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Localisation of states in quantum mechanics

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Abstract. A theory is presented to describe the possible simultaneous localisation of states, to arbitrary accuracy, in position and total energy $H = H_0 + V$, where V is locally singular and decays at infinity. The theory is entirely time-independent; that is, the time evolution of states in such potentials is not considered. Examples of localising potentials in this sense are relatively simple, and may be written down in closed form.

1. Introduction

In Quantum Mechanics, the Heisenberg uncertainty principle gives an absolute limit to the degree to which states may be localised simultaneously in position and momentum. One mathematical expression of this limit to localisability lies in the fact that $E_{x\in\Sigma_1} E_{p\in\Sigma_2}$ is *compact*, for any pair of finite intervals Σ_1, Σ_2. (Here $E_{T\in\Sigma}$ denotes the spectral projection of the self-adjoint operator T associated with the interval Σ.) This compactness implies that the norm of $E_{x\in\Sigma_1}E_{p\in\Sigma_2}$ converges to zero as the lengths of Σ_1, Σ_2 approach zero. Indeed, an estimate of this norm may be used to derive a lower bound for $(\delta x)(\delta P)$. (Here δT denotes the uncertainty, in a particular state, of the observable corresponding to T.)

This paper is devoted to exploring the possibility of localising states simultaneously in *position* and *total energy* H by means of a localising potential $V(\mathbf{r})$ which decays at infinity but which is locally singular. For simplicity, we shall suppose that V is locally regular away from the single point $\mathbf{r} = 0$; this condition could be relaxed to allow, for example, bounded singular surfaces.

As a measure of the degree to which states may be localised, we shall consider the function of energy $\gamma(\lambda)$ defined by

$$\gamma(\lambda) = \lim_{\substack{R\to 0\\ \varepsilon\to 0}} \|E_{|\mathbf{r}|<R}E_{|H-\lambda|<\varepsilon}\|,$$

where we shall show (Theorem 1) that $\gamma(\lambda)$ is always 0 or 1 at a given energy λ. If $\gamma(\lambda) = 0$, λ is called a regular point (Section 3), and if $\gamma(\lambda) = 1$, λ is called a singular point. Section 4 is devoted to abstract characterisations of regular and singular points, and of their distribution. It is shown in particular (Corollary 1 to Theorem 5) that the localisation implied by the existence of singular points manifests itself in a very clear violation of the uncertainty relation between position and total energy, and that this can happen for potentials which may be written down quite easily in closed form.

A subsequent paper will deal exclusively with short range potentials, and will provide a complete characterisation in that case of the types of localisation which can occur, together with an analysis of the consequences for Scattering Theory.

2. Mathematical preliminaries

Let H_0 be the unique self-adjoint extension, in $L^2(\mathbb{R}^3)$, of $-\Delta$, the negative Laplacian defined on $C_0^\infty(\mathbb{R}^3)$. Let V be a real potential which is locally square integrable away from the single point $\mathbf{r}=0$, and assume that V approaches zero in the limit $|\mathbf{r}|\to\infty$. (It is sufficient to assume that $V=V_s+V_L$, where, for any $R>0$, V_s and V_L are respectively square integrable and bounded in the region $|\mathbf{r}|>R$, with $\lim_{|\mathbf{r}|\to\infty} V_L(\mathbf{r})=0$.)

Define $\hat{H}=-\Delta+V$ with domain $C_0^\infty(\mathbb{R}^3\backslash\{0\})$, and let H be a self-adjoint extension of $\hat{H}$. If $\hat{H}$ is not essentially self-adjoint, the definition of H will involve boundary conditions at $\mathbf{r}=0$, but we shall not need to consider these boundary conditions explicitly.

Locally, away from $\mathbf{r}=0$, the domains $D(H_0)$, $D(H)$, of H_0 and H look the same. Let $\rho(r)$ be a non-decreasing function, infinitely differentiable for $0\le r<\infty$, such that $\rho(r)\equiv 0$ for all r sufficiently small, and $\rho(r)\equiv 1$ for all r sufficiently large. We shall use the same symbol ρ for the *function* $\rho(|\mathbf{r}|)$ as for the *operator*, in $L^2(\mathbb{R}^3)$, of multiplication by $\rho(|\mathbf{r}|)$. Then $f\in D(H)\Rightarrow \rho f\in D(H_0)$. Thus $\rho D(H)\subseteq D(H_0)$, and similarly

$$\rho D(H_0)\subseteq D(H),\qquad \rho D(H_0)\subseteq D(H_0),\qquad \rho D(H)\subseteq D(H).$$

It is often useful to note that, for example, $(H_0+1)\rho E_{H\in\Sigma}$ is bounded by the closed graph theorem, where Σ is a finite interval and $E_{H\in\Sigma}$ is the spectral projection of H associated with the interval Σ.

We shall make considerable use of compactness. The fact that $E_{|\mathbf{r}|<R}E_{H_0\in\Sigma}$ is compact (even Hilbert–Schmidt), where $E_{|\mathbf{r}|<R}$ denotes multiplication by the characteristic function of the ball $|\mathbf{r}|<R$, implies that $\lim_{R\to 0}\|E_{|\mathbf{r}|<R}E_{H_0\in\Sigma}\|=0$, so that states cannot be localised simultaneously in position near $\mathbf{r}=0$ and in kinetic energy.

For $\operatorname{Im} z\neq 0$, we have the identity

$$\rho(H_0-z)^{-1}-(H-z)^{-1}\rho=(H-z)^{-1}([H_0,\rho]+V\rho)(H_0-z)^{-1}.$$

Using $[H_0,\rho]=-\Delta\rho-2i\,(\nabla\rho)\cdot\mathbf{P}$, with $\mathbf{P}=$ momentum operator, one verifies that $[H_0,\rho]\;(H_0-z)^{-1}$ is compact. Since $V\rho$ is nonsingular, $V\rho(H_0-z)^{-1}$ is also compact. Hence $\rho(H_0-z)^{-1}-(H-z)^{-1}\rho$ is compact. Taking norm limits, for different z, of this result, it follows that

$$\rho\phi(H_0)-\phi(H)\rho$$

is compact for any $\phi\in C_0^\infty(\mathbb{R})$.

From the corresponding result with $V=0$, we know also that $\rho\phi(H_0)-\phi(H_0)\rho$ is compact, and hence so is $(\phi(H)-\phi(H_0))\rho$.

The method of Dirichlet decoupling ([1], [2], [3]) has previously been used to study the effect of local singularities of the potential. We shall denote by H_D the operator $-\Delta+V$ with Dirichlet boundary conditions at the surface of the sphere

$|\mathbf{r}|=L$, and with the same boundary conditions at $\mathbf{r}=0$ as for H. Then H_D is a self-adjoint operator in $L^2(\mathbb{R}^3)$ which "decouples" the regions $|\mathbf{r}|<L$ and $|\mathbf{r}|>L$. We shall denote by H_L the operator $-\Delta+V$ acting in $L^2(B)$, where B is the ball $|\mathbf{r}|<L$, with Dirichlet boundary conditions at $|\mathbf{r}|=L$ and again the same boundary conditions at $\mathbf{r}=0$ as for H. Then H_L is a self-adjoint operator in $L^2(B)$, and may be thought of as the part of H_D which acts in $L^2(B)$.

Lemma 1. *For* $\operatorname{Im} z\neq 0$, $(H-z)^{-1}-(H_D-z)^{-1}$ *is compact.*

Proof. Let $\rho_0(r)$ be a smooth, non-increasing function such that $\rho_0\equiv 1$ for $0\leq r\leq L/3$ and $\rho_0\equiv 0$ for $r\geq 2L/3$. Let $\rho_\infty(r)$ be a smooth, non-decreasing function such that $\rho_\infty(r)\equiv 0$ for $0\leq r\leq 2L$ and $\rho_\infty(r)\equiv 1$ for $r\geq 3L$. Define corresponding multiplication operators ρ_0, ρ_∞ with $r=|\mathbf{r}|$, and set $\rho_L=1-\rho_0-\rho_\infty$. Then ρ_L localises near $|\mathbf{r}|=L$, and

$$\rho_L(H-z)^{-1}=\rho_L(H_0-z)^{-1}(H_0-z)\rho(H-z)^{-1} \tag{1}$$

where ρ is smooth, non-decreasing, with $\rho\equiv 0$ near $r=0$ and $\rho\equiv 1$ on the support of ρ_L. On the r.h.s. of (1), $(H_0-z)\rho(H-z)^{-1}$ is bounded (closed graph theorem) and $\rho_L(H_0-z)^{-1}$ is compact. Hence $\rho_L(H-z)^{-1}$ is compact. Moreover, $(H_D-z)^{-1}\rho_L$ is compact. (For the part of this operator in $|\mathbf{r}|<L$ use local domain properties together with the compactness of the resolvent of $-\Delta$ with Dirichlet boundary conditions at $|\mathbf{r}|=L$. For the part in $|\mathbf{r}|>L$ use local domain properties together with the compactness of the resolvent of $-\Delta$ with Dirichlet boundary conditions at $|\mathbf{r}|=L$ and at $\mathbf{r}=4L$, acting in L^2 of the region $L<|\mathbf{r}|<4L$.)

Writing

$$\begin{aligned}(H-z)^{-1}-(H_D-z)^{-1}&=\rho_L(H-z)^{-1}-(H_D-z)^{-1}\rho_L\\&\quad+(1-\rho_L)(H-z)^{-1}-(H_D-z)^{-1}(1-\rho_L),\end{aligned}$$

it remains only to prove compactness of

$$\rho_0(H-z)^{-1}-(H_D-z)^{-1}\rho_0$$

and of

$$\rho_\infty(H-z)^{-1}-(H_D-z)^{-1}\rho_\infty.$$

But this follows as for the proof in the case of the operator $\rho(H_0-z)^{-1}-(H-z)^{-1}\rho$, using commutation relations for H and H_D with ρ_0 and ρ_∞ and noting that locally H and H_D have the same domains away from $|\mathbf{r}|=L$. Hence the result.

A final technical result which we shall need is as follows.

Lemma 2. *In* $L^2(B)$, *where* B *is the ball* $|\mathbf{r}|<L$, *let* $\mathcal{D}$ *denote the set of elements belonging to* $D(H_L)$ *which have compact support in* $|\mathbf{r}|<L$. *(Such elements are of the form* $(1-\rho)f$ *for some* $f\in D(H_L)$, *where* $\rho(r)$ *is smoothly non-decreasing with* $\rho\equiv 0$ *near* $|\mathbf{r}|=0$ *and* $\rho\equiv 1$ *near* $|\mathbf{r}|=L$.) *For* $\lambda\in\mathbb{R}$, *let* $P_{(\lambda)}$ *denote the projection onto the closure of* $(H_L-\lambda)\mathcal{D}$.

Then, if Σ *is any finite interval with* λ *not in the closure of* Σ, $E_{H_L\in\Sigma}(1-P_{(\lambda)})$ *is compact.*

Proof. Define ρ_0 as in the proof of Lemma 1. Then

$$(H_D-\lambda)\rho_0 E_{H_D\in\Sigma}-\rho_0(H_D-\lambda)E_{H_D\in\Sigma}=-(\Delta\rho_0+2i\nabla\rho_0\cdot\mathbf{P})\rho_1 E_{H_D\in\Sigma} \tag{2}$$

where $\rho_1(r)\in C_0^\infty(0,L)$ and $\rho_1\equiv 1$ on the support of $\nabla\rho_0$. Using the facts that $(H_0+1)\rho_1 E_{H_D\in\Sigma}$ is bounded and $(\Delta\rho_0+2i\,\nabla\rho_0\cdot\mathbf{P})(H_0+1)^{-1}$ is compact, we see that the r.h.s. of (2) is compact. Projecting equation (2) onto the subspace of $L^2(\mathbb{R}^3)$ corresponding to $L^2(B)$, we have that

$$(H_L-\lambda)\rho_0 E_{H_L\in\Sigma}-\rho_0(H_L-\lambda)E_{H_L\in\Sigma}$$

is compact. Now the range of $\rho_0 E_{H_L\in\Sigma}$ is contained in $\mathscr{D}$, so that $(1-P_{(\lambda)})\times(H_L-\lambda)\rho_0 E_{H_L\in\Sigma}=0$. Hence $\{(1-P_{(\lambda)})\rho_0 E_{H_L\in\Sigma}(H_L-\lambda)\}^*$ is compact. Since λ is not in the closure of Σ, the restriction of $H_L-\lambda$ to the range of $E_{H_L\in\Sigma}$ is an operator with a bounded inverse, so that $E_{H_L\in\Sigma}\rho_0(1-P_{(\lambda)})$ is compact.

The conclusion of the lemma now follows from the observation that $E_{H_L\in\Sigma}(1-\rho_0)$ is compact. (Local domain properties plus compactness of the resolvent of $-\Delta$ with Dirichlet boundary conditions at $|\mathbf{r}|=L$.)

Remark (i) The orthogonal subspace to $(H_L-\lambda)\mathscr{D}$ consists of those $f\in L^2(B)$ which satisfy both the equation $(-\Delta+V)f=\lambda f$ and the boundary condition for H_L (equivalently H) at $\mathbf{r}=0$. Thus $(1-P_{(\lambda)})$ is the projection onto such f.

Remark (ii) The condition that λ not lie in the closure of Σ is intended to rule out the cases where λ is a limit point of eigenvalues, or an eigenvalue of infinite multiplicity. These cases can indeed occur for Hamiltonians of the generality considered here.

3. Localisation of states; regular and singular points

As a measure of the degree to which states can be localised simultaneously in position (near $\mathbf{r}=0$) and total energy H, we define, for finite intervals Σ of energy, the function $\gamma(\Sigma)$ by

$$\gamma(\Sigma)=\lim_{R\to 0}\|E_{|\mathbf{r}|<R}E_{H\in\Sigma}\| \tag{3}$$

If we are to consider localisation at a single energy λ rather than a range of energies Σ, we define

$$\gamma(\lambda)=\lim_{\substack{R\to 0\\ \varepsilon\to 0}}\|E_{|\mathbf{r}|<R}E_{|H-\lambda|<\varepsilon}\| \tag{3$'$}$$

where $E_{|H-\lambda|<\varepsilon}$ is the spectral projection of H associated with the interval $(\lambda-\varepsilon,\lambda+\varepsilon)$. The limits (3), (3)′ always exist and in (3)′ the $\gamma(\lambda)$ is independent of the manner in which the limits are taken. (This follows from the fact that

$$\gamma(\lambda)=\inf_{\substack{R>0\\ \varepsilon>0}}\|E_{|\mathbf{r}|<R}E_{|H-\lambda|<\varepsilon}\|.)$$

Clearly in each case $0\leq\gamma\leq 1$. It is sometimes convenient to replace $E_{|H-\lambda|<\varepsilon}$ in (3)′ by a smooth function of H. Define a function $\phi_\varepsilon(x)$, infinitely differentiable, increasing in the interval $[\lambda-2\varepsilon,\lambda-\varepsilon]$ and decreasing in $[\lambda+\varepsilon,\lambda+2\varepsilon]$, such that

$\phi_\varepsilon(x) \equiv 1$ for $|x-\lambda| \le \varepsilon$ and $\equiv 0$ for $|x-\lambda| \ge 2\varepsilon$. Then

$$\chi_\varepsilon(x) \le \phi_\varepsilon(x) \le \chi_{2\varepsilon}(x),$$

where χ_ε is the characteristic function of $(\lambda-\varepsilon, \lambda+\varepsilon)$. It follows from (3)′ that we also have

$$\gamma(\lambda) = \lim_{\substack{R\to 0\\ \varepsilon\to 0}} \|E_{|\mathbf{r}|<R}\phi_\varepsilon(H)\|. \tag{4}$$

The following lemma shows that localisation in position may be replaced by localisation at large kinetic energy.

Lemma 3. *For finite intervals* Σ,

$$\gamma(\Sigma) = \lim_{M\to\infty} \|E_{H_0>M}E_{H\in\Sigma}\|. \tag{5}$$

Proof. In (5), $E_{H_0>M}$ is the spectral projection of H_0 for the interval (M, ∞). Let $\gamma'(\Sigma)$ be the limit on the r.h.s. of (5). We show first $\gamma \le \gamma'$; then $\gamma \ge \gamma'$.
(i) $\gamma \le \gamma'$: We have

$$E_{|\mathbf{r}|<R}E_{H\in\Sigma} = E_{|\mathbf{r}|<R}E_{H_0>M}E_{H\in\Sigma} + E_{|\mathbf{r}|<R}E_{H_0<M}E_{H\in\Sigma}. \tag{6}$$

Given $\delta>0$, choose M such that $\|E_{H_0>M}E_{H\in\Sigma}\| \le \gamma'+\delta$. Then $\lim_{R\to 0}\|E_{|\mathbf{r}|<R}E_{H_0<M}\| = 0$ by compactness, so that applying the triangle inequality to (6) we have

$$\gamma = \lim_{R\to 0}\|E_{|\mathbf{r}|<R}E_{H\in\Sigma}\| \le \gamma'+\delta.$$

Since δ was arbitrary, this yields $\gamma \le \gamma'$.

(ii) $\gamma \geqslant \gamma'$: Define as before a multiplication operator ρ with $\rho(r)\equiv 0$ for small r and $\rho(r)\equiv 1$ for $r \ge R$, with R sufficiently small that $\|(1-\rho)E_{H\in\Sigma}\| \le \gamma+\delta$. Then $\|E_{H_0>M}E_{H\in\Sigma}\| \le \gamma+\delta+\|E_{H_0>M}\rho E_{H\in\Sigma}\|$, where we have

$$\begin{aligned}\|E_{H_0>M}\rho E_{H\in\Sigma}\| &= \|E_{H_0>M}(H_0+1)^{-1}(H_0+1)\rho E_{H\in\Sigma}\|\\ &\le \|E_{H_0>M}(H_0+1)^{-1}\| \times \|(H_0+1)\rho E_{H\in\Sigma}\|\\ &\le \text{const}\,(M+1)^{-1} \to 0 \quad \text{as} \quad M\to\infty.\end{aligned}$$

Hence $\gamma' = \lim_{M\to\infty}\|E_{H_0>M}E_{H\in\Sigma}\| \le \gamma+\delta$. So $\gamma' \le \gamma$, and we have finally $\gamma' = \gamma$. Taking a second limit we also obtain, from (3)′,

$$\gamma(\lambda) = \lim_{\substack{M\to\infty\\ \varepsilon\to 0}} \|E_{H_0>M}E_{|H-\lambda|<\varepsilon}\| \tag{7}$$

where again the manner in which the limits are taken is immaterial. We now have our first basic result on localisation.

Theorem 1. *For any given* λ, $\gamma(\lambda)$ *is either* 0 *or* 1.

Proof. Let ρ be a monotonic multiplication operator as before, vanishing near $r=0$, with $\rho\equiv 1$ for large enough r. Suppose that ρ has support in $[1, \infty)$.

Define $\phi_\varepsilon(H)$ as in (4). Then $E_{|\mathbf{r}|<1}\rho=0$. Moreover

$$E_{|\mathbf{r}|<1}\phi_\varepsilon(H)\rho E_{H_0<M}=-E_{|\mathbf{r}|<1}\{\rho\phi_\varepsilon(H_0)-\phi_\varepsilon(H)\rho\}E_{H_0<M}$$

is compact, by compactness of the operator in curly brackets. On the other hand, $(1-\rho)E_{H_0<M}$ is compact, and hence

$$E_{|\mathbf{r}|<1}\phi_\varepsilon(H)E_{H_0<M} \tag{8}$$

is compact. Now write, for $R<1$,

$$\begin{aligned}E_{|\mathbf{r}|<R}\phi_\varepsilon^2(H)&=E_{|\mathbf{r}|<R}\{E_{|\mathbf{r}|<1}\phi_\varepsilon^2(H)E_{H_0<M}\}\\&\quad+E_{|\mathbf{r}|<R}\{E_{|\mathbf{r}|<1}E_{H_0<M}\}\phi_\varepsilon^2(H)E_{H_0>M}\\&\quad+E_{|\mathbf{r}|<R}E_{H_0>M}\phi_\varepsilon^2(H)E_{H_0>M}.\end{aligned} \tag{9}$$

The terms in curly brackets are compact, and give norm convergence to zero when we take the limit $R\to 0$, so that

$$\lim_{R\to 0}\|E_{|\mathbf{r}|<R}\phi_\varepsilon^2(H)\|\leq\|E_{H_0>M}\phi_\varepsilon^2(H)E_{H_0>M}\|=\|E_{H_0>M}\phi_\varepsilon(H)\|^2. \tag{10}$$

Now take the limits $\varepsilon\to 0$, $M\to\infty$, using (4) (with ϕ_ε^2 for ϕ_ε), and (7) with $E_{|H-\lambda|<\varepsilon}$ replaced by $\phi_\varepsilon(H)$. Then (10) gives $\gamma(\lambda)\leq(\gamma(\lambda))^2$. But certainly $\gamma(\lambda)\geq(\gamma(\lambda))^2$, since $0\leq\gamma(\lambda)\leq 1$. So $\gamma(\lambda)=(\gamma(\lambda))^2$, and the result follows.

Corollary. *Let P_0 be any projection commuting with H, such that*

$$\lim_{\varepsilon\to 0}\|E_{|\mathbf{r}|>R}E_{|H-\lambda|<\varepsilon}(1-P_0)\|=0, \tag{11}$$

for some (equivalently all) $R>0$. Define $\gamma_0(\lambda)$ by

$$\gamma_0(\lambda)=\lim_{\substack{R\to 0\\ \varepsilon\to 0}}\|E_{|\mathbf{r}|<R}E_{|H-\lambda|<\varepsilon}P_0\| \tag{12}$$

Then, for any given λ, $\gamma_0(\lambda)$ is either 0 *or* 1.

Proof. Use the identity (9) with $\phi_\varepsilon(H)$ replaced by $\phi_\varepsilon(H)P_0$. (Analogous results to, e.g., (7), may be proved for $\gamma_0(\lambda)$.) On the r.h.s. of this modified identity write, for the first term,

$$\begin{aligned}E_{|\mathbf{r}|<1}\phi_\varepsilon^2(H)P_0E_{H_0<M}&=\{E_{|\mathbf{r}|<1}\phi_\varepsilon^2(H)E_{H_0<M}\}\\&\quad-E_{|\mathbf{r}|<1}\phi_\varepsilon^2(H)(1-P_0)\{(1-\rho)E_{H_0<M}\}\\&\quad-E_{|\mathbf{r}|<1}\phi_\varepsilon^2(H)(1-P_0)\rho E_{H_0<M}.\end{aligned}$$

Operators in curly brackets are compact, so that proceeding as before we obtain

$$\begin{aligned}\lim_{R\to 0}\|E_{|\mathbf{r}|<R}\phi_\varepsilon^2(H)P_0\|&\leq\|E_{H_0>M}\phi_\varepsilon^2(H)P_0E_{H_0>M}\|\\&\quad+\|\phi_\varepsilon^2(H)(1-P_0)\rho E_{H_0<M}\|\end{aligned}$$

where by (11) the second norm on the r.h.s. goes to zero in the limit $\varepsilon\to 0$. Take, then, the successive limits $\varepsilon\to 0$, then $M\to\infty$, and $\gamma_0\leq\gamma_0^2$ as before, from which the result follows.

Definition. λ is a *regular point* if $\gamma(\lambda)=0$, and a *singular point* if $\gamma(\lambda)=1$.

A similar result to Theorem 1 holds for intervals.

Theorem 2. *Let $\Sigma=[a,b]$ be a finite interval, and suppose that a and b are regular points. Then $\gamma(\Sigma)=0$ or 1, with $\gamma(\Sigma)=0$ if and only if Σ contains no singular points.*

Proof. Define a smooth function $\psi_\varepsilon(x)$, increasing in $[a-\varepsilon,a]$ and decreasing in $[b,b+\varepsilon]$, such that $\psi_\varepsilon\equiv 1$ for $x\in[a,b]$ and $\psi_\varepsilon\equiv 0$ in the complement of $(a-\varepsilon,b+\varepsilon)$. Then ψ_ε differs from the characteristic function of $[a,b]$ only on $(a-\varepsilon,a)\cup(b,b+\varepsilon)$, and since a, b are regular points this implies

$$\lim_{\substack{\varepsilon\to 0\\ R\to 0}}\|E_{|\mathbf{r}|<R}(E_{H\in\Sigma}-\psi_\varepsilon(H)\|=0.$$

As in the proof of Theorem 1, $E_{|\mathbf{r}|<1}\psi_\varepsilon(H)E_{H_0<M}$ is compact, so that, for fixed ε,

$$\lim_{R\to 0}\|E_{|\mathbf{r}|<R}\psi_\varepsilon(H)E_{H_0<M}\|=0.$$

Combining these two results gives

$$\lim_{R\to 0}\|E_{|\mathbf{r}|<R}E_{H\in\Sigma}E_{H_0<M}\|=0.$$

The proof that $\gamma(\Sigma)=0$ or 1 now proceeds as for Theorem 1, starting from (9) with everywhere $\phi_\varepsilon(H)$ replaced by $E_{H\in\Sigma}$.

Now suppose Σ contains a singular point λ. Then $\gamma(\Sigma)\geq\gamma(\lambda)=1$, so that $\gamma(\Sigma)=1$.

On the other hand, suppose $\gamma(\Sigma)=1$ but that Σ contains no singular point. In that case, if $\Sigma_1=[a,(a+b)/2]$ and $\Sigma_2=[(a+b)/2,b]$, then either $\gamma(\Sigma_1)=1$ or $\gamma(\Sigma_2)=1$, since $\gamma(\Sigma_1)=\gamma(\Sigma_2)=0$ would imply $\gamma(\Sigma)=0$. Proceeding to subdivide the interval, we can construct a sequence $\{\Sigma_{n_i}\}$ of intervals, converging on a single point λ, such that $\gamma(\Sigma_{n_i})=1$. We have, then, $\gamma(\lambda)=1$ for this limiting point, in contradiction with our assumption. Hence $\gamma(\Sigma)=1\Leftrightarrow\Sigma$ contains at least one singular point, and the proof is complete.

Corollary. *With the same assumptions as for the Theorem,*

(i) $\gamma(\Sigma)=0\Leftrightarrow E_{|\mathbf{r}|<R}E_{H\in\Sigma}$ is compact ($R>0$).
(ii) $E_{|\mathbf{r}|<R}(H-z)^{-1}$ is compact ($\operatorname{Im} z\neq 0$)$\Leftrightarrow$there are no singular points.

Proof. (i) If $E_{|\mathbf{r}|<R}E_{H\in\Sigma}$ is compact, we immediately deduce $\gamma(\Sigma)=0$. Conversely, suppose $\gamma(\Sigma)=0$. For $0<R<1$, one may use local domain properties to show that $E_{R<|\mathbf{r}|<1}E_{H\in\Sigma}$ is compact. Hence

$$E_{|\mathbf{r}|<1}E_{H\in\Sigma}=E_{R<|\mathbf{r}|<1}E_{H\in\Sigma}+E_{|\mathbf{r}|<R}E_{H\in\Sigma}$$

and is the sum of a compact operator and an operator norm convergent to zero. It follows that this operator is compact, and similarly for $E_{|\mathbf{r}|<R}E_{H\in\Sigma}$.

(ii) Use $E_{|\mathbf{r}|<R}(H-z)^{-1}=\lim_{M\to\infty}E_{|\mathbf{r}|<R}E_{|H|<M}(H-z)^{-1}$.

Remark. Notice that (i) the set of singular points is closed, and (ii) each singular point λ belongs to $\sigma_{\text{ess}}(H)$.

To verify (i), observe that if λ is a *regular* point, $\|E_{|\mathbf{r}|<R}E_{|H-\lambda|<\varepsilon}\|<\frac{1}{2}$ for R, ε sufficiently small. Hence, for any fixed $\lambda' \in (\lambda-\varepsilon, \lambda+\varepsilon)$, $\gamma(\lambda') \leq \|E_{|\mathbf{r}|<R}E_{|H-\lambda|<\varepsilon}\| < \frac{1}{2}$, so that $\gamma(\lambda')=0$. Thus regular points form an open set, and the result follows.

To verify (ii), observe that if $\lambda \notin \sigma_{ess}(H)$ then $E_{|H-\lambda|<\varepsilon}$ is compact for small ε, and it follows that λ is a regular point.

4. Characterisation of singular points

It is simplest to characterise the *negative* singular points, and we have

Theorem 3. *The set of negative singular points is* $\sigma_{ess}(H) \cap (-\infty, 0)$.

Proof. We have seen that singular points belong to $\sigma_{ess}(H)$. It remains to prove that $\lambda \in \sigma_{ess}(H)$, $\lambda<0$, $\Rightarrow \lambda$ is a singular point.

Construct an orthonormal sequence $\{f_n\}$ of vectors, such that $E_{|H-\lambda|>(1/n)}f_n = 0$. (Thus each f_n has H-spectral support contained in $[\lambda-(1/n), \lambda+(1/n)]$.) If λ is an eigenvalue of infinite multiplicity, let $\{f_n\}$ be orthonormal sequence of eigenvectors. Otherwise, choose spectral supports for different n to be non-overlapping.)

Find $\phi \in C_0^\infty(\mathbb{R})$ with $\phi(\lambda)=1$ such that the support of ϕ is contained in $(-\infty, 0)$. Now $\rho\phi(H_0)-\phi(H)\rho$ is compact. But $\sigma(H_0)=[0,\infty)$, so that $\rho\phi(H)$ is compact on taking adjoints.

Since $f_n \to 0$ weakly, we have $\rho\phi(H)f_n \to 0$ strongly. But $(\phi(H)-1)f_n \to 0$ strongly. Hence $\rho f_n \to 0$ strongly.

Since the support of $1-\rho$ can be taken to lie in an arbitrarily small neighbourhood of $\mathbf{r}=0$, we see that the sequence $\{f_n\}$ asymptotically localises in position near $\mathbf{r}=0$. Clearly the sequence also localises in energy at λ, and it follows that $\gamma(\lambda)=1$.

Remark. One can define $\gamma(\lambda)$ for $\lambda=-\infty$ by

$$\gamma(-\infty) = \lim_{\substack{R\to 0 \\ K\to\infty}} \|E_{|\mathbf{r}|<R}E_{H<-K}\| \tag{13}$$

It may be shown that $\gamma(-\infty)=0$ or 1, with $\gamma(-\infty)=0$ if and only if H is semi-bounded. One can also set

$$\gamma(\infty) = \lim_{\substack{R\to 0 \\ K\to\infty}} \|E_{|\mathbf{r}|<R}E_{H>K}\|. \tag{13'}$$

It is not clear, in this case, whether always $\gamma(\infty)=0$ or 1. However, one can show that if there are no (finite) singular points then either $\gamma(-\infty)=1$ or $\gamma(+\infty)=1$. In this sense, if we extend the notion of singular points to include $\lambda=\pm\infty$, then H *always* has singular points (which may be infinite). For most Hamiltonians considered in scattering theory one has $\lambda=+\infty$ as the only singular point.

A characterisation which applies also to *positive* singular points is as follows.

Theorem 4. *The set of (finite) singular points is* $\sigma_{ess}(H_L)$.

Proof. Define $\phi_\varepsilon(H)$ as in equation (4). Lemma 1 implies that $\phi_\varepsilon(H)-\phi_\varepsilon(H_D)$ is compact. We have, then, from equation (4),

$$\gamma(\lambda)=\lim_{\substack{R\to 0\\ \varepsilon\to 0}}\|E_{|\mathbf{r}|<R}\phi_\varepsilon(H_D)\|. \tag{14}$$

(Thus H and H_D have the same singular points.) Since H_L is the part of H_D in $L^2(B)$, where B is the ball $|\mathbf{r}|<L$, it follows from (14) that

$$\gamma(\lambda)=\lim_{\substack{R\to 0\\ \varepsilon\to 0}}\|E_{|\mathbf{r}|<R}E_{|H_L-\lambda|<\varepsilon}\|. \tag{14$'$}$$

(i) Consider first the case where λ is an eigenvalue of $H_{L'}$ with infinite multiplicity. Then certainly $\lambda\in\sigma_{\text{ess}}(H_L)$, and we have to show $\gamma(\lambda)=1$.

Define a smooth, non-decreasing multiplication operation ρ on $L^2(B)$, with $\rho\equiv 0$ near $r=0$ and $\rho\equiv 1$ near $r=L$. Then $\rho E_{|H_L-\lambda|<\varepsilon}$ is compact, and as in the proof of Theorem 3 we can show that an orthonormal sequence $\{g_n\}$ of eigenvectors with eigenvalue λ localises asymptotically near $\mathbf{r}=0$. Hence $\gamma(\lambda)=1$ as required.

(ii) Now suppose either that λ is not on eigenvalue of H_L, or that λ is an eigenvalue of finite multiplicity. Let $P^{(\lambda)}$ denote the projection onto the eigenspace, with $P^{(\lambda)}=0$ if λ is not an eigenvalue.

Since $P^{(\lambda)}$ is compact,

$$\lim_{\substack{R\to 0\\ \varepsilon\to 0}}\|E_{|\mathbf{r}|<R}E_{|H_L-\lambda|<\varepsilon}P^{(\lambda)}\|=0,$$

so that (14)′ gives

$$\gamma(\lambda)=\lim_{\substack{R\to 0\\ \varepsilon\to 0}}\|E_{|\mathbf{r}|<R}E_{|H_L-\lambda|<\varepsilon}(1-P^{(\lambda)})\|. \tag{15}$$

But $E_{|\mathbf{r}|>R}E_{|H_L-\lambda|<\varepsilon}$ is compact, and $s-\lim_{\varepsilon\to 0}E_{|H_L-\lambda|<\varepsilon}(1-P^{(\lambda)})=0$, so that

$$\lim_{\varepsilon\to 0}\|E_{|\mathbf{r}|>R}E_{|H_L-\lambda|<\varepsilon}(1-P^{(\lambda)})\|=0.$$

Equation (15) now implies that

$$\gamma(\lambda)=\lim_{\substack{R\to 0\\ \varepsilon\to 0}}\|E_{|H_L-\lambda|<\varepsilon}(1-P^{(\lambda)})\|,$$

and it follows easily that

$$\gamma(\lambda)=1\Leftrightarrow\lambda\in\sigma_{\text{ess}}(H_L).$$

We now introduce some further definitions which will allow us to study more closely the distribution of singular points.

For given $L>0$, define $\mathcal{D}$ as in Lemma 2, and for any $\lambda\in\mathbb{R}$ define $\beta(\lambda, L)$ by

$$\beta(\lambda, L)=\inf_{f\in\mathcal{D}}\|(H_L-\lambda)f\|/\|f\|. \tag{16}$$

Since, locally in $|\mathbf{r}|<L$, H and H_L have the same domain, we could equivalently

write

$$\beta(\lambda, L) = \inf_{f \in \mathscr{D}} \|(H-\lambda)f\|/\|f\|, \tag{16$'$}$$

where $\mathscr{D}$ is regarded now as the subset of $L^2(\mathbb{R}^3)$ consisting of those $f \in D(H)$ having compact support in $|\mathbf{r}| < L$.

It is easy to verify that (i) $\beta(\lambda, L)$ is monotonic non-decreasing as L decreases, (ii)

$$|\beta(\lambda_1, L) - \beta(\lambda_2, L)| \leq |\lambda_1 - \lambda_2|. \tag{17}$$

We now define $\beta(\lambda)$ by

$$\beta(\lambda) = \lim_{L \to 0} \beta(\lambda, L), \tag{18}$$

allowing always the possibility $\beta(\lambda) = +\infty$.

We now have

Theorem 5.

(i) $\beta(\lambda) = 0 \Leftrightarrow \lambda$ *is a singular point.*

(ii) $\beta(\lambda)$ *is the distance from* λ *to the nearest singular point; in particular* $\beta(\lambda) = \infty \Leftrightarrow$ *there are no (finite) singular points.*

Proof. (i) Suppose $\beta(\lambda) = 0$. Then $\exists$ a normalised sequence $\{f_n\}$ of vectors, asymptotically localised near $\mathbf{r} = 0$, and such that $s - \lim_{n \to \infty} (H-\lambda)f_n = 0$. For any $\alpha > 0$, we have

$$\|E_{|H-\lambda|>\alpha} f_n\| \leq \frac{1}{\alpha} \|(H-\lambda)f_n\| \to 0,$$

so that the sequence localises asymptotically at energy λ. Hence $\gamma(\lambda) = 1$; we prove the converse as part of (ii).

(ii) Suppose $\beta(\lambda) > 0$. Given $\varepsilon > 0$, arbitrarily small, find L (depending on ε) sufficiently small that $\beta(\lambda) > 2\varepsilon$ and

$$\|(H_L - \lambda)f\| \geq (\beta(\lambda) - \varepsilon)\|f\|, \tag{19}$$

for all $f \in \mathscr{D}$. From now on, L will be fixed. Then

$$\begin{aligned} \|E_{|H_L-\lambda|<\beta(\lambda)-2\varepsilon}(H_L - \lambda)f\| &\leq (\beta(\lambda) - 2\varepsilon)\|E_{|H_L-\lambda|<\beta(\lambda)-2\varepsilon} f\| \\ &\leq (\beta(\lambda) - 2\varepsilon)\|f\| \leq \frac{\beta(\lambda) - 2\varepsilon}{\beta(\lambda) - \varepsilon}\|(H_L - \lambda)f\|, \end{aligned} \tag{20}$$

for all $f \in \mathscr{D}$. Hence the restriction of $E_{|H_L-\lambda|<\beta(\lambda)-2\varepsilon}$ to $(H_L - \lambda)\mathscr{D}$ has norm strictly smaller that 1.

Now define $P_{(\lambda)}$ as in Lemma 2, and we have shown that

$$\|E_{|H_L-\lambda|<\beta(\lambda)-2\varepsilon} P_{(\lambda)}\| < 1. \tag{21}$$

Let Σ be any subinterval of $(\lambda - \beta(\lambda) + 2\varepsilon, \lambda + \beta(\lambda) - 2\varepsilon)$ not containing λ in its closure. Then (21) implies

$$\|E_{|\mathbf{r}|<R} E_{H_L \in \Sigma} P_{(\lambda)}\| < 1,$$

whereas Lemma 2 implies

$$\lim_{R\to 0} \|E_{|\mathbf{r}|<R} E_{H_L \in \Sigma}(1-P_{(\lambda)})\| = 0.$$

Combining these results, we have, then

$$\lim_{R\to 0} \|E_{|\mathbf{r}|<R} E_{H_L \in \Sigma}\| < 1.$$

It follows that $\lim_{R\to 0} \|E_{|\mathbf{r}|<R} E_{H_D \in \Sigma}\| < 1$, and that the interval $(\lambda - \beta(\lambda) + 2\varepsilon, \lambda + \beta(\lambda) - 2\varepsilon)$ can contain no singular point (of H_D, and hence of H). (The possibility that λ itself might be singular can be ruled out, by applying the same argument to a point λ' very close to λ, and using the fact that, from (17) in the limit $L \to 0$, $\beta(\lambda)$ is continuous.)

Since ε was arbitrary, the nearest singular point to λ is at distance at least $\beta(\lambda)$. We have verified in particular that λ is singular implies $\beta(\lambda) = 0$, completing the proof of (i).

It remains to show that there is a singular point within, say, distance $\beta(\lambda) + 2\varepsilon$ of λ. Suppose again $\beta(\lambda) > 0$.

Let $\{g_n\}$ be a normalised sequence asymptotically approaching $\mathbf{r} = 0$, such that

$$\|(H-\lambda)g_n\| \le \beta(\lambda) + \varepsilon. \tag{22}$$

Then

$$\begin{aligned}\|E_{|H-\lambda|>\beta(\lambda)+2\varepsilon} g_n\| &\le \frac{1}{\beta(\lambda)+2\varepsilon} \|E_{|H-\lambda|>\beta(\lambda)+2\varepsilon}(H-\lambda)g_n\| \\ &\le \frac{\beta(\lambda)+\varepsilon}{\beta(\lambda)+2\varepsilon} < 1.\end{aligned}$$

We cannot have $\lim_{R\to 0} \|E_{|\mathbf{r}|<R} E_{|H-\lambda| \le \beta(\lambda)+2\varepsilon}\| = 0$, since this would imply, for n large enough,

$$\|g_n\| = \|E_{|H-\lambda|\le\beta(\lambda)+2\varepsilon} g_n + E_{|H-\lambda|>\beta(\lambda)+2\varepsilon} g_n\| < 1.$$

So, by Theorem 2, $[\lambda - \beta(\lambda) - 2\varepsilon, \lambda + \beta(\lambda) + 2\varepsilon]$ contains a singular point for any $\varepsilon > 0$, and this completes the proof.

Corollary 1. *Suppose $H \upharpoonright C_0^\infty(\mathbb{R}^3\backslash\{0\})$ is essentially self-adjoint. Let λ be a singular point. Then $\exists$ a normalised sequence $\{\phi_n\}$ in $C_0^\infty(\mathbb{R}^3\backslash\{0\})$ such that the support of ϕ_n is contained in $|\mathbf{r}| < 1/n$, and such that $s-\lim_{n\to\infty}(H-\lambda)\phi_n = 0$.*

(That is an asymptotically localising sequence can be found of C_0^∞ functions, such that the uncertainty in H approaches zero.)

Proof. Let ρ_0 be smooth, non-increasing, with $\rho_0(r) \equiv 1$ near $r = 0$ and $\rho_0(r) \equiv 0$ near $r = L$.

Given $f \in \mathcal{D}$, $\exists$ sequence $\{\psi_n\} \in C_0^\infty(\mathbb{R}^3\backslash\{0\})$ such that $\psi_n \to f$ and $H\psi_n \to Hf$. (Strong limits.) Using the commutation relation of H with ρ_0, one also finds $(H\rho_0)\psi_n \to H\rho_0 f$. It follows that equation (16)′ may be replaced by

$$\beta(\lambda, L) = \inf_{\phi \in \mathcal{D}'} \|(H-\lambda)\phi\|/\|\phi\|,$$

where $\mathscr{D}'$ is the set of infinitely differentiable functions having compact support in $0<|\mathbf{r}|<L$. The result then follows from the fact that $\beta(\lambda)=0$.

Corollary 2. *Suppose* $\exists$ *no solution in* $L^2(B)$ *of the equation* $(-\Delta+V)h=\lambda h$, *such that the boundary condition at* $\mathbf{r}=0$ *is satisfied. Then* λ *is a singular point.*

Proof. Suppose the hypothesis, and that λ is a regular point. Then $\beta(\lambda)>0$. In Lemma 2, we have $P_{(\lambda)}=1$, so that (21) implies $\lambda\notin\sigma(H_L)$. Since $(H_L-\lambda)\mathscr{D}$ is dense in $L^2(B)$, it follows that $(H_L-\lambda)^{-1}$ is essentially self-adjoint on $(H_L-\lambda)\mathscr{D}$. Hence $(H_L-\lambda)$ is e.s.a. on $\mathscr{D}$. But this leads to a contradiction, since elements of $\mathscr{D}$ vanish near $|\mathbf{r}|=L$, and infinitely many self-adjoint extensions of $H_L\restriction\mathscr{D}$ can be found. It follows that λ is a singular point.

Examples of localising potentials

So called 'absorbing" potentials, which in Scattering Theory may give rise to violations of asymptotic completeness and of unitarity of the scattering operator [4], and locally singular short range potentials for which the associated total Hamiltonian has a spectrally singular continuous component [5], [6], are two classes of potential which lead to localisation of states in the sense described above. In this connection, it is important to realise that there is no *necessary* link between the phenomenon of localisation and "unusual" spectral properties of H. For example it is known [7], at least in the one-dimensional case, that singular spectrum of H_D at positive energies, for a short range potential, will not generate singular spectrum of H, despite the fact that localisation will occur for such a total Hamiltonian. We shall deal with this point in a further publication, which will explore the relation between localisability for H_D and H respectively, and the consequences for Scattering Theory.

From neither of the two classes of potential mentioned above is it easy to construct examples in closed form. To remedy this we put forward the following example of a localising potential which, however, belongs to a different class and is illustrative of quite different phenomena: for $0<r<1$, define $u(r)$ by

$$u(r)=\frac{1}{r}\sin^2\left(\frac{1}{r}\right)+r^\beta,$$

for some $\beta>1$, and for some fixed λ_0 define $V(r)$ $(0<r<1)$ by

$$-\frac{d^2u}{dr^2}+V(r)u(r)=\lambda_0u(r),$$

with $V(r)=0$ for $r>1$. It is not difficult to check that

$$\int_0^1 u^2(t)\,dt=\infty \quad\text{and that}\quad \int_0^1\frac{1}{u^2(t)}\,dt=\infty.$$

The point of this choice of $u(r)$ is that the differential equation $-d^2\psi/dr^2+V(r)\psi=\lambda_0\psi$ has no non-trivial solution in $L^2(0,1)$. For such a solution would need to be a linear combination of $u(r)$ and $u(r)\int_r^1 1/u^2(t)\,dt$, whereas no such linear combination can be square integrable. By Corollary 2 (or rather a one-dimensional statement of this result), it follows that λ_0 is a singular point of the differential operator $-d^2/dr^2 + V(r)$ in $L^2(0, \infty)$, and so also of $-\Delta + V(|\mathbf{r}|)$ in $L^2(\mathbb{R}^3)$.

The function $u(r)$ in this example approaches, for large β, a function (viz. $1/r \sin^2 1/r$) which, while non-negative, has a graph which repeatedly touches the $u = 0$ axis. One can study analytically what happens to solutions $\psi(r)$ in this limit, for a general class of functions $u(r)$, and finds that one is dealing, canonically, with H_D having a limit point of eigenvalues at threshold. (In other words, λ_0 is a limit point of eigenvalues, and there is no spectrum below λ_0.) Further results for potentials generated in this way will be given elsewhere.

As a final example, albeit an artificial one, of a localising potential, take $V(\mathbf{r}) = -1/r^3$. The restriction of $-\Delta + V$ to each angular momentum partial wave subspace $\mathcal{H}(l, m)$ is then an ordinary differential operator having deficiency indices (1, 1). In each partial wave subspace, a boundary condition at $r = 0$ can be found to ensure, either that a given value λ_0 is an an eigenvalue of H_L in each subspace, or that λ_0 is a limit point of such eigenvalues, as the quantum numbers l and m are varied. This family of boundary condition will define a particular self-adjoint extension H of $-\Delta + V$, and again H will be a localising Hamiltonian, at energy λ_0. A localising sequence of states in this instance will be characterised by asymptotically large angular momentum quantum numbers.

The brief catalogue of various classes of localising potentials which we have presented here is by no means a complete list of all the possibilities that may occur. Rather I have tried to indicate a few avenues that might usefully be explored, and to lay down in this paper the beginnings of a theoretical framework within which such exploration might take place.

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