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Weak-field magnetic bands in superlattices and the single-band approximation

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Abstract. We prove the existence and we give the semiclassical magnetic asymptotics of the magnetic bands in superlattices. We use the Wannier single-band approximation which leads to a *dual* semiclassical Bloch model with a band function as potential. A picture of x-dependent bands suggests exponentially small magnetic gap widths as given by the beating effect of a Zener double well.

1. Introduction

Recently considerable interest has centred on the problem of a two-dimensional electron moving in a periodic potential $V(x, y)$ in the presence of a perpendicular magnetic field of strength B. The problem was studied particularly as a starting point for the quantum Hall effect (see for instance Aizim and Volkov 1984, 1985, Avron and Simon 1985). In particular the magnetic bands have been considered for a strong magnetic field (Aizim and Volkov 1984, 1985) and a one-dimensional superlattice potential $V(x)$. In this case the solution to the problem is simply given by considering the potential as a perturbation. More complciated and interesting also for its connections with the Stark–Wannier problem is, as we shall see in the following, the weak-field case. In the Landau gauge (with x in the place of y) we have the Hamiltonian

$$\mathscr{H}(\omega) = \left(\frac{h}{\mathrm{i}}\frac{\partial}{\partial y} + \omega x\right)^2 + \left(\frac{h}{\mathrm{i}}\frac{\partial}{\partial x}\right)^2 + V(x) \qquad \text{in } L^2(\mathbb{R}^2) \tag{1.1}$$

which, restricted to the vectors $\psi(x, y) = \psi(x)\exp(\mathrm{i}yk_y/h)$, becomes the one-dimensional Hamiltonian:

$$H_{x_0} = H_{\mathrm{B}} + \omega^2(x - x_0)^2 = p^2 + V(x) + \omega^2(x - x_0)^2 \qquad \text{in } L^2(\mathbb{R}) \tag{1.2}$$

where

$$p = -\mathrm{i}h\frac{\mathrm{d}}{\mathrm{d}x} \qquad h = \frac{\hbar}{\sqrt{2m}} \qquad \omega = \sqrt{\frac{m}{2}}\,\omega_{\mathrm{c}} \qquad \omega_{\mathrm{c}} = \frac{eB}{mc}$$

ω_{c} being the cyclotronic frequency,

$$x_0 = -\lambda^2 k_y \qquad \lambda = \sqrt{\frac{\hbar c}{eB}}$$

λ being the magnetic length. Here $V(x)$ is the superlattice's potential with period π and is even, i.e. $V(x) = V(-x)$. Moreover we suppose $V \in C^2$, $V(x) \geqslant 0$, $V(0) = V'(0) = 0$, $V''(0) > 0$.

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Let us call $E_n(k)$ the band function of the original Bloch operator H_B and let $E_n^b = \min\ E_n(k)$, $E_n^t = \max\ E_n(k)$ be the band endpoints. As a further hypothesis about the potential $V(x)$ we suppose in the following that all the gaps (E_n^t, E_{n+1}^b), $n \geqslant 1$, are not empty. On the other side, the bidimensional Bloch operator $\mathscr{H}(0)$ has band functions

$$\tilde{E}_n(k_x, k_y) = E_n(k_x) + h^2 k_y^2 = E_n(k_x) + \omega^2 x_0^2. \tag{1.3}$$

The magnetic band functions are defined as $\tilde{\varepsilon}_n(k_y) = \varepsilon_n(x_0)$, $x_0 = -\lambda^2 k_y$, where $\varepsilon_n(x_0)$ are the eigenvalues of H_{x_0}. In the following we shall consider only the functions $\varepsilon_n(x_0) = \varepsilon_n(-x_0) = \varepsilon_n(x_0 + \pi)$, also called magnetic band functions.

Hence the spectrum of the operator defined by the Hamiltonian $\mathscr{H}(\omega)$ is continuous and is the union of the magnetic bands B_n, $n \geqslant 1$, $B_n = \{\varepsilon_n(x_0) | x_0 \in \mathscr{B}'\} = [\varepsilon_n^b, \varepsilon_n^t]$; here $\mathscr{B}' = (-\pi/2, +\pi/2]$ is the *dual* Brillouin zone.

Actually, for ω small (definitely not for ω large) such magnetic band functions $\varepsilon_n(x_0)$ have most of the general properties of the Bloch band functions.

In our case, fixing $k_y = -x_0/\lambda^2$ and making the single-band approximation, from $\mathscr{H}(\omega)$ we get

$$P_1 H_{x_0} P_1 = H_{SB}(x_0). \tag{1.4}$$

If we consider, by unitary equivalence, $H_{SB}(x_0)$ in the crystal momentum representation we have the operator

$$\tilde{H}_{SB}(x_0) = P_1 \tilde{E}_1(\boldsymbol{k} + h^{-1}\boldsymbol{A}) P_1 \tag{1.5}$$

where $\boldsymbol{A} = (0, \omega x)$ in the Landau gauge and $\boldsymbol{k} = (k_x, -x_0/\lambda^2)$, in agreement with the Peierls substitution rule (see for instance Claro and Wannier 1979). By a further simple approximation we obtain the *dual* Bloch operator

$$\tilde{H}_D(x_0) = -\omega^2 \frac{d^2}{dk^2} + E_1(k) \qquad E_1(k) = E_1(k+2) \tag{1.6}$$

with $x_0 \in \mathscr{B}'$ as crystal momentum.

In the energy region $E_1^b \leqslant \varepsilon < E_1^t$ (§ 3) the semiclassical quantisation rule of Bohr-Sommerfield applied to (1.6) gives the Onsager-type relation (see for instance Pippard 1969 and Guillot *et al* 1988):

$$A_C(\varepsilon_n(x_0)) = 2(n - \tfrac{1}{2})\pi\omega + O(\omega^2) \qquad \text{as } \omega \downarrow 0 \tag{1.7}$$

where $A_C(\varepsilon) = \oint \sqrt{\varepsilon - E_1(k)}\, dk$ is the action area or, equivalently,

$$\varepsilon_n(x_0) = A_C^{-1}[2(n - \tfrac{1}{2})\pi\omega] + O(\omega^2) \qquad \omega \downarrow 0,\ n = 1, 2, \ldots. \tag{1.8}$$

In this way, fixing n and letting $\omega \downarrow 0$, we have the rigorous behaviour:

$$\varepsilon_n(x_0) = E_1^b + \omega(n - \tfrac{1}{2})\sqrt{2E_1''(0)} + O(\omega^2) \qquad n = 1, 2, \ldots, x_0 \in \mathscr{B}'. \tag{1.9}$$

Even more interesting is the energy region $[E_1^t + \delta, E_2^b - \delta]$, $\delta > 0$, (§ 2) where we have the similar quantisation rule, for $0 \leqslant x_0 \leqslant \pi/2$, applied to (1.6):

$$A_C(\varepsilon_{2n+1/2\pm 1/2}(x_0)) = 2\omega(n\pi \pm x_0) + O(\omega^2) \qquad \text{as } \omega \downarrow 0 \tag{1.10}$$

where now $A_C(\varepsilon) = \int_{-1}^{+1} \sqrt{\varepsilon - E_1(k)}\, dk$. Equation (1.10) gives the existence and the semiclassical estimate for the magnetic band function. In particular, for $x_0 \in [0, \pi/2]$ fixed, we have the $\omega \downarrow 0$ behaviour:

$$\begin{aligned}\varepsilon_{2n+1/2\pm 1/2}(x_0) &= \varepsilon(2n\pi\omega \pm x_0\omega) + O(\omega^2) \\ &= \varepsilon(2n\pi\omega) \pm x_0\omega\varepsilon'(2n\pi\omega) + O(\omega^2) \qquad \omega \downarrow 0\end{aligned} \tag{1.11}$$

where $\varepsilon(\cdot) = A_C^{-1}(\cdot)$ and $\varepsilon(2n\pi\omega) \in [E_1^t + \delta, E_2^b - \delta]$.

The small x_0 ($x_0 \approx \pi/2$) monotone behaviour is given by a degenerate perturbation formula:

$$\varepsilon_{2n+1/2\pm1/2}(x_0) = \frac{\varepsilon_{2n+1}(0)+\varepsilon_{2n}(0)}{2} + x_0^2\omega^2$$
$$\pm\left(\frac{(\varepsilon_{2n+1}(0)-\varepsilon_{2n}(0))^2}{4} + 4\omega^2 x_0^2|\omega\hat{x}|^2\right)^{1/2} + \mathrm{O}(\omega x_0^2) \qquad (1.12)$$

where $|\omega\hat{x}| = |\langle\phi_{2n+1}(0), \omega x\phi_{2n}(0)\rangle| = \varepsilon'(2\pi\omega) + \mathrm{O}(\omega)$.

Collecting the rigorous results for ω small enough, we have as many simple magnetic bands as we want in the energy region $(E_1^{\mathrm{t}}, E_2^{\mathrm{b}})$ defined by the band functions $\varepsilon_n(x_0) = \varepsilon_n(x_0+\pi) = \varepsilon_n(-x_0)$. The extreme band values $\varepsilon_n(0)$ ($\varepsilon_n(\pi/2)$) are given by H_0 on $L^2(\mathbb{R}^+)$ ($H_{\pi/2}$ on $L^2(\pi/2, \infty)$) with Dirichlet–Neumann boundary conditions at $x = 0(\pi/2)$; and, since $\varepsilon_n'(0) = \varepsilon_n'(\pi/2) = 0$, we have the divergence of the density of states at these energy values. The best method for understanding some of the above-mentioned results and to obtain other heuristic estimates is the picture of x-dependent bands. Let $E_n^{\mathrm{b/t}}(x) = E_n^{\mathrm{b/t}} + \omega^2(x-x_0)^2$, $|x_0| \leq \pi/2$ (see figure 1). For $E_2^{\mathrm{b}} > E > E_1^{\mathrm{t}}$ we have a double well model with wavefunctions concentrated in the region $[x_+^1, x_+^2] \cup [x_-^2, x_-^1]$, where

$$x_\pm^1 = x_0 \pm \sqrt{E - E_1^{\mathrm{b}}}/\omega \qquad \text{and} \qquad x_\pm^2 = x_0 \pm \sqrt{E - E_1^{\mathrm{t}}}/\omega.$$

Let us note that the sign of $\varepsilon_n'(x_0)$ gives the concentration of the state in the two possible regions (wells) defined in figure 1 for x positive or negative; in fact we have:

$$\varepsilon_n'(x_0) = -2\omega^2\langle\phi_n(x_0), (x-x_0)\phi_n(x_0)\rangle \qquad (1.13)$$

and the sign of $\varepsilon_n'(x_0)$ determines the direction of the 'propagation' of the states in the y direction along a series of 'reflected arcs' (see for instance Pippard 1969, p 121, figure 3.2). For $x_0 = 0$, $\pi/2$ we have no propagation at all because both the opposite motions are allowed (with tunnelling between). In this case $H(x_0)$ is a symmetric double well Hamiltonian and we have a splitting of the levels of the order of the square

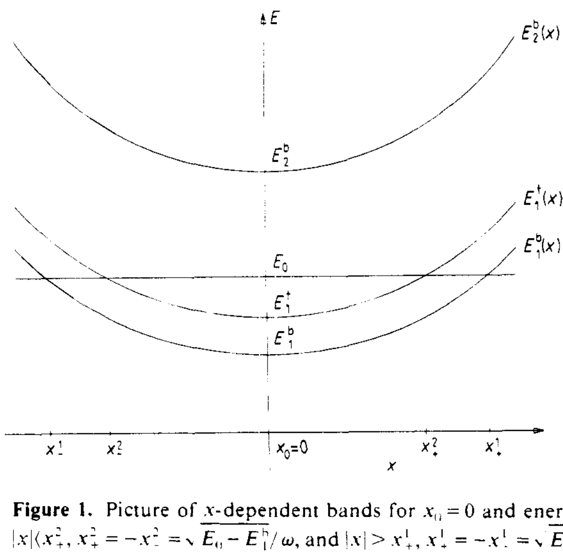

Figure 1. Picture of x-dependent bands for $x_0 = 0$ and energy $E_0 \in (E_1^{\mathrm{t}}, E_2^{\mathrm{b}})$. The regions $|x| < x_+^2$, $x_+^2 = -x_-^2 = \sqrt{E_0 - E_1^{\mathrm{b}}}/\omega$, and $|x| > x_+^1$, $x_+^1 = -x_-^1 = \sqrt{E_0 - E_2^{\mathrm{b}}}/\omega$, are *classically forbidden*; so that we have a double-well model.

of the Zener transmission amplitude through half a barrier. Such splitting is by definition the gap width and it turns out to be exponentially small:

$$\Delta E = |G(E)| = O(\exp\{-C(E)/\omega\}) \qquad \omega \downarrow 0 \tag{1.14}$$

where

$$C(E) = \int_{E_1^{\rm t}}^{E} \frac{\chi(E)\,\mathrm{d}E}{\sqrt{E - E_1^{\rm t}}} \qquad \chi(E) = |\Im k(E)|$$

$k(E)$ is the crystal momentum in the first gap for the original Bloch operator $H_{\rm B}$.

We consider the limit of small h (true semiclassical limit) only for the purpose of completeness. All the main results are valid for $h = 1$ as well.

We also consider (in § 3) a partially solvable model given by the operators:

$$H'_{x_0} = H_{\rm B} + \omega^2(x - x_0)^2 + \omega(x - x_0)\cos 2x \qquad x_0 \in \mathscr{B}' \tag{1.15}$$

where

$$H_{\rm B} = -h^2\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\cos^2 2x}{4} + h(1 + \sin 2x).$$

The first eigenvalue of H'_{x_0} is exactly given by

$$\varepsilon_1(x_0) = E_1^{\rm b} + \omega h = h + \omega h.$$

As announced above, we do not consider the case of large ω since, as noted by Aizim and Volkov (1984, 1985), the magnetic bands are given by a perturbation of the degenerate Landau eigenvalues $\varepsilon_n(x_0) = (2n - 1)h\omega$, $n \geqslant 1$. In this case the perturbation is the bounded operator $V(x)$ and the unperturbed one is $p^2 + \omega^2(x - x_0)^2$, so that the perturbation theory of Kato applies for $\omega > \max|V(x)|/h$.

We have not exploited here the promising connections of the single-band approximation of the magnetic field case with the electric field case of Stark–Wannier.

After the completion of this work we received a very interesting paper by Helffer and Sjöstrand where magnetic fields in crystals are rigorously treated (Helffer and Sjöstrand 1989).

2. Magnetic bands in the first gap of the zero-field one-dimensional Bloch model

Let $\mathscr{H}(\omega)$ be the self-adjoint operator (Cycon *et al* 1987) obtained by the closure of the formal operator (1.1) defined on $C_0^\infty(\mathbb{R}^2)$. By a Fourier transform in the y variable it becomes the direct integral $\mathscr{H}(\omega) = \int_{\mathscr{B}'}^{\oplus} H_{x_0}\,\mathrm{d}x_0$ of the one-dimensional positive operator

$$H_{x_0} = p^2 + V(x) + \omega^2(x - x_0)^2 \qquad x_0 \in \mathscr{B}' = \left(-\frac{\pi}{2}, +\frac{\pi}{2}\right] \qquad \omega > 0 \tag{2.1}$$

with domain $\mathbf{D}(H_{x_0}) = \mathbf{D}(p^2) \cap \mathbf{D}(x^2)$; here $p = -\mathrm{i}h\,\mathrm{d}/\mathrm{d}x$ and $h > 0$ (for a definition of direct integral decomposition see Reed and Simon (1978) ch XIII § 16).

Since the potential goes to ∞ as $x \to \pm\infty$, the eigenvalues of H_{x_0} are simple (ch III § 3 of Voros 1982, ch 24 § 1–§ 5 of Naimark 1968). Moreover, H_{x_0} is an analytic operator family in $x_0 \in \mathbb{C}$, ω in the sector $\Re\omega^2 > 0$, so that the nth magnetic band function $\varepsilon_n(x_0)$ is analytic in a strip around the real axis.

In this section we prove (theorem 2.6 and remark 2.7) the existence of the magnetic band functions $\varepsilon_n(x_0)$ in the interval $[E_1^t+\delta, E_2^b-\delta]$, $\delta>0$, which are approximated, modulo $O(\omega^{(1+\alpha)})$, $0<\alpha<1$, $\omega\downarrow 0$, for $x_0\in\mathscr{B}'$, by the band functions $\varepsilon_n^D(x_0)$ of the Bloch operator obtained by the single-band approximation.

We now briefly recall the crystal momentum representation (CMR, see Bentosela *et al* 1988) which will be used in the following.

Let us consider the unitary transformation

$$U: L^2(\mathbb{R})\to\int_{\mathscr{B}}^{\oplus}\mathscr{H}'(k)\,\mathrm{d}k \qquad \mathscr{H}'(k)=l^2$$

$$\psi\to(U\psi)(k,K)=\varphi(k,K)=\hat{\psi}(k+K) \qquad k\in\mathscr{B} \qquad K\in\mathbb{Z}$$

where $\hat{\psi}$ denotes the Fourier transform of ψ. The sequence $\{\varphi(k,K)\}_{K\in\mathbb{Z}}$ belongs to $\mathscr{H}'(k)=l^2$, for almost all $k\in\mathscr{B}$, where $\mathscr{B}$ is the Brillouin zone $(-1,+1]$.

Under this transformation the operator $H_B=p^2+V(x)$ becomes

$$UH_BU^{-1}=\int_{\mathscr{B}}^{\oplus}H(k)\,\mathrm{d}k$$

where

$$\begin{aligned}(H(k)a)(K)&=(T(k)a)(K)+(\tilde{V}a)(K)\\&=h^2(k+K)^2\cdot a(K)+\sum_{j\in\mathbb{Z}}V_ja(K-j)\end{aligned}$$

for any $a(K)$ of the form $a(K)=(U\psi)(k,K)$ for some $\psi\in D(H_B)$ and for k fixed. Here V_j denotes the jth Fourier coefficient of V ($V_j\in\mathbb{R}$ because V is even, i.e. $V(x)=V(-x)$). $H(k)$ has compact resolvent for any k and there exists a sequence of eigenvalues $0<E_1(k)\leqslant E_2(k)\leqslant\ldots\leqslant E_n(k)\leqslant\ldots$ with real-valued orthonormal eigenvectors $\{\omega_1^{(k)}(K)\}_{K\in\mathbb{Z}},\ldots,\{\omega_n^{(k)}(K)\}_{K\in\mathbb{Z}},\ldots$ analytic in k if $E_n(k)$ is simple, with the property $\omega_n^{-k}(-K)=\omega_n^k(K)$.

For k fixed $\{E_n(k)\}_{n=1}^{\infty}$ is the discrete spectrum of the operator formally defined by H_B with the boundary conditions $\psi(\pi)=\mathrm{e}^{ik\pi}\psi(0)$ and $\psi'(\pi)=\mathrm{e}^{ik\pi}\psi'(0)$.

Such eigenvalues, as functions of k, are called band functions and are analytic, even and periodic with period 2; moreover they are strictly monotone in $[0,1]$. In particular, in the open interval $(0,1)$, the derivatives of $E_n(k)$ are positive for n odd and negative for n even. Let

$$E_n^t=\max_{k\in\mathscr{B}}E_n(k) \qquad E_n^b=\min_{k\in\mathscr{B}}E_n(k)$$

then $\sigma(H_B)=\bigcup_{n=1}^{\infty}[E_n^b,E_n^t]$ is purely absolutely continuous. The closed interval $[E_n^b,E_n^t]$is the nth band and the open intervals $(-\infty,E_1^b)$ and (E_n^t,E_{n+1}^b) are the 0th and nth gaps. Now let us consider the unitary transformation

$$\tilde{U}: L^2(\mathbb{R})\to\bigoplus_{n=1}^{\infty}L^2(\mathscr{B})$$

defined by

$$\begin{aligned}\psi\to(\tilde{U}\psi)_n(k)&=\langle\omega_n^{(k)}(\cdot),(U\psi)(k,\cdot)\rangle_{l^2}\\&=\sum_{j\in\mathbb{Z}}\overline{\omega_n^{(k)}(j)}\cdot(U\psi)(k,j)\equiv\sum_{j\in\mathbb{Z}}\omega_n^{(k)}(j)\cdot(U\psi)(k,j).\end{aligned}$$

Let us define the unitary transformation $\tilde{H}_0$ of H_0 ($H_0=H_{x_0}$ for $x_0=0$ fixed) given by

$$\tilde{H}_0=\tilde{U}H_0\tilde{U}^{-1}=\tilde{H}_B+\omega^2\tilde{U}x^2\tilde{U}^{-1}$$

where $\tilde{H}_0$ is self-adjoint with compact resolvent on the domain $\mathbf{D}(\tilde{H}_0) = \tilde{U}(\mathbf{D}(x^2) \cap \mathbf{D}(p^2))$. Formally, we have:

$$\tilde{H}_0 = \tilde{H}_B + \omega^2(\mathrm{i}D + X)^2$$

acting on the vectors $a = (a_n)_n \in \bigoplus_{n=1}^{\infty} L^2(\mathscr{B})$ such that $a_n \in C^2(\mathscr{B})$ $\forall n$, and only a finite number of the a_n are not identically zero, where:

$$(\tilde{H}_B a)_n(k) = E_n(k) \cdot a_n(k)$$

$$(Xa)_n(k) = \sum_{m=1}^{\infty} X_{n,m}(k) \cdot a_m(k)$$

$$(Da)_n(k) = \frac{\mathrm{d}a_n(k)}{\mathrm{d}k}$$

$$X_{n,m}(k) = \mathrm{i}\left\langle \omega_n^{(k)}(\cdot), \frac{\mathrm{d}\omega_m^{(k)}(\cdot)}{\mathrm{d}k} \right\rangle_{l^2} = -X_{m,n}(k) = -X_{n,m}(-k).$$

Then the unitary transformation $\tilde{H}_{x_0}$ of H_{x_0} is defined by:

$$\tilde{H}_{x_0} = \tilde{H}_B + \omega^2(\mathrm{i}D + X - x_0)^2.$$

Let us split the interband operator X into two terms:

$$X = X' + \tilde{W}_1$$

where $\tilde{W}_1 = \tilde{U} W_1 \tilde{U}^{-1}$ and

$$W_1 = P_1' x P_1 + P_1 x P_1' = P_1' x P_1 + (P_1' x P_1)^* = P_1'[x, P_1]_- + (P_1'[x, P_1]_-)^*.$$

Here P_1 denotes the orthogonal projection on the first band:

$$P_1 = -\frac{1}{2\pi\mathrm{i}} \oint_{\Gamma_1} (p^2 + V - z)^{-1}\, \mathrm{d}z$$

where Γ_1 is the positively oriented contour around the spectrum of the first band:

$$\Gamma_1 = \left\{ z \in \mathbb{C} \,\middle|\, \mathrm{dist}(z, [E_1^b, E_1^t]) = d = \frac{E_2^b - E_1^t}{2} > 0 \right\}$$

and $P_1' = 1 - P_1$.

Lemma 2.1. W_1 is bounded and its norm L_1 satisfies the following estimate:

$$L_1 = \| W_1 \| \leqslant C_1 h^{1/2} \qquad \text{if } h < h_0 \tag{2.2}$$

where $C_1 > 0$ and $h_0 > 0$ are suitable constants.

Proof. Relation (2.2) follows immediately, in fact (Avron 1979 and Bentosela *et al* 1988):

$$[x, P_1]_- = \frac{h}{\pi} \oint_{\Gamma_1} (p^2 + V - z)^{-1} p (p^2 + V - z)^{-1}\, \mathrm{d}z.$$

Since V is positive we have that

$$p^2 \leqslant p^2 + V \leqslant \nu^2 (p^2 + V)^2 + \frac{1}{\nu^2} \qquad \forall \nu > 0$$

so p is relatively bounded by p^2+V with relative bound $\nu>0$ arbitrary. Then:

$$\|[x, P_1]_-\| \leq h \frac{\text{length}(\Gamma_1)}{d\pi}\left(\nu(1+E_2^b d^{-1})+\frac{1}{\nu d}\right)$$

where $d=(h/2)\sqrt{2V''(0)}+O(h^2)$, $\text{length}(\Gamma_1)=\pi h\sqrt{2V''(0)}+O(h^2)$ and $E_2^b=(3h/2)\sqrt{2V''(0)}+O(h^2)$ if $h<h_0$ for suitable $h_0>0$ (see Harrell 1979 and Weinstein and Keller 1985).

If we choose $\nu=h^{-1/2}$ we have (2.2) with $C_1=8[2+1/\sqrt{2V''(0)}]$. □

Let us define the symmetric operator formally given by

$$S_{x_0}=\frac{1}{\omega}(P_1\tilde{H}_{x_0}P_1'+P_1'\tilde{H}_{x_0}P_1)=\omega[\mathrm{i}D+X'-x_0,\ \tilde{W}_1]_+ \tag{2.3}$$

acting on the vectors $a=(a_n)_n\in\bigoplus_{n=1}^{\infty}L^2(\mathscr{B})$ such that $a_n\in C^2(\mathscr{B})\ \forall n$, and only a finite number of a_n is not identically zero. Obviously S_{x_0} is the term coupling the first band with the others in the operator $\tilde{H}_{x_0}$. We have the following result.

Theorem 2.2. (i) S_{x_0} is infinitesimally form-bounded with respect to $\tilde{H}_{x_0}$, i.e. $\mathbf{Q}(\tilde{H}_{x_0})\subset\mathbf{Q}(S_{x_0})$ and

$$|\langle u, S_{x_0}u\rangle|\leq\left(\frac{(L_1)^2}{\mu}-\mu E_1^b\right)\langle u,u\rangle+\mu\langle u,\tilde{H}_{x_0}u\rangle \qquad \forall u\in\mathbf{Q}(\tilde{H}_{x_0})\quad\forall\mu>0 \tag{2.4}$$

where $\langle\cdot,\cdot\rangle$ is the inner product in $\bigoplus_{n=1}^{\infty}L^2(\mathscr{B})$.

(ii) The sum in the form sense

$$T_{x_0}(\eta)=\tilde{H}_{x_0}\dot{+}(\eta-\omega)S_{x_0}$$

is an analytic family of type (B) in the complex η plane.

(iii) $T_{x_0}(\eta)$ has compact resolvent for any η in the complex plane.

(iv) $T_{x_0}(0)=P_1\tilde{H}_{x_0}P_1+P_1'\tilde{H}_{x_0}P_1'$.

Proof. (i) Let $\mathbf{Q}(\tilde{H}_{x_0})$ be the domain of the form defined by $\tilde{H}_{x_0}$. Since $\tilde{H}_B\geq 0$ then

$$\mathbf{Q}(\tilde{H}_{x_0})\subset\mathbf{Q}([\mathrm{i}D+X'-x_0+\tilde{W}_1]^2).$$

Let $\mathbf{Q}(S_{x_0})$ be the domain of the form defined by S_{x_0}. Since $S_{x_0}\leq\omega[\mathrm{i}D+X'-x_0+\tilde{W}_1]^2$, it follows that

$$\mathbf{Q}(\tilde{H}_{x_0})\subset\mathbf{Q}([\mathrm{i}D+X'-x_0+\tilde{W}_1]^2)\subset\mathbf{Q}(S_{x_0}).$$

Moreover, (2.4) follows from the positiveness of the operators $(\tilde{W}_1)^2$ and $\tilde{H}_B-E_1^b$, and the following estimates:

$$\begin{aligned}|\langle u, S_{x_0}u\rangle| &= 2|\langle\omega(\mathrm{i}D+X'-x_0)u,\ \tilde{W}_1u\rangle|\\ &\leq 2(\langle u,\omega^2(\mathrm{i}D+X'-x_0)^2u\rangle)^{1/2}(\langle u,(\tilde{W}_1)^2u\rangle)^{1/2}\\ &\leq\frac{1}{\mu}\langle u,(\tilde{W}_1)^2u\rangle+\mu\omega^2\langle u,(\mathrm{i}D+X'-x_0)^2u\rangle\\ &\leq\left(\frac{(L_1)^2}{\mu}-\mu E_1^b\right)\langle u,u\rangle+\mu\langle u,(\tilde{H}_{x_0}-\omega S_{x_0})u\rangle.\end{aligned}$$

(ii) This follows from theorem 4.8 in ch VII of Kato (1984).

(iii) This follows from (ii) and theorem 4.3 in ch VII of Kato (1984) since $T_{x_0}(\omega)=\tilde{H}_{x_0}$ has compact resolvent too.

(iv) This follows immediately from the definition of S_{x_0} in (2.3). □

Let us call $\varepsilon_n(x_0, \eta)$ the eigenvalues of $T_{x_0}(\eta)$. Since $T_{x_0}(\omega) = \tilde{H}_{x_0}$ the eigenvalues $\varepsilon_n(x_0, \omega)$ coincide with the magnetic band functions $\varepsilon_n(x_0)$.

Now, we calculate the eigenvalues $\varepsilon_n^{SB}(x_0)$ of the unperturbed operator $T_{x_0}(0)$ in the interval $[E_1^t+\delta, E_2^b)$, $0<\delta<E_2^b-E_1^t$. In particular we prove that they are the eigenvalues of the operator given by the single-band approximation.

Theorem 2.3. For any $x_0 \in \mathscr{B}'$, $\delta = K\omega^\beta$, $0<\beta<1$ and $K>0$, the spectrum of $T_{x_0}(0)$ contained in the interval $[E_1^t+\delta, E_2^b)$ is not empty and consists of the eigenvalues $\varepsilon_n^{SB}(x_0)$, where $\varepsilon_n^{SB}(x_0)$ is the nth band function of a Bloch model.

Let $A = 2n\pi\omega$ so that

$$A_C(E_2^b) > A > A_C(E_1^t+\delta) \geq A_C(E_1^t) + C\omega^\beta \qquad \omega<\omega_0 \tag{2.5}$$

where $C>0$ is proportional to K, $\omega_0>0$ and $A_C(\mathscr{E})$ is the classical action defined below. Then the eigenvalues $\varepsilon^{SB}_{2n+1/2\pm1/2}(x_0)$ must satisfy the following:

$$A \pm 2x_0\omega = A_C(\varepsilon^{SB}_{2n+1/2\pm1/2}(x_0)) + O(\omega^2) \qquad \omega\downarrow 0,\ x_0\in\mathscr{B}' \tag{2.6}$$

and in particular:

$$\varepsilon^{SB}_{2n+1/2\pm1/2}(x_0) = \varepsilon(A) \pm \frac{4\omega x_0 + O(\omega^2)}{\int_{\mathscr{B}} [\varepsilon(A) - E_1(k)]^{-1/2}\, dk} \qquad \omega\downarrow 0,\ x_0\in\mathscr{B}' \tag{2.7}$$

where $\varepsilon(\cdot)$ is defined by the inverse function $\varepsilon^{-1}(E) = A_C(E)$.

Proof. Let us define the single-band operator: $\tilde{H}_{SB}(x_0) \equiv P_1\tilde{H}_{x_0}P_1$. Since $T_{x_0}(0) = P_1\tilde{H}_{x_0}P_1 + P_1'\tilde{H}_{x_0}P_1'$ we have

$$\sigma(T_{x_0}(0)) = \sigma(\tilde{H}_{SB}(x_0)) \cup \sigma(P_1'\tilde{H}_{x_0}P_1').$$

Since $\Theta\ (P_1'\tilde{H}_{x_0}P_1') \subset [E_2^b, \infty)$ we have $\sigma(T_{x_0}(0)) \cap (-\infty, E_2^b) = \sigma(\tilde{H}_{SB}(x_0)) \cap (-\infty, E_2^b)$. Hence to calculate the spectrum of $T_{x_0}(0)$ in the interval $(-\infty, E_2^b)$ it is sufficient to consider the single-band approximation:

$$\begin{aligned}
\tilde{H}_{SB}(x_0) &\equiv P_1\tilde{H}_{x_0}P_1 = P_1T_{x_0}(0)P_1 \\
&= \omega^2(-D^2 + (\tilde{W}_1^2)_{1,1}(k) + (X_{1,1}(k)-x_0)^2 + i[D, X_{1,1}(k)-x_0]_+) + E_1(k) \\
&= \exp\left(i\int_{-1}^{k} (X_{1,1}(\nu)-x_0)\, d\nu\right)(-\omega^2D^2 + E_1(k) \\
&\quad + \omega^2(\tilde{W}_1^2)_{1,1}(k)) \exp\left(-i\int_{k} (X_{1,1}(\nu)-x_0)\, d\nu\right) \\
&= \exp[-ix_0(k+1)](-\omega^2D^2 + E_1(k) + \omega^2(\tilde{W}_1^2)_{1,1}(k)) \exp[ix_0(k+1)]
\end{aligned} \tag{2.8}$$

with periodic boundary conditions, where $X_{1,1} \equiv 0$ and $(\tilde{W}_1^2)_{1,1}(k)$ is the multiplication operator $\Sigma_{l\neq1} X_{1,l}(k) \cdot X_{l,1}(k)$.

Equation (2.8) is equivalent to the operator defined by

$$-\omega^2D^2 + E_1(k) + \omega^2(\tilde{W}_1^2)_{1,1}(k) \qquad k\in[-1,+1] = \tilde{\mathscr{B}} \tag{2.9}$$

with boundary conditions

$$\psi(1) = e^{i2x_0}\psi(-1) \qquad \psi'(1) = e^{i2x_0}\psi'(-1). \tag{2.10}$$

Therefore for fixed ω and $x_0 \in \mathscr{B}'$ we have another band function sequence $\{\varepsilon_n^{\mathrm{SB}}(x_0)\}_n$; $\mathscr{B}' = (-\pi/2, +\pi/2]$ is the *dual* Brillouin zone. Hence for the implicit determination of such bands we shall use the analyticity and monotonicity properties of the band functions. Since $(\tilde{W}_1^2)_{1,1}(k)$ is bounded, we treat each operator (2.9), (2.10) as a regular perturbation of the following operator:

$$\tilde{H}_{\mathrm{D}}(x_0) = -\omega^2 D^2 + E_1(k) \tag{2.11}$$

with boundary conditions (2.10). Hence we have again a band function sequence $\varepsilon_n^{\mathrm{D}}(x_0)$, $x_0 \in \mathscr{B}'$, of $H_{\mathrm{D}}(x_0)$, with monotonicity in x_0, $0 \leqslant x_0 \leqslant \pi/2$.

It is well known (ch IV § 3 of Erdelyi (1956) and ch IV §§ 1, 2 of Voros (1982)) that the differential equation

$$\frac{\mathrm{d}^2\psi(k)}{\mathrm{d}k^2} + \frac{\mathscr{E} - E_1(k)}{\omega^2}\psi(k) = 0 \qquad \text{for } \mathscr{E} > E_1(k) \quad \forall k \in \bar{\mathscr{B}} \tag{2.12}$$

has two linearly independent solutions ψ_-, $\psi_+ = \overline{\psi_-}$ asymptotic to all orders to the formal solutions:

$$\Psi_\pm(k) = u^{-1/2} \exp\left(\pm \frac{\mathrm{i}}{\omega} \int_{-1}^{k} u(\tau)\, \mathrm{d}\tau\right). \tag{2.13}$$

Here $u(k)$ is a formal real function $u(k) = \sum_{j=0}^{\infty} u_{2j}(k)\omega^{2j}$, uniformly over $\bar{\mathscr{B}}$, where u_0 is given by $u_0(k) = \sqrt{\mathscr{E} - E_1(k)}$. Moreover the coefficients $u_{2j}(k)$ are periodic as $E_1(k)$ and

$$u(-1) = u(1) \qquad \text{and} \qquad u'(-1) = u'(1).$$

Let us set $A_{\mathrm{SC}}^N = \sum_{j=0}^{N} \int_{\mathscr{B}} u_{2j}(k)\omega^{2j}\, \mathrm{d}k$, where

$$A_{\mathrm{SC}}^0 = \int_{\mathscr{B}} u_0(k)\, \mathrm{d}k = \int_{-1}^{1} \sqrt{\mathscr{E} - E_1(k)}\, \mathrm{d}k \equiv A_C(\mathscr{E})$$

is the classical action function.

Now let $\psi = a\psi_+ + b\psi_-$ be a generic solution of (2.12) with $(a, b) \neq (0, 0)$. By the torus conditions (2.10) on ψ we have that a and b must satisfy the following system of formal equations:

$$a[\Psi_+(1) - \mathrm{e}^{2\mathrm{i}x_0}\Psi_+(-1)] + b[\Psi_-(1) - \mathrm{e}^{2\mathrm{i}x_0}\Psi_-(-1)] = 0$$

$$a[\Psi_+'(1) - \mathrm{e}^{2\mathrm{i}x_0}\Psi_+'(-1)] + b[\Psi_-'(1) - \mathrm{e}^{2\mathrm{i}x_0}\Psi_-'(-1)] = 0.$$

Since $(a, b) \neq (0, 0)$ the determinant of the system must be zero so that, by some calculations, we obtain the asymptotic formula:

$$\cos(2x_0) - \cos\left(\frac{A_{\mathrm{SC}}^N}{\omega}\right) = \mathrm{O}(\omega^{(2N+1)}) \qquad \omega \downarrow 0,\ N \geqslant 1 \text{ arbitrary}. \tag{2.14}$$

Thus we obtain

$$A_{\mathrm{SC}}^N = 2n\pi\omega \pm 2x_0\omega + \mathrm{O}(\omega^{N+2}) \qquad \omega \downarrow 0 \text{ uniformly for } x_0 \in [\gamma_1, \pi/2 - \gamma_1]$$

$$A_{\mathrm{SC}}^N = 2n\pi\omega \pm \mathrm{O}(\omega^{N+1}) \qquad \omega \downarrow 0 \text{ uniformly for } x_0 \in [0, \gamma_1] \cup [\pi/2 - \gamma_1, \pi/2]$$

where $\gamma_1 = \mathrm{O}(\omega^N)$, whence the following asymptotic equation in $\mathscr{E}$:

$$A \pm 2x_0\omega + \mathrm{O}(\omega^2) = A_C(\mathscr{E}) \qquad \omega \downarrow 0.$$

Therefore the hypothesis (2.5) and the monotonicity of the band functions $\mathscr{E}_{\pm}(n, x_0)$ in $0 \leq x_0 \leq \pi/2$, yield the asymptotic behaviour:

$$\begin{aligned}\mathscr{E}_{\pm}(n, x_0) &= \varepsilon(A \pm 2x_0\omega + O(\omega^2)) \\ &= \varepsilon(A) + \frac{\pm 4\omega x_0 + O(\omega^2)}{\int_{\mathscr{B}} [\varepsilon(A) - E_1(k)]^{-1/2}\, dk} \qquad \omega \downarrow 0. \end{aligned} \tag{2.15}$$

Then the spectrum of $\tilde{H}_D(x_0)$ and $\tilde{H}_{SB}(x_0)$ in the interval $[E_1^t + \delta, E_2^b)$, is not empty and we have the asymptotics of the eigenvalues. From the band theory, applied to the operators (2.9) and (2.11), we have the monotonicity of $\varepsilon_n^D(x_0)$ and $\varepsilon_n^{SB}(x_0)$ in x_0 with $0 \leq x_0 \leq \pi/2$ and the following asymptotic behaviour of the band functions:

$$\varepsilon_{2n+1}^{SB}(x_0) = \varepsilon_{2n+1}^D(x_0) + O(\omega^2) = \mathscr{E}_+(n, x_0) + O(\omega^2) \qquad \omega \downarrow 0$$

$$\varepsilon_{2n}^{SB}(x_0) = \varepsilon_{2n}^D(x_0) + O(\omega^2) = \mathscr{E}_-(n, x_0) + O(\omega^2) \qquad \omega \downarrow 0. \qquad \square$$

Remark 2.4. For $x_0 = 0$ the eigenfunctions and their derivatives are even or odd, hence the asymptotics:

$$\begin{aligned}\psi_{2n}^{SB}(k) &= \frac{u_0^{-1/2}(k) \cos(\omega^{-1} \int_{-1}^{k} u_0(\tau)\, d\tau)}{(\int_{\mathscr{B}} u_0^{-1}(k)\, dk)^{1/2}} + O(\omega) \\ \psi_{2n+1}^{SB}(k) &= \frac{u_0^{-1/2}(k) \sin(\omega^{-1} \int_{-1}^{k} u_0(\tau)\, d\tau)}{(\int_{\mathscr{B}} u_0^{-1}(k)\, dk)^{1/2}} + O(\omega) \\ \omega \frac{d\psi_{2n}^{SB}}{dk} &= -u_0(k)\psi_{2n+1}^{SB}(k) + O(\omega) \\ \omega \frac{d\psi_{2n+1}^{SB}}{dk} &= u_0(k)\psi_{2n}^{SB}(k) + O(\omega). \end{aligned} \tag{2.16}$$

From (2.7) we get immediately the following estimate for the isolation distance $d_n(x_0)$ of the nth eigenvalue:

$$\begin{aligned} d_n(x_0) &= C_2\omega[\min\{x_0, \pi/2 - x_0\} + O(\omega)] \qquad \omega \downarrow 0 \\ C_2 &= 8\left(\int_{\mathscr{B}} \frac{dk}{\sqrt{\varepsilon(A) - E_1(k)}}\right)^{-1} \geq 4\delta^{1/2} > 0 \qquad \varepsilon(A) > E_1^t + \delta \end{aligned} \tag{2.17}$$

uniformly for $x_0 \in (\gamma_2, \pi/2 - \gamma_2)$ where $\gamma_2 = \omega^{\alpha}$, $0 < \alpha < 1$, and $A = 2[\frac{n}{2}]\pi\omega$. Moreover we have the following estimate of the gap width:

$$G_n^{SB} = G_n^D + O(\omega^2) = O(\omega^2) \quad \omega \downarrow 0 \tag{2.18}$$

where

$$G_{2n}^{SB/D} = \varepsilon_{2n+1}^{SB/D}(0) - \varepsilon_{2n}^{SB/D}(0) \qquad G_{2n-1}^{SB/D} = \varepsilon_{2n}^{SB/D}(\pi/2) - \varepsilon_{2n-1}^{SB/D}(\pi/2) \quad n \geq 1.$$

The estimate of the instability gap and the asymptotic expansion for the eigenvalues $\varepsilon_n^{SB}(x_0)$, $x_0 = 0$, $\pi/2$, can be also obtained starting from the ones given in Weinstein and Keller (1987). In particular, they proved that the eigenvalue $\varepsilon_n^D(x_0)$, for $x_0 = 0$, of the operator defined in (2.11) with periodic boundary conditions has the following asymptotic expansion:

$$\varepsilon_n^D(0) \approx \varepsilon(A) - \frac{(-1)^n}{\pi}\left(\int_{\mathscr{B}} \frac{dk}{\sqrt{\varepsilon(A) - E_1(k)}}\right)^{-1} \exp\left(-\frac{1}{\omega}\int_{-m(A)}^{+m(A)} \sqrt{\varepsilon(A) - E_1(1 + i\sigma)}\, d\sigma\right)$$

where $\pm m(A)$ are the imaginary parts of the solutions $E_1(k)=\varepsilon(A)$, $\varepsilon(A)\geq E_1^{\text{t}}+K\omega^{\beta}$, $K>0$, $0<\beta<1$. Hence the nth gap width G_n^{D} is exponentially small for small ω (a similar behaviour is obtained for $x_0=\pi/2$).

Thus, introducing the bounded perturbation $\omega^2(\tilde{W}_1^2)_{1,1}(k)$, we obtain a gap estimate in agreement with the one given in (2.18).

Now we are ready to describe the behaviour of the magnetic band function $\varepsilon_n(x_0)$, $\varepsilon_n(x_0)\in[E_1^{\text{b}}+\delta,\ E_2^{\text{b}}-\delta]$. In particular we prove theorem 2.6 and remark 2.7, the existence of the eigenvalues $\varepsilon_n(x_0)$, $x_0\in\mathscr{B}'$, and we approximate them, modulo $\mathrm{O}(\omega^{1+\alpha})$, $0<\alpha<1$, $\omega\downarrow 0$, by the unperturbed one.

Let us state the following technical lemma.

Lemma 2.5. For any $\omega>0$, $\omega<\omega_0$, there exist $\eta_0>\omega$, $K>0$ such that for any α, $0<\alpha<1$, and for any $x_0\in(\gamma_2,\pi/2-\gamma_2)$, $\gamma_2=\omega^{\alpha}$, the resolvent $R(z,\eta)=[T_{x_0}(\eta)-z]^{-1}$ is analytic in η for $|\eta|<\eta_0$, for any $z\in\Gamma$ fixed, if the unperturbed eigenvalue $\varepsilon_n^{\text{SB}}(x_0)$ lies in $[E_1^{\text{t}}+\delta,\ E_2^{\text{b}}-\delta]$. Here $\delta=K\omega^{2(1-\alpha)/3}$ and Γ is the circle around $\varepsilon_n^{\text{SB}}(x_0)$ with radius $d_n=\mathrm{O}(\omega^{(1+\alpha)})$.

Moreover, there exist $h_0>0$, $C_3>0$ such that $K=(C_3h^2)^{2/3}$ for $h<h_0$.

Proof. Let us consider the resolvent

$$R(z,\eta)=[T_{x_0}(\eta)-z]^{-1}\qquad z\in\Gamma$$

where Γ is the circle around $\varepsilon_n^{\text{SB}}(x_0)$ with radius (see 2.17)

$$d_n=\tfrac{1}{2}\inf_{x_0\in(\gamma_2,\pi/2-\gamma_2)} d_n(x_0)=\tfrac{1}{2}C_2(\omega^{(1+\alpha)}+\mathrm{O}(\omega^2))=\mathrm{O}(\omega^{(1+\alpha)})\qquad \omega\downarrow 0.$$

The resolvent admits the following power series expansion in η (see Kato (1984) ch VII, formula 4.20):

$$\begin{aligned}R(z,\eta)=R(z,0)&+[T_{x_0}(0)+\rho]^{-1/2}[T_{x_0}(0)+\rho]R(z,0)\\&\times\left(\sum_{j=1}^{\infty}(-\eta)^j(S'_{x_0}[T_{x_0}(0)+\rho]R(z,0))^j\right)[T_{x_0}(0)+\rho]^{1/2}\end{aligned}\tag{2.19}$$

where $\rho=(1/\mu)(L_1^2/\mu-\mu E_1^{b})+\sigma$, $\mu>0$, $\sigma>0$ arbitrary and S'_{x_0} is the bounded operator defined by

$$S'_{x_0}=[T_{x_0}(0)+\rho]^{-1/2}S_{x_0}[T_{x_0}(0)+\rho]^{-1/2}$$

with bound $\|S'_{x_0}\|\leq 2\mu$ from (2.4). Notice that S'_{x_0} is the only operator in (2.19) coupling the first band with the others.

Hence, the convergence radius r_0 of the series (2.19) is given by

$$r_0=\sup\{|\eta|\,|\,\eta\in\mathbb{C},\ |\eta|^2\|(S'_{x_0}[T_{x_0}(0)+\rho]R(z,0))^2\|<1\}.$$

We have the following estimates for any $x\in\Gamma$:

$$\begin{aligned}&\|(S'_{x_0}[T_{x_0}(0)+\rho]R(z,0))^2\|\\&\quad\leq 2\|P_1'S'_{x_0}P_1[T_{x_0}(0)+\rho]R(z,0)P_1\|\,\|P_1S'_{x_0}P_1'[T_{x_0}(0)+\rho]R(z,0)P_1'\|\\&\quad\leq 8\mu^2\|P_1[T_{x_0}(0)+\rho]R(z,0)P_1\|\,\|P_1'[T_{x_0}(0)+\rho]R(z,0)P_1'\|\\&\quad\leq 32\left[\frac{\mu^{-1}L_1^2+\mu(\varepsilon_n^{\text{SB}}-E_1^{\text{b}})}{d_n(x_0)}+\mu\right]\left[\frac{\mu^{-1}L_1^2+\mu(\varepsilon_n^{\text{SB}}-E_1^{\text{b}})}{E_2^{b}-\varepsilon_n^{\text{SB}}}+\mu\right]\\&\quad\leq\frac{C_4}{\delta d_n}\end{aligned}\tag{2.20}$$

where $C_4 = C_3 h^2$ for $h < h_0$ as in lemma 2.1,

$$C_3 = 32\left(\mu^{-1}C_1^2 + \mu\frac{\varepsilon_n^{\rm SB}(x_0) - E_1^{\rm b}}{h}\right)^2.$$

Now, lemma 2.5 follows immediately from the above estimates. In fact we fix $\eta_0 = \sqrt{\delta d_n / C_4}$, so that, by (2.20),

$$r_0 \geqslant \eta_0 = \sqrt{\frac{\delta d_n}{C_4}}.$$

Now we impose the condition $\eta_0 > \omega$, obtaining the following inequality:

$$\eta_0^2 = \frac{\delta d_n}{C_4} = \frac{C_2\delta(\omega^{1+\alpha} + {\rm O}(\omega^2))}{2C_4} > \omega^2. \tag{2.21}$$

Equation (2.21) is satisfied if we choose $\delta C_2/2C_4 > \omega^{1-\alpha}$ for $\omega < \omega_0$, $\omega_0 > 0$ small, i.e.

$$\delta = (\omega^{1-\alpha}C_3 h^2)^{2/3} \qquad h < h_0 \quad 0 < \alpha < 1. \qquad \square$$

Our main result is the following.

Theorem 2.6. There exist $\omega_0 > 0$, $K > 0$ such that for any α, $0 < \alpha < 1$, $x_0 \in (\gamma_2, \pi/2 - \gamma_2)$, $\gamma_2 = \omega^\alpha$, $\omega < \omega_0$, the spectrum of $\tilde{H}_{x_0}$ in $[E_1^{\rm t} + \delta, E_2^{\rm b} - \delta]$, $\delta = K\omega^{2(1-\alpha)/3}$, consists of the eigenvalues:

$$\varepsilon_n(x_0) = \varepsilon_n^{\rm SB}(x_0) + {\rm O}(\omega^{1+\alpha}) = \varepsilon_n^{\rm D}(x_0) + {\rm O}(\omega^{(1+\alpha)}) \qquad \omega \downarrow 0$$

$$= \varepsilon(A) - (-1)^n 4\omega x_0\left(\int_{\mathcal{B}} [\varepsilon(A) - E_1(k)]^{-1/2}\,{\rm d}k\right)^{-1} + {\rm O}(\omega^{(1+\alpha)}) \qquad \omega \downarrow 0 \tag{2.22}$$

where $A = 2[\frac{n}{2}]\pi\omega$ is such that $A_{C}(E_2^{\rm b} - \delta) \geqslant A \geqslant A_{C}(E_1^{\rm t} + \delta)$. Here $\varepsilon(A)$ is the inverse function of the classical action $A_{C}(\mathscr{E})$.

Moreover there exists $h_0 > 0$ such that for $h < h_0$, $K = (C_3 h^2)^{2/3}$.

Proof. Let $\varepsilon_n^{\rm SB}(x_0) \in [E_1^{\rm t} + \delta, E_2^{\rm b} - \delta]$ as we have shown in theorem 2.3. From lemma 2.5 the resolvent $R(z, \eta)$ is analytic in η, $|\eta| < \eta_0$, $\eta_0 > \omega$, for any fixed $x \in \Gamma$. Hence Γ encloses $\varepsilon_n(x_0)$ and $\varepsilon_n^{\rm SB}(x_0)$, so that:

$$|\varepsilon_n(x_0) - \varepsilon_n^{\rm SB}(x_0)| \leqslant d_n = {\rm O}(\omega^{(1+\alpha)}) \qquad \omega \downarrow 0$$

and so (2.22) follows from formula (2.7) given in theorem 2.3. $\square$

Remark 2.7. For any $x_0 \in [0, \gamma_2] \cup [\pi/2 - \gamma_2, \pi/2]$ we have similar results for the couple of eigenvalues $\varepsilon_{2n+1}(x_0)$, $\varepsilon_{2n}(x_0)$, for $x_0 \in [0, \gamma_2]$($\varepsilon_{2n}(x_0)$, $\varepsilon_{2n-1}(x_0)$, for $x_0 \in [\pi/2 - \gamma_2, \pi/2]$), as can be seen from the degenerate pertrubation theory applied to a couple of eigenvalues enclosed in a path Γ with its points separated by at least ${\rm O}(\omega^{(1+\alpha)})$, $0 < \alpha < 1$, from both eigenvalues.

In particular we obtain the following asymptotic behaviour for any $x_0 \in \mathscr{B}'$:

$$\varepsilon_n(x_0) = \varepsilon_n^{\rm SB}(x_0) + {\rm O}(\omega^{(1+\alpha)}) = \varepsilon_n^{\rm D}(x_0) + {\rm O}(\omega^{(1+\alpha)}) \qquad \omega \downarrow 0$$

$$= \varepsilon(A) - (-1)^n 4\omega x_0\left(\int_{\mathcal{B}} [\varepsilon(A) - E_1(k)]^{-1/2}\,{\rm d}k\right)^{-1} + {\rm O}(\omega^{(1+\alpha)}) \qquad \omega \downarrow 0. \tag{2.23}$$

The two eigenvalues in the couple can approach without crossing each other for $0 \leq \eta \leq \omega$. By (2.23) we have an upper bound for the minimal distance of the eigenvalues of the order of $O(\omega^{(1+\alpha)})$, $\omega \downarrow 0$. In particular we estimate the magnetic gap width as

$$G_n = O(\omega^{(1+\alpha)}) \quad \omega \downarrow 0 \qquad \text{where } G_n = \varepsilon_{n+1}^{\mathrm{b}} - \varepsilon_n^{\mathrm{t}}.$$

The small ω asymptotics at $x_0 = 0$ of the eigenfunctions ψ_{2n} (ψ_{2n+1}) are given by

$$(\psi_{2n})(m,k) = \delta_1^m \psi_{2n}^{\mathrm{SB}}(k) + O(\omega) \qquad (\psi_{2n+1})(m,k) = \delta_1^m \psi_{2n+1}^{\mathrm{SB}}(k) + O(\omega)$$

where the asymptotics of $\psi_{2n}^{\mathrm{SB}}(k)$ ($\psi_{2n+1}^{\mathrm{SB}}(k)$) are given in (2.16).

Moreover, for $x_0 \in \mathscr{B}'$ fixed and $\varepsilon(A) \in [E_1^{\mathrm{t}} + \delta, E_2^{\mathrm{b}} - \delta]$, $\delta > 0$ fixed, we have the better estimates:

$$\begin{aligned} \varepsilon_n(x_0) &= \varepsilon_n^{\mathrm{SB}}(x_0) + O(\omega^2) = \varepsilon_n^{\mathrm{D}}(x_0) + O(\omega^2) \qquad \omega \downarrow 0 \\ &= \varepsilon(A) - (-1)^n 4\omega x_0 \left(\int_{\mathscr{B}} [\varepsilon(A) - E_1(k)]^{-1/2}\, \mathrm{d}k \right)^{-1} + O(\omega^2) \qquad \omega \downarrow 0. \end{aligned}$$

Remark 2.8. The estimate of the gap width G_n given in remark 2.7 is far from being optimal; in fact the following heuristic calculus proves that the magnetic gap width $G_{2n} \leq G(E) = \varepsilon_{2n+1}(0) - \varepsilon_{2n}(0)$, $E = \varepsilon_{2n+1}(0)$, is of order $O(\mathrm{e}^{-C/\omega})$ (or equivalently $G_{2n+1} \leq G(E) = \varepsilon_{2n+2}(\pi/2) - \varepsilon_{2n+1}(\pi/2)$, $E = \varepsilon_{2n+1}(\pi/2)$) as the unperturbed one (remark 2.4) where $C = C(E) > 0$, $\omega \downarrow 0$ and $E \in (E_1^{\mathrm{t}}, E_2^{\mathrm{b}})$.

This estimate comes from the x-dependent band picture as illustrated in the introduction and in figure 1: we consider the problem at $x_0 = 0$ as *locally* Bloch with x-dependent bands: $E^{\mathrm{t/b}}(x) = E_1^{\mathrm{t/b}} + \omega^2 x^2$, so that a gap acts locally as a potential barrier with Zener exponential behaviour of the solution ϕ, i.e.

$$\phi(x_2) \approx \phi(x_1) \exp[\pm\chi(E(x_2))(x_2 - x_1)] \qquad x_2 - x_1 = n\pi,\ E(x_2) \in (E_1^{\mathrm{t}}, E_2^{\mathrm{b}}), \text{ as } \omega \downarrow 0$$

where $\chi(E) = |\Im k(E)|$, $k(E)$ being the crystal momentum in the gap. Hence the exponential decay of the wavefunction, i.e. the transmission amplitude $T(E)$, from the extreme $\bar{x}$ to the middle of the barrier is given by $\exp(-\int_0^{\bar{x}} \chi(E(x))\, \mathrm{d}x)$ where $\bar{x} = \sqrt{E - E_1^{\mathrm{t}}}/\omega$. So we estimate the gap as the splitting of the double-well beating effect:

$$G(E) \approx T^2(E) \approx \exp\left(-2 \int_0^{\bar{x}} \chi(E(x))\, \mathrm{d}x \right) \approx \mathrm{e}^{-C(E)/\omega} \qquad \omega \downarrow 0 \tag{2.24}$$

where

$$C(E) = \int_{E_1^{\mathrm{t}}}^{E} \frac{\chi(E)\, \mathrm{d}E}{\sqrt{E - E_1^{\mathrm{t}}}}.$$

Remark 2.9. Using the degenerate perturbation theory applied to the analytic family of type (A) $H_0 + W_{x_0}$, $W_{x_0} = \omega x_0(2\omega x) + \omega^2 x_0^2$, we can control the magnetic band functions for x_0 in a neighbourhood of 0 ($\pi/2$).

We use the degenerate perturbation theory, for $|x_0| \ll (\pi\varepsilon'(A)/2\sqrt{\varepsilon(A)})$, for the two states $2n+1$ and $2n$ since

$$|\varepsilon_{2n+1}(0) - \varepsilon_{2n}(0)| = O(\omega^2)$$

and

$$|\varepsilon_{2n}(0) - \varepsilon_{2m}(0)| \geq 2\pi\varepsilon'(A)\omega + O(\omega^2) \qquad m \neq n,\ A = 2n\pi\omega.$$

Up to the first order in x_0, we have all the 'avoided crossings' of $\varepsilon_{2n+1}(x_0)$, $\varepsilon_{2n}(x_0)$ near $x_0=0$. In particular, if we call $\lambda_+(x_0)=\varepsilon_{2n+1}(x_0)$, $\lambda_-(x_0)=\varepsilon_{2n}(x_0)$, $\omega\hat{x}=\langle\phi_{2n+1}(0), \omega x\phi_{2n}(0)\rangle$, where $\phi_n(x_0)$ is the normalised eigenvector associated with the eigenvalue $\varepsilon_n(x_0)$, we have

$$\lambda_\pm(x_0)=\frac{\lambda_+(0)+\lambda_-(0)+2x_0^2\omega^2}{2}\pm\left(\frac{(\lambda_+(0)-\lambda_-(0))^2}{4}+4\omega^2x_0^2|\omega\hat{x}|^2\right)^{1/2}+\mathrm{O}(\omega x_0^2) \tag{2.25}$$

with the two behaviours:

$$\lambda_\pm(x_0)=\begin{cases}\lambda_\pm(0)+x_0^2\omega^2\pm 4\dfrac{\omega^2x_0^2|\omega\hat{x}|^2}{\lambda_+(0)-\lambda_-(0)}+\mathrm{O}(\omega x_0^2) & |x_0|\ll\dfrac{\lambda_+(0)-\lambda_-(0)}{4\omega|\omega\hat{x}|} \quad (2.26)\\[2ex] \left(\dfrac{\lambda_+(0)+\lambda_-(0)}{2}+x_0^2\omega^2\pm 2\omega|x_0||\omega\hat{x}|^2+\mathrm{O}(\omega x_0^2)\right. & |x_0|\gg\dfrac{\lambda_+(0)-\lambda_-(0)}{4\omega|\omega\hat{x}|} \quad (2.27)\end{cases}$$

where (2.27) is in agreement with (2.22) for $|x_0|\geq\omega^\alpha$, $0<\alpha<1$, if (as can be easily checked by (2.16)):

$$\begin{aligned}|\omega\hat{x}|&=|\langle\phi_{2n+1}(0),\omega x\phi_{2n}(0)\rangle|\\&=\left|\left\langle\psi_{2n+1}^{\mathrm{SB}},\mathrm{i}\omega\frac{\partial}{\partial k}\psi_{2n}^{\mathrm{SB}}\right\rangle_{L^2(\mathscr{B})}\right|+\mathrm{O}(\omega)\\&=\varepsilon'(A)+\mathrm{O}(\omega)\qquad \omega\downarrow 0\end{aligned} \tag{2.28}$$

where

$$\varepsilon'(A)=\left(\int_{\mathscr{B}}\frac{\mathrm{d}k}{2\sqrt{\varepsilon(A)-E_1(k)}}\right)^{-1}.$$

From (2.25) and (2.28) we obtain the monotonicity of $\lambda_\pm(x_0)$ for $|x_0|\leq\omega^\alpha$, $0<\alpha<1$. Similarly we can control the magnetic band function in a neighbourhood of $\pi/2$.

From (2.22) and remark 2.9 we can state the following.

Proposition. The magnetic band functions satisfy the following equations for ω small enough:

$$\varepsilon_n^{\mathrm{b}}=\min_{x_0\in\mathscr{B}'}\varepsilon_n(x_0)=\begin{cases}\varepsilon_n(0) & n\text{ odd}\\ \varepsilon_n(\pi/2) & n\text{ even}\end{cases}$$

$$\varepsilon_n^{\mathrm{t}}=\max_{x_0\in\mathscr{B}'}\varepsilon_n(x_0)=\begin{cases}\varepsilon_n(\pi/2) & n\text{ odd}\\ \varepsilon_n(0) & n\text{ even}\end{cases}$$

with all the magnetic gaps $(\varepsilon_n^{\mathrm{t}},\varepsilon_{n+1}^{\mathrm{b}})$, $n\geq 1$, not empty since H_{x_0} has simple eigenvalues.

Remark 2.10. For reasons of completeness we give the following upper bound for $\varepsilon_n'(x_0)$ ($'$ means $\mathrm{d}/\mathrm{d}x_0$, ω fixed), very similar to the estimate given for the band function of a Bloch operator (see theorem 2.1 of Avron and Simon 1981):

$$|\varepsilon_n'(x_0)|\leq 2\omega\sqrt{\varepsilon_n(x_0)-E_1^b}\qquad x_0\in\mathscr{B}',\ \omega>0. \tag{2.29}$$

In fact, by the Schwarz inequality

$$\begin{aligned}|\varepsilon_n'(x_0)|&=2\omega^2|\langle\phi_n(x_0),(x-x_0)\phi_n(x_0)\rangle|\\&\leq 2\omega\sqrt{\varepsilon_n(x_0)-\langle\phi_n(x_0),(p^2+V)\phi_n(x_0)\rangle}\\&\leq 2\omega\sqrt{\varepsilon_n(x_0)-\langle(\tilde{U}\phi_n(x_0)),\tilde{H}_{\mathrm{B}}(\tilde{U}\phi_n(x_0))\rangle_{\oplus_m L^2(\mathscr{B})}}\\&\leq 2\omega\sqrt{\varepsilon_n(x_0)-E_1^b}.\end{aligned}$$

Moreover, we can also obtain an upper bound for $\partial\varepsilon_n(x_0)/\partial\omega$ for $x_0\in\mathscr{B}'$ and $\omega>0$:

$$
\begin{aligned}
0\leqslant\frac{\omega}{2}\frac{\partial\varepsilon_n(x_0)}{\partial\omega}&=\langle\phi_n(x_0),\,(x-x_0)^2\phi_n(x_0)\rangle\\
&=\varepsilon_n(x_0)-\langle(\tilde U\phi_n(x_0)),\,\tilde H_{\mathrm B}(\tilde U\phi_n(x_0))\rangle_{L^2(\mathscr{B})}\\
&\leqslant\varepsilon_n(x_0)-E_1^{\mathrm b}.
\end{aligned}\tag{2.30}
$$

3. Magnetic bands in the first band energy region of the Bloch model

For small ω there are magnetic bands in the first band region $[E_1^{\mathrm b}, E_1^{\mathrm t}]$ of the Bloch model. We recall that for small h the band width is exponentially small: $E_1^{\mathrm t}-E_1^{\mathrm b}=\mathrm e^{-C/h}$, $C>0$ (see Harrell 1979), so that for the asymptotic estimates below (equation (3.1)) we should take $\omega\ll\mathrm e^{-C/h}$ for small h.

As above, the union of the magnetic bands is the spectrum of the operator

$$\mathscr{H}(\omega)=\int_{\mathscr{B}'}^{\oplus}H_{x_0}\,\mathrm dx_0.$$

The bands are completely given by the perturbation theory, but not explicitly as in the gap region. Only for n fixed do we give an explicit asymptotic behaviour (equation (3.2)). In the case of a particular model we give explicitly the h, ω behaviour of the first magnetic band.

Theorem 3.1. For any $x_0\in\mathscr{B}'$, the spectrum of H_{x_0} in the interval $[E_1^{\mathrm b}, E_1^{\mathrm t}]$, is given by the magnetic band function satisfying the following asymptotic behaviour:

$$\varepsilon_n(x_0)=\varepsilon_n^{\mathrm D}(x_0)+\mathrm O(\omega^2)=\varepsilon_n^{\mathrm{SB}}(x_0)+\mathrm O(\omega^2)\qquad\omega\downarrow0,\,x_0\in\mathscr{B}'.\tag{3.1}$$

Each magnetic band in $[E_1^{\mathrm b}, E_1^{\mathrm t}-K\omega^{\beta}]$, $0<\beta<1$, $K>0$, has band width vanishing at least as $\mathrm O(\omega^2)$ and the isolation distance vanishing as $\mathrm O(\omega)$ for $\omega\downarrow0$.

Moreover, for n fixed we have the following asymptotic behaviour:

$$\varepsilon_n(x_0)=E_1^{\mathrm b}+\omega(n-\tfrac12)\sqrt{2E_1''(0)}+\mathrm O(\omega^2)\qquad\omega\downarrow0,\,n\geqslant1.\tag{3.2}$$

Proof. Mimicking the proof of theorem 2.3, we give the single-band approximation of the operator (2.1):

$$\tilde H_{\mathrm{SB}}(x_0)=-\omega^2\frac{\mathrm d^2}{\mathrm dk^2}+E_1(k)+\omega^2(\tilde W_1^2)_{1,1}(k)$$

with boundary conditions (2.10). Since $(\tilde W_1^2)_{1,1}(k)$ is bounded, the band functions of the single-band approximation in the interval $[E_1^{\mathrm b}, E_1^{\mathrm t}]$ are, modulo $\mathrm O(\omega^2)$, given by the Bloch operator

$$\tilde H_{\mathrm D}(x_0)=-\omega^2\frac{\mathrm d^2}{\mathrm dk^2}+E_1(k)\qquad\text{with boundary conditions (2.10).}\tag{3.3}$$

Its band functions are calculated by Harrell (1979) and Weinstein and Keller (1985, 1987). In particular Harrell (1979) and Weinstein and Keller (1985) prove, under some hypothesis on the potential, that the mean values of the band functions for n fixed are asymptotically given by

$$\overline{\varepsilon_n^{\mathrm{D}}} = E_1^{\mathrm{b}} + \omega(n-\tfrac{1}{2})\sqrt{2E_1''(0)} + \mathrm{O}(\omega^2) \qquad \omega\downarrow 0,\ n<N(\omega)$$

and the band width is exponentially small: $|\varepsilon_n^{\mathrm{D}}(0)-\varepsilon_n^{\mathrm{D}}(\pi/2)| \approx \mathrm{O}(\mathrm{e}^{-C/\omega})$, $C>0$.

Hence

$$\begin{aligned}\varepsilon_n^{\mathrm{SB}}(x_0) &= \overline{\varepsilon_n^{\mathrm{D}}} + \mathrm{O}(\omega^2)\\ &= E_1^{\mathrm{b}} + \omega(n-\tfrac{1}{2})\sqrt{2E_1''(0)} + \mathrm{O}(\omega^2) \qquad \omega\downarrow 0,\ n<N(\omega),\ x_0\in\mathscr{B}'\end{aligned} \tag{3.4}$$

and

$$G_n^{\mathrm{SB}} = G_n^{\mathrm{D}} + \mathrm{O}(\omega^2) = \omega\sqrt{2E_1''(0)} + \mathrm{O}(\omega^2) \qquad \omega\downarrow 0,\ n<N(\omega).$$

Since the isolation distance is of the order of $\omega\sqrt{2E_1''(0)}$, we can apply the perturbation theory as in lemma 2.5 and theorem 2.6, choosing the radius of the circle Γ as $d_n = \mathrm{O}(\omega^2)$, for $\omega\downarrow 0$, without any discussion at the endpoints of the interval $[0, \pi/2]$. In particular, the series (2.19) is convergent for η such that $|\eta|<\eta_0$, $\eta_0>\omega$, uniformly for $x_0\in\mathscr{B}'$. Hence, by (3.4), we obtain the asymptotic expansions (3.2).

We must only require that our potential $E_1(k)$ in (3.3) satisfies the hypothesis of the theorems given in Harrell (1979) and Weinstein and Keller (1985) cited above. This is easily proved; in fact $E_1(k)$ is analytic in a strip around the real axis, it is even and satisfies the inequality (see Avron and Simon 1981):

$$E_1''(0) \geqslant \frac{\pi^2}{2h^2}\exp\left[-\frac{\pi}{h}\left(h+\sqrt{E_1(0)}+\sqrt{\|V\|_\infty}\right)\right] > 0.$$

Now, let us consider all the magnetic band functions in the interval $[E_1^{\mathrm{b}}, E_1^{\mathrm{t}}]$. As above, we use the semiclassical results (see Weinstein and Keller 1987) for the operator (3.3).

If n satisfies the inequalities

$$C'\omega^{\beta'-1} \leqslant n \leqslant \frac{1}{\pi\omega}\int_{\mathscr{B}} \sqrt{E_1^{\mathrm{t}} - E_1(k)}\,\mathrm{d}k - C\omega^{\beta-1}$$

for some $C>0$, $C'>0$, $0<\beta<1$, $0<\beta'<1$, then the band functions $\varepsilon_n^{\mathrm{D}}(x_0)$ at the endpoints satisfy the asymptotic inequalities

$$E_1^{\mathrm{b}} + K'\omega^{\beta'} \leqslant \varepsilon_n^{\mathrm{D}}(x_0) \leqslant E_1^{\mathrm{t}} - K\omega^{\beta} \qquad x_0 = 0, \pi/2$$

where $K>0$ is proportional to C, $K' = C'\sqrt{2E_1''(0)}>0$, and the gap width G_n^{D} has the following behaviour as $\omega\downarrow 0$:

$$G_n^{\mathrm{D}} \approx C_5\omega \qquad C_5 = 2\pi\left(\int_{-\bar{k}}^{\bar{k}} [\varepsilon_n^{\mathrm{D}} - E_1(k)]^{-1/2}\,\mathrm{d}k\right)^{-1}$$

where $\pm\bar{k}$ are the classical turning points, i.e. $E_1(\pm\bar{k}) = \varepsilon_n^{\mathrm{D}}$.

Hence $G_n^{\mathrm{SB}} = G_n^{\mathrm{D}} + \mathrm{O}(\omega^2) \approx C_5\omega$.

Since the isolation distance of the eigenvalue $\varepsilon_n^{\mathrm{SB}}(x_0)$ is greater than $C_5\omega$, we obtain the asymptotic behaviour (3.1) applying the perturbation theory as done in lemma 2.5 and theorem 2.6 with the choice $d_n = \mathrm{O}(\omega^2)$.

Moreover, since the unperturbed band function $\varepsilon_n^{\mathrm{D}}(x_0)$ has exponentially small band width, we can estimate, by (3.1), the band width as $\mathrm{O}(\omega^2)$ and the gap width as $\mathrm{O}(\omega)$.

Finally, we can also estimate the band functions $\varepsilon_n^{D}(x_0)$, $x_0 = 0, \pi/2$, near the top E_1^t starting from the result that: if $n \approx (1/\pi\omega)\int_{\mathcal{B}} \sqrt{E_1^t - E_1(k)}\,dk$ then $\varepsilon_n^{D}(x_0) \approx E_1^t$ and the gap is estimated as:

$$G_n^{D} \approx C_6\omega \qquad C_6 = 2\pi E_1^t\left(\int_{\mathcal{B}} \sqrt{E_1^t - E_1(k)}\,dk\right)^{-1}.$$

Hence $\varepsilon_n^{SB}(x_0) \approx E_1^t$ and $G_n^{SB} = G_n^{D} + O(\omega^2) = O(\omega)$, $\omega \downarrow 0$, and using the perturbation theory we complete the proof of estimate (3.1). □

We conclude the present section by considering a solvable problem giving a totally flat first magnetic band:

$$H'_{x_0} = -h^2\frac{d^2}{dx^2} + \omega^2(x-x_0)^2 + \frac{\cos^2 2x}{4} + h(1+\sin 2x) + \omega(x-x_0)\cos 2x$$

$$= \left(-h\frac{d}{dx} + \omega(x-x_0) + \frac{\cos 2x}{2}\right)\left(h\frac{d}{dx} + \omega(x-x_0) + \frac{\cos 2x}{2}\right) + h + h\omega$$

with x_0-independent first eigenvalue $h + h\omega$ and eigenvector

$$\psi(x) = \exp\left(-\frac{\omega(x-x_0)^2}{2h} - \frac{\sin 2x}{4h}\right).$$

Here $V(x) = \frac{1}{4}\cos^2 2x + h(1+\sin 2x)$. Thus we have a flat first magnetic band function

$$\varepsilon_1(x_0) = E_1^b + h\omega = h + h\omega$$

in agreement with the behaviour given in theorem 3.1.

Actually, the term $\omega(x-x_0)\cos 2x$ enables the model to only asymptotically approach the class considered above as $\omega \downarrow 0$. We recall that each true magnetic band is flat in the $\omega \downarrow 0$ limit.

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