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LETTER TO THE EDITOR

On the adiabatic theorem of quantum mechanics

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Abstract. Let $H(t)$ be a Hamiltonian whose spectrum has for all t a finite number of disjoint components $\sigma_j(t)$. It is proved that when the change of $H(t)$ is made infinitely slow the system, when started from a state corresponding to $\sigma_k(0)$, passes through states corresponding to $\sigma_k(t)$, for all t.

Let us consider the family of self-adjoint operators $H(s)$, $s \in [0, 1]$, satisfying the following conditions.

(i) For all $T \in \mathbb{R}$, the equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s} U_T(s) = TH(s)U_T(s), \qquad U_T(0) = 1, \tag{1}$$

has a unique solution with $U_T(s)$ being a strongly continuous family of unitary operators.

(ii) There exist real continuous functions on $[0, 1]$, $a_j(s)$, $b_j(s)$, $j = 1, \ldots, N-1 < \infty$, with the properties

$$a_j(s) < b_j(s) \leqslant a_{j+1}(s) \qquad \min_j \inf_s (b_j(s) - a_j(s)) \geqslant d > 0$$

such that

$$\sigma(H(s)) = \bigcup_{j=1}^{N} \sigma_j(s)$$

$$\sigma_1(s) \subset (-\infty, a_1(s)]$$

$$\sigma_j(s) \subset [b_{j-1}(s), a_j(s)], \qquad j = 2, \ldots, N-1$$

$$\sigma_N(s) \subset [b_{N-1}(s), \infty).$$

(iii) Let $P_j(s)$ be the spectral projections of $H(s)$ corresponding to $\sigma_j(s)$. $P_j(s)$ are norm twice differentiable on $[0, 1]$.

(iv) $(H(s)-z)^{-1}$ is norm differentiable with respect to s on $[0, 1]$, and for every $\delta > 0$ there exists a $K_\delta < \infty$ such that

$$\left\|\frac{\mathrm{d}}{\mathrm{d}s}(H(s)-z)^{-1}\right\| \leqslant \frac{K_\delta}{\operatorname{dist}\{z, \sigma[H(s)]\}} \tag{2}$$

for all z satisfying $\operatorname{dist}\{z, \sigma[H(s)]\} > \delta$.

Under the above conditions we prove the following theorem.

Theorem (*the adiabatic theorem*).

$$\lim_{T\to\infty} \|U_T(s)P_j(0)-P_j(s)U_T(s)\|=0 \tag{3}$$

for all $s\in[0, 1]$ and $j=1, \ldots, N$.

Remarks.

(1) If for some $j=j_0$, $\sigma_{j_0}(s)$ consists of a single point, $\sigma_{j_0}(s)=\{\lambda(s)\}$, then (3) written for $j=j_0$ reduces to the standard adiabatic theorem (see Kato (1950) for the proof and Bohm (1954), Messiah (1960) for further references and the physical discussion). Our interest in generalising the adiabatic theorem came from relativistic quantum mechanics, where the spectrum of the relevant operators has two disjoint continuous parts (Nenciu 1978, 1980 On the adiabatic limit for Dirac particles in external fields (to be published)). Our result might be relevant also in solid state physics, due to the band structure of the spectrum of the Hamiltonians involved.

(2) For sufficient conditions to ensure (i) we refer to Reed and Simon (1975).

(3) The condition (ii) can be relaxed, allowing a finite number of eigenvalues belonging to $\sigma_j(s)$ to cross a finite number of eigenvalues belonging to $\sigma_{j+1}(s)$ or $\sigma_{j-1}(s)$. We imposed (ii) in order not to obscure the simple idea of the proof.

(4) It is not necessary for $H(s)$ to be independent of T. The result also holds true for general $H_T(s)$, as far as (i)–(iii) are fulfilled uniformly as $T\to\infty$.

(5) There are two steps in proving the adiabatic theorem. The first one is the construction of the adiabatic transformation $A(s)$. We add nothing to this step and we shall sketch, for completeness, the construction of $A(s)$, following closely Messiah (1960). The second step is to prove that the subspaces corresponding to $P_j(0)$ are invariant under $A^*(s)U_T(s)$ in the limit $T\to\infty$. This is the point where the previous proofs cannot be applied to our general case, and a different proof is needed.

Proof of the theorem.

1st step. Let $K(s)$ be defined by

$$K(s)=-\mathrm{i}\sum_{j=1}^{N} P_j(s)\frac{\mathrm{d}}{\mathrm{d}s}P_j(s). \tag{4}$$

The $K(s)$ are bounded and (Messiah 1960)

$$K(s)=K^*(s) \tag{5}$$

$$P_j(s)K(s)-K(s)P_j(s)=-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s}P_j(s). \tag{6}$$

Let $A(s)$ be defined by

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s}A(s)=K(s)A(s), \qquad A(0)=1. \tag{7}$$

Equation (7) has a unique solution satisfying $A^{-1}(s)=A^*(s)$ (Reed and Simon (1975) theorem X69). Using (6) and (7) one can verify that

$$\frac{\mathrm{d}}{\mathrm{d}s}[A^*(s)P_j(s)A(s)]=0, \qquad j=1, \ldots, N, \tag{8}$$

which implies that

$$P_j(0)=A^*(s)P_j(s)A(s), \qquad j=1,\ldots,N;\ s\in[0,1]. \tag{9}$$

$A(s)$ is the so-called adiabatic transformation.

2nd step. Consider the operator

$$\tilde{U}_T(s)=A^*(s)U_T(s). \tag{10}$$

By direct computation we have

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s}\tilde{U}_T(s)=\tilde{H}_T(s)\tilde{U}_T(s), \qquad \tilde{U}_T(0)=1, \tag{11}$$

$$\tilde{H}_T(s)=A^*(s)[TH(s)-K(s)]A(s). \tag{12}$$

Since $A^*(s)=A^{-1}(s)$ it follows that $\sigma[A^*(s)H(s)A(s)]=\sigma[H(s)]$ and then $\sigma[A^*(s)TH(s)A(s)]=\{T\lambda|\lambda\in\sigma[H(s)]\}$. Moreover, by (9), the $P_j(0)$ are the spectral projections of $A^*(s)H(s)A(s)$ corresponding to $\sigma_j(s)$. Because of (iii), $\|A^*(s)K(s)A(s)\|\leqslant M<\infty$ and then, for big enough T, $\sigma(\tilde{H}_T(s))$ has N disjoint components $\tilde{\sigma}_j(s)$.

The idea of the proof is to iterate the above procedure, defining $B(s)$ by

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s}B(s)=L(s)B(s), \qquad B(0)=1, \tag{13}$$

$$L(s)=-\mathrm{i}\sum_{j=1}^{N}Q_j(s)\frac{\mathrm{d}}{\mathrm{d}s}Q_j(s) \tag{14}$$

where $Q_j(s)$ are the spectral projections of $\tilde{H}_T(s)$ corresponding to $\tilde{\sigma}_j(s)$.

As for $A(s)$, one has

$$Q_j(0)=B^*(s)Q_j(s)B(s), \qquad j=1,\ldots,N;\ s\in[0,1]. \tag{15}$$

Now let $\Phi_T(s)$, $S_T(s)$ be defined by

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s}\Phi_T(s)=B^*(s)\tilde{H}_T(s)B(s)\Phi_T, \qquad \Phi_T(0)=1, \tag{16}$$

$$S_T(s)=\Phi_T^*(s)B^*(s)\tilde{U}_T(s). \tag{17}$$

By construction

$$\Phi_T(s)Q_j(0)=Q_j(0)\Phi_T(s), \qquad j=1,\ldots,N;\ s\in[0,1], \tag{18}$$

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}s}S_T(s)=-\Phi_T^*(s)B^*(s)L(s)B(s)\Phi_T(s)S_T(s), \qquad S_T(0)=1, \tag{19}$$

$$U_T(s)=A(s)B(s)\Phi_T(s)S_T(s). \tag{20}$$

Using (9), (18) and (20) one obtains the following identity:

$$\begin{aligned}U_T(s)P_j(0)-P_j(s)U_T(s)&\\ =A(s)B(s)\Phi_T(s)(S_T(s)-1)P_j(0)&+A(s)B(s)\Phi_T(s)(P_j(0)-Q_j(0))\\ +A(s)(Q_j(s)-P_j(0))B(s)\Phi_T(s)&+P_j(s)A(s)B(s)\Phi_T(s)(1-S_T(s)).\end{aligned} \tag{21}$$

Due to (21), the proof of the theorem is complete if

$$\lim_{T\to\infty} \|Q_j(s)-P_j(0)\|=0, \qquad j=1,\ldots,N;\ s\in[0,1], \tag{22}$$

$$\lim_{T\to\infty} \|S_T(s)-1\|=0, \qquad s\in[0,1]. \tag{23}$$

Writing (19) as an integral equation, (23) is implied by

$$\lim_{T\to\infty} \left\|\frac{\mathrm{d}}{\mathrm{d}s} Q_j(s)\right\|=0, \qquad j=1,\ldots,N;\ s\in[0,1]. \tag{24}$$

The proof of (22) and (24) rests in the following formula relating the spectral projections and the resolvent of self-adjoint operators:

$$\begin{aligned} Q_j(s)-P_j(0) &\\ &=(2\pi\mathrm{i})^{-1}\int_{C_j(s)} [(\tilde{H}_T(s)-z)^{-1}-(TA^*(s)H(s)A(s)-z)^{-1}]\,\mathrm{d}z\\ &=A^*(s)\left((2\pi\mathrm{i})^{-1}\int_{C_j(s)} (TH(s)-K(s)-z)^{-1}K(s)(TH(s)-z)^{-1}\,\mathrm{d}z\right)A(s) \end{aligned} \tag{25}$$

where $C_j(s)$ are contours surrounding $\sigma_j(s)\cup\tilde{\sigma}_j(s)$. We shall take $C_j(s)$ to be composed of straight lines of the form $x+\mathrm{i}y$, where x are the midpoints of the spectral gaps of $TH(s)$.

Taking the norms under the integral sign in the RHS of equation (26) and the fact that for a self-adjoint operator N

$$\|(N-z)^{-1}\|\leq 1/\mathrm{dist}(z,\sigma(N)),$$

one obtains for sufficiently large T

$$\|Q_j(s)-P_j(0)\|\leq \text{constant} \int_{-\infty}^{\infty} \left(y^2+T^2\frac{d^2}{16}\right)^{-1} \mathrm{d}y,$$

which proves (22).

Differentiating (25), and estimating as above using also (iv), one can prove (24), and the proof of the adiabatic theorem is complete.

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