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THE FREE LAPLACIAN WITH ATTRACTIVE BOUNDARY CONDITIONS

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1. Introduction

It is well known[1] that the motion of a free Schroedinger particle on a half line $R_+ = [0,\infty)$ is described by an one-parameter family of Hamiltonians H_σ

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

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

(The family H_σ, $\sigma \in \mathbb{R} \cup \{\infty\}$ represents all possible self-adjoint extensions of a half line "Hamiltonian" H_0 with the boundary point 0 removed

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

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

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

Since H_σ is the norm-resolvent limit of Schroedinger operators with local short-range potentials[2,3]

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

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 quantum particle on a 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.)
The deficiency indices of H_0 are not finite for $n > 1$ and this makes the situation very complicated.

The aim of our paper is to study Hamiltonians of a free particle on half space $R^{n-1} \times R_+$ which are defined by local b.c.

$$\frac{\partial}{\partial x_n} f(x_1,\dots,x_n) \Big/_{x_n=0} = \sigma(x_1,\dots,x_{n-1}) \cdot f(x_1,\dots,x_{n-1},0) \quad (2)$$

(The corresponding operator is denoted as H_σ .)
In the contrary to the one-dimensional case the local b.c. do not represent all possible ones. There are also non-local b.c. , cf. ref./4/.

The homogeneous b.c. with σ = const. were already considered in connection with the Bose condensation (ref./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

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

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

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

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

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

similarities. Thus it seems that the influence of the boundary can be modelled by the appropriate boundary conditions of the type (2) 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 at 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 $E \geq 0$ construct a function $\Psi \in C_0^\infty(R^{n-1} \times R_+)$ such that

$$\|-\Delta\Psi - E\Psi\| < \varepsilon \|\Psi\|$$

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 is $K_{0,0}$ - bounded with a 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 Hamiltonian with the rest mass equal to the binding energy -E we can simply investigate the negative part of $\sigma(H_\sigma)$.

The min-max-principle (ref. /10/ § XIII.1) yields that the m-th eigenvalue of $H_{\sigma=0} + V_1$ is less then the m-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 also for H_σ

Proposition 2: If $\sigma_1(x) \leq \sigma_2(x)$ for all $x \in R^{n-1}$ then

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

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

Conclusion: For the ground state of H_σ holds

$$E_1(H_\sigma) \geq -(\min\{0, \inf \sigma(x)\})^2 \qquad (4)$$

Remark: If H_σ has only $1 < m$ eigenvalues bellow its essential spectrum $E_m(H_\sigma)$ denotes $\inf \sigma_{ess}(H_\sigma)$ for all $m > 1$.

Proof of the conclusion: Take $\sigma_1(x) = \min\{0, \inf \sigma(x)\}$. Then $\sigma_1(x) \leq \sigma(x)$ and

$$E_1(H_\sigma) \geq E_1(H_{\sigma_1}) = \inf \sigma_{ess}(H_{\sigma_1}) = -\sigma_1^2 .$$

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 ref. /11/.) Conversly for bounded V holds

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

i.e. the asymptotical behaviour of $E_1(H_{\sigma=0} + \lambda V)$ is only linear. This difference between $H_{\sigma,\lambda}$ and $H_{\sigma=0} + \lambda V$ is observable already in the explicitely solvable one-

dimensional case. But it is not surprizing , since if we approximate the operator $H_{\sigma,\lambda}$ by $H_{\sigma=0} + (\lambda/\varepsilon) V(x_1,..,x_{n-1},x_n/\varepsilon)$ then

$$\inf_{\varepsilon\to 0} \frac{\lambda}{\varepsilon} V(x_1,...,x_{n-1},x_n/\varepsilon) = -\infty .$$

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 V 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 $\sigma \in L^p(R^{n-1}) + L^\infty_\varepsilon(R^{n-1})$ with $2 \leq p < \infty$ and $p > n-1$. (i.e. for any $\varepsilon > 0$ there is a decomposition $\sigma = \sigma_{1,\varepsilon} + \sigma_{2,\varepsilon}$ with $\sigma_{1,\varepsilon} \in L^p(R^{n-1})$ and $\|\sigma_{2,\varepsilon}\| < \varepsilon$) 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 $\sigma \in C_0^\infty(R^{n-1})$ the proposition was already proved by Povzner and Krein /13,14/

2/ The proposition 3 is an analogue of the fact that

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

for $V \in L^p(R^{n-1} \times R_+) + L^\infty_\varepsilon(R^{n-1} \times R_+)$, $2 \leq p < \infty$, $p > n/2$ (cf. ref. /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 $1 < p \leq 2$ and $p' > 1$. Then for the m-th eigenvalue of H_σ holds

$$E_m(H_\sigma) \geq -((1/\pi)\|K_0\|_g \|\sigma_-\|_p)^{2g} m^{-g} \qquad (5)$$

where $1/p + 1/g = 1$ 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 (ref. /10/, theorem XIII.10) and replacing the Green's function of $-\Delta$ by the Green's function of $K_{0,E}$ we get

$$N_0(K_{\sigma,E}) \leq (1/\pi^2)\int_{R\times R} K_0^2(\sqrt{-E}|x-y|)\,\sigma_-(x)\,\sigma_-(y)\,dxdy \qquad (6)$$

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

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

2/ The condition $\sigma \in L^p(R)$, $p > 1$ implies that σ is infinitely small with respect to $K_{0,0}$ /9/ what enables us apply the 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. It is therefore impossible 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 the direct integral decomposition of $L^2(R^{n-1})$ outlined in ref. /10/, § XIII.10.

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

$$Q = \Big\{ \sum_{i=1}^{n-1} t_i a_i \ , \ t_i \in [0,1] \ , \ i=1,2,\dots,n-1 \Big\}$$

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

$$x^{2l} := |x|^{2l} \ ; \quad x^{2l+1} := x\,|x|^{2l} \ .$$

Now we can state

Proposition 5: Let σ be a periodic function

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

Suppose that σ is l times differentiable with

$$l \geq \frac{(n-1)(n-3)}{2(n-2)}$$ for $n > 2$ or $l \geq 1$ for $n = 2$ respectively and that

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

for

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

for $n = 2$. Then the spectrum of H_σ is absolutely continuous.

Proof: We note at the beginning that under these assumptions is σ infinitely small with respect to $K_{0,0}$. Thus the proposition 1 is applicable /9/.

Let us now 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

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

and

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

($\tilde{\sigma}_m$ 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

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

The assumption (7) implies that 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 $s \leq 2$ for $n = 2$.

Now we will follow the standard direct integral decomposition technique /10/. We denote

$$\mathcal{E}_m(z) = \left[\left((a + zb) + \sum_{i=1}^{n-1} m_i \tilde{a}_i\right)^2 - E\right]^{1/2}$$

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

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

(For the analytic continuation into the complex plane the branch with $\mathrm{Re}(\mathcal{E}_m(z)) \geq 0$ is choosen.) Since

$$|\xi^2 + 1| \leq |\xi + 1|^2 \quad \text{for all } \xi \in C,\ \mathrm{Re}\,\xi \geq 0$$

we get

$$|\mathcal{E}_m(z) + 1| \geq |\mathcal{E}_m(z)^2 + 1|^{1/2} .$$

This allows us to use step by step the method of the proof of the theorem XIII.100 of ref. /10/. We get

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

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

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

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 $e_j(k,E)$ decreasing functions of E for k fixed.

Decomposing the operator H_σ we get

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

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

$$\tilde{H}_\sigma(k) : f_m(x) \longrightarrow -(m+k)^2 f''(x) ; \quad m \in Z^{n-1}$$

and defined by boundary conditions

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

Using the arguments of the proposition 1 we get

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

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

Let us now investigate what happens when σ is not $K_{0,0}$ bounded.

4. An example:

We show that for σ singular enough a collapse at the boundary occurs.

We start with n = 2 . In order to make the life easy we choose

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

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

$$H^{(0)}_{\sigma_c} = H_{\sigma_c} \upharpoonright D_0$$

$$D_0 = \left\{ f \in D(H_{\sigma_c}),\ f = 0 \text{ in some neighbourhood of } 0 \right\}$$

The operator $H^{(0)}_{\sigma_c}$ is symmetric but it is not self adjoint. The original Hamiltonian H_{σ_c} represents one of its self - adjoint extensions. We show that all the self-adjoint exten - sions of $H^{(0)}_{\sigma_c}$ are not bellow bounded for $c < 0$.

Introducing polar coordinates

$$x_1 = r \sin\varphi$$
$$x_2 = r \cos\varphi \quad ; \ r \in R_+ ,\ \varphi \in [0,\pi]$$

we get

$$L^2(R \times R_+) = L^2(R_+\, r dr) \otimes L^2(0,\pi) \tag{9}$$

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

$$H^{(0)}_{\sigma_c} = -\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \left(\frac{1}{r^2}\right) \cdot B$$

where B denotes the modified "angular momentum" operator

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

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

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

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

$$B \cdot \chi_n = \varkappa_n \cdot \chi_n \quad , \quad n = 1,2,\dots$$

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

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

Using the decomposition (10) we get finally for $H^{(o)}_{\sigma_c}$.

$$H^{(o)}_{\sigma_c} = \bigoplus_{m=1}^{\infty} h_n^{(o)} \otimes I \tag{11}$$

where $h_n^{(o)}$ are operators acting on $L^2(R_+;rdr)$

$$h_n^{(o)} = - \frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{\varkappa_n}{r^2} \tag{12}$$

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

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

$$(n-1)^2 \leqslant \varkappa_n \leqslant n^2 \quad , \quad n = 1,2,\dots$$

But for $c < 0$ there are also negative eigenvalues of B and we have

$$\varkappa_1 \leqslant - c^2$$

$$\varkappa_n \geqslant 0 \ ; \ n = 2,3,\dots \qquad \text{for } -2/\pi < c < 0$$

resp.

$$\varkappa_1 \leqslant - c^2$$

$$- c^2 \leqslant \varkappa_2 \leqslant 0$$

$$\varkappa_n > 0 \ ; \ n = 3,4,\dots \qquad \text{for } c < -2/\pi \ .$$

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

For $c < 0$ the situation changes. We have now $\varkappa_1 < 0$ and this implies that the operator $h_1^{(o)}$ is

not semibounded. Using the formula (11) we find that $H^{(o)}_{\sigma_c}$ is not semibounded. Since $H^{(o)}_{\sigma_c}$ is an operator with finite deficiency indices we get finally that all its self - adjoint extensions are not bellow bounded.

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 $\sigma_c(x)$ is not $K_{0,0}$ bounded. But nevertheless the corresponding Klein-Gordon operator $K_{\sigma_c,E}$ is also not bellow bounded for $c < 0$ (cf. ref. /17/, theorems 2.1 and 2.5).

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Свободный оператор Лапласа
с притягивающими граничными условиями

Обсуждается движение свободной квантовой частицы на полупространстве $R^{n-1} \times R_+$. Изучается зависимость поверхностных состояний от граничных условий и полученные результаты сравниваются с результатами, которые получаются при использовании оператора Шредингера с притягивающим потенциалом короткого действия. Показано также, что в случае достаточно притягивающей границы появляется падение системы на границу.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Englisch H., Schröder M., Šeba P. E5-86-524
The Free Laplacian
with Attractive Boundary Conditions

We consider the motion of a free quantum particle on the 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 Schroedinger operator with attractive short-range potential in the neighbourhood of the boundary. It is also shown that for a sufficiently attractive boundary a colapse of the system occurs.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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