

MAXIMALLY RESONANT POTENTIALS SUBJECT TO p -NORM CONSTRAINTS

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We prove the existence of and characterize quantum-mechanical potentials within certain L^p -classes that produce maximally sharp resonances. The best results are obtained in the spherically symmetric case where it is shown that, roughly speaking, maximally sharp resonances are caused by barrier confinement of a metastable state, although in some cases there is interaction in the interior of the confining barrier.

I. Introduction. The question of optimizing various spectral properties of Schrödinger operators has recently received attention in several articles [2, 5, 6]. For example in [2] Ashbaugh and Harrell consider (among other things) various self-adjoint realizations of $H = -\Delta + V(x)$ (or more generally $A + V(x)$ where A is a uniformly elliptic operator) on bounded regions in \mathbf{R}^n for $n = 1, 2, 3$. The potential V satisfies the constraint $\|V\|_p \leq M$ for fixed $p(n)$, M but otherwise is unspecified. The authors show the existence and analyze potentials V that maximize or minimize eigenvalues of H . In particular such potentials are supported everywhere in the region and are connected with their wave functions by the algebraic relation

$$(1.1) \quad |\psi|^2 = cV^{p-1}$$

for some constant c (which can be assumed equal to 1 by renormalizing ψ if necessary). This can then be substituted into the eigenvalue equation and will yield the following non-linear differential equation characterizing the wave function of such an optimal potential:

$$(1.2) \quad A\psi \pm |\psi|^{(p+1)/(p-1)} \operatorname{sgn}(\psi) = E\psi.$$

In the one-dimensional specialization (1.2) can be integrated and interpreted as a problem in classical dynamics. Optimizing potentials in that case are characterized quite explicitly.

The basic ideas in [2] can also be used to analyze potentials optimizing eigenvalue gaps or resonance widths. This paper is devoted to the latter question. The motivation comes from quantum mechanical considerations. A particle surrounded by a large potential barrier might move inside the barrier for a considerable period of time before penetrating it (or tunnelling through it) and escaping to infinity. The system behaves

almost as if it were in a bound state. The effect of the penetration can show up in scattering as a sharp resonance. Resonances can be conveniently defined as nonreal eigenvalues of the complex-scaled Schrödinger operator. The real part, E , of the resonance eigenvalue roughly corresponds to the energy at which resonance is observed and the minus imaginary part ε measures the width of the resonance in units of energy. A sharp resonance is one with small ε , and by the uncertainty principle ε may be inversely proportional to the lifetime of a metastable state, i.e. to the time spent by the particle in the interior of the barrier.

While barrier confinement is known to produce sharp resonances, it is by no means obvious that this is the only physical mechanism capable of producing this phenomenon. This provides a motivation for the question we are asking: to what degree sharp resonances are due to tunnelling? The answer is that essentially barrier confinement of a metastable state produces the sharpest possible resonances although in certain situations there are also interactions in the interior of the confining barrier.

The problem has already been studied in [6]. There we considered the differential equation

$$(1.3) \quad -d^2\psi/dr^2 + V\psi = k^2\psi$$

on the interval $[0, L] \supset \text{supp } V$. In (1.3) $k^2 = E - i\varepsilon$ ($E, \varepsilon > 0$) is the resonance eigenvalue, V is presumed bounded, and the wave function ψ satisfies the Dirichlet boundary condition at 0 and the outgoing condition at L :

$$(1.4) \quad \psi(0) = 0; \quad \frac{\psi'}{\psi}(L) = ik.$$

Generalizations of (1.3), (1.4) to higher dimension were also considered in which case the equation

$$(1.5) \quad -\Delta\psi + V\psi = k^2\psi$$

holds in a bounded domain $\Omega \subset \mathbf{R}^2$ or \mathbf{R}^3 .

Note that one can think of the one-dimensional problem as coming from separation of variables in a spherically symmetric three-dimensional problem, in which case it describes S -wave resonances. We shall therefore refer to the one-dimensional problem as the (totally) spherically symmetric case. Resonances for subspaces of nonzero angular momentum correspond to the outgoing condition of the form

$$\frac{\psi'}{\psi}(L) \rightarrow ik \quad \text{as } L \rightarrow \infty$$

and are discussed in [11].

In [6] we were concerned with the problem of minimizing ϵ within the class of potentials

$$S_\infty(\Omega) = \{ V: V \geq 0, \text{supp } V \subset \Omega, \|V\|_\infty \leq M \}$$

for a fixed domain $\Omega \subset \mathbf{R}^+, \mathbf{R}^2$ or \mathbf{R}^3 and a large fixed number M . All such potentials are exteriorly dilation analytic as defined in [4, 10] with dilation taking place outside a ball containing Ω , and equations (1.3), (1.4) and (1.5) are equivalent to the operator eigenvalue problem for the complex-scaled Hamiltonian. An optimal potential is called maximally resonant and denoted by $V_\#$.

In the totally spherically symmetric case a quite detailed description of such a potential was obtained. In particular, it was proved that it can only equal M on its support which consists of a finite number of closed intervals (barriers). Moreover, the last barrier stretches all the way to the right most point of $\Omega = [0, L]$. This shows that maximally sharp resonances are due at least in part to barrier confinement of a metastable state. Another property of a maximally resonant potential is the fact that the intervals on which it is supported are characterized by the sign of $\text{Im } \psi_\#^2$ in the sense that $\text{Im } \psi_\#^2 \geq 0$ on the support and $\text{Im } \psi_\#^2 \leq 0$ outside of the support of $V_\#$ in Ω .

This paper extends the results in [6] to the class of potentials

$$S_p(\Omega) = \{ V: V \geq 0, \text{supp } V \subset \Omega, \|V\|_p \leq M \}$$

for $p \geq 2$ if $n = 2$ or 3 and $p > 1$ if $n = 1$. Moreover, in the latter case we also consider the class

$$S_1(\Omega) = \left\{ V: \text{positive bounded Borel measures in } \Omega \text{ with } \int_0^L V(dx) \leq M \right\}.$$

All such potentials are once again exteriorly dilation analytic with respect to a dilation taking place outside any ball containing Ω . It turns out that for every p maximally resonant potentials exist within the classes $S_p(\Omega)$ and just as in the case of $p = \infty$, the sign of $\text{Im } \psi_\#^2$ determines the intervals on which they are supported. However, unlike the previous case, each maximally resonant potential is now a smooth function characterized by a nonlinear second order differential equation that contains the corresponding wave function as the inhomogeneous term.

The results are somewhat different when $p = 1$. In this case elliptic functions arise. We shall discuss this in the last section.

II. Existence of maximally resonant potentials. The existence proof closely follows that in [6] with only minor changes. Since it very much depends on compactness arguments, we first prove the existence of

maximally resonant potentials within those producing resonances in a fixed energy range.

Thus given C and D satisfying $0 \leq C < D < \infty$ for every allowed p , we define classes

$$(2.1) \quad S_p^{(C,D)}(\Omega) = S_p(\Omega) \cap \{V: C \leq E(V) \leq D\}$$

where C and D are chosen so that $S_p^{(C,D)}$ is not empty.

THEOREM II.1. *For fixed Ω , M , p , C , D , let $\varepsilon_{\#} = \inf\{\varepsilon(V): V \in S_p^{(C,D)}(\Omega)\}$. Then the infimum is attained, i.e. there is $V_{\#} \in S_p^{(C,D)}(\Omega)$ such that $\varepsilon(V_{\#}) = \varepsilon_{\#}$ and moreover $\varepsilon_{\#} > 0$.*

REMARKS.

(1) Just as in [6] there is no guarantee of uniqueness.

(2) We shall prove the theorem under the assumption $p \geq 2$. As one can see from the proof it works for every such p and is independent of dimension n as long as $n \leq 3$. The proof for $1 \leq p < 2$ is similar and can be found in [11].

Proof. Let Ω_1 be an arbitrary finite ball containing Ω . Let $\{V_n\}$ be a minimizing sequence of potentials, i.e. $\varepsilon(V_n) \downarrow \varepsilon_{\#}$. Let $\{\psi_n\}$ and $\{k_n^2\}$ be sequences of associated eigenfunctions and eigenvalues, respectively.

Now we start extracting subsequences. First of all, by the compactness of $[C, D]$, there is a subsequence of $\{k_n^2\}$ that converges to some limit $k_{\#}^2$. We may also normalize $\{\psi_n\}$ such that $\|\psi_n\|_{\infty} = 1$. It then follows from

$$-\Delta\psi_n + V_n\psi_n = k_n^2\psi_n$$

that $\{\psi_n\}$ is bounded in $W_2^2(\Omega_1)$. By Rellich's Theorem, $\{\psi_n\}$ is compactly embedded into $C(\Omega_1)$, so we can pass to a subsequence converging uniformly to some limit $\psi_{\#}$. Finally, by the Banach-Alaoglu Theorem, we can extract a subsequence of $\{V_n\}$ converging weakly in $L^p(\Omega_1)$ to some limit $V_{\#}$. Moreover, $\|V_{\#}\|_p \leq M$ and $V_{\#} \geq 0$.

Now for every $f \in C_0^{\infty}(\Omega_1)$ and each n

$$(f, (-\Delta + V_n)\psi_n) = (f, k_n^2\psi_n).$$

Letting $n \rightarrow \infty$ we find that in the sense of distributions

$$(-\Delta + V_{\#})\psi_{\#} = k_{\#}^2\psi_{\#}.$$

Thus $V_{\#} \in S_p^{(C,D)}(\Omega)$.

It remains to show that $\varepsilon_{\#} > 0$. Suppose $\varepsilon_{\#} = 0$. Then either $E_{\#} > 0$ or $k_{\#}^2 = 0$. If $E_{\#} > 0$, this would imply by the usual argument of dilation analyticity that $k_{\#}^2$ is a positive embedded eigenvalue of the self-adjoint realization of the problem. Embedded positive eigenvalues however are impossible for the potentials under consideration [3, 7, 9].

The other possibility is also easily ruled out: if $k_{\#}^2 = 0$, then $\psi_{\#}$ satisfies

$$(-\Delta + V_{\#})\psi_{\#} = 0$$

without complex scaling. In particular,

$$0 = (\psi_{\#}, -\Delta\psi_{\#}) + (\psi_{\#}, V_{\#}\psi_{\#}) = \int_{\mathbb{R}^r} |\nabla\psi_{\#}|^2 dx + (\psi_{\#}, V_{\#}\psi_{\#}) > 0$$

contradiction. □

Now in order to show the existence of maximally resonant potentials in $S_p(\Omega)$ (for every p) we let $C \downarrow 0$ and $D \uparrow \infty$ and prove that at least in the totally spherically symmetric case there are no sharp resonances in either low or high energy regimes. Thus we need an idea of how small ε can be for fixed L and M , the length of the support of the potential and its L^p -norm, respectively. The simplest case is that of a square barrier of length L and height M (i.e. when $p = \infty$). In that case one can easily find a resonance with width $\varepsilon = O(\exp(-L\sqrt{M}))$. This shows that when these two quantities are sufficiently large there are indeed very sharp resonances. The following proposition shows that in the totally spherically symmetric case, ε cannot be too small when the energy E is either very high or very low.

PROPOSITION II.2. *Every resonance with $\varepsilon < \max(1/2L^2, 1/L^3)$ satisfies $\pi^2/4L^2 < E < CM^2L^{2-2/p}$, where the constant C can be chosen arbitrarily close to 1 by choosing M or L sufficiently large.*

REMARKS. (1) For the proof of the lower bound see [6]. The upper bound on E is obtained using a variation of parameters argument. For details see [11].

(2) The proof of the lower bound uses the fact that $\psi \in C^1[0, L]$ and thus we cannot immediately extend it to the case $p = 1$. However, as we show in the last section any maximally resonant measure in $S_1(\Omega)$ has to be absolutely continuous in $[0, L]$. That would imply that even in this case the bound remains valid.

COROLLARY II.3. *In the totally spherically symmetric case if M and L are sufficiently large, there exists a potential $V_{\#}$ in every $S_p(\Omega)$ for $1 \leq p < \infty$ that is maximally resonant for the entire energy range $0 \leq E(V) \leq \infty$. Moreover, $\pi^2/4L^2 \leq E(V_{\#}) \leq CM^2L^{2-2/p}$ where the constant C can be taken arbitrarily close to 1 by choosing L or M appropriately large.*

III. Characterization of maximally resonant potentials. Now that the existence of maximally resonant potentials has been proved, the next step is to attempt to characterize them. We remark that just as in the case $p = \infty$ potentials under consideration are relatively form compact with respect to the exteriorly complex scaled free Hamiltonian. Thus resonances associated with $V_{\#}$ are all finitely degenerate and can accumulate only at 0 or ∞ . They will always be nondegenerate in the totally spherically symmetric case and in general we shall restrict ourselves to characterizing those maximally resonant potentials whose resonance eigenvalues are nondegenerate.

The basic idea is to perturb the maximally resonant potential $V_{\#}$ slightly by appropriate functions and analyze the first order change in $k_{\#}^2$. This method will characterize not only the global minimum of the functional $\epsilon(V)$ but other local extrema as well. Thus, just as in [6] we make the following

DEFINITION. For any fixed Ω , M and p , $1 < p \leq \infty$, the potential $V_{\#}$ is locally maximally resonant for the set $S_p(\Omega)$ if it has a resonance eigenvalue $k^2(V_{\#})$ such that for sufficiently small δ ,

$$\epsilon(V_{\#}) = \min_V \left\{ \epsilon(V) : V \in S_p(\Omega), \|V - V_{\#}\|_p < \delta \text{ and } |k^2(V) - k^2(V_{\#})| < \delta \right\}.$$

The definition is similar when $p = 1$. If $p \geq 2$, the basic formula for the first order change in $k_{\#}^2$ corresponding to the small perturbation of $V_{\#}$ by a bounded function P supported in Ω ($V_{\#} \rightarrow V_{\#} + \lambda P$ for small $\lambda \in \mathbf{R}$) is

$$(3.1) \quad \frac{dk^2}{d\lambda} = \frac{\int_{\Omega} P\psi_{\theta}^2 dx}{\int_{\mathbf{R}^n} \psi_{\theta}^2 dx} \equiv \alpha \int_{\Omega} P\psi_{\theta}^2 dx$$

where ψ_{θ} is the exteriorly complex scaled wave function and $\alpha \equiv 1/\int_{\mathbf{R}^n} \psi_{\theta}^2 dx$ is independent of P [6]. When $1 \leq p < 2$ Formula (3.1) is only slightly modified by putting everything in the language of quadratic forms [11]. (We shall drop the subscript θ in the future).

We shall now consider the case $p \geq 2$ (or $p > 1$ when $n = 1$). The remaining case $p = 1$ is considered separately in the last section. Suppose now for some fixed Ω , M and p , $V_{\#}$ is maximally resonant in $S_p(\Omega)$.

A perturbation $V_{\#} \rightarrow V_{\#} + \lambda P$ will be called admissible iff the perturbed potential remains in $S_p(\Omega)$, i.e. $\|V_{\#} + \lambda P\|_p \leq M$ and $V_{\#} + \lambda P \geq 0$. There will be several such admissible perturbations. Using Formula (3.1) for each of them will yield the basic relation between $\psi_{\#}$ and $V_{\#}$ which is the analog of (1.1) in the self-adjoint case. Our first result is

PROPOSITION III.1. *Either $\|V_{\#}\|_p = M$ or otherwise $\psi_{\#} \equiv 0$ on $\text{supp } V_{\#}$.*

REMARKS. (1) The support of $V_{\#}$ is defined as for generalized functions and not in the classical sense.

(2) It follows from above proposition and the unique continuation property [7] that if $\|V_{\#}\|_p < M$, then $\text{supp } V_{\#}$ is a nowhere dense set. While we cannot rule out the possibility that in higher dimensions maximally resonant potentials might be supported on such a set, we conjecture, however, that this does not occur. It is also clear that in the spherically symmetric case one must have $\|V_{\#}\|_p = M$: if $\psi_{\#}(r_0) = 0$ for some $r_0 > 0$, then on the interval $[0, r_0]$ we have a self-adjoint problem with Dirichlet boundary conditions at the end points. This forces $\varepsilon = 0$ which contradicts Theorem II.1. Thus the nodal surface of $\psi_{\#}$ in the spherically symmetric case is of measure zero. Moreover, we show below (cf. Proposition III.3) that in the spherically symmetric case $\text{supp } V_{\#}$ consists of a finite number of closed intervals and thus nowhere dense sets are ruled out.

Proof. We will only sketch the proof since it is similar to the one in [6]. Suppose $\|V_{\#}\|_p < M$. Let T be a small set in $\text{supp } V_{\#}$. The perturbation $V_{\#} \rightarrow V_{\#} + \lambda \chi_T$ is then admissible for small λ . Formula (3.1) implies that $\text{Im } \alpha \psi^2 \equiv 0$ on $\text{supp } V$ which in turn implies $\psi \equiv 0$ on $\text{supp } V$. \square

THEOREM III.2. *Let $V_{\#}$ denote a maximally resonant potential in $S_p(\Omega)$ for some fixed Ω , M and p . Then*

(a) $\text{Im } \alpha \psi_{\#}^2 / V_{\#}^{p-1} = c \geq 0$ a.e. on $Y \equiv \text{supp } V_{\#}$. Moreover, $c > 0$ unless $\psi \equiv 0$ on Y .

(b) $\text{Im } \alpha \psi_{\#}^2 \leq 0$ outside $\text{supp } V_{\#}$ in Ω .

In particular $\text{Im } \alpha \psi_{\#}^2 \geq 0$ on Y and $\text{Im } \alpha \psi_{\#}^2 \leq 0$ on the complement of Y in Ω .

Proof.

(a) Let $T_2, T_2 \subset \text{supp } V_{\#}$ be two small sets of equal Lebesgue measure centered at y_1 and y_2 respectively. For small real λ let

$$(3.2) \quad V(\lambda) = V_{\#} + \lambda(\chi_{T_1} - \eta_1 \chi_{T_2})$$

where $\eta_1 = \eta_1(\lambda, T_1, T_2)$ is chosen so that $\|V(\lambda)\|_p = \|V_{\#}\|_p \leq M$. One can easily show by expanding the integral for $\|V(\lambda)\|_p^p$ that the last condition is insured iff for almost every $y_1, y_2 \in \text{supp } V_{\#}$, $\eta_1(\lambda) \rightarrow V_{\#}^{p-1}(y_1)/V_{\#}^{p-1}(y_2)$ as $\lambda \rightarrow 0$ and the sets T_1 and T_2 converge to their centers y_1 and y_2 .

Substituting (3.2) into (3.1) we get:

$$\frac{d\varepsilon}{d\lambda} \Big|_{\lambda=0} = -\text{Im} \alpha \left[\psi_{\#}^2(y_1) - \frac{V_{\#}^{p-1}(y_1)}{V_{\#}^{p-1}(y_2)} \psi_{\#}^2(y_2) \right] = 0.$$

This implies that a.e. on $\text{supp } V_{\#}$

$$(3.3) \quad \frac{\text{Im} \alpha \psi_{\#}^2}{V_{\#}^{p-1}} = \text{const} \equiv c.$$

To show that $c \geq 0$ we notice that $V_{\#} \rightarrow V_{\#} + \lambda \chi_{T_1}$ is an admissible perturbation for $\lambda \leq 0$. Using (3.1) once again we find that

$$\frac{d\varepsilon}{d\lambda} \Big|_{\lambda=0} = -\text{Im} \alpha \psi_{\#}^2 \leq 0.$$

If we assume that $c = 0$, then $\text{Im} \alpha \psi_{\#}^2 \equiv 0$ on $\text{supp } V_{\#}$ and this once again would imply $\psi_{\#} \equiv 0$ on $\text{supp } V_{\#}$.

(b) If T_1 still denotes a small set in the support of $V_{\#}$ centered at y_1 and S_1 small set of equal Lebesgue measure in the complement of the support in Ω centered at z_1 , then the perturbation

$$(3.4) \quad V(\lambda) = V_{\#} + \lambda(\chi_{S_1} - \eta_2 \chi_{T_1})$$

(where $\eta_2 = \eta_2(\lambda, T_1, S_1)$ is chosen so that $\|V(\lambda)\|_p = \|V_{\#}\|_p \leq M$) is admissible if $\lambda \geq 0$. One can show just as before, that $\eta_2 \rightarrow 0$ as $\lambda \rightarrow 0$, and Formula (3.1) will then yield the remaining part of the theorem. \square

In the rest of the paper we consider only the totally spherically symmetric case. We have shown that just as for $p = \infty$, the sign of $\text{Im} \alpha \psi_{\#}^2$ (or $\text{Im} \psi_{\#}^2$ if we normalize $\psi_{\#}$ so that $\alpha = 1$) determines the set on which $V_{\#}$ is supported. Moreover, $\arg \psi$ is a monotone increasing function for any resonance wave function:

$$(3.5) \quad \frac{d}{dr} \arg \psi = \frac{\varepsilon}{|\psi(r)|^2} \int_0^r |\psi(y)|^2 dy.$$

(for the proof see [6].) These two facts combined show that maximally resonant potentials in $S_p(\Omega)$ for all $1 < p < \infty$ (just as for $p = \infty$) possess the ‘switching property’. By this we mean that the potential switches on and off as soon as $\arg \psi$ has increased by $\pi/2$. More precisely:

PROPOSITION III.3. *If $V_{\#} \in S_p(\Omega)$ for any $1 < p \leq \infty$ is maximally resonant and spherically symmetric, then $Y \equiv \text{supp } V_{\#}$ is a finite union of disjoint intervals. That is for some integer $N \geq 1$, there are points*

$$0 \leq r_1 < r_2 < \dots < r_{2N} \leq L$$

for which, if we let $B(j) = [r_{2j-1}, r_{2j}]$ and $G(j) = [r_{2j}, r_{2j+1}]$, then $\text{supp } V_{\#} \equiv Y = \bigcup_{j=1}^N B(j)$. In addition, we have lower bounds on the lengths of $B(j)$ and $G(j)$ for all j except (i) when $j = 1$, i.e. $r_1 = 0$ or (ii) $j = N$ when the associated interval or gap includes the point L :

$$|B(j)| \geq \pi \min_{B(j)} |\psi_{\#}^2| / 2K$$

$$|G(j)| \geq \pi \min_{G(j)} |\psi_{\#}^2| / 2K.$$

For the proof see [6].

DEFINITION. We call the intervals $B(j)$ the ‘‘barriers,’’ and the intervals $G(j)$ the ‘‘gaps’’.

The above proposition shows that the switching property is common to all spherically symmetric maximally resonant potentials in $S_p(\Omega)$ for all $1 < p \leq \infty$. However, what is peculiar to the case $p = \infty$ is the discontinuity and two-valuedness of $V_{\#}$. As we show next, for each $1 < p < \infty$, each maximally resonant potential in $S_p(\Omega)$ has a smooth representative in the interior of its support.

THEOREM III.4. *In the spherically symmetric case, $V_{\#}$ has a continuous representative in $[0, L)$. Moreover, $V_{\#} \in C^{\infty}(\overset{\circ}{B}(j))$ for all $1 \leq j \leq N$, where $\overset{\circ}{B}(j) = (r_{2j-1}, r_{2j})$.*

Proof. Relation (3.3) shows that in the interior of every barrier

$$V_{\#}^{p-1} = \frac{1}{c} \text{Im } \alpha \psi_{\#}^2.$$

The continuity of $V_{\#}$ on $\overset{\circ}{B}(j)$ for any $1 \leq j \leq N$ follows immediately by the continuity of $\text{Im } \alpha \psi_{\#}^2$. Moreover, discontinuities cannot occur at the boundary, i.e. at points $\{r_i\}_{i=1}^{2N}$ (with the possible exception of $r_{2N} = L$,

where the potential is switched off automatically). For $\text{Im } \alpha \psi_{\#}^2 \geq 0$ on $B(j)$ and $\text{Im } \alpha \psi_{\#}^2 \leq 0$ on $G(j)$, so $\text{Im } \alpha \psi_{\#}^2(r_i) = 0$ for all $1 \leq i \leq 2N$. But also

$$\frac{\text{Im } \alpha \psi_{\#}^2(r_i)}{V_{\#}^{p-1}(r_i)} = c > 0.$$

Hence $V_{\#}^{p-1}(r_i) = 0$.

To prove the second part of the theorem, we substitute $V_{\#} = [(1/c) \text{Im } \alpha \psi_{\#}^2]^{1/(p-1)}$ into the eigenvalue equation.

$$-\psi_{\#}'' + \left[\frac{1}{c} \text{Im } \alpha \psi_{\#}^2 \right]^{1/(p-1)} \psi_{\#} = k_{\#}^2 \psi_{\#}.$$

It follows now that $V_{\#} \in C^{\infty}(\dot{B}(j))$ for any $1 \leq j \leq N$ by elliptic regularity. □

Formula (3.3):

$$\text{Im } \alpha \psi_{\#}^2 = c V_{\#}^{p-1}$$

gives the relation between the optimal potential and the imaginary part of its wave function. Can one find a relation between $V_{\#}$ and $\psi_{\#}$ itself rather than its imaginary part? The answer is yes but unlike (1.1) for the self-adjoint case it is not an algebraic relation (when $p > 1$) but a differential equation.

PROPOSITION III.5. *If $V_{\#}$ is a maximally resonant potential in $S_p(\Omega)$ for some $1 < p < \infty$ and $\psi_{\#}$ is its wave function, then they are related via the second order nonlinear differential equation*

$$(3.6) \quad 4\epsilon \alpha \psi_{\#}^2 = \frac{d^2}{dr^2} [c V_{\#}^{p-1}] - 2 \left[\left(2 - \frac{1}{p} \right) V_{\#} - 2 \bar{k}_{\#}^2 \right] [c V_{\#}^{p-1}] + \text{const}$$

that holds on each $B(j)$. Moreover, unless $r_{2N} = L \in B(N)$, $V_{\#}$ satisfies the boundary condition at the end points of each barrier $V_{\#}(r_{2j-1}) = V_{\#}(r_{2j}) = 0$.

Proof. For uncluttered notation we drop the subscript $\#$. We start differentiating (3.3) remembering that

$$\psi'' = (V - k^2)\psi.$$

Thus we find

$$\begin{aligned} 2 \text{Im } \alpha \psi \psi' &= (d/dr) [c V^{p-1}], \\ (*) \quad 2 [\text{Im } \alpha \psi'^2 + \text{Im } \alpha \psi \psi''] &= 2 [\text{Im } \alpha \psi'^2 + \text{Im } \alpha (V - k^2) \psi^2] \\ &= (d^2/dr^2) [c V^{p-1}]. \end{aligned}$$

Now

$$\begin{aligned} \operatorname{Im} \alpha(V - k^2)\psi^2 &= \operatorname{Im} \alpha(V - E)\psi^2 + \operatorname{Im} \alpha(i\varepsilon)\psi^2 \\ &= (V - E) \operatorname{Im} \alpha\psi^2 + \varepsilon \operatorname{Re} \alpha\psi^2 = (V - E)[cV^{p-1}] + \varepsilon \operatorname{Re} \alpha\psi^2. \end{aligned}$$

So (*) becomes

$$2[\operatorname{Im} \alpha\psi'^2 + (V - E)[cV^{p-1}] + \varepsilon \operatorname{Re} \alpha\psi^2] = \frac{d^2}{dr^2} [cV^{p-1}].$$

After we differentiate one more time and simplify, we find that

$$2\left[2 \frac{d}{dr} (V - E)[cV^{p-1}] - \frac{d}{dr} \left[\frac{c}{p} V^p\right] + 4\varepsilon \operatorname{Re} \alpha\psi\psi'\right] = \frac{d^3}{dr^3} [cV^{p-1}].$$

Integrating the last relation and solving for $4\varepsilon \operatorname{Re} \alpha\psi^2$ we find:

$$4\varepsilon \operatorname{Re} \alpha\psi^2 = \frac{d^2}{dr^2} [cV^{p-1}] - 2\left[\left(2 - \frac{1}{p}\right)V - 2E\right][cV^{p-1}] + \text{const}$$

and

$$i4\varepsilon \operatorname{Im} \alpha\psi^2 = i4\varepsilon [cV^{p-1}].$$

Adding these two equations yields (3.6). In particular, when $p = 2$, (3.6) becomes

$$4\varepsilon \alpha\psi^2 = cV'' - [3V - 4\bar{k}^2]cV + \text{const}. \quad \square$$

REMARK. If $V_{\#}$ is a maximally resonant potential in $S_p(\Omega)$ for fixed L , M and p can it also be maximally resonant in some other class $S_{p'}(\Omega)$ for $p' \neq p$ and $M' \neq M$? The answer is no, which can be easily seen from Relation (3.3): suppose $V_{\#}$ is maximally resonant in $S_p(\Omega)$ and $S_{p'}(\Omega)$, and $\|V_{\#}\|_p = M$ and $\|V_{\#}\|_{p'} = M'$. Then by (3.3) $(\operatorname{Im} \alpha\psi_{\#}^2)/V_{\#}^{p-1} = c$ and $(\operatorname{Im} \alpha\psi_{\#}^2)/V_{\#}^{p'-1} = c'$. Hence, $V_{\#}^{p-p'} = \text{const}$ which implies $V_{\#} = \text{const}$ since $p' \neq p$. But then $\operatorname{Im} \alpha\psi_{\#}^2 = \text{const}$ on $\operatorname{supp} V_{\#}$. This constant has to be zero since $\operatorname{Im} \alpha\psi_{\#}^2 = 0$ on the boundary of the support of $V_{\#}$. We have thus once again arrived at a familiar contradiction.

We close this section with the figure depicting a typical maximally resonant potential in $S_p(\Omega)$ for some fixed p , $1 < p < \infty$. The gaps $G(j)$ are the closed intervals on which $\operatorname{Im} \alpha\psi_{\#}^2 \leq 0$. The barriers $B(j)$ are the closed intervals where $\operatorname{Im} \alpha\psi_{\#}^2 \geq 0$. Inside the barriers the potential $V_{\#}$ is a smooth function connected with its wave function through the second-order non-linear equation (3.6). The question of how many times the switch occurs remains open. We expect that the same situation holds here as in the $p = \infty$ case. The potential will switch on inside the outer barrier if the resonance wave function has a sufficiently small modulus

over a given region (see Formula (3.5).) In this case, the wave function resembles an excited state of the associated problem with some self-adjoint boundary condition at L . Moreover, we expect that when the resonance width is small, resonances are localized near and asymptotically in one-to-one correspondence with the bound state energies of the related self-adjoint problem. The reason for this conjecture is provided, for example, in [1]. The sharpest resonance seems to be generally associated with the ground state eigenfunction, and its potential contains a confining barrier but no other pieces.

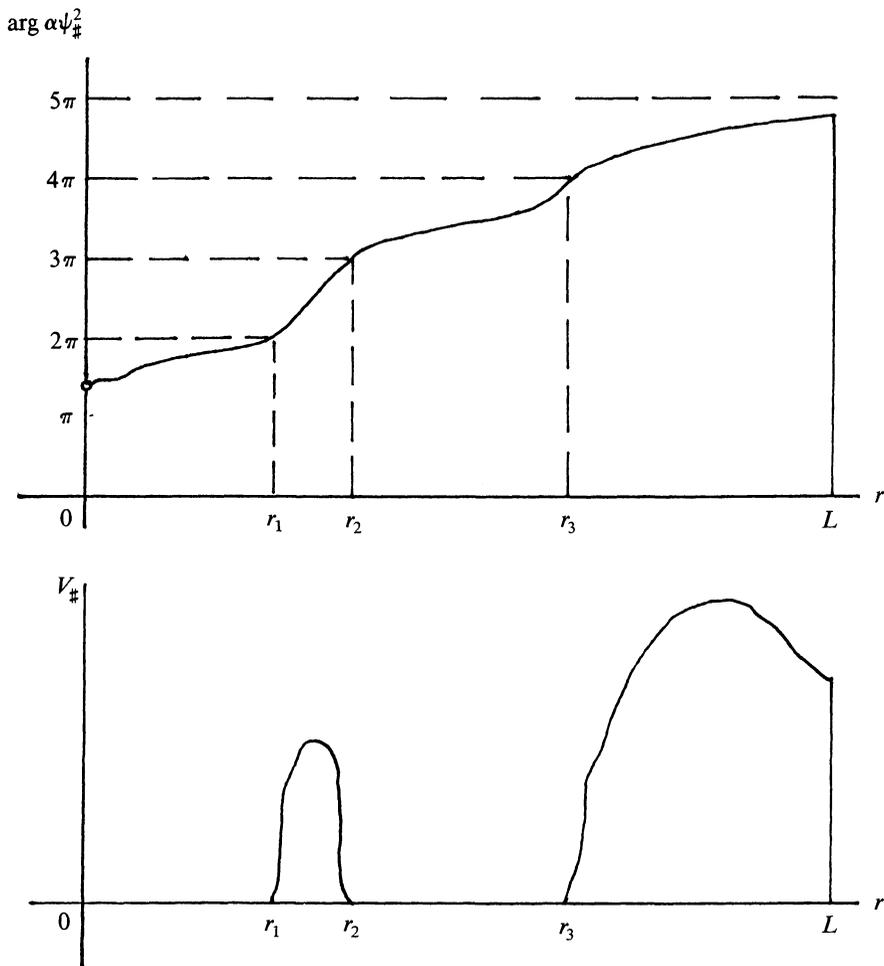


FIGURE 1

The relation between the argument of the resonance wave function and the on and off intervals of the maximally resonant potential.

IV. Case $p = 1$. In this last section we discuss the remaining case. In the proof of Theorem II.1 we use the duality of L^p -spaces for $p > 1$. Since for $p = 1$ the space $L^1(\Omega)$ is not a dual of any space, we do not define $S_1(\Omega)$ as the ball or radius M in $L^1(\Omega)$. Rather, we define $S_1(\Omega)$ to be the set of non-negative Borel measures on Ω of total mass at most M . Thus $S_1(\Omega) \subset C(\Omega)^*$.

As we have already noted, in one dimension any $V \in S_1(\Omega)$ is relatively form compact with respect to $-d^2/dr^2$ on $[0, \infty)$ with the Dirichlet boundary condition at 0. Thus from now on $\Omega \equiv [0, L]$, the Hamiltonian $H = -(d^2/dr^2) + V$ is defined as a sum of quadratic forms by the KLMN Theorem [9]. The measure V is associated with a quadratic form by the formula

$$V(f, g) = \int_{\Omega} \bar{f}gV(dx).$$

An argument similar to the one in Theorem II.1 proves the existence of a maximally resonant potential $V_{\#}$ in $S_1(\Omega)$. The characterization of $V_{\#}$ is along similar lines as for $p > 1$. The only difference is that a priori $V_{\#} = V_{\#}^{ac} \oplus V_{\#}^{sc} \oplus V_{\#}^{pp}$, where $V_{\#}^{ac}$, $V_{\#}^{sc}$ and $V_{\#}^{pp}$ denote the absolutely continuous, the singular continuous and the pure point measures respectively. Once again we perturb $V_{\#}$ slightly and study the effect of the perturbation on the first-order terms. Just as before, a perturbation is admissible if the resulting measure remains in $S_1(\Omega)$. For example,

$$(4.1) \quad V_{\#} \rightarrow V_{\#} + \lambda(\chi_{T_1}(r) - \chi_{T_2}(r)) \quad T_1, T_2 \subset \text{supp } V_{\#}^{ac}$$

and $|T_1| = |T_2|$, where $|T|$ denotes Lebesgue measure on the set is admissible for small λ iff $\text{supp } V_{\#}^{ac} \neq \{\emptyset\}$. Analogously for some singular continuous measure

$$(4.2) \quad V_{\#} \rightarrow V_{\#} + \lambda(V_{T_3}^{sc}(r) - V_{T_4}^{sc}(r)),$$

$$T_3, T_4 \subset \text{supp } V_{\#}^{sc}, V^{sc}(T_3) = V^{sc}(T_4)$$

is admissible for small λ iff $\text{supp } V_{\#}^{sc} \neq \{\emptyset\}$, and

$$(4.3) \quad V_{\#} \rightarrow V_{\#} + \lambda(\delta(r - a) - \delta(r - b)), \quad a, b \in \text{supp } V_{\#}^{pp},$$

is admissible for small λ iff $\text{supp } V_{\#}^{pp}$ contains more than one point. Obviously one could also use

$$(4.4) \quad V_{\#} \rightarrow V_{\#} + \lambda(\chi_{T_1} - |T_1| \delta(r - a)), \text{ etc.}$$

Either $\text{supp } V_{\#}$ consists of only one point or at least one of perturbations above is admissible. In the first case it is trivial to show that $V_{\#} = M\delta(r - L)$, i.e. the most resonant δ -function is one with the maximal weight supported at the right most point—a hardly surprising result.

Let us now assume that $\text{supp } V_{\#}$ contains more than one point. While we do not prove that this second possibility holds rather than the first one, the numerical evidence suggests that this is indeed the case. We have the following analog of Theorem III.2.

THEOREM IV.1. *If $V_{\#}$ is maximally resonant in $S_1(\Omega)$ and $\text{supp } V_{\#}$ contains more than one point, then*

$$(4.5) \quad (a) \quad \text{Im } \alpha \psi_{\#}^2 = c > 0 \text{ on } \text{supp } V_{\#};$$

$$(4.6) \quad (b) \quad \text{Im } \alpha \psi_{\#}^2 \leq c \text{ on the complement of } \text{supp } V_{\#} \text{ in } \Omega.$$

Proof. The most general assumption is that $V_{\#}$ contains all three parts. Then using perturbations (4.1), (4.2) and (4.3) and Formula (3.1) (or its quadratic form analog) we show that

$$\begin{aligned} \text{Im } \alpha \psi_{\#}^2 = c_1 \quad \text{on } \text{supp } V_{\#}^{\text{ac}}, \quad \text{Im } \alpha \psi_{\#}^2 = c_2 \quad \text{on } \text{supp } V_{\#}^{\text{sc}} \quad \text{and} \\ \text{Im } \alpha \psi_{\#}^2 = c_3 \quad \text{on } \text{supp } V_{\#}^{\text{pp}}. \end{aligned}$$

Moreover, $c_1 = c_2 = c_3 \equiv c$ which can be easily seen by using a perturbation like (4.4).

To show that $c \geq 0$ we observe that

$$V_{\#} \rightarrow V_{\#} + \lambda \chi_{T_1}(r)$$

is an admissible perturbation for $\lambda \leq 0$.

To prove (b) let S_1 be a set in the complement of $\text{supp } V_{\#}^{\text{ac}}$ such that $|S_1| = |T_1|$. Then the perturbation

$$V_{\#} \rightarrow V_{\#} + \lambda (\chi_{S_1}(r) - \chi_{T_1}(r))$$

is admissible iff $\lambda \geq 0$. Relation (3.1) implies that (b) holds in the complement of $V_{\#}^{\text{ac}}$. To complete the proof of (b) we repeat the same trick with the set S_2 in the complement of $\text{supp } V_{\#}^{\text{sc}}$ and the set S_3 in the complement of $\text{supp } V_{\#}^{\text{pp}}$.

All that is left to show now is that $c > 0$. Suppose $c = 0$. Then $\text{Im } \alpha \psi_{\#}^2 = 0$ on $\text{supp } V_{\#}$, but this can only occur at a finite number of points. (Otherwise, there is an accumulation point r_0 at which we can differentiate to obtain $\psi_{\#}(r_0) = 0$; then once again we have a self-adjoint problem on the interval $[0, r_0]$ which forces $\varepsilon = 0$ and this is impossible). So if $c = 0$, then $\text{Im } \alpha \psi_{\#}^2 \leq 0$ on $[0, L]$ and $\text{Im } \alpha \psi_{\#}^2 = 0$ on $\text{supp } V_{\#}$. But this contradicts (3.5) according to which $\arg \psi_{\#}$ is monotonically increasing. \square

COROLLARY IV.2. $\text{Supp } V_{\#} \subseteq [0, L]$. In particular, $0 \notin \text{supp } V_{\#}$.

Proof. This follows immediately by observing that $\text{Im } \alpha \psi_{\#}^2(0) = 0 < c$. □

REMARK. It follows from (3.5), (4.5) and (4.6) that the switching property is modified. We can still say that $V_{\#} \equiv 0$ on the sets where $\text{Im } \alpha \psi_{\#}^2 \leq 0$. However, the potential does not switch on at the points where $\text{Im } \alpha \psi_{\#}^2$ changes sign from minus to plus. The first possible point at which the switch can occur is when $\text{Im } \alpha \psi_{\#}^2$ reaches c .

We are now going to exploit Relation (4.5) firstly to rule out singular continuous and pure point measures on $[0, L)$ and secondly, to obtain more information about $V_{\#}^{\text{ac}}$.

PROPOSITION IV.3. For any maximally resonant $V_{\#} \in S_1(\Omega)$

- (a) $\text{supp } V_{\#}^{\text{pp}} \cap [0, L) = \emptyset$ and
- (b) $\text{supp } V_{\#}^{\text{sc}} \cap [0, L) = \emptyset$.

Proof. (a) Suppose that $V_{\#}^{\text{pp}}$ contains an isolated δ -function supported at some point $r_0 \in (0, L)$. Then $\text{Im } \alpha \psi_{\#}^2(r_0) = c$ and $\text{Im } \alpha \psi_{\#}^2 \leq c$ in some small neighborhood around r_0 . So

$$(\text{Im } \alpha \psi_{\#}^2)'(r_0 -) \geq 0 \quad \text{and} \quad (\text{Im } \alpha \psi_{\#}^2)'(r_0 +) \leq 0.$$

Also $\psi'(r_0 +) - \psi'(r_0 -) = \beta \psi_{\#}(r_0)$, where β is the coefficient of the δ -function. Multiplying both sides of the last expression by $\alpha \psi_{\#}(r_0)$ and taking imaginary parts we obtain:

$$0 \geq \text{Im } \alpha \psi_{\#} \psi'_{\#}(r_0 +) - \text{Im } \alpha \psi_{\#} \psi'_{\#}(r_0 -) = \beta \text{Im } \alpha \psi_{\#}^2(r_0) = \beta c > 0$$

contradiction.

If we now have a sequence of δ -functions supported on a Cantor-like set or a δ -function embedded in $V_{\#}^{\text{ac}}$ or $V_{\#}^{\text{sc}}$, the proof proceeds similarly.

(b) Suppose $V_{\#}^{\text{sc}} \neq 0$. Then $\text{Im } \alpha \psi_{\#}^2 = c$ on some perfect set F which is of Lebesgue measure zero and nowhere dense. We can always differentiate on such set by considering sequences of points of F . Thus after second differentiation we obtain:

$$\text{Im } \alpha \psi_{\#}^2 + \text{Im } \alpha \psi_{\#} \psi''_{\#} = 0 \quad \text{a.e. } [V_{\#}] \text{ on } \text{supp } V_{\#}.$$

Hence, for almost every $r \in [0, L)$ (with respect to $V_{\#}$), $\text{Im } \alpha \psi_{\#} \psi''_{\#}$ is defined as a function. On the other hand, multiplying both sides of the Schrödinger equation by $\alpha \psi_{\#}$ and extracting the imaginary parts we obtain

$$cV_{\#} = \text{Im } \alpha \psi_{\#} \psi''_{\#} + \text{Im } \alpha k_{\#}^2 \psi_{\#}^2.$$

The right hand side is determined pointwise a.e. $[V_{\#}]$, so the left hand side has to be. Hence, $V_{\#}^{\text{sc}} = 0$. \square

REMARK. The argument in part (a) of the proposition does not rule out a point measure supported at L , since we know nothing about $\text{Im } \alpha \psi_{\#}^2(r)$ for $r > L$.

Hence, now we can identify $V_{\#}$ on $[0, L)$ with an L^1 -function. Further analysis of $V_{\#}$ becomes a special case of the results for $p > 1$. In particular $\text{Im } \alpha \psi_{\#}^2 = c$ is a special case of $(\text{Im } \alpha \psi_{\#}^2)/V_{\#}^{p-1} = c$ for $p > 1$. The differential equation (3.6) turns into a simple algebraic relation that holds on $\text{supp } V_{\#}^{\text{ac}}$:

$$(4.7) \quad 2\varepsilon\alpha\psi_{\#}^2 + cV_{\#} = \text{const.}$$

Let us denote this constant by A . Equation (4.7) can be differentiated further yielding our final result.

THEOREM IV.4. (a) *On $\text{supp } V_{\#}$, $\psi_{\#}$ satisfies the non-linear Schrödinger equation (4.8) below.*

(b) *Let $\zeta = -4(E + (\text{Re } A)/2c)$ and $\tilde{V}_{\#} = \frac{1}{2}(V_{\#} + \zeta/6)$. Then $\tilde{V}_{\#}$ satisfies Equation (4.10') for the Weierstrass \mathbf{P} -function.*

Proof. (a) For convenience we drop the ‘ $\#$ ’ sign. From (4.7)

$$V = \frac{A}{c} - \frac{2\varepsilon\alpha}{c}\psi^2.$$

Substituting this into $-\psi'' + V\psi = k^2\psi$ we find:

$$(4.8) \quad -\psi'' + \left(\frac{A}{c} - k^2\right)\psi - \frac{2\varepsilon\alpha}{c}\psi^3 = 0$$

or multiplying by ψ' and integrating:

$$(4.8') \quad -\frac{1}{2}\psi'^2 + \frac{1}{2}\left(\frac{A}{c} - k^2\right)\psi^2 - \frac{\varepsilon\alpha}{2c}\psi^4 = \text{const.}$$

(b) We start by differentiating (4.5) and substitute for ψ'' from the Schrödinger equation in the same way it was done in Proposition III.5. After several steps we arrive at the equation

$$(4.9) \quad V'' - 6VV' + 4(E + D_1)V' = 0$$

with $D_1 = (\text{Re } A)/2c$. Note that V can be thought of as a traveling wave solution of the KdV equation

$$W_t = 6WW_r - W_{rrr}$$

where $W(r, t) = V(r - \zeta t)$ provided that $\zeta = -4(E + D_1) > 0$ [8]. Equation (4.9) can be integrated, then multiplied by V' and integrated again. We then obtain:

$$(4.10) \quad (V')^2 = 2V^3 - 4(E + D_1)V^2 + 2D_2V + 2D_3.$$

Here D_2 and D_3 are constants of integration. Now let $V = a\tilde{V} + b$, where we choose constants a and b so that \tilde{V} satisfies the equation for the **P**-function:

$$(4.10') \quad (\tilde{V}')^2 = 4\tilde{V}^3 - g_2\tilde{V} - g_3.$$

Substituting $a\tilde{V} + b$ into (4.10) we easily find that $a = 2$; $b = \frac{2}{3}(E + D_1) - \zeta/6$;

$$g_2 = \frac{4}{3}(E + D_1)^2 - D_2 \quad \text{and}$$

$$g_3 = \frac{8}{27}(E + D_1)^3 - \frac{D_2}{3}(E + D_1) - \frac{D_3}{2}.$$

\tilde{V} is indeed a **P**-function provided that $\Delta = g_2^3 - 27g_3^2 \neq 0$. In principle D_2 and D_3 are just constants of integration and they can always be chosen so that $\Delta \neq 0$. If however we let $D_2 = D_3 = 0$, then $\Delta = 0$ and instead of being an elliptic function $V(r) = (\zeta/2) \operatorname{csch}^2(\sqrt{\zeta}/2)r$ provided $\zeta > 0$ and $V(r) = -\zeta/2 \operatorname{sec}^2(\sqrt{-\zeta}/2)r$ if $\zeta < 0$. \square

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