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Periodic Schrödinger Operators with Constant Weak Magnetic Fields

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Periodic Schrödinger operators with constant weak magnetic fields.

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The aim of this talk is to decribe a mathematically rigorous justification of the Peierls substitution. In this written version of the talk we do not include the very preliminary discussion of the Haas Van Alphen effect, but refer to [HS2,3] for more definite results. A part from the classical work of Peierls [P], we have been inspired by several mathematical works: such as Avron-Simon [ASi], Nenciu [N1-3], Bellissard [B1,2], Guillot-Ralston-Trubowitz [GuRT]. (Some references to the physical litterature are also given below.) We learned about the use of Wannier functions from [B1,2],[N1-3], and in our earlier paper [HS1], we used such functions in the case when the periodic Schrödinger operator has a single band in its spectrum. In that case we obtained a reduction of the study of the spectrum and of the density of states to that of corresponding quantities for a certain effective Hamiltonian which is a pseudodifferential operator, "obtained by Peierls substitution". In [B1,2],[N1-3] such reductions to an infinite matrix were given. Such infinite matrices also play a role as an intermediate step in our approach. In the work [GuRT] certain approximate solutions of the magnetic Schrödinger equation are constructed by means of WKB-methods and some discussion of the Haas Van Alphen effect is also given. Since only special solutions are constructed, only some partial results about the spectrum are obtained.

More recently, we managed to improve the results of [HS1] (see [HS2]), by eliminating the assumption that we work with energies close to a single band for the zero field case, and this talk will give an outline of this more general case. The usual Wannier functions have then dissappeared, but they are reminiscent in the choice of certain auxiliary operators:

Let $V\in C^\infty(\mathbb{R}^n;\mathbb{R})$ be periodic with respect to the lattice, $\Gamma=\bigoplus_1^n \mathbb{Z}e_j$, where the e_j form a basis in $\mathbb{R}^n$, so that $V(x+\gamma)=V(x)$ for every $\gamma\in\Gamma$. Let $A_1,..,A_n\in C^\infty(\mathbb{R}^n;\mathbb{R})$, and assume that the corresponding exterior differential or "magnetic field", $B=d(\Sigma A_j dx_j)$ is constant on $\mathbb{R}^n$. We are then interested in the spectrum and in the density of states for the magnetic Schrödinger operator (m.S.o.):

(1) $$P_{B,V}=\Sigma(D_{x_j}+A_j(x))^2+V(x).$$

By simple conjugations of the operator by exponential factors, we know that only B and not the special choice of A is important here, and since we assume that B is constant, we may take $A_k(x)=\frac{1}{2}\Sigma b_{j,k}x_j$, where $B=\frac{1}{2}\Sigma\Sigma b_{j,k}dx_j\wedge dx_k$ and $b_{j,k}=-b_{k,j}$.

In the case $B=0$ we can use the Bloch-Floquet theory: Let Γ^* be the dual lattice, $\{\gamma^*\in\mathbb{R}^{n*};\ \gamma\gamma^*\in 2\pi\mathbb{Z}\}$, and put $\mathcal{H}_\theta=\{u\in L^2_{loc}(\mathbb{R}^n);\ u(x+\gamma)=e^{i\gamma\theta}u(x)$ for all $\gamma\in\Gamma\}$, for $\theta\in\mathbb{R}^{n*}/\Gamma^*$ (which is a Hilbert space equipped with the standard L^2 inner product over a fundamental domain of Γ.) The operator U, defined by $Uu(x,\theta)=\sum_\Gamma u(x-\gamma)e^{i\gamma\theta}$ is unitary from $L^2(\mathbb{R}^n)$ to $\int^\oplus\mathcal{H}_\theta d\theta$ and the inverse is given by

$$U^{-1}v(x)=(\mathrm{Vol}(\mathbb{R}^{n*}/\Gamma^*))^{-1}\int v(x,\theta)d\theta.$$

$P=P_{0,V}$ is then unitarily equivalent to $\int^\oplus P_\theta d\theta$, where P_θ is the (essentially self-adjoint) operator on $\mathcal{H}_\theta$ defined as $P_{0,V}$ in the sense of distributions. We also know that the spectrum of $P_{0,V}$ is purely absolutely continuous and of the form $\bigcup_0^\infty J_k$, where $J_k=\{E_k(\theta);\ \theta\in\mathbb{R}^{n*}/\Gamma^*\}$. Here $E_0(\theta)\le E_1(\theta)\le..$ are the eigenvalues of P_θ. In the case of a simple band, J_{k_0}, (disjoint from J_k when $k\neq k_0$) the Peierls substitution says that when B is small and for energies close to J_{k_0}, the operator is "well approximated" by the pseudodifferential operator, $E_{k_0}(D_{x_1}+A_1(x),..,D_{x_n}+A_n(x))$.

We fix some $z_0\in\mathbb{R}$. Our aim is to study the spectrum and the density of states near the energy z_0, when B is small. We start with the case $B=0$:

<u>Proposition 1.</u> There exists an integer $N\ge 0$, and analytic functions, $\varphi_j:\mathbb{R}^{n*}/\Gamma^*\to\mathcal{H}_\theta$, for $j=1,..,N$, such that for every $\theta\in\mathbb{R}^{n*}/\Gamma^*$ and for every z in a complex neighborhood of z_0, the operator

$$\mathcal{P}(z,\theta)=\begin{pmatrix}P_\theta-z & R_-\\ R_+ & 0\end{pmatrix}\ :\ \mathcal{H}^2_\theta\times\mathbb{C}^N\to\mathcal{H}_\theta\times\mathbb{C}^N$$

is bijective. Here $\mathcal{H}^2_\theta$ is the intersection of $\mathcal{H}_\theta$ and the space of functions belonging locally to the standard Sobolev space H^2. Moreover, $R_+u(j)=(u|\varphi_j)_{\mathcal{H}_\theta}$, $R_-=R_+^*$.

If z_0 belongs to a simple band, J_{k_0}, then one can prove that $\mathrm{Ker}(P_\theta - E_{k_0}(\theta))$ is a trivial line bundle over $\mathbb{R}^{n*}/\Gamma^*$ (See [N1],[HS1]), and it follows in that case that we can take N=1, and $\varphi_1(\theta)=\varphi(\theta)$, a normalized analytic section of $\mathrm{Ker}(P_\theta - E_{k_0}(\theta))$.

Let

$$\mathcal{E}(z,\theta)=\begin{pmatrix} E(z,\theta) & E_+(z,\theta) \\ E_-(z,\theta) & E_{-+}(z,\theta)\end{pmatrix}$$

denote the inverse of $\mathcal{P}(z,\theta)$. (We notice that in the simple band case, we get $E_{-+}(z,\theta)=z-E_{k_0}(\theta)$, provided that we choose $R_\pm$ as above.) An important observation is that z belongs to the spectrum of P_θ if and only if 0 belongs to the spectrum of $E_{-+}(z,\theta)$. This is due to the formulas,

$$(P_\theta - z)^{-1}=E(z,\theta)-E_+(z,\theta)(E_{-+}(z,\theta))^{-1}E_-(z,\theta),$$

$$E_{-+}(z,\theta)^{-1}=-R_+(P_\theta - z)^{-1}R_-$$

We now add a weak constant magnetic field, B. For some suitable m, let $l_1(x,\xi),..,l_n(x,\xi)$ be linearly independent real linear forms on $T^*\mathbb{R}^m=\mathbb{R}^m\times\mathbb{R}^{m*}$ with the property that,

(2) $\{l_j,l_k\}=\langle B,e_j\wedge e_k\rangle$, for j,k=1,..,n.

Here {a,b} denotes the Poisson bracket; $\Sigma(\partial_{\xi_j}a)(\partial_{x_j}b)-(\partial_{x_j}a)(\partial_{\xi_j}b)$, for $a=a(x,\xi)$, $b=b(x,\xi)$ in $C^\infty(T^*\mathbb{R}^m)$. As an example, we can always take m=n and $l_j(x,\xi)=\xi_j+A_j(x)$ (and this corresponds to the classical Peierls substitution), but it is also of interest that we can sometimes take m<n. Let $\theta=(\theta_1,..,\theta_n)$, where $\theta_j=\langle\theta,e_j\rangle$, so that θ_j are the dual coordinates on $\mathbb{R}^{n*}$ and using these coordinates, we define $l(x,\xi)=(l_1(x,\xi),..,l_n(x,\xi))$ as a point of $\mathbb{R}^{n*}/\Gamma^*$. We then have:

<u>Theorem 2.</u> There exists a smooth function $g=g(B,z;\theta)$ with values in the N×N matrices, defined in a neighborhood of $\{0\}\times\{z_0\}\times(\mathbb{R}^{n*}/\Gamma^*)$ in $\mathbb{R}^{n(n-1)/2}\times\mathbb{C}\times(\mathbb{C}^{n*}/\Gamma^*)$, holomorphic with respect to z,θ, such that for z,B in a neighborhood of $(z_0,0)$ in $\mathbb{C}\times\mathbb{R}^{n(n-1)/2}$, we have the equivalence:

(3) $z\in\sigma(P_{B,V})\Leftrightarrow 0\in\sigma(\mathrm{Op}^W(g(B,z;l(x,\xi))).$

Moreover, $g(0,z;\theta)=E_{-+}(z,\theta)$.

Here "σ" denotes "spectrum of", and $\mathrm{Op}^W(a)$ denotes the peudodifferential operator obtained by Weyl quantization of a (assumed to belong to some suitable space of symbols on $T^*\mathbb{R}^m$):

(4) $\mathrm{Op}^W(a)u(x)=\iint e^{i(x-y)\eta}\, a((x+y)/2,\eta)u(y)\, dy d\eta/(2\pi)^m,$

for u in the Schwarz space, $\mathscr{S}(\mathbb{R}^m)$. (It follows from standard results on pseudodifferential opertors, that $Op^W(g\circ l)$ is bounded on $L^2(\mathbb{R}^m)$.)

<u>Brief outline of the proof.</u> We first return to the case $B=0$, and put $\Phi_{0,j}(x)=U^{-1}(\varphi_j)(x)$, $\Phi_{\gamma,j}(x)=\Phi_{0,j}(x-\gamma)$. In the case of a single band, and with the special choice indicated after Proposition 1, the functions $\Phi_\gamma=\Phi_{\gamma,1}$ form an orthonormal basis of the spectral subspace associated to $P_{0,V}$, J_{k_0}. These are the Wannier functions, used by Bellissard [B1,2] and Nenciu [N1-3]. In the general case, the analyticity of φ_j with respect to θ, implies that $\Phi_{0,j}$ is exponentially decreasing: There exists a constant $C>0$ such that, $|\Phi_{0,j}(x)|\leq Ce^{-|x|/C}$ for all $x\in\mathbb{R}^n$, and we have the same type of estimate for every derivative of $\Phi_{0,j}$. (Here we actually need that φ_j is smooth in x, but this property can easily be added to the conclusion of Proposition 1.)

Using U^{-1}, we find that

$$\mathscr{P}^0(z)=\begin{pmatrix} P_{0,V}-z & R_-^0 \\ R_+^0 & 0 \end{pmatrix} : H^2(\mathbb{R}^n)\times l^2(\Gamma;\mathbb{C}^N)\rightarrow L^2\times l^2,$$

is bijective, where $(R_+^0u)(\gamma)_j=(u|\Phi_{\gamma,j})_{L^2(\mathbb{R}^n)}$, and $R_-^0=(R_+^0)^*$ (the complex adjoint of R_+^0) . If

$$\mathscr{E}^0(z)=\begin{pmatrix} E^0(z) & E_+^0(z) \\ E_-^0(z) & E_{-+}^0(z) \end{pmatrix}$$

denotes the inverse, then $E_{-+}^0(z)$ is given by the (block) matrix, $E_{-+}^0(z;\alpha,\beta)=\mathscr{F}(E_{-+}(z,.))(\beta-\alpha)$, where we let $\mathscr{F}(f)(\alpha)$ denote the Fourier coefficient at $\alpha\in\Gamma$, of the function $f\in C^\infty(\mathbb{R}^{n*}/\Gamma^*)$. Thanks to the exponential decrease of the function $\Phi_{0,j}$, one can show that $\mathscr{E}^0(z)$ remains bounded also on certain exponentially weighted spaces.

For $B\neq 0$, one has to consider $P_{B,V}$ as a singular perturbation of $P_{0,V}$. Moreover, $P_{B,V}$ will not in general commute with translations by elements of Γ, but with certain modified "magnetic" translations (see Zak [Z], Luttinger [L], Bellissard [B1,2] and Nenciu [N1-3]): For $\alpha\in\Gamma$, we put $T_\alpha^Bu(x)=e^{(i/2)\langle B,x\wedge\alpha\rangle}u(x-\alpha)$ and check that:

(4) $\qquad [P_{B,V},T_\alpha^B]=0.$

We can not use Floquet theory (in general) since the T_α^B do not necessarily form a commutative group:

(5) $\qquad T_\alpha^BT_\beta^B=e^{-i\langle B,\alpha\wedge\beta\rangle}T_\beta^BT_\alpha^B.$

We put $\Phi^B_{\alpha,j}=T^B_\alpha\Phi_{0,j}$. $R^B_+u(\alpha)_j=(u|\Phi^B_{\alpha,j})$, $u\in L^2(\mathbb{R}^n)$, $R^B_-=R^{B*}_+$,

$$\mathcal{P}^B(z)=\begin{pmatrix} P_{B,V}-z & R^B_- \\ R^B_+ & 0\end{pmatrix} .$$

Let $H^2_B=\{u\in L^2(\mathbb{R}^n)$; such that $(D_{x_j}+A_j)u$, $(D_{x_j}+A_j)(D_{x_k}+A_k)u$ belong to L^2 for all $j,k\}$. This is a Hilbert space with the natural norm.

<u>Proposition 3.</u> For (z,B) in a neighborhood of $\{z_0\}\times\{0\}$ in $\mathbb{C}\times\mathbb{R}^{n(n-1)/2}$, the operator $\mathcal{P}_B(z)$ is bijective from $H_B{}^2\times l^2$ onto $L^2\times l^2$. If we let

$$\mathcal{E}^B(z)=\begin{pmatrix} E^B(z) & E^B_+(z) \\ E^B_-(z) & E^B_{-+}(z)\end{pmatrix}$$

be the corresponding inverse, then the matrix of $E^B_{-+}(z)$ is of the form, $E^B_{-+}(z)=e^{(i/2)\langle B,\alpha\wedge\beta\rangle}f(B,z;\alpha-\beta)$, where f is smooth in B,z and holomorphic in z, with

(6) $|\partial^\gamma_B f(B,z;\alpha)|\leq C_\gamma\, e^{-\eta|\alpha|}$ for some $\eta>0$, independent of γ,

(7) $f(0,z;\alpha)=\mathcal{F}(E_{-+}(z,.))(-\alpha)$.

Moreover, $z\in\sigma(P_{B,V})$ if and only if $0\in\sigma(E^B_{-+}(z))$.

The idea of the proof is that although $P_{B,V}$ is a singular perturbation of $P_{0,V}$, the two operators are close in any fixed compact set, when B is small enough. The same can be said about $\mathcal{P}^B$ and $\mathcal{P}^0$ and it turns out that we can form approximate inverses by using suitable partitions of unity, the magnetic translation operators and $\mathcal{E}^0$.

The matrices of the form $\mathcal{M}_B(f)(\alpha,\beta)=e^{(i/2)\langle B,\alpha\wedge\beta\rangle}f(\alpha-\beta)$ with $f\in l^1(\Gamma)$ form an algebra. We can write $\mathcal{M}_B(f)=\Sigma\, f(\alpha)\tau_\alpha^{-B}$, $\tau_\alpha^{-B}=\mathcal{M}_B(\delta_\alpha)$ where $\delta_\alpha(\beta)=1$ if $\beta=\alpha$, and $=0$ otherwise. We have,

(8) $$\tau_\alpha^{-B}\tau_\beta^{-B}=e^{i\langle B,\alpha\wedge\beta\rangle}\tau_\beta^{-B}\tau_\alpha^{-B}.$$

Thanks to the choice of the l_j, one verifies that,

(9) $e^{i\langle\alpha,l(x,D_x)\rangle}\, e^{i\langle\beta,l(x,D_x\rangle}=e^{i\langle B,\alpha\wedge\beta\rangle}\, e^{i\langle\beta,l(x,D_x)\rangle}\, e^{i\langle\alpha,l(x,D_x\rangle}$.

In fact $e^{i\langle\alpha,l(x,D_x)\rangle}=\mathrm{Op}^W(e^{i\langle\alpha,l(x,\xi)\rangle})$ so we can use the calculus of Weyl quantizations. (See [BoGH], [Hö].) To $\mathcal{M}_B(f)$ we can then associate the pseudodifferential operator, $\mathrm{Op}^W(\Sigma f(\alpha)e^{i\langle\alpha,l(x,\xi)\rangle})=\mathrm{Op}^W(g\circ l)$, where g is the function on $\mathbb{R}^{n*}/\Gamma^*$ with $f=\mathcal{F}(g)$. This correspondence commutes with composition of the operators.

In the case, when f is of exponential decrease, one can show, using a theorem of R.Beals [Be], that

(10) $$\sigma(\mathcal{M}_B(f))=\sigma(\mathrm{Op}(g\circ l)).$$

Applying this to the function, f, given in Proposition 3, we obtain Theorem 2.

Remark 4. In order to apply semiclassical analysis, we can fix a field B_0, put $B=hB_0$ and let $h\to 0$. If $l_1,..,l_n$ are adapted to B_0 as above, then to B we can associate the linear forms $l_j(x,h\xi)$, and the study of the spectrum of $P_{B,V}$ is then reduced to the study of the "semiclassical" pseudodifferential operator, $Op^W(g(hB,z;l(x,h\xi)))$.

Not only the spectrum, but the density of states, can be reduced in the same way. Let $F\in C_0^\infty(\mathbb{R})$. Then $F(P_{B,V})$ is a smoothing operator, and the (smooth) distribution kernel, $K(x,y)$ satisfies: $K(x+\gamma,x+\gamma)=K(x,x)$. Following Shubin [Sh], and several other authors, we introduce the averaged trace,

(11) $\tilde{tr}\, F(P_{B,V})=\int_\Omega K(x,x)dx/Vol(\Omega)$,

where Ω is some fundamental domain of Γ. If $F\geq 0$, then $\tilde{tr}\, F(P_{B,V})\geq 0$, so there is a unique Radon measure, $\rho_{B,V}$ (the so called density of states) such that,

(12) $\tilde{tr}\, F(P_{B,V})=\int F(z)\,\rho_{B,V}(dz)$.

Let $\tilde{F}\in C_0^\infty(\mathbb{C})$ be an extension of F such that $\bar{\partial}\tilde{F}=\mathcal{O}(|Im(z)|)$. Then,

(13) $F(P_{B,V})=-(1/\pi)\int \dfrac{\partial\tilde{F}(z)}{\partial\bar{z}}\,(z-P_{B,V})^{-1}\,L(dz)$,

where L denotes the Lebesgue measure on $\mathbb{C}\simeq\mathbb{R}^2$. If F and $\tilde{F}$ have their support in a sufficiently small neighborhood of $\{z_0\}$, we can exploit the formula $(z-P_{B,V})^{-1}=-E^B(z)+E_+^B(z)(E_{-+}^B(z))^{-1}E_-^B(z)$, and that $E^B(z)$ is holomorphic in z, to get,

(14) $F(P_{B,V})=-(1/\pi)\int \dfrac{\partial\tilde{F}(z)}{\partial\bar{z}}\,E_+^B(z)(E_{-+}^B(z))^{-1}E_-^B(z)\,L(dz)$.

Next, we take the trace of this relation. One can show that,

(15) $\tilde{tr}\, E_+^B(E_{-+}^B)^{-1}E_-^B=\hat{tr}(E_-^BE_+^B(E_{-+}^B)^{-1})$,

where,

(16) $\hat{tr}(\mathcal{M}_B(f))=(Vol(\Omega))^{-1}\,tr(f(0))=(2\pi)^{-n}\int_{\mathbb{R}^{n*}/\Gamma^*} tr\, g(\theta)\,d\theta,\ f=\mathcal{F}g$.

Moreover,

(17) $E_-^BE_+^B=\partial E_{-+}^B/\partial z$.

If $Q=Op^W(g\circ l)$ is the operator in Theorem 2, we get:

$$(18)\quad \tilde{tr}\, F(P_{B,V}) = -(1/\pi)\int \frac{\partial F(z)}{\partial \bar{z}}\, \tilde{tr}((\partial Q/\partial z)\circ Q^{-1})\, L(dz)/\mathrm{Vol}(\Omega)$$

Here, in the case of Weyl-quantizations, we define $\tilde{tr}(Op^W(q))$ as the mean value of the trace of the symbol q. (This mean value exists in the case of $(\partial Q/\partial z)\circ Q^{-1}$). Further developments will appear in [HS2,3].

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