The behaviour of the three-dimensional Hamiltonian $-\Delta + \lambda [\delta(x + x_0) + \delta(x - x_0)]$ as the distance between the two centres vanishes

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In this note, we continue our analysis of the behavior of self-adjoint Hamiltonians with symmetric double wells given by twin point interactions perturbing various types of “free Hamiltonians” as the distance between the two centers shrinks to zero. In particular, by making the coupling constant to be renormalized and also dependent on the separation distance between the two impurities, we prove that it is possible to rigorously define the unique self-adjoint Hamiltonian that, differently from the one studied in detail by Albeverio and collaborators, behaves smoothly as the separation distance between the impurities shrinks to zero. In fact, we rigorously prove that the Hamiltonian introduced in this note converges in the norm resolvent sense to that of the negative three-dimensional Laplacian perturbed by a single attractive point interaction situated at the origin having double strength, thus making this three-dimensional model more similar to its one-dimensional analog (not requiring the renormalization procedure) as well as to the three-dimensional model involving impurities given by potentials whose range may even be physically very short but non-zero.

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1. Introduction

In this brief presentation, we wish to further investigate the phenomenon that had been first observed in [1] for the one-dimensional Salpeter Hamiltonian perturbed by a pair of identical Dirac distributions symmetrically situated around the origin and later in [2, 3] for the Hamiltonian of the three-dimensional isotropic harmonic oscillator with the same perturbation: as the distance between the two centers shrinks to zero, the Hamiltonian does not approach the Hamiltonian with a single $\delta$-perturbation centered at the origin and having twice the strength. Here, we consider the model that can be regarded as the most pedagogical one, that is to say the three-dimensional Hamiltonian $-\Delta + \lambda [\delta(x + x_0) + \delta(x - x_0)]$.

As stated in those papers, such a problematic behavior does not occur in the case of one-dimensional Schrödinger Hamiltonians with the same singular double well, as attested by the findings of [4, 5]. The absence of the aforementioned phenomenon in this case is due to the fact that the $\delta$-perturbation need not be defined by means of the coupling constant renormalization, since it is an infinitesimally small perturbation of the one-dimensional negative Laplacian due to the KLMN theorem.

2. The rigorous definition of the three-dimensional Hamiltonian $-\Delta + \lambda [\delta(x + x_0) + \delta(x - x_0)]$

As is well known (see, e.g., the references in [6]), the Dirac measure in three dimensions was seen to be far more singular as a perturbation of the negative Laplacian than its one-dimensional counterpart even in the early days of Quantum Mechanics. In fact, one has that the matrix element:

$$(f, \delta)(\delta, f) = \left(\hat{f}, \hat{1}\right) \left(\hat{\delta}, 1\right) = \frac{1}{(2\pi)^3} \left(\hat{f}, 1\right) = \frac{1}{(2\pi)^3} \left(\left(|p|^2 + 1 \right)^{1/2}\hat{f}, \left(|p|^2 + 1 \right)^{-1/2}\right) \left(\left(|p|^2 + 1 \right)^{-1/2}, \left(|p|^2 + 1 \right)^{1/2}\hat{f}\right),$$
diverges since the function \((|p|^2 + 1)^{-1}\) is not in \(L^1(\mathbb{R}^3)\) because the integral

\[
4\pi \int_0^{+\infty} p^2 (p^2 + 1)^{-1} \, dp,
\]

is clearly divergent.

As a consequence, the coupling constant renormalization will have to be exploited. In view of the detailed study of the important phenomenon mentioned earlier, the case of a singular double well consisting of two Dirac distributions symmetrically centered around the origin will be considered, precisely at the points:

\[
\pm \tilde{z}_0 = (\pm x_0, 0, 0), \quad x_0 > 0.
\]

Therefore, after introducing the ultraviolet cut-off given by \(k > 0\), i.e.:

\[
|\tilde{p}| = \sqrt{p_x^2 + p_y^2 + p_z^2} \leq k,
\]

the resolvent limit, as \(k \to +\infty\), of the Hamiltonian describing in momentum space the negative Laplacian plus a sum of symmetric \(\delta\)-potentials at \(\pm \tilde{z}_0\), with cut-off \(k\) and coupling constant \(\lambda(k) \neq 0\) depending on it:

\[
h(k, x_0) = |\tilde{p}|^2 + \frac{\lambda(k)}{(2\pi)^3} \left[ |x|_{|\tilde{p}| \leq k} e^{-i\tilde{z}_0 \cdot \tilde{p}} \left( |\tilde{p}|^2 + |E| \right)^{-1} \chi_{|\tilde{p}| \leq k} e^{-i\tilde{z}_0 \cdot \tilde{p}} \right],
\]

is to be studied (\(\chi(\cdot)\) denoting the indicator function of the set \((\cdot)\)). As the intermediate steps are essentially along the same lines of those in the three aforementioned papers [1–3], it is quite straightforward to obtain the expression for the resolvent of \(H(k, x_0)\) for any \(E < 0\):

\[
\left[ h(k, x_0) + |E| \right]^{-1} = \left[ |\tilde{p}|^2 + |E| \right]^{-1} -
\]

\[
\frac{2}{(2\pi)^3} \left| \chi_{|\tilde{p}| \leq k} \cos(\tilde{z}_0 \cdot \tilde{p}) \cdot \left( |\tilde{p}|^2 + |E| \right)^{-1} \chi_{|\tilde{p}| \leq k} \sin(\tilde{z}_0 \cdot \tilde{p}) \cdot \left( |\tilde{p}|^2 + |E| \right)^{-1} \right|^2
\]

\[
\left[ \frac{1}{\lambda(k)} + \frac{2}{(2\pi)^3} \left| \chi_{|\tilde{p}| \leq k} \cos(\tilde{z}_0 \cdot \tilde{p}) \cdot \left( |\tilde{p}|^2 + |E| \right)^{-1/2} \right|^2 \right]^2
\]

\[
\left[ \frac{2}{(2\pi)^3} \left| \chi_{|\tilde{p}| \leq k} \sin(\tilde{z}_0 \cdot \tilde{p}) \cdot \left( |\tilde{p}|^2 + |E| \right)^{-1} \chi_{|\tilde{p}| \leq k} \sin(\tilde{z}_0 \cdot \tilde{p}) \cdot \left( |\tilde{p}|^2 + |E| \right)^{-1} \right|^2 \right]^2
\]

Furthermore,

\[
\frac{2}{(2\pi)^3} \left| \chi_{|\tilde{p}| \leq k} \cos(\tilde{z}_0 \cdot \tilde{p}) \cdot \left( |\tilde{p}|^2 + |E| \right)^{-1/2} \right|^2 = \frac{2}{(2\pi)^3} \int_{|\tilde{p}| \leq k} \cos(\tilde{z}_0 \cdot \tilde{p}) \cdot \left( |\tilde{p}|^2 + |E| \right)^{-1} d^3 p =
\]

\[
\frac{1}{(2\pi)^3} \int_{|\tilde{p}| \leq k} \frac{1 + \cos(2\tilde{z}_0 \cdot \tilde{p})}{|\tilde{p}|^2 + |E|} \, d^3 p = \frac{1}{(2\pi)^3} \int_{|\tilde{p}| \leq k} \frac{4\pi}{|\tilde{p}|^2} \, d |\tilde{p}| + \frac{\cos(2\tilde{z}_0 \cdot \tilde{p})}{|\tilde{p}|^2 + |E|} \, d^3 p =
\]

\[
\frac{1}{(2\pi)^3} \left[ 4\pi k - 4\pi |E| \int_{|\tilde{p}| \leq k} \frac{1}{|\tilde{p}|^2 + |E|} \, d |\tilde{p}| + \frac{\cos(2\tilde{z}_0 \cdot \tilde{p})}{|\tilde{p}|^2 + |E|} \, d^3 p \right] =
\]

\[
\frac{4\pi}{(2\pi)^3} \left[ k - |E|^{1/2} \tan^{-1} \left( \frac{k}{|E|^{1/2}} \right) \right] + \frac{1}{(2\pi)^3} \int_{|\tilde{p}| \leq k} \frac{\cos(2\tilde{z}_0 \cdot \tilde{p})}{|\tilde{p}|^2 + |E|} \, d^3 p.
\]

Similarly,

\[
\frac{2}{(2\pi)^3} \left| \chi_{|\tilde{p}| \leq k} \sin(\tilde{z}_0 \cdot \tilde{p}) \cdot \left( |\tilde{p}|^2 + |E| \right)^{-1/2} \right|^2 =
\]

\[
\frac{4\pi}{(2\pi)^3} \left[ k - |E|^{1/2} \tan^{-1} \left( \frac{k}{|E|^{1/2}} \right) \right] - \frac{1}{(2\pi)^3} \int_{|\tilde{p}| \leq k} \frac{\cos(2\tilde{z}_0 \cdot \tilde{p})}{|\tilde{p}|^2 + |E|} \, d^3 p.
\]
The removal of the cut-off, that is to say the limit \( k \to +\infty \), does not constitute a problem for the two rank one operators in the last two terms of (2.3) since:

\[
\left\| \cos(\vec{x}_0 \cdot \vec{p}) \cdot \left( |\vec{p}|^2 + |E| \right)^{-1} \right\|_2 < \infty, \quad \left\| \sin(\vec{x}_0 \cdot \vec{p}) \cdot \left( |\vec{p}|^2 + |E| \right)^{-1} \right\|_2 < \infty.
\]

Then, it is clear that the reciprocal of \( \lambda(k) \) is to be chosen in such a way as to get the cancellation of the divergent quantity proportional to \( k \). In fact, by setting:

\[
\frac{1}{\lambda(k, \beta)} = -\frac{1}{\beta} \left( \frac{1}{2\pi^3} \int_{|\vec{p}| \leq k} \frac{1}{|\vec{p}|^2} d^3p - \frac{1}{\beta} = -\frac{k}{2\pi^3} \frac{1}{\beta}, \right.
\]

or equivalently:

\[
\lambda(k, \beta) = \frac{\beta}{1 + \frac{1}{(2\pi)^3} \int_{|\vec{p}| \leq k} \frac{1}{|\vec{p}|^2} d^3p},
\]

for any real \( \beta \), the limit of the right hand side of (2.3), as \( k \to +\infty \), is given by:

\[
R(|E|, \beta, x_0) = \left[ \frac{2}{(2\pi)^3} \frac{1}{|\vec{p}|^2 + |E|} \right] \left( \frac{\cos(\vec{x}_0 \cdot \vec{p})}{|\vec{p}|^2 + |E|} \right) + \left[ \frac{2}{(2\pi)^3} \frac{1}{|\vec{p}|^2 + |E|} \right] \left( \frac{\sin(\vec{x}_0 \cdot \vec{p})}{|\vec{p}|^2 + |E|} \right) = \frac{\beta}{4\pi} + \frac{1}{(2\pi)^3} \lim_{k \to +\infty} \int_{|\vec{p}| \leq k} \frac{1}{|\vec{p}|^2 + |E|} d^3p.
\]

At this stage, one should prove that \( R(|E|, \beta, x_0) \) is the resolvent of a self-adjoint operator \( h(\beta, x_0) \). However, such a proof will be omitted here given that it would be almost identical to the one provided in [6] in the case of a single point perturbation centered at the origin, the only difference represented by the possibility of having a second point to be excluded along the negative energy semiaxis, namely the possible zero of the denominator of the last term in (2.6).

The above findings can be summarized in the following theorem:

**Theorem 2.1.** The Hamiltonian of the three-dimensional negative Laplacian perturbed by two identical attractive point interactions situated symmetrically with respect to the origin at the points \( \pm \vec{x}_0 = (\pm x_0, 0, 0) \), \( x_0 = |\vec{x}_0| > 0 \), making sense of the merely formal expression:

\[
h(\lambda(\beta), x_0) = -\Delta + \lambda(\beta) \left[ \delta(\vec{z} - \vec{x}_0) + \delta(\vec{z} + \vec{x}_0) \right],
\]

with:

\[
\lambda(\beta) = \frac{\beta}{1 + \frac{1}{(2\pi)^3} \int_{|\vec{p}| \leq k} \frac{1}{|\vec{p}|^2} d^3p},
\]

being the self-adjoint operator \( h(\beta, x_0) \) whose resolvent is given by the bounded operator (2.6). The latter is the limit of the resolvents (2.3) of the Hamiltonians (2.2) (with the energy cut-off \( k \) defined by (2.1)) in the norm topology of bounded operators on \( L^2(\mathbb{R}^3) \) once the energy cut-off is removed, i.e. for \( k \to +\infty \). Furthermore, \( h(\beta, x_0) \) regarded as a function of \( \beta \) is an analytic family in the sense of Kato.

Hence, the equation leading to the calculation of the ground state energy is:

\[
\alpha + \frac{|E|^{1/2}}{4\pi} - \frac{1}{4\pi} e^{-2|E|^{1/2}x_0} = 0, \quad \alpha = \frac{1}{\beta},
\]

while the one leading to the calculation of the energy of the other bound state is:

\[
\alpha + \frac{|E|^{1/2}}{4\pi} + \frac{1}{4\pi} e^{-2|E|^{1/2}x_0} = 0.
\]
These two equations are exactly those thoroughly studied at the end of section II.1 in [6]: as shown graphically in Fig. 1 below for $x_0 = 1/2$.

i) both eigenvalues are absent if $4\pi \alpha \geq (2x_0)^{-1}$;
ii) the ground state is the only bound state if $-(2x_0)^{-1} \leq \pi \alpha < (2x_0)^{-1}$;
iii) there are two bound states if $4\pi \alpha < -(2x_0)^{-1}$.

![Spectral curves](image)

**Fig. 1.** The spectral curves of the two eigenvalues of $h(1/\alpha, x_0)$ as functions of the extension parameter $\alpha$ for $x_0 = 1/2$

As can be seen in the above plot, whilst the excited state energy gets absorbed into the absolutely continuous spectrum at the point $\alpha = -(4\pi)^{-1}$, the ground state energy gets absorbed into the absolutely continuous spectrum at the opposite value $\alpha = (4\pi)^{-1}$. This is entirely consistent, of course, with the fact that, for any fixed value of $x_0$, as $\alpha \to +\infty$, $h(1/\alpha, x_0)$ approaches the free Hamiltonian in the norm resolvent sense.

The interesting phenomenon previously anticipated is that, as $x_0 \to 0_+$, the two eigenvalues exhibit different behaviors: whilst the second eigenvalue gets absorbed into the absolutely continuous spectrum, the magnitude of the ground state energy diverges, clearly implying that the Hamiltonian does not converge to the one in which the perturbation is represented by a single point interaction having double the strength. As mentioned earlier, the same phenomenon was observed in [1] dealing with the one-dimensional Salpeter Hamiltonian perturbed by a pair of twin Dirac distributions symmetrically situated with respect to the origin, the spectrum of which also consists of two eigenvalues below the absolutely continuous spectrum, as well as in [2, 3] dealing instead with an operator having only infinitely many eigenvalues, namely the Hamiltonian of the three-dimensional harmonic oscillator perturbed by a pair of twin Dirac distributions symmetrically situated with respect to the origin. Such a singular behavior is in contrast with the smooth one of one-dimensional Schrödinger Hamiltonians with or without the harmonic confinement under the same perturbation (see [4, 5]), as well as with that exhibited by three-dimensional Hamiltonians with perturbations whose range might be even very short but non-zero.

The strategy needed to regularize this singular behavior, thus making three-dimensional zero range perturbations behave like positive range ones, is the one adopted in the aforementioned papers, that is to say the coupling constant to be renormalized must also suitably depend on $x_0$. It is quite instructive to see how this works in the case of the model analyzed in this note.

By setting:

$$
\frac{1}{\lambda(k, \beta, x_0)} = -\frac{k}{(2\pi)^2} + \frac{1}{\beta} + \frac{1}{(2\pi)^3} \int_{|\vec{p}| \leq k} \frac{\cos(2\vec{x}_0 \cdot \vec{p})}{|\vec{p}|^2} d^3 p, 
$$

(2.9)

and

$$
H(k, x_0) = |p|^2 + \frac{\lambda(k, \beta, x_0)}{(2\pi)^3} \left[ |\chi|_{|\vec{p}| \leq k e^{-i\vec{x}_0 \cdot \vec{p}}} \langle \chi | \vec{p} \leq k e^{-i\vec{x}_0 \cdot \vec{p}} | \chi \rangle + |\chi|_{|\vec{p}| \leq k e^{i\vec{x}_0 \cdot \vec{p}}} \langle \chi | \vec{p} \leq k e^{i\vec{x}_0 \cdot \vec{p}} | \chi \rangle \right],
$$

(2.10)
it is rather straightforward to obtain the new limit of the resolvent of (2.10) once the ultraviolet cut-off gets removed, namely:

\[
\tilde{R}(\{E\}; \beta, x_0) = \left(\frac{2}{(2\pi)^3} \frac{1}{|p|^2 + |E|} \right)^{-1} \left(\frac{2}{(2\pi)^3} \frac{\cos(\vec{x}_0 \cdot \hat{p})}{|p|^2 + |E|} \right) \left(\frac{1}{|p|^2} - \frac{1}{|p|^2 + |E|} \right) d^3p + \frac{1}{\beta} \frac{|E|^{1/2}}{4\pi} \left(\frac{2}{(2\pi)^3} \right) \lim_{|p| \to k} \left(\frac{\sin(\vec{x}_0 \cdot \hat{p})}{|p|^2 + |E|} \right) d^3p
\]

\[
\tilde{R}(\{E\}; \beta, x_0) = \frac{1}{\beta} + \frac{|E|^{1/2}}{4\pi} \left(\frac{2}{(2\pi)^3} \right) \lim_{|p| \to k} \left(\frac{\sin(\vec{x}_0 \cdot \hat{p})}{|p|^2 + |E|} \right) d^3p = \left[\frac{|p|^2 + |E|}{k} \right]^{-1} + \frac{2}{(2\pi)^3} \frac{\cos(\vec{x}_0 \cdot \hat{p})}{|p|^2 + |E|} \left(\frac{1}{|p|^2} - \frac{1}{|p|^2 + |E|} \right) d^3p + \frac{2}{(2\pi)^3} \frac{\sin(\vec{x}_0 \cdot \hat{p})}{|p|^2 + |E|} \left(\frac{1}{|p|^2} - \frac{1}{|p|^2 + |E|} \right) d^3p
\]

This operator can be rigorously shown to be the resolvent of another self-adjoint operator \(H(\beta, x_0) = H(1/\alpha, x_0)\) by means of a proof again patterned after the aforementioned one in [6]. Therefore, also in this case our findings can be summarized in the following theorem:

**Theorem 2.2.** The Hamiltonian of the three-dimensional negative Laplacian perturbed by two identical attractive point interactions situated symmetrically with respect to the origin at the points \(\pm \vec{x}_0 = (\pm x_0, 0, 0)\), \(x_0 = |\pm x_0| > 0\), making sense of the merely formal expression:

\[
H(\lambda(\beta, x_0), x_0) = -\Delta + \lambda(\beta, x_0) \left[\delta(\vec{x} - \vec{x}_0) + \delta(\vec{x} + \vec{x}_0)\right],
\]

with:

\[
\lambda(\beta, x_0) = \frac{\beta}{1 + \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{1 + \cos(2\vec{x} \cdot \hat{p})}{|p|^2} d^3p},
\]

is the self-adjoint operator \(H(\beta, x_0)\) whose resolvent is given by the bounded operator (2.11). The latter is the limit of the resolvents of the Hamiltonians (2.10) (with the energy cut-off \(k\) defined by (2.1)) in the norm topology of bounded operators on \(L^2(\mathbb{R}^3)\) once the energy cut-off is removed, i.e. for \(k \to +\infty\). Furthermore, \(H(\beta, x_0)\) regarded as a function of \(\beta\) is an analytic family in the sense of Kato.

The discrete spectrum of \(H(\beta, x_0) = H(1/\alpha, x_0)\) may also have up to two eigenvalues, namely the solutions of:

\[
\alpha + \frac{|E|^{1/2}}{4\pi} + \frac{1}{4\pi} \frac{1 - e^{-2|E|^{1/2}x_0}}{2x_0} = 0, \quad \alpha = \frac{1}{\beta} \quad \text{(ground state energy equation)},
\]

\[
\alpha + \frac{|E|^{1/2}}{4\pi} + \frac{1}{4\pi} \frac{1 + e^{-2|E|^{1/2}x_0}}{2x_0} = 0, \quad \alpha = \frac{1}{\beta} \quad \text{(excited state energy equation)}.
\]

The solutions of both equations are plotted below in Fig. 2 as functions of \(\alpha = 1/\beta\), for \(x_0 = 1/2\), for the sake of comparison with those of \(h(1/\alpha, x_0)\) shown earlier in Fig. 1.

The above plot shows that the ground state energy gets absorbed into the absolutely continuous spectrum exactly at \(\alpha = 0\), thus implying \(\epsilon_0(0) = 0\). This is entirely consistent with the expectation that this operator should approach, as \(x_0 \to 0_+\), the negative Laplacian perturbed by a single point interaction centred at the origin which is known to have a zero energy resonance at \(\alpha = 0\), characterised by the fact that the corresponding x-space wave function is only locally square integrable (see [6]).
Fig. 2. The spectral curves of the two eigenvalues of $H(1/\alpha, x_0)$ as functions of the extension parameter $\alpha$ for $x_0 = 1/2$

The norm resolvent limit of $H(\beta, x_0)$, as $x_0 \to 0_+$, is clearly given by:

$$
\left(\frac{1}{|p|^2 + |E|}\right)^{-1} + \frac{1}{(2\pi)^3} \frac{1}{|p|^2 + |E|} \left(\frac{1}{|p|^2 + |E|^{1/2}}\right) \cdot \frac{1}{2\beta + \frac{|E|^{1/2}}{4\pi}}.
$$

(2.14)

The latter is nothing else but the resolvent in momentum space of the negative Laplacian perturbed by a single point interaction centered at the origin having double strength, as can be understood by looking at either (1.1.21), its $x$-space counterpart, in Section I.1 of [6] or (1.1.24) in Section II.1 of the same monograph for $N = 1$ with the origin being the location of the single point perturbation, taking into account that the extension parameter $\alpha$ used therein is the reciprocal of the strength. Apart from the absolutely continuous spectrum $[0, +\infty)$, if $\beta < 0$, there is an isolated eigenvalue below the absolutely continuous spectrum, namely:

$$
E_0(2\beta) = \left(\frac{2\pi}{\beta}\right)^2.
$$

3. Final remarks

In this brief note, we have considered the most pedagogical three-dimensional model involving a symmetric double well consisting of two identical Dirac distributions, whose Hamiltonian is heuristically given by $-\Delta + \lambda [\delta(x + x_0) + \delta(x - x_0)]$. We have first reviewed the coupling constant renormalization procedure leading to the rigorous definition of the self-adjoint operator fully investigated in [6] as well as the two ensuing equations determining the two possible eigenvalues generated by the perturbation. Since the ground state eigenenergy does not converge to the single eigenvalue of the self-adjoint Hamiltonian $-\Delta_{1/2\beta, 0}$, defined in [6] (with $\beta < 0$) as the distance between the two centres shrinks to zero, an alternative renormalization procedure has been adopted in order to regularise this problematic behavior. By making the coupling constant suitably dependent also on $x_0 = |\pm \tilde{x}_0| > 0$, in addition to the usual momentum cut-off, it has been possible to define a new self-adjoint Hamiltonian whose resolvent converges in norm to that of $-\Delta_{1/2\beta, 0}$ as $x_0 \to 0_+$. The crucial difference between the discrete spectra of the two operators is that, whilst the ground state eigenenergy of the former Hamiltonian gets absorbed into the absolutely continuous spectrum at $\alpha = (8\pi x_0)^{-1}$ ($\alpha = 1/\beta$ being the extension parameter), the ground state eigenenergy of the latter gets absorbed into the absolutely continuous spectrum at $\alpha = 0$ independently of $x_0$. As pointed out earlier, this is entirely consistent with the fact that the limiting operator, that is to say the negative Laplacian perturbed by a single point interaction centered at the origin, is known to have a zero energy resonance at $\alpha = 0$, so that the corresponding $x$-space wave function is only locally square integrable (see [6]).

This might have some relevant implications in the study of quantum three-body models consisting of two heavy particles and a light one interacting with each other via two-body zero range interactions, at least in the adiabatic approximation, as might be implied by the findings of [7].

We also intend to extend the analysis of the singular phenomenon carried out in this note and in the aforementioned papers [1-3] to another type of quantum oscillator with a different confinement, namely the one whose Hamiltonian is given by:

$$
H_0 = \frac{1}{2} (-\Delta + |\tilde{x}|),
$$
even though the resolvent of this three-dimensional operator will have to be determined first since, differently from its one-dimensional counterpart (see [10, 11]), it is not yet explicitly known.

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