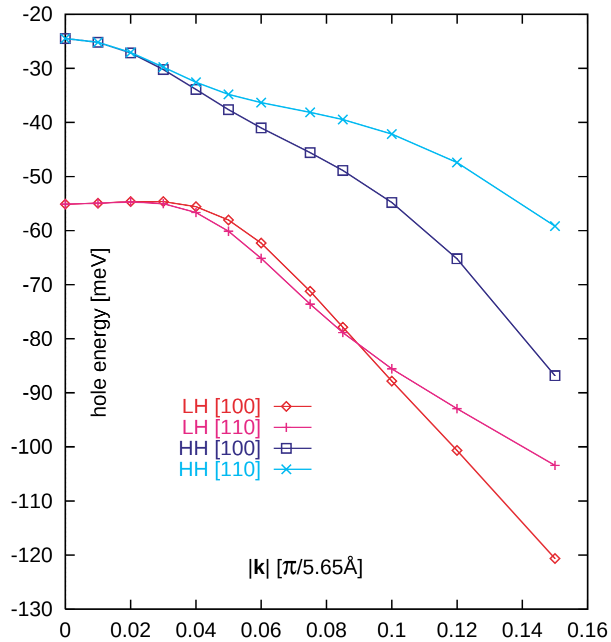

Figure 1: Subband structure for different directions in **k**–space.

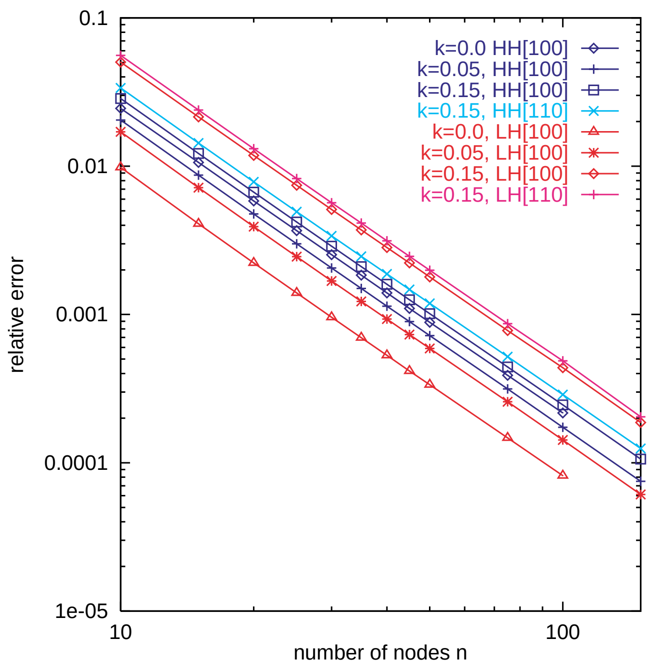

Figure 2: Relative error of the eigenvalues.

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