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The free Laplacian with attractive boundary conditions

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ABSTRACT. — We consider the motion of a free quantum particle in a half space $R^{n-1} \times R_+$. The dependence of surface states on the boundary conditions is investigated and the results are compared with those obtained by a Schrödinger operator with attractive short-range potential in the neighbourhood of the boundary. It is also shown that for boundary conditions sufficiently singular a collapse on the boundary occurs.

RÉSUMÉ. — On considère le mouvement d'une particule libre quantique dans un demi espace $\mathbb{R}^{n-1} \times \mathbb{R}_+$. On étudie la dépendance des états de surface par rapport aux conditions aux limites et on compare les résultats avec ceux qu'on obtient avec un opérateur de Schrödinger comportant un potentiel attractif à courte durée au voisinage de la frontière. On montre aussi que pour des conditions aux limites suffisamment singulières, il se produit un effondrement sur la frontière.

1. INTRODUCTION

It is well known that the motion of a free Schrödinger particle on a half line $R_+ = [0, \infty)$ is described by a one parameter family of Hamiltonians H_σ ([*1*]; § X.1)

$$H_\sigma = -\frac{d^2}{dx^2}$$

$$D(H_\sigma) = \{ f \in L^2(R_+) ; f, f' \in AC(R_+), f'' \in L^2(R_+), f'(0_+) = \sigma f(0_+) \}$$
$$\sigma \in R \cup \{ \infty \}.$$

(The family H_σ represents all possible self adjoint extensions of a half line « Hamiltonian » H_0 with the boundary point removed

$$H_0 = -\frac{d^2}{dx^2} \restriction C_0^\infty(R_+).\Big)$$

The interaction of the particle with the point 0 is modelled here by the boundary condition (b. c.)

$$f'(0_+) = \sigma f(0_+). \tag{1}$$

Since H_σ is the norm resolvent limit of Schrödinger operators with short-range potentials [2] [3].

$$H_\sigma = \text{N. R.} \lim_{\varepsilon \to 0} H_{\sigma=0} + (1/\varepsilon)V(x/\varepsilon)$$

with $\sigma = \int_0^\infty V(y)dy$; $V \in L(R_+)$, describes (1) with $\sigma < 0$ an attractive interaction with the boundary. Analogously (1) with $\sigma > 0$ describes a repulsive interaction while the free endpoint is modelled by $\sigma = 0$ (Neumann b. c.).

In the multidimensional case the situation becomes more complicated. Considering the motion of a free particle on a n-dimensional half space $R^{n-1} \times R_+$ we have to construct all possible self-adjoint extensions of the half space Laplacian H_0 with the boundary removed

$$H_0 = -\Delta \restriction C_0^\infty(R^{n-1} \times R_+).$$

(These extensions represent the admissible quantum Hamiltonians of the system.)

But now the deficiency indices of H_0 are not finite and this makes the situation very complicated.

The aim of our paper is to study self adjoint extensions of H_0 defined by local b. c.

$$\frac{\partial}{\partial x_n} f(x_1, \ldots, x_n)/_{x_n=0} = \sigma(x_1, \ldots, x_{n-1}) f(x_1, \ldots, x_{n-1}, 0) \tag{2}$$

for $n \geqslant 2$. (The corresponding operator is denoted as H_σ.) In contrary to the one dimensional case the local b. c. do not represent all possible ones (there are also nonlocal b. c., cf. [4]).

The homogeneous b. c. with $\sigma = \text{const.}$ were already considered in connection with the Bose condensation [5]-[7]. It was remarked in [3] that it is possible to describe such an operator as a norm resolvent limit of

$$H_{\sigma=0} + (1/\varepsilon)V(x_n/\varepsilon); \qquad V \in L(R_+).$$

The constant σ is then determined by

$$\sigma = \int_0^\infty V(y)dy .$$

Therefore one should expect that also for the more general case (2) holds

$$H_\sigma = \lim_{\varepsilon \to 0} H_{\sigma=0} + (1/\varepsilon)V(x_1, x_2, \ldots, x_{n-1}, x_n/\varepsilon) \tag{3}$$

where $\sigma(x_1, \ldots, x_{n-1}) = \int_0^\infty V(x_1, \ldots, x_{n-1}, y)dy$.

But up to now we do not know any proof of (3) in the general case. Nevertheless a comparison of properties of H_σ with those of

$$H_{\sigma=0} + (1/\varepsilon)V(x_1, \ldots, x_{n-1}, x_n/\varepsilon)$$

shows many similarities. Thus it seems that the influence of the boundary can be modelled by an appropriate boundary condition of the type (3) as well as by an additive short-range potential.

In the next section we study the spectral properties of H_σ by an ansatz leading to a Klein-Gordon pseudodifferential operator. In the section 3 σ is taken to be a L^p function or a periodic function respectively. In the first case we find that at most a finite number of negative eigenvalues of H_σ appear. For σ periodic the spectrum of H_σ is absolutely continuous only. In section 4 we discuss the properties of H_σ with σ singular. We show that for σ negative and singular enough a collapse on the boundary occurs. In a forthcoming paper [*8*] random b. c. are considered.

2. TRANSFORMATION TO A KLEIN-GORDON HAMILTONIAN

The interval $[0, \infty)$ belongs to the spectrum of H_σ for any σ, since one can for any $\varepsilon > 0$ and $E \geqslant 0$ construct functions $\psi \in C_0^\infty(R^{n-1} \times R_+)$ such that

$$\| (-\Delta - E)\psi \| < \varepsilon \| \psi \| .$$

This is why we are interested only in the negative part of $\sigma(H_\sigma)$. Introducing for $E < 0$ an operator

$$K_{\sigma,E} = \sqrt{-\Delta - E} + \sigma(x)$$

defined on the Hilbert space $L^2(R^{n-1})$ we get the following proposition [*9*].

PROPOSITION 1. — Let σ be a $K_{0,0}$ bounded function with the relative bound less then 1. Then for $E < 0$ holds

a) $E \in \sigma(H_\sigma)$ if and only if $0 \in \sigma(K_{\sigma,E})$
b) $E \in \sigma_{disc}(H_\sigma)$ if and only if $0 \in \sigma_{disc}(K_{\sigma,E})$
c) $E \in \sigma_{ess}(H_\sigma)$ if and only if $0 \in \sigma_{ess}(K_{\sigma,E})$.

Thus using the Klein-Gordon operator with a rest mass corresponding to the binding energy $-E$ we can simply investigate the negative part of $\sigma(H_\sigma)$.

The min-max-principle ([*10*], § XIII.1) yields that the n-th eigenvalue of $H_{\sigma=0} + V_1$ is less then the n-th eigenvalue of $H_{\sigma=0} + V_2$ if $V_1(x) < V_2(x)$ for any x. The approximation argument (3) let us expect the same for H_σ.

PROPOSITION 2. — If $\sigma_1(x) \leqslant \sigma_2(x)$ for all $x \in R^{n-1}$ then

$$E_m(H_{\sigma_1}) \leqslant E_m(H_{\sigma_2})$$

where $E_m(H_\sigma)$ denotes the m-th eigenvalue of H_σ.

CONCLUSION. — For the ground state of H_σ holds

$$E_1(H_\sigma) \geqslant -(\min\{0, \inf \sigma(x)\})^2. \tag{4}$$

Remark. — If H_σ has only $k < m$ eigenvalues bellow its essential spectrum then $E_m(H_\sigma)$ denotes $\inf \sigma_{ess}(H_\sigma)$ for all $m > k$.

Proof of the Conclusion. — Take $\sigma_1(x) = \min(0, \inf \sigma(x)) \leqslant \sigma(x)$. Then $E_1(H_\sigma) \geqslant E_1(H_{\sigma_1}) = \inf \sigma_{ess}(H_{\sigma_1}) = -\sigma_1^2$.

Proof of the Proposition 2. — The min-max-principle yields that $E_m(K_{\sigma,E})$ is increasing in σ and decreasing in E. Thus the solution $E = E(\sigma)$ of

$$E_m(K_{\sigma,E}) = 0$$

is decreasing in σ.

For $H_{\lambda\sigma}$, $\lambda \to \infty$ the estimate (4) becomes exact in the sense that

$$\lim_{\lambda \to \infty} E_1(H_{\lambda\sigma})/\lambda^2 = -(\min\{0, \inf \sigma(x)\})^2.$$

(For the proof take trial functions for $K_{\sigma,E}$ as in [*11*].)

Conversely for bounded V

$$\lim_{\lambda \to \infty} E_1(H_{\sigma=0} + \lambda V)/\lambda = \inf V$$

i. e. the asymptotical behaviour of $E_1(H_{\sigma=0} + \lambda V)$ is only linear. This difference between $H_{\lambda\sigma}$ and $H_{\sigma=0} + \lambda V$ is observable already in the explicitely solvable one dimensional case. But it is not surprizing since approximating $H_{\lambda\sigma}$ by $H_{\sigma=0} + (\lambda/\varepsilon)V(x_1, \ldots, x_{n-1}, x_n/\varepsilon)$ (cf. (3)) we get

$$\inf (\lambda/\varepsilon)V(x_1, \ldots, x_{n-1}, x_n/\varepsilon) \to -\infty$$

in the $\varepsilon \to 0$ limit for negative V.

3. SHORT AND LONG RANGE BOUNDARY CONDITIONS

Let us first investigate the spectrum of H_σ when σ is a short-range function. Since $H_{\sigma=0} + V$ has only discrete spectrum bellow 0 for short-range potentials one would expect the same also for H_σ with σ short-range. Proposition 1 of the present paper and theorem 4.2 of ref. [*12*] imply immediately.

PROPOSITION 3. — Let $\sigma \in L^p(R^{n-1}) + L_\varepsilon^\infty(R^{n-1})$ with $2 \leqslant p < \infty$ and $p > n - 1$ (i. e. for any $\varepsilon > 0$ there is a decomposition

$$\sigma = \sigma_{1,\varepsilon} + \sigma_{2,\varepsilon}$$

with $\sigma_{1,\varepsilon} \in L^d(R^{n-1})$ and $\| \sigma_{2,\varepsilon} \|_\infty < \varepsilon$). Then

$$\sigma_{ess}(H_\sigma) = [0, \infty)$$

and the negative part of $\sigma(H_\sigma)$ consists of isolated eigenvalues of finite multiplicity.

Remarks. 1) For $\sigma \in C_0^\infty(R^{n-1})$ a similar proposition was already proved in [*13*] [*14*].

2) Proposition 3 is an analogue of the fact that

$$\sigma_{ess}(H_{\sigma=0} + V) = [0, \infty)$$

for $V \in L^p(R^{n-1} \times R_+) + L_\varepsilon^\infty(R^{n-1} \times R_+)$; $2 \leqslant p < \infty$, $p > n/2$. (Cf. [*10*], § XIII.4).

In the case $n = 2$ it is possible to get some more detailed information on the eigenvalues of H_σ.

PROPOSITION 4. — Let $\sigma \in L^p(R)$ and $\sigma_+ \in L^{p'}(R)$ where $1 \leqslant p < 2$ and $p' > 1$. Then for the m-th eigenvalue of H_σ holds

$$E_m(H_\sigma) \geqslant - ((1/\pi) \| K_0 \|_q \| \sigma_- \|_p)^{2q} m^{-q} \tag{5}$$

where $1/p + 1/q = 1$ and K_0 denotes the modified Hankel function of order zero. (σ_-, σ_+ are the negative and positive parts of σ respectively.)

Proof. — Let $N_0(K_{\sigma,E})$ denotes the number of nonpositive eigenvalues of $K_{\sigma,E}$. Using the Birman-Schwinger argument ([*10*], theorem XIII.10) and replacing the Green's function of $-\Delta$ by the Green's function of $K_{0,E}$ we get

$$N_0(K_{\sigma,E}) \leqslant (1/\pi^2) \int_{\mathbb{R}^2} K_0^2(\sqrt{-E} \, | x-y |) \sigma_-(x) \sigma_-(y) dx dy . \tag{6}$$

The fact that $K_0 \in L^p(R)$ for any $p \geqslant 1$ [*15*] and the Young inequality imply (5).

Remarks. — 1) In the case of higher dimensions this technique is not applicable since the kernel of $K_{0,E}$ becomes too singular. Consequently the integrals corresponding to (6) are divergent.

2) The condition $\sigma \in L^p(R)$ for $p > 1$ implies that σ is infinitely small with respect to $K_{0,0}$ (cf. [*9*]) what enables us apply proposition 1.

It is rather difficult to investigate the spectrum of $K_{\sigma,E}$ in the general case. This difficulty is connected with the nonlocality of this operator. Therefore it is not possible to use standard arguments based on differential equations. Nevertheless one can prove that the spectrum of $K_{\sigma,E}$ is absolutely continuous for σ periodic (and hence for H_σ) using the technique based on direct integral decomposition of $L^2(R^{n-1})$ outlined in ([*10*], § XIII.10).

Let $(a_1, \ldots, a_{n-1})$ be a basis in R^{n-1}. We denote

$$Q = \left\{ \sum_{j=1}^{n-1} t_j a_j \, ; \, t_m \in [0,1], \, m = 1, 2, \ldots, n-1 \right\}.$$

Moreover we define for $x \in R^{n-1}$ and $k \in N$

$$x^{2k} := |x|^{2k}; \qquad x^{2k+1} := x\,|x|^{2k}.$$

Now we can state

PROPOSITION 5. — Let σ be a periodic function

$$\sigma\left(x + \sum_{j=1}^{m-1} m_j a_j\right) = \sigma(x), \qquad m \in Z^{n-1}.$$

Suppose that σ is 1 times differentiable with

$$1 > \frac{(n-1)(n-3)}{2(n-2)} \quad \text{for} \quad n > 2 \quad \text{or} \quad 1 \geqslant 1 \quad \text{for} \quad n = 2$$

and that

$$|\nabla^l \sigma| \in L^p(Q)$$

$$\text{for } 2 \geqslant p > \frac{2(n-1)(n-2)}{2l(n-2)+n-1} \text{ for } n>2 \text{ resp. } 2 \geqslant p \geqslant 1 \text{ for } n=2. \qquad (7)$$

Then the spectrum of H_σ is absolutely continuous.

Proof. — We note at the beginning that under these assumptions σ is infinitely small with respect to $K_{0,0}$. Thus the proposition 1 is applicable. We introduce

$$g = |\nabla^l \sigma|$$

Since $g \in L^p(Q)$ the Hausdorff-Young inequality yields

$$\tilde{g} \in l_{p/p-1}(Z^{n-1})$$

where $\tilde{g}_m$, $m \in Z^{n-1}$ are the Fourier coefficients of g. Let us now define

$$f_m = \begin{cases} 1/|m|^l & m \neq 0 \\ 1 & m = 0 \end{cases}$$

$$h_m = \begin{cases} |\tilde{g}_m| & m \neq 0 \\ \tilde{\sigma}_0 & m = 0 \end{cases}$$

($\tilde{\sigma}_m$ denotes the Fourier coefficients of σ). Since

$$|\tilde{\sigma}_m| = h_m f_m$$

and $f \in l_r(Z^{n-1})$ for all $r > (n-1)/l$ the Hölder inequality yields

$$\tilde{\sigma} \in l_s(Z^{n-1}) \quad \text{for} \quad s > \frac{n-1}{(1-1/p)(n-1)+1}. \tag{8}$$

The assumption (7) implies that the right hand side of (8) is less then $(2n-4)/(2n-5)$. Thus we can choose $s < (2n-4)/(2n-5)$. Analogously we get $\tilde{\sigma} \in l_s(Z)$ with $s \leqslant 2$ for $n = 2$.

From now on we will follow the proof of the theorem XIII.100, ref. [*10*]. We denote

$$\mathscr{C}_m(z) = \left(\left(a + zb + \sum_{j=1}^{n-1} m_j \tilde{a}_j\right)^2 - E\right)^{1/2}$$

where $a, b \in R^{n-1}$ and $(\tilde{a}_j)$ denotes the basis reciprocal to (a_j)

$$(a_i ; \tilde{a}_j) = 2\pi\delta_{ij}.$$

(For the analytic continuation into the complex plane the branch with $\operatorname{Re} \mathscr{C}_m(z) > 0$ is choosen.) Since

$$|\xi^2 + 1| \leqslant |\xi + 1|^2$$

for all $\xi \in C$, $\operatorname{Re} \xi \geqslant 0$ we get

$$|\mathscr{C}_m(z) + 1| \geqslant |\mathscr{C}_m(z)^2 + 1|^{1/2}.$$

This allows us to follow completely the proof of the theorem XIII.100 of ref. [*10*]. We get

$$K_{\sigma,E} = F^{-1} \int_{[0,2\pi]^{n-1}}^{\oplus} \hat{K}_{\sigma,E}(k) d^{n-1}k F.$$

where F denotes the Fourier transform and $\hat{K}_{\sigma,E}(k)$ is an operator acting on $l_2(Z^{n-1})$

$$(\tilde{K}_{\sigma,E}(k)f)_m = ((m+k)^2 - E)^{1/2} f_m + \sum_{j \in \mathbb{Z}^{n-1}} \tilde{\sigma}_j f_{m-j}.$$

It is simple to show that the eigenvalues $e_j(k, E)$ of the operator $\tilde{K}_{\sigma,E}(k)$

are nonconstant analytic functions of k for $k \in [0, 2\pi]^{n-1}$. At the same time are $e_j(k, \mathrm{E})$ decreasing functions of E for k fixed.

Let us now decompose the operator H_σ. Here we get

$$\mathrm{H}_\sigma = \mathrm{F}^{-1} \int_{(0,2\pi)^{n-1}}^{\oplus} \tilde{\mathrm{H}}_\sigma(k) d^{n-1}k \mathrm{F}$$

where $\tilde{\mathrm{H}}_\sigma(k)$ is an operator acting on $l_2(\mathrm{Z}^{n-1}) \otimes \mathrm{L}^2(\mathrm{R}_+)$

$$\tilde{\mathrm{H}}_\sigma(k) : f_m(x) \to -(m+k)^2 f''(x), \qquad m \in \mathrm{Z}^{n-1}$$

defined by boundary condition

$$f_m'(0) = \sum_{j \in \mathbb{Z}^{n-1}} \tilde{\sigma}_j f_{m-j}(0) .$$

Using the argument of the proposition 1 we get

$$\mathrm{E}(k) \in \sigma(\tilde{\mathrm{H}}_\sigma(k)) \cap (-\infty, 0] \Leftrightarrow 0 \in \sigma(\tilde{\mathrm{K}}_{\sigma,\mathrm{E}}(k)) .$$

Hence the eigenvalues $\mathrm{E}(k)$ of $\tilde{\mathrm{H}}_\sigma(k)$ are nonconstant functions of k and theorem XIII.86, ref. [*10*] implies the absolute continuity of $\sigma(\mathrm{H}_\sigma)$.

4. AN EXAMPLE

Let us now investigate what happens when σ is not $\mathrm{K}_{0,0}$ bounded. In order to make the life easy we start with $n = 2$ and we choose

$$\sigma(x_1) = \sigma_c(x_1) = c/|x_1| .$$

The function σ_c is singular at 0 and it is not $\mathrm{K}_{0,0}$ bounded. In order to define the operator H_{σ_c} we remove the singularity by defining an operator

$$\mathrm{H}_{\sigma_c}^{(0)} = \mathrm{H}_{\sigma_c} \upharpoonright \mathrm{D}_0$$

$$\mathrm{D}_0 = \{ f \in \mathrm{D}(\mathrm{H}_{\sigma_c}) ; f = 0 \text{ in some neighbourhood of } 0 \} .$$

The operator $\mathrm{H}_{\sigma_c}^{(0)}$ is symmetric but it is not self adjoint and the original Hamiltonian H_{σ_c} represents one of its self adjoint extensions.

Introducing the polar coordinates

$$x_1 = r \sin \varphi$$

$$x_2 = r \cos \varphi ; \qquad r \in \mathrm{R}_+, \quad \varphi \in [0, \pi]$$

the Hilbert space decomposes as

$$\mathrm{L}^2(\mathrm{R} \times \mathrm{R}_+) = \mathrm{L}^2(\mathrm{R}_+, rdr) \otimes \mathrm{L}^2(0, \pi) . \tag{9}$$

The operator $\mathrm{H}_{\sigma_c}^{(0)}$ decomposes with respect to (9) as

$$\mathrm{H}_{\sigma_c}^{(0)} = -\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2} . \mathrm{B}$$

where B denotes the modified « angular momentum » operator

$$B = -\frac{\partial^2}{\partial \varphi^2}$$

which is defined on $L^2(0, \pi)$ by boundary conditions

$$f'(0_+) = -cf(0_+)$$
$$f'(\pi_-) = cf(\pi_-).$$

Let now $\varkappa_n$ and χ_n denote the eigenvalues and eigenvectors of B

$$B\chi_n = \varkappa_n \chi_n, \qquad n = 1, 2, \ldots$$

Because $\{ \chi_n \}_{n=1}^{\infty}$ form an orthogonal basis in $L^2(0, \pi)$ we get from (9)

$$L^2(R \times R_+) = \bigoplus_{m=1}^{\infty} L^2(R_+, rdr) \otimes \{ \chi_m \}. \tag{10}$$

$$H_{\sigma_c}^{(0)} = \bigoplus_{m=1}^{\infty} h_m^{(0)} \otimes I, \tag{11}$$

where

$$h_m^{(0)} = -\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{1}{r^2} \cdot \varkappa_m \tag{12}$$

$D(h_m^{(0)}) = \{ f \in L^2(R_+, rdr) ; f, f' \in AC(R_+), f = 0$ in some neighbourhood of 0 and $h_m^{(0)} f \in L^2(R_+, rdr) \}$.

Estimating the eigenvalues of B we get for $c > 0$

$$(n-1)^2 \leqslant \varkappa_n \leqslant n^2, \qquad n = 1, 2, \ldots$$

For $c < 0$ also negative eigenvalues occur and we obtain

$$\varkappa_1 \leqslant -c^2$$
$$\varkappa_n \geqslant 0, \qquad n = 2, 3, \ldots \quad \text{for} \quad -2/\pi \leqslant c < 0$$

resp.

$$\varkappa_1 \leqslant -c^2$$
$$-c^2 \leqslant \varkappa_2 < 0$$
$$\varkappa_n \geqslant 0, \qquad n = 3, 4, \ldots \quad \text{for} \quad c < -2/\pi.$$

Inserting these values into (12) we find ([*1*], appendix to § X.1) that for $c > 0$ the operators $h_n^{(0)}$ are positive and essentially self adjoint for $n > 1$. Moreover $h_1^{(0)}$ has deficiency indices (1, 1) and all its self adjoint extensions are semibounded. Consequently $H_{\sigma_c}^{(0)}$ is an operator with deficiency indices (1, 1) and all its self adjoint extensions are bounded from below.

For $c < 0$ the situation changes. We have now $\varkappa_1 < 0$ and this implies that the operator $h_1^{(0)}$ is not semibounded. Using the formula (11) we find that $H_{\sigma_c}^{(0)}$ is not bounded from below. Since $H_{\sigma_c}^{(0)}$ is an operator with finite deficiency indices we get finally that all its self adjoint extensions are not bounded from below. This mathematical fact has a simple physical interpretation. It means that for $c < 0$ a collapse of the system on the boundary occurs [*16*].

The proposition 1 cannot be applied in this case since σ_c is not $K_{0,0}$ bounded. But nevertheless the corresponding Klein-Gordon operator $K_{\sigma_c,E}$ is also not bounded from below for $c < 0$. (Cf. [*17*], theorems 2.1 and 2.5).

The situation is similar also for $n > 2$. Introducing $\sigma_c = c' | x |$ we get that the operator H_{σ_c} is not bounded from below for all $c < c_n$, where c_n is some negative constant. (For instance for $n = 4$ we get $c_4 = -2/\pi$.)

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