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Spectral properties of a symmetric three-dimensional quantum dot with a pair of identical attractive δ-impurities symmetrically situated around the origin II

S. Albeverio[1,2,3], S. Fassari[2,4], and F. Rinaldi[2,4]

[1]Institut für Angewandte Mathematik, HCM, IZKS, BiBoS, Universität Bonn, Endenicheralee 60, D-53115 Bonn, Germany

[2]CERFIM, PO Box 1132, CH-6601 Locarno, Switzerland

[3]Chair Professorship, Department of Mathematics and Statistics, King Fahd University of Petroleum and Minerals, Dhahran, KSA

[4]Università degli Studi Guglielmo Marconi, Via Plinio 44, I-00193 Rome, Italy

sifassari@gmail.com

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In this note, we continue our analysis (started in [1]) of the isotropic three-dimensional harmonic oscillator perturbed by a pair of identical attractive point interactions symmetrically situated with respect to the origin, that is to say, the mathematical model describing a symmetric quantum dot with a pair of point impurities. In particular, by making the coupling constant (to be renormalized) dependent also upon 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 introduced in [1], 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 isotropic three-dimensional harmonic oscillator 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 different from zero. Moreover, we show the manifestation of the Zeldovich effect, known also as level rearrangement, in the model investigated herewith. More precisely, we take advantage of our renormalization procedure to demonstrate the possibility of using the concept of 'Zeldovich spiral', introduced in the case of perturbations given by rapidly decaying potentials, also in the case of point perturbations.

Keywords: level crossing, degeneracy, point interactions, renormalisation, Schrödinger operators, quantum dots, perturbed quantum oscillators, Zeldovich effect, level rearrangement.

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1. Introduction

The main purpose of this note is to extend the results of [1] by fixing the problematic behavior of the Hamiltonian $H_{\{\beta,\vec{x}_0\}}$ studied therein in the limit $x_0 = |\pm\vec{x}_0| \to 0_+$, that is to say as the distance between the two twin point perturbations shrinks to zero. As was noticed in [1], the Hamiltonian $H_{\{\beta,\vec{x}_0\}}$, the self-adjoint energy operator of the three-dimensional isotropic harmonic oscillator perturbed by a pair of identical point interactions symmetrically situated around the origin defined rigorously by means of a 'coupling constant renormalization', does not converge to $H_{2\beta}$, the one of the three-dimensional isotropic harmonic oscillator perturbed by a single point interaction situated at the origin having double strength. Such a singular behavior manifested by singular double wells with point interactions in three dimensions is in sharp contrast with conventional double wells generated by potentials, whose range may even be very short but non-zero. By citing [1] it is important to recall that *'as is well known to Quantum Chemistry students, three-dimensional interactions with a nonzero range do not manifest this singular behavior in the limit of the distance between the two centers shrinking to zero, as the classical textbook example of* H_2^+ *smoothly approaching* He^+ *in the limit* $R \to 0_+$ *clearly shows'* (see [2–4]). The same phenomenon had been observed in [5] (see also [6–10]) dealing with another model involving a pair of identical point interactions symmetrically situated around the origin defined rigorously by using a 'coupling constant renormalization' as well, namely the one-dimensional energy operator in which the kinetic component is given by the Salpeter free Hamiltonian $\sqrt{p^2+m^2}$, $m>0$.

As was fully proved in [10], this singular behavior does not occur in the one-dimensional analog of the model given that the Dirac distribution is an infinitesimally small perturbation of the Laplacian in one dimension, which implies that the renormalization procedure is not required at all in that case to define a self-adjoint Hamiltonian (obtained instead by means of the KLMN theorem, see [11]).

Here, in the next section, we adopt the same strategy used in [5] to regularize the behavior in the limit $x_0 \to 0_+$: we make the coupling constant to be renormalized dependent also on x_0, in addition to the two standard parameters, namely the positive integer labeling the ultraviolet energy cut-off and the real number whose reciprocal represents the extension parameter (see [5–7]). The new self-adjoint Hamiltonian $\mathrm{H}_{\{\beta,\vec{x}_0\}}$, clearly dependent on x_0 and obtained as the norm resolvent limit after removing the energy cut-off (Theorem 2.1), is shown to approach smoothly $H_{2\beta}$ in the norm resolvent limit as $x_0 \to 0_+$ (Theorem 2.2). We would like to stress that, although this is exactly the strategy employed also in papers such as [12–14] to obtain the self-adjoint operator with the δ'-interaction perturbing either the negative Laplacian or the Hamiltonian of the harmonic oscillator in one dimension as the norm resolvent limit of Hamiltonians with the perturbation consisting of a triple of δ-interactions, the dependence on x_0 is completely different.

We also carry out the detailed spectral analysis of the lowest lying eigenvalues of $\mathrm{H}_{\{\beta,\vec{x}_0\}}$ as functions of α, the parameter labeling the self-adjoint extensions. Although the analysis could be extended to higher eigenvalues at the conceptual level, we have decided to restrict our investigation because of its increasing operational complexity (the same restriction had also been adopted in [1, 8–10, 15, 16]). The latter analysis shows that the spectrum of $\mathrm{H}_{\{\beta,\vec{x}_0\}}$, similarly to that of the operator $H_{\{\beta,\vec{x}_0\}}$ investigated in [1], exhibits the rather remarkable phenomenon of having a range of values of the parameter where the $2S$ state is more tightly bound than the $2P$ one.

In the third section, we revisit the spectral analysis of the lowest lying eigenvalues by regarding them as functions of β, the parameter appearing explicitly in the coupling constant to be renormalized. Our main motivation for this further analysis has been the fact that, following [17], the latter parameter is the conventional one used to study the manifestation of the Zeldovich effect (see [18]), widely known also as level rearrangement. We are going to show that the phenomenon, studied by the authors of that article when the perturbation of the three-dimensional isotropic harmonic oscillator is represented by a potential whose range is physically very short but different from zero, does manifest itself also in the case of point perturbations. In particular, it is our intention to demonstrate that the structure of the discrete spectrum of operators like $H_{2\beta}$ and $\mathrm{H}_{\{\beta,\vec{x}_0\}}$ can be better understood by adopting the cylindrical mapping based on the Cartesian product $\mathbb{R} \times S^1$, with E, the energy parameter, drawn along the real line (the symmetry axis of the cylinder) and the extension parameter along the unit circle identifying $\pm\infty$, instead of the traditional $\mathbb{R}^2$. This alternative representation was first introduced in [19], in which the rather intriguing concept of 'Zeldovich spiral' was proposed investigating the 3D-isotropic harmonic oscillator perturbed by three rapidly decaying potentials, even though their plots are of the type E vs. $\alpha = 1/\beta$. In the third section of the current note, we will show that, as a result of our renormalization procedure (which is different from the one adopted in [20] and leads to the spectral requirement $E_0(\alpha = 0, x_0) = 0 = E_0(\beta = +\infty, x_0)$ for the ground state energy of $\mathrm{H}_{\{\beta,\vec{x}_0\}}$), the Zeldovich spiral can also be visualized in the case of point perturbations of the three-dimensional isotropic harmonic oscillator directly on plots of the type E vs. β.

Finally, in the last section we review the key results of this note and outline prospective avenues of further research work.

2. The regularized three-dimensional isotropic harmonic oscillator perturbed by two twin attractive point perturbations symmetrically situated with respect to the origin

Given that all the steps preceding the introduction of the coupling constant are identical to those from (3.1) up to (3.10) in [1], we omit them here and refer the reader to that paper. As anticipated earlier and following the strategy used in [5], the coupling constant will be made dependent on the magnitude of the position vectors of the twin point impurities, namely $x_0 = |\pm\vec{x}_0|$, $x_0 = (x_0, 0, 0)$, $x_0 > 0$, as follows:

$$\frac{1}{\mu(\ell,\beta;x_0)} = \frac{1}{\beta} + 2\sum_{|\vec{n}|=0}^{\ell} \frac{\Psi^2_{2\vec{n}}(\vec{x}_0)}{|2\vec{n}| + \frac{3}{2}}, \tag{2.1}$$

or equivalently

$$\mu(\ell,\beta;x_0) = \beta\left[1 + 2\beta\sum_{|\vec{n}|=0}^{\ell} \frac{\Psi^2_{2\vec{n}}(\vec{x}_0)}{|2\vec{n}| + \frac{3}{2}}\right]^{-1} \tag{2.1b}$$

with $\beta \in \mathbb{R}^3\backslash\{0\}$.

In perfect accordance with the use of the term 'attractive' in [1, 5, 8, 9], it is clear that $\mu(\ell,\beta;x_0) > 0$ for the large values of ℓ involved in the limit $\ell \to +\infty$ regardless of the sign of β, making the singular interaction attractive because of the presence of the negative sign in the second term in (3.2) in [1].

Hence, for any $E < 3/2$:

$$\frac{1}{2\mu(\ell,\beta;x_0)} - (H_0^\ell - E)_s^{-1}(\vec{x}_0,\vec{x}_0) = \frac{1}{2\beta} + \sum_{|\vec{n}|=0}^{\ell} \frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}| + \frac{3}{2}} - \sum_{|\vec{n}|=0}^{\ell} \frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}| + \frac{3}{2} - E} \tag{2.2}$$

and

$$\frac{1}{2\mu(\ell,\beta;x_0)} - (H_0^\ell - E)_{as}^{-1}(\vec{x}_0,\vec{x}_0) = \frac{1}{2\beta} + \sum_{|\vec{n}|=0}^{\ell} \frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}| + \frac{3}{2}} - \sum_{|\vec{n}|=0}^{\ell} \frac{\psi(x_0)_{2n_1+1}^2 \psi_{2n_2}^2(0)\psi_{2n_3}^2(0)}{2n_1 + 2n_2 + 2n_3 + \frac{5}{2} - E}. \tag{2.3}$$

Therefore, we need only mimic what was done in [1] to get that, after removing the ultraviolet cut-off, i.e. in the limit $\ell \to +\infty$, the norm resolvent limit of our net of Hamiltonians

$$\begin{aligned}\left(\mathrm{H}_{\{\ell,\beta,\vec{x}_0\}} - E\right)^{-1} &= (H_0 - E)^{-1} \\ &+ \frac{1}{\frac{1}{2\mu(\ell,\beta;x_0)} - (H_0^\ell - E)_s^{-1}(\vec{x}_0,\vec{x}_0)} \big|(H_0^\ell - E)_s^{-1}(\cdot,\vec{x}_0)\big\rangle\big\langle(H_0^\ell - E)_s^{-1}(\vec{x}_0,\cdot)\big| \\ &+ \frac{1}{\frac{1}{2\mu(\ell,\beta;x_0)} - (H_0^\ell - E)_{as}^{-1}(\vec{x}_0,\vec{x}_0)} \big|(H_0^\ell - E)_{as}^{-1}(\cdot,\vec{x}_0)\big\rangle\big\langle(H_0^\ell - E)_{as}^{-1}(\vec{x}_0,\cdot)\big| \end{aligned} \tag{2.4}$$

is given by:

$$\begin{aligned} &(H_0 - E)^{-1} + \frac{\big|(H_0 - E)_s^{-1}(\cdot,\vec{x}_0)\big\rangle\big\langle(H_0 - E)_s^{-1}(\vec{x}_0,\cdot)\big|}{\frac{1}{2\beta} + \lim_{\ell\to+\infty}\left[\sum_{|\vec{n}|=0}^{\ell} \frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}| + \frac{3}{2}} - \sum_{|\vec{n}|=0}^{\ell} \frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}| + \frac{3}{2} - E}\right]} \\ &\quad + \frac{\big|(H_0 - E)_{as}^{-1}(\cdot,\vec{x}_0)\big\rangle\big\langle(H_0 - E)_{as}^{-1}(\vec{x}_0,\cdot)\big|}{\frac{1}{2\beta} + \lim_{\ell\to+\infty}\left[\sum_{|\vec{n}|=0}^{\ell} \frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}| + \frac{3}{2}} - \sum_{|\vec{n}|=0}^{\ell} \frac{\psi(x_0)_{2n_1+1}^2 \psi_{2n_2}^2(0)\psi_{2n_3}^2(0)}{2n_1 + 2n_2 + 2n_3 + \frac{5}{2} - E}\right]} \\ &= (H_0 - E)^{-1} + \frac{\big|(H_0 - E)_s^{-1}(\cdot,\vec{x}_0)\big\rangle\big\langle(H_0 - E)_s^{-1}(\vec{x}_0,\cdot)\big|}{\frac{1}{2\beta} - E\sum_{|\vec{n}|=0}^{\infty} \frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{(|2\vec{n}| + 3/2)(|2\vec{n}| + 3/2 - E)}} \\ &\quad + \frac{\big|(H_0 - E)_{as}^{-1}(\cdot,\vec{x}_0)\big\rangle\big\langle(H_0 - E)_{as}^{-1}(\vec{x}_0,\cdot)\big|}{\frac{1}{2\beta} + \lim_{\ell\to+\infty}\left[\sum_{|\vec{n}|=0}^{\ell} \frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}| + \frac{3}{2}} - \sum_{|\vec{n}|=0}^{\ell} \frac{\psi(x_0)_{2n_1+1}^2 \psi_{2n_2}^2(0)\psi_{2n_3}^2(0)}{2n_1 + 2n_2 + 2n_3 + \frac{5}{2} - E}\right]}. \end{aligned} \tag{2.5}$$

As can be immediately noticed, the series in the denominator of the second term on the right hand side is convergent for any fixed $x_0 > 0$ and any $E < 3/2$ as an easy consequence of an estimate similar to (3.8) in [1] (see also (2.2) in [9]).

We can also analyze the limits appearing in both denominators in (2.5) by means of a suitable modification of the method used in [1] (essentially based on the properties of the semigroup of the three-dimensional harmonic oscillator, as seen in [1, 9, 20]). In fact, for any $E < 3/2$, the limit in the first denominator of (2.5) is given by:

$$\begin{aligned} &-E\sum_{|\vec{n}|=0}^{\infty} \frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{(|2\vec{n}| + 3/2)(|2\vec{n}| + 3/2 - E)} = \lim_{\ell\to+\infty}\left[\sum_{|\vec{n}|=0}^{\ell} \frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}| + \frac{3}{2}} - \sum_{|\vec{n}|=0}^{\ell} \frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}| + \frac{3}{2} - E}\right] = \\ &\frac{1}{2\pi^{3/2}}\left[\int_0^1 \frac{\xi^{\frac{1}{2}}}{(1-\xi^2)^{3/2}}d\xi - \int_0^1 \frac{\xi^{\frac{1}{2}-E}\left[e^{-x_0^2\frac{1-\xi}{1+\xi}} + e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi\right] = \\ &\frac{1}{2\pi^{3/2}}\int_0^1 \frac{\left(\xi^{\frac{1}{2}} - \xi^{\frac{1}{2}-E}\right)\left[e^{-x_0^2\frac{1-\xi}{1+\xi}} + e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi < \infty. \end{aligned} \tag{2.6}$$

The second one, well defined even for any $E < 5/2$, is instead equal to:

$$\frac{1}{2\pi^{3/2}}\left[\int_0^1 \frac{\xi^{\frac{1}{2}}\left[e^{-x_0^2\frac{1-\xi}{1+\xi}}+e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi-\int_0^1 \frac{\xi^{\frac{1}{2}-E}\left[e^{-x_0^2\frac{1-\xi}{1+\xi}}-e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi\right]<\infty. \tag{2.7}$$

Hence, for any $E < 3/2$, the norm limit of the resolvents for $\ell \to +\infty$ (i.e after removing the ultraviolet cut-off) can be written as:

$$(H_0-E)^{-1}+\frac{\left|(H_0-E)_s^{-1}(\cdot,\vec{x}_0)\right\rangle\left\langle(H_0-E)_s^{-1}(\vec{x}_0,\cdot)\right|}{\frac{1}{2\beta}+\frac{1}{2\pi^{3/2}}\int_0^1\frac{\left(\xi^{\frac{1}{2}}-\xi^{\frac{1}{2}-E}\right)\left[e^{-x_0^2\frac{1-\xi}{1+\xi}}+e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi}$$
$$+\frac{\left|(H_0-E)_{as}^{-1}(\cdot,\vec{x}_0)\right\rangle\left\langle(H_0-E)_{as}^{-1}(\vec{x}_0,\cdot)\right|}{\frac{1}{2\beta}+\frac{1}{2\pi^{3/2}}\left[\int_0^1\frac{\xi^{\frac{1}{2}}\left[e^{-x_0^2\frac{1-\xi}{1+\xi}}+e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi-\int_0^1\frac{\xi^{\frac{1}{2}-E}\left[e^{-x_0^2\frac{1-\xi}{1+\xi}}-e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi\right]}. \tag{2.8}$$

The final part of the proof meant to show that the limiting operator (2.8) is indeed the resolvent of a self-adjoint operator is omitted, as was also done in the case of its counterpart in [1], since it is exactly along the same lines of its analogs in the aforementioned papers [5, 8, 9].

The results obtained so far can thus be summarized in the following theorem.

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

$$\mathrm{H}_{\{\mu(\beta;x_0),\vec{x}_0\}} = H_0 - \mu(\beta;x_0)\left[\delta(\vec{x}-\vec{x}_0)+\delta(\vec{x}+\vec{x}_0)\right]$$

with

$$\mu(\beta;x_0) = \beta\left[1+2\beta\sum_{|\vec{n}|=0}^{\infty}\frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{|2\vec{n}|+\frac{3}{2}}\right]^{-1}$$

is the self-adjoint operator $\mathrm{H}_{\{\beta,\vec{x}_0\}}$ *whose resolvent is given by the bounded operator (2.8). The latter is the limit of the resolvents of the Hamiltonians (with the energy cut-off* ℓ *defined by (2.4)) in the norm topology of bounded operators on* $L^2(\mathbb{R}^3)$ *once the energy cut-off is removed, i.e. for* $\ell \to +\infty$. *Furthermore,* $\mathrm{H}_{\{\beta,\vec{x}_0\}}$ *regarded as a function of* β *is an analytic family in the sense of Kato.*

Before moving forward, it may be worth noticing the close analogy between the denominator of the second term in (2.5) (and its other representation in (2.8)) and its counterpart in the case of the spherically symmetric quantum dot with a single point impurity centered at the origin appearing in (2.4) in [1] (see also (2.5) in [9]). As a result of this analogy, even before getting into the detailed spectral analysis of the operator, we can already anticipate that, as was pointed out in [1,9] for the spectrum of the Hamiltonian of the isotropic harmonic oscillator perturbed by a single point impurity, also in the case of the operator introduced in Theorem 2.1 the ground state energy for $\alpha = 0$, where $\alpha = 1/\beta$ (corresponding to the limiting case of point impurities of infinite strength), is equal to zero for any $x_0 > 0$ (α is sometimes called, in the literature on point interactions, see e.g. [6], 'extension parameter').

The ground state energy of the operator $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$, denoted by $E_0(\alpha;x_0)$, can be determined for any fixed value of $x_0 > 0$ by solving the equation:

$$\frac{\alpha}{2} = E\sum_{|\vec{n}|=0}^{\infty}\frac{\Psi_{2\vec{n}}^2(\vec{x}_0)}{(|2\vec{n}|+3/2)(|2\vec{n}|+3/2-E)}, \tag{2.9}$$

solving with respect to E, or equivalently:

$$\alpha = \frac{1}{\pi^{3/2}}\int_0^1\frac{\left(\xi^{\frac{1}{2}-E}-\xi^{\frac{1}{2}}\right)\left[e^{-x_0^2\frac{1-\xi}{1+\xi}}+e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi. \tag{2.9a}$$

The plot of $E_0(\alpha; x_0 = 0.2)$, shown below in Fig. 1, can be compared with both Fig. 1 in [1], the one of the ground state energy of the Hamiltonian of the 3D-isotropic harmonic oscillator perturbed by a single point impurity centered at the origin, and Fig. 3 in the same paper, the corresponding one of the ground state energy of the operator with the symmetrical configuration of point impurities investigated therein obtained for the same value of the separation distance ($x_0 = 0.2$). As was to be expected, the anticipated similarity of the ground state energy of the Hamiltonian introduced in the above theorem with the one considered in the second section of [1] and in [9] is rather striking: both curves intersect the vertical axis at the origin, in agreement with the spectral requirement mentioned earlier at the end of the introduction.

The asymptotic approach to $E_0 = 3/2$, as $\alpha = 1/\beta \to +\infty$, is a straightforward consequence of the fact that the operator converges to the Hamiltonian of the unperturbed harmonic oscillator in the norm resolvent sense.

In the graph shown below (Fig. 2), we also provide the analogous graph for the other value of the distance between each center and the origin considered in [1], that is to say $x_0 = 0.4$.

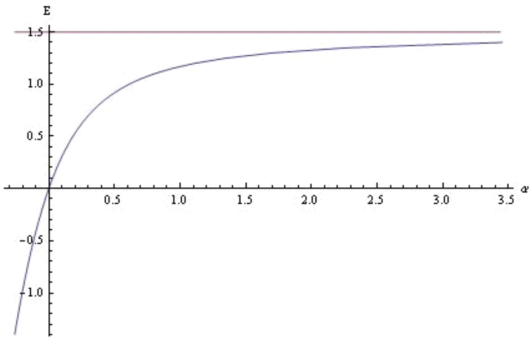

FIG. 1. The ground state energy E_0 of the operator $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$, with $x_0 = 0.2$, as a function of the extension parameter $\alpha = 1/\beta$

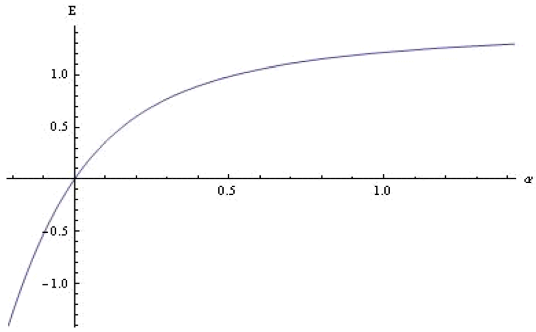

FIG. 2. The ground state energy E_0 of the operator $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$, with $x_0 = 0.4$, as a function of the extension parameter $\alpha = 1/\beta$

In Fig. 3, in order to make more evident the role played by the separation distance x_0, we provide a visual comparison between $E_0(\alpha; x_0 = 0.2)$ and $E_0(\alpha; x_0 = 1)$.

Finally, we show the comparison between $E_0(\alpha; x_0 = 0.2)$ and $E_0(\alpha; x_0 = 0))$ in Fig. 4.

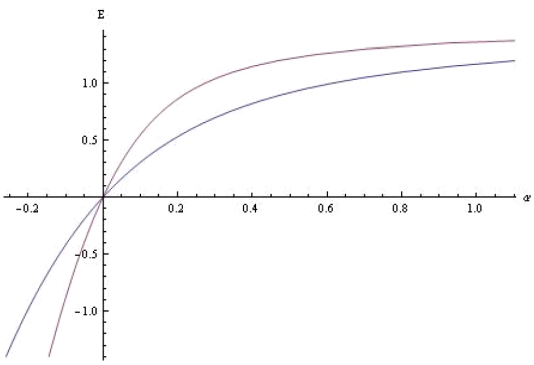

FIG. 3. Comparison between $E_0(\alpha; x_0 = 0.2)$ (blue curve) and $E_0(\alpha; x_0 = 1)$ (violet curve)

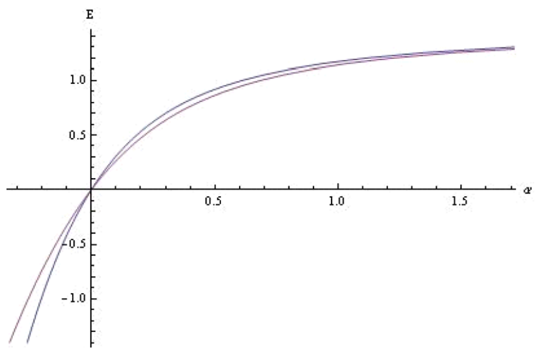

FIG. 4. Comparison between $E_0(\alpha; x_0 = 0.2)$ (blue curve) and $E_0(\alpha; x_0 = 0)$ (violet curve)

As can be noticed from the last two graphs, the behavior of the ground state energy $E_0(\alpha; x_0)$ as a function of x_0 changes remarkably in the vicinity of $\alpha = 0$ ($E = 0$): whilst for positive parameter values, the energy increases as the distance increases, conforming to the expected pattern in terms of the 'positional disorder' (see [1, 20]), the opposite occurs for negative values of α.

Therefore, it is worth computing the derivative of $E_0(\alpha;x_0)$ with respect to x_0 in order to get a better understanding of this phenomenon. By means of implicit differentiation, we can write for any $E < 3/2$:

$$\frac{dE}{dx_0} = -\frac{\dfrac{\partial}{\partial x_0}\int_0^1 \dfrac{(\xi^{\frac{1}{2}-E} - \xi^{\frac{1}{2}})\left[e^{-x_0^2\frac{1-\xi}{1+\xi}} + e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi}{\dfrac{\partial}{\partial E}\int_0^1 \dfrac{(\xi^{\frac{1}{2}-E} - \xi^{\frac{1}{2}})\left[e^{-x_0^2\frac{1-\xi}{1+\xi}} + e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi}, \tag{2.10}$$

having simplified the factor $1/\pi^{3/2}$.

After computing the two partial derivatives (by moving the derivatives inside the integrals, using dominated convergence) we get:

$$\frac{dE}{dx_0} = -\frac{2x_0\int_0^1 \dfrac{(\xi^{\frac{1}{2}-E} - \xi^{\frac{1}{2}})\left[\frac{1-\xi}{1+\xi}e^{-x_0^2\frac{1-\xi}{1+\xi}} + \frac{1+\xi}{1-\xi}e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi}{\int_0^1 \dfrac{\xi^{\frac{1}{2}-E}\left[e^{-x_0^2\frac{1-\xi}{1+\xi}} + e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]\ln\xi}{(1-\xi^2)^{3/2}}d\xi}. \tag{2.11}$$

Given that $\ln\xi \le 0$ over the interval $(0,1]$, the denominator is always negative. With regard to the sign of the numerator, we notice that for $\alpha > 0$ (resp. $\alpha < 0$) the energy belongs to the interval $(0,3/2)$ (resp. $(-\infty,0)$), so that the integral, and therefore the numerator, is positive (resp. negative). Hence, the whole expression on the right hand side is positive for $\alpha > 0$ and negative for $\alpha < 0$.

The lowest antisymmetric eigenvalue of the operator $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$, created by the twin point perturbations and emerging out of the eigenvalue $5/2$ (which stays in the spectrum but with its degeneracy lowered to two) will be denoted by $E_1(\alpha;x_0) < 5/2$. It can be determined for any fixed value of $x_0 > 0$ by solving the equation:

$$\alpha = \frac{1}{\pi^{3/2}}\int_0^1 \frac{\left(\xi^{\frac{1}{2}-E} - \xi^{\frac{1}{2}}\right)e^{-x_0^2\frac{1-\xi}{1+\xi}} - \left(\xi^{\frac{1}{2}-E} + \xi^{\frac{1}{2}}\right)e^{-x_0^2\frac{1+\xi}{1-\xi}}}{(1-\xi^2)^{3/2}}d\xi \tag{2.12}$$

with $E = E_1(\alpha;x_0)$.

The resulting graph of $E_1(\alpha;x_0 = 0.2)$ is provided below in Fig. 5.

As can be noticed, the asymptotic approach to the unperturbed antisymmetric energy level $E = 5/2$, as the parameter $\alpha = 1/\beta \to \infty$, is a straightforward consequence of the fact that the operator converges to the Hamiltonian of the unperturbed harmonic oscillator in the norm resolvent sense.

The lowest excited symmetric eigenvalue of the operator $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$, created by the twin point perturbations and emerging out of the eigenvalue $7/2$ (which stays in the spectrum but with its degeneracy lowered to five) will be denoted by $E_2(\alpha;x_0) < 7/2$ (see [1,9]).

By essentially mimicking again what was done in [1] to determine the equation enabling us to compute the second symmetric eigenvalue, which was in turn based on the techniques used in [8–10, 15, 16], we get that $E_2(\alpha;x_0)$ is the solution of the following equation:

$$\alpha = \frac{4Ee^{-x_0^2}}{3\,(3-2E)\,\pi^{3/2}} + \frac{1}{\pi^{3/2}}\int_0^1 \frac{(\xi^{\frac{1}{2}-E} - \xi^{\frac{1}{2}})\left[e^{-x_0^2\frac{1-\xi}{1+\xi}} + e^{-x_0^2\frac{1+\xi}{1-\xi}} - 2e^{-x_0^2}(1-\xi^2)^{3/2}\right]}{(1-\xi^2)^{3/2}}d\xi \tag{2.13}$$

with $E = E_2(\alpha;x_0)$.

In Fig. 6 shown below, we have plotted the three lowest eigenvalues created by the twin point perturbations, namely $E_0(\alpha;0.2)$, $E_1(\alpha;0.2)$ and $E_2(\alpha;0.2)$, as well as the two other eigenvalues $E = 5/2$ and $E = 7/2$ still present in the spectrum but with their degeneracy lowered by one due to the emergence of $E_1(\alpha;0.2)$ and $E_2(\alpha;0.2)$. The energy level $E = 3/2$ is no longer in the spectrum but has nevertheless been plotted since it is the lower horizontal asymptote of $E_2(\alpha;0.2)$ in addition to being the upper one of the ground state energy $E_0(\alpha;0.2)$.

As is evident from the graph, the striking spectral feature observed in [1] for the Hamiltonian $H_{\{1/\alpha,\vec{x}_0\}}$ studied therein, that is to say the existence of a range of values of the extension parameter for which the lowest excited symmetric eigenstate is more tightly bound than the lowest excited antisymmetric one due to the double level crossing between $E_1(\alpha;0.2)$ and $E_2(\alpha;0.2)$, is present also in the spectrum of our 'regularized' operator $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$. We avoid producing the analog of Table 1 in [1] since it would be perfectly identical apart from the numerical values of the points $\alpha_i, i = 1,2,3,4$. However, it is certainly worth making a comparison between the

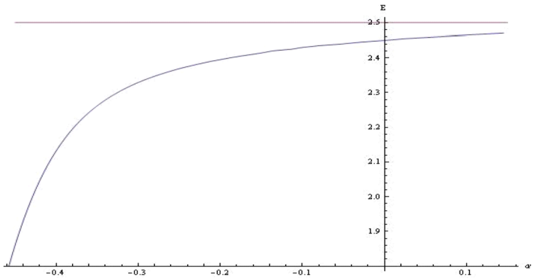

FIG. 5. The lowest antisymmetric eigenvalue of the operator $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$, with $x_0 = 0.2$, as a function of the extension parameter $\alpha = 1/\beta$

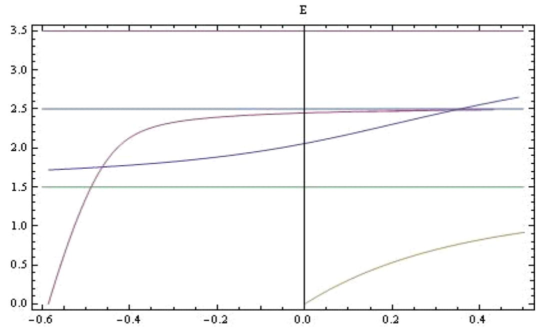

FIG. 6. The ground state energy and the next two eigenenergies of the Hamiltonian $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$, with $x_0 = 0.2$, as functions of the extension parameter $\alpha = 1/\beta$

interval $[\alpha_2, \alpha_3]$ (the range of values of the parameter over which $2S < 2P$, adopting the widely used notation adopted in atomic physics, as is done in [17]), for $\sigma\left(H_{\{1/\alpha,0.2\}}\right)$ investigated in [1] and for $\sigma\left(\mathrm{H}_{\{1/\alpha,0.2\}}\right)$ being studied here: whilst in the former case the interval was approximately $[-0.126478, 0.309201]$, here the interval has expanded to become $[-0.462637, 0.339]$. We will come back to this point in the next section of this note.

On the other hand, as was the case for the operator $H_{\{1/\alpha,\vec{x}_0\}}$ studied in [1], the increase of the separation distance between the two centers leads to the 'disentanglement' between the two spectral curves in the sense that the two level crossings disappear and $E_1(\alpha; 0.2) < E_2(\alpha; 0.2)$ for any value of the extension parameter α and any value of x_0 beyond a certain threshold X_0. In Fig. 7 shown below we provide the reader with the visualization of the latter spectral phenomenon for $x_0 = 0.45$.

Therefore, in complete analogy with what was done in [1], it is entirely possible to determine the solution of the system:

$$\begin{cases} E_1(\alpha, x_0) = E_2(\alpha, x_0), \\ \dfrac{\partial}{\partial\alpha} E_1(\alpha, x_0) = \dfrac{\partial}{\partial\alpha} E_2(\alpha, x_0). \end{cases} \tag{2.14}$$

in order to locate the value of x_0 and the corresponding coordinates (α, E) of the point where we have the tangential contact between the two spectral curves. The numerical solution of (2.14) is the point with coordinates $E = E_t$ (approximately equal to 2.17509732), $x_0 = X_t$ (approximately equal to 0.31558276), and $\alpha = \alpha_t$ (approximately equal to 0.04957412). The plot of the tangential contact between the two spectral curves for $x_0 = X_t$ is provided below in Fig. 8.

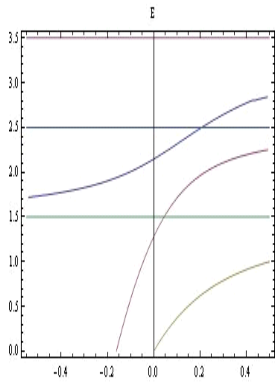

FIG. 7. The ground state energy and the next two eigenenergies of the Hamiltonian $\mathrm{H}_{\{1/\alpha,\vec{x}_0\}}$, with $x_0 = 0.45$, as functions of the extension parameter $\alpha = 1/\beta$

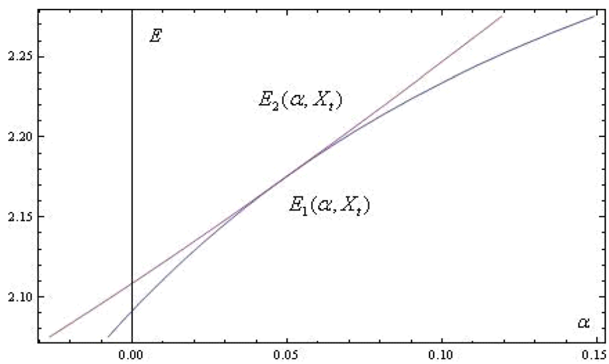

FIG. 8. The curves of the two eigenenergies $E_1(\alpha, X_t)$ and $E_2(\alpha, X_t)$ (X_t being approximately equal to 0.31558276) intersecting each other tangentially at $\alpha = \alpha_t$ (approximately equal to 0.04957412)

We can also visualize the intersection between the two eigenenergies as three-dimensional surfaces (Fig. 9).

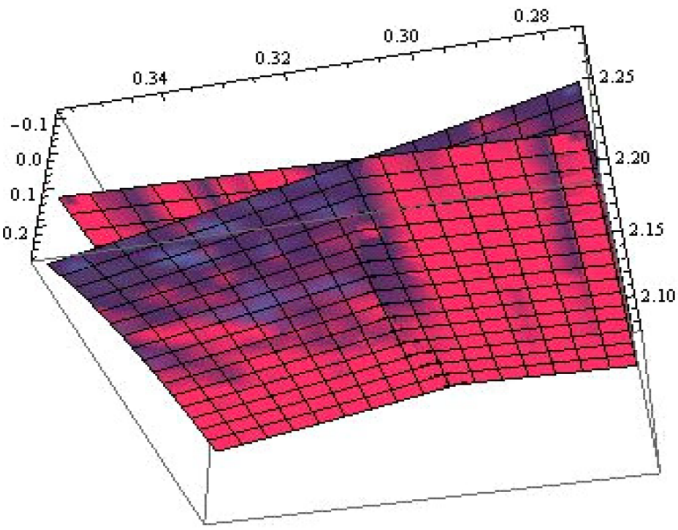

FIG. 9. The two eigenenergies $E_1(\alpha; x_0)$ and $E_2(\alpha; x_0)$ as three-dimensional surfaces

Before ending this section, we wish to state and prove the theorem showing that the singular double well Hamiltonian, defined in the previous theorem, differently from the one considered in [1], behaves smoothly as the distance between the two attractive point interactions shrinks to zero, which fully explains our extensive use of the term 'regularization' throughout this note.

Theorem 2.2. *The resolvents of the self-adjoint Hamiltonians*

$$\mathrm{H}_{\{\beta,\vec{x}_0\}}$$

converge, as the distance $x_0 \to 0_+$ *(the magnitude of the vectors giving the location of the centres of the twin point impurities), in the norm topology of bounded operators on* $L^2(\mathbb{R}^3)$ *to*

$$(H_{2\beta} - E)^{-1} = (H_0 - E)^{-1} + \frac{\big|(H_0 - E)^{-1}(\cdot, 0)\big\rangle\big\langle(H_0 - E)^{-1}(0, \cdot)\big|}{(2\beta)^{-1} - E \displaystyle\sum_{|\vec{n}|=0}^{\infty} \frac{\Psi^2_{2\vec{n}}(0)}{(|2\vec{n}| + 3/2)(|2\vec{n}| + 3/2 - E)}}, \tag{2.15}$$

namely the one of the self-adjoint Hamiltonian of the three-dimensional isotropic harmonic with an attractive point interaction centred at the origin having double strength.

Proof. We start by noting that, because of the local nature of the limit procedure, it is not restrictive at all to consider only those values of x_0 in a suitable right neighbourhood of zero, i.e. $(0, X_0]$. Moreover, without any loss of generality, we may also restrict the proof to $\beta > 0$.

As shown earlier, for any $\beta > 0$, $E_0(\beta; x_0)$ is an increasing function of x_0, which implies that $E_0(\beta; 0) < E_0(\beta; x_0)$. Furthermore, given that for both operators $E_0(+\infty; 0) = 0$ and $E_0(\infty; x_0) = 0$, any negative E will belong to the resolvent set of both operators.

Therefore, by referring to (2.5), what is to be shown here for all $E < 0$ is simply:

$$\big\|(H_{2\beta} - E)^{-1} - (\mathrm{H}_{\{\beta,\vec{x}_0\}} - E)^{-1}\big\|_\infty \le \big\|(H_{2\beta} - E)^{-1} - (\mathrm{H}_{\{\beta,\vec{x}_0\}} - E)^{-1}\big\|_p =$$

$$\Bigg\| \left[\frac{\big|(H_0-E)^{-1}(\cdot,0)\big\rangle\big\langle(H_0-E)^{-1}(0,\cdot)\big|}{(2\beta)^{-1}-E\sum\limits_{|\vec n|=0}^{\infty}\frac{\Psi_{2\vec n}^2(0)}{(|2\vec n|+3/2)(|2\vec n|+3/2-E)}} - \frac{\big|(H_0-E)_s^{-1}(\cdot,\vec x_0)\big\rangle\big\langle(H_0-E)_s^{-1}(\vec x_0,\cdot)\big|}{(2\beta)^{-1}-E\sum\limits_{|\vec n|=0}^{\infty}\frac{\Psi_{2\vec n}^2(\vec x_0)}{(|2\vec n|+3/2)(|2\vec n|+3/2-E)}} \right]$$

$$\oplus \frac{\big|(H_0-E)_{as}^{-1}(\cdot,\vec x_0)\big\rangle\big\langle(H_0-E)_{as}^{-1}(\vec x_0,\cdot)\big|}{(2\beta)^{-1}+\lim\limits_{\ell\to+\infty}\left[\sum\limits_{|\vec n|=0}^{\ell}\frac{\Psi_{2\vec n}^2(\vec x_0)}{|2\vec n|+3/2}-\sum\limits_{|\vec n|=0}^{\ell}\frac{\psi(x_0)_{2n_1+1}^2\psi_{2n_2}^2(0)\psi_{2n_3}^2(0)}{2n_1+2n_2+2n_3+5/2-E}\right]} \Bigg\|_p \to 0, \quad (2.16)$$

as $x_0 \to 0_+$, for any Schatten norm of index $p > 3$ (the fact that the resolvent of H_0 belongs to any Schatten ideal with index $p > 3$ is shown in [9]). Since both direct summands inside the norm are operators of finite rank, the left hand side of (2.16) is bounded from above by:

$$\left\| \frac{\big|(H_0-E)^{-1}(\cdot,0)\big\rangle\big\langle(H_0-E)^{-1}(0,\cdot)\big|}{(2\beta)^{-1}-E\sum\limits_{|\vec n|=0}^{\infty}\frac{\Psi_{2\vec n}^2(0)}{(|2\vec n|+3/2)(|2\vec n|+3/2-E)}} - \frac{\big|(H_0-E)_s^{-1}(\cdot,\vec x_0)\big\rangle\big\langle(H_0-E)_s^{-1}(\vec x_0,\cdot)\big|}{(2\beta)^{-1}-E\sum\limits_{|\vec n|=0}^{\infty}\frac{\Psi_{2\vec n}^2(\vec x_0)}{(|2\vec n|+3/2)(|2\vec n|+3/2-E)}} \right\|_1$$

$$+\left\| \frac{\big|(H_0-E)_{as}^{-1}(\cdot,\vec x_0)\big\rangle\big\langle(H_0-E)_{as}^{-1}(\vec x_0,\cdot)\big|}{(2\beta)^{-1}+\lim\limits_{\ell\to+\infty}\left[\sum\limits_{|\vec n|=0}^{\ell}\frac{\Psi_{2\vec n}^2(\vec x_0)}{|2\vec n|+3/2}-\sum\limits_{|\vec n|=0}^{\ell}\frac{\psi(x_0)_{2n_1+1}^2\psi_{2n_2}^2(0)\psi_{2n_3}^2(0)}{2n_1+2n_2+2n_3+5/2-E}\right]} \right\|_1. \quad (2.17)$$

Let us deal with the limit of the first summand. Of course, if we can prove that the second term inside the norm converges to the first one in $T_1(L^2(\mathbb{R}^3))$ (the norm on the trace class operators acting on $L^2(\mathbb{R}^3)$), then the norm of their difference will necessarily converge to zero.

As can be guessed, the proof is bound to be rather similar to the one of Theorem 2.2(b) in [10] for the one-dimensional analog of the model since the behavior of the following series will play a crucial role:

$$\big((H_0)_s^{-1}(\vec x_0,\cdot),(H_0-E)_s^{-1}(\cdot,\vec x_0)\big) = \sum_{|\vec n|=0}^{\infty}\frac{\Psi_{2\vec n}^2(\vec x_0)}{(|2\vec n|+3/2)(|2\vec n|+3/2-E)}, \quad (2.18)$$

$$\big\|(H_0-E)_s^{-1}(\vec x_0,\cdot)\big\|_2^2 = \sum_{|\vec n|=0}^{\infty}\frac{\Psi_{2\vec n}^2(\vec x_0)}{(|2\vec n|+3/2-E)^2} = (H_0-E)_s^{-2}(\vec x_0,\vec x_0). \quad (2.19)$$

As a consequence of the estimate (3.8) in [1], it is evident that, in order to take advantage of the dominated convergence theorem, it will not be possible to use the square of the uniform norm $\|\psi_{2n}\|_\infty^2$, as was done in the one-dimensional case, since the latter decays only like $1/(2n)^{1/6}$ (see [21, 22]), a decay not sufficiently rapid to ensure the convergence of

$$\sum_{n=0}^{\infty}\frac{\|\psi_{2n}\|_\infty^2}{(2n+1/2)^{2/3}}.$$

However, given that the limit procedure involves only those x_0's in $(0, X_0]$ for some suitable $X_0 > 0$, we need not use the global maximum of ψ_{2n} in our quest for a dominating ℓ_1-sequence but rather the one over such a right vicinity of zero. Then, we can take advantage of the estimates (21) in [23] in order to state that, by choosing any $X_0 \leq \sqrt{3}-1$, we are guaranteed that there exists a constant C such that:

$$\sum_{n=0}^{\infty}\frac{\psi_{2n}^2(x_0)}{(2n+1/2)^{2/3}} \leq \frac{2^{2/3}}{\sqrt{\pi}} + \sum_{n=1}^{\infty}\frac{C^2}{(2n)^{1/2}(2n+1/2)^{2/3}} < \infty, \quad (2.20)$$

which ensures, together with the fact that

$$\sum_{n=0}^{\infty} \frac{\psi_{2n}^2(0)}{(2n+1/2)^{2/3}} < \infty,$$

the possibility of exploiting the dominated convergence for the three-dimensional series (2.18) and (2.19). Having established this technical subtlety, the remainder of the proof can mimic the aforementioned one for the one-dimensional analog almost word by word. As to the second summand of (2.17), since

$$\left\|(H_0-E)_{as}^{-1}(\vec{x}_0,\cdot)\right\|_2^2 = \sum_{|\vec{n}|=0}^{\infty} \frac{\psi_{2n_1+1}^2(x_0)\psi_{2n_2}^2(0)\psi_{2n_3}^2(0)}{\left(2n_1+2n_2+2n_3+\frac{5}{2}-E\right)^2} = (H_0-E)_{as}^{-2}(\vec{x}_0,\vec{x}_0), \tag{2.21}$$

it is clear that a dominating ℓ_1-sequence can be found also in this case such that:

$$\left|(H_0-E)_{as}^{-1}(\cdot,\vec{x}_0)\right\rangle\left\langle(H_0-E)_{as}^{-1}(\vec{x}_0,\cdot)\right| \to 0_+$$

in $T_1(L^2(\mathbb{R}^3))$ as $x_0 \to 0_+$. The latter convergence to zero is further enhanced by the divergence of the denominator since, as $x_0 \to 0_+$, we have:

$$\int_0^1 \frac{\xi^{\frac{1}{2}}\left[e^{-x_0^2\frac{1-\xi}{1+\xi}}+e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi - \int_0^1 \frac{\xi^{\frac{1}{2}-E}\left[e^{-x_0^2\frac{1-\xi}{1+\xi}}-e^{-x_0^2\frac{1+\xi}{1-\xi}}\right]}{(1-\xi^2)^{3/2}}d\xi \to 2\int_0^1 \frac{\xi^{\frac{1}{2}}}{(1-\xi^2)^{3/2}}d\xi = +\infty,$$

differently from its one-dimensional counterpart which stays finite. This concludes the proof of the theorem.

3. Manifestation of the Zeldovich effect (level rearrangement)

Although we might return to the issue in a separate paper in the near future, we cannot help anticipating here that it is possible to reinterpret the results of the spectral analysis carried out in this note from a slightly different point of view in order to discuss the manifestation of the Zeldovich effect (see [18]) in the case of the three lowest eigenvalues of the self-adjoint operator being analyzed in this note taking account of the results outlined in [17,19].

By citing [17], *'in 1959, Zeldovich discovered an interesting phenomenon while considering an excited electron in a semiconductor. The model describing the electron-hole system consists of a Coulomb attraction modified at short-distance. A similar model is encountered in the physics of exotic atoms: if an electron is substituted by a negatively charged hadron, this hadron feels both the Coulomb field and the strong interaction of the nucleus'*. Moreover, *'Zeldovich and later Shapiro and his collaborators look at how the atomic spectrum evolves when the strength of the short-range interaction is increased, so that it becomes more and more attractive. The first surprise, when this problem is encountered, is that the atomic spectrum is almost unchanged even though the nuclear potential at short distance is much larger than the Coulomb one. When the strength of the short-range interaction reaches a critical value, the ground state of the system leaves suddenly the domain of typical atomic energies, to become a nuclear state, with large negative energy. The second surprise is that, simultaneously, the first radial excitation leaves the range of values very close to the pure Coulomb 2S energy and drops towards (but slightly above) the 1S energy. In other words, the "hole" left by the 1S atomic level becoming a nuclear state is immediately filled by the rapid fall of the 2S. Similarly, the 3S state replaces the 2S, etc. This is why the process is named level rearrangement'*.

In their paper, the authors extend their analysis from exotic atoms to quantum dots which are mathematically modelled by Hamiltonians with the harmonic confinement perturbed by an attractive interaction whose action is strong only in the short range.

Although only attractive perturbations of the 3D-isotropic harmonic oscillator represented by square wells are considered, the authors of [17] observe, in addition to the aforementioned level rearrangement (Zeldovich effect), the same remarkable spectral phenomenon noticed by us in this note and its predecessor [1] dealing with point perturbations, namely the double level crossing because of which the level ordering becomes $1S < 2S < 2P$ over a certain range of values of the appropriate parameter, the coupling constant (resp. the extension parameter) in the case of [17] (resp. our model with point interactions).

Therefore, in order to investigate the manifestation of the Zeldovich effect in our model, it makes sense to plot the curves representing the energy levels as functions of the parameter β instead of α, the extension parameter. By citing [1], we wish to remind the reader that the latter '*is physically characterized by being proportional to the inverse scattering length*'.

We first plot the equivalent of Fig. 2 in [1], that is to say the graph of the ground state energy and the eigenenergy pertaining to the next symmetric bound state ($2S$) created by the point perturbation of the Hamiltonian H_β, the one of the 3D-isotropic harmonic oscillator perturbed by a single attractive point perturbation centred at the origin, as functions of the parameter β. Of course, if $\beta = 0$, we have the unperturbed Hamiltonian H_0 of the 3D-isotropic harmonic oscillator. We have also plotted the horizontal lines $E = 3/2$, no longer in the spectrum except for $\beta = 0$, and $E = 5/2$, the eigenenergy of the $2P$ state, clearly not affected by the central point perturbation.

Furthermore, we draw the reader's attention to the two horizontal asymptotes appearing in the plot, the lower one for the ground state $(1S)$ energy obviously situated at $E = 0$, and the upper one for the energy of the next symmetric bound state $(2S)$ located approximately at 2.307876 (Fig. 10(a)).

By comparing the above graph to Fig. 2 in [1], in which the energy is plotted against the extension parameter α, we cannot refrain from pointing out the analysis carried out in [19] to the interested reader. Although the spectral analysis therein pertains to three Hamiltonians with potentials whose range is short but different from zero (the finite square well, the modified Poshl-Teller potential and an exponential one), the ideas put forward in that article are relevant also in the case of point perturbations of the isotropic harmonic oscillator in three dimensions.

First of all, as is stressed in that note, from the point of view of the experimental observation of this intriguing physical phenomenon '*currently available experimental techniques in cold-atoms research offer an exciting opportunity for a direct observation of the Zeldovich effect without the difficulties imposed by conventional condensed matter and nuclear physics studies'*.

It is important to remind the reader that the typical graphs used to describe the level rearrangement phenomenon are drawn assuming the presence of the negative sign multiplying the coupling constant in the interaction term of the Hamiltonian so that the interaction becomes increasingly attractive as the coupling goes from negative to positive infinity, which might look a bit unusual since it is exactly the opposite of the standard plots based on the presence of the positive sign in front of the coupling constant in the interaction term of the Hamiltonian.

By looking at the above graph, it is crucial to realize that, differently from the plots in [17, 19] and because of our renormalization, the manifestation of the Zeldovich effect occurs in the vicinity of $\beta = 0$ whilst the left boundary of the graph is instead $\beta = -\infty$.

As stated at the beginning of this section, here, it is not our intention to dwell on an extensive discussion of the level rearrangement phenomenon based on the ideas proposed in [19]. We simply wish to stress that we certainly agree with the authors that the Zeldovich effect implied by the plots of the energy versus either α or β can be better understood by adopting the cylindrical mapping based on the Cartesian product $\mathbb{R} \times S_1$, with the energy E drawn along the real line (the symmetry axis of the cylinder) and either parameter along the unit circle identifying $\pm\infty$, which naturally leads them to the introduction of the denomination 'Zeldovich spiral'.

In order to show the 'flow' of the spectrum along the Zeldovich spiral, we plot again the above graph with the arrows showing that in the E vs. β plot the spectral flow goes from top to bottom vertically and counter clockwise along S_1 (Fig. 10(b)).

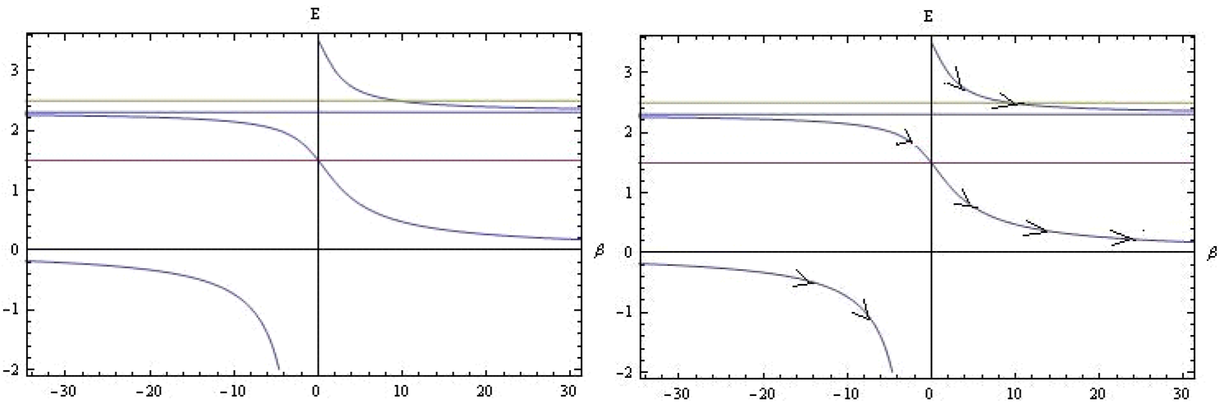

FIG. 10. The ground state energy and the next eigenenergy of the Hamiltonian H_β as functions of the strength parameter β

The analogous graph of $\mathrm{H}_{\{\beta,\vec{x}_0\}}$, with $x_0 = 0.2$, shows, in addition to similar features, the presence of the curve pertaining to the $2P$ eigenenergy with its horizontal asymptote located slightly below the energy level $5/2$ at approximately 2.450008. The horizontal asymptote of the curve of the $2S$ eigenenergy is situated instead at approximately 2.058391.

Furthermore, as pointed out in the comments on the E vs. α plot, there is a range of values of the parameter over which the $2S$ eigenenergy falls below the $2P$ eigenenergy, namely $(-\infty, \beta_2)$ (with $\beta_2 = 1/\alpha_2$ approximately equal to -2.161522) along the negative semiaxis and $(\beta_3, +\infty)$ (with $\beta_3 = 1/\alpha_3$ approximately equal to 2.949853) along the positive one.

Hence, we can infer that, as we rotate counter clockwise along the Zeldovich spiral from the angle corresponding to β_3 to the one corresponding to β_2, the $2S$ state is more tightly bound than the $2P$ one (Fig. 11).

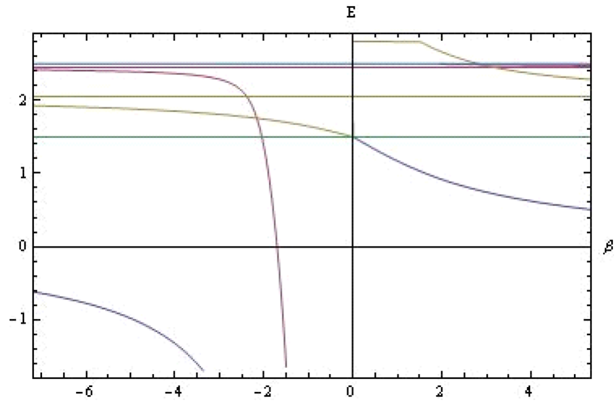

FIG. 11. The ground state energy and the next two eigenenergies of the Hamiltonian $\mathrm{H}_{\{\beta,\vec{x}_0\}}$, with $x_0 = 0.2$, as functions of the parameter β

4. Final remarks

The main goal of this note has been to show that, by renormalizing the coupling constant in a way that is dependent on x_0 (the distance between each point interaction center and the origin), the self-adjoint Hamiltonian modeling an isotropic three-dimensional harmonic oscillator perturbed by two twin attractive point interactions symmetrically situated around the origin can be rigorously defined in such a way to avoid the problem encountered in our previous paper [1]: the self-adjoint Hamiltonian investigated therein did not converge to the one with a single point interaction located at the origin having double strength.

By citing [1], it is important to recall that *'as is well known to Quantum Chemistry students, three-dimensional interactions with a nonzero range do not manifest this singular behavior in the limit of the distance R between the two centers shrinking to zero, as the classical textbook example of* H_2^+ *smoothly approaching* He^+ *in the limit* $R \to 0_+$ *clearly shows*' (see [2–4]). Hence, the regularization being proposed here should make such singular double wells more similar to conventional double wells generated by rapidly decaying potentials.

We remind the reader that this singular behavior seems to be a general feature of models with double singular wells represented by point interactions requiring the renormalization of the coupling constant, as has also recently been noticed in the case of the one-dimensional Salpeter Hamiltonian studied in [5].

Furthermore, we have carried our spectral analysis not only in terms of α, the extension parameter physically related to the inverse scattering length, but also in terms of β, the strength parameter directly involved in the renormalization procedure. Our main motivation for this further analysis has been the fact that, following [17], the latter parameter is the conventional one used to study the manifestation of the Zeldovich effect, known also as level rearrangement. We have been able to show that the phenomenon, studied by the authors when the perturbation of the three-dimensional isotropic harmonic oscillator is represented by a potential whose range is physically very short but different from zero, does manifest itself also in the case of point perturbations.

We wish to stress that a remarkable advantage resulting from our renormalization procedure, uniquely associated to the fundamental spectral condition $E_0(\alpha = 0, x_0) = 0 = E_0(\beta = +\infty, x_0)$, is that the Zeldovich spiral, introduced by Farrell et al. in [19] by adopting the cylindrical mapping based on the Cartesian product $\mathbb{R} \times S^1$, with E along the real line (the symmetry axis of the cylinder) and the parameter α along the unit circle identifying $\pm\infty$, can be visualized directly in a plot of the energy vs. β as well.

Acknowledgements

We wish to thank Prof. Igor Yu. Popov (Chair of Higher Mathematics, ITMO University, St. Petersburg, Russian Federation) for his kind invitation to contribute to this special issue dedicated to the memory of our dear friend Boris Pavlov. The first author had the great luck to meet him in the 80s, first during a meeting in Dubna, and was greatly impressed by his bright mind, his contagious enthusiasm for mathematics, that he transmitted to a large

number of students. One of the topics we discussed was the subject of point interactions. He gave fundamental contributions to this area and, more generally, to spectral theory. The contacts with him and his research associates happily accompanied our further scientific life.

The second author had the privilege of meeting him in February 1991 as we were both visiting Prof. Albeverio in Bochum. It was a great pleasure, shared also by the third author, to see him twenty-four years later in St. Petersburg on the occasion of the international conference 'Mathematical Challenge of Quantum Transport in Nanosystems', held at ITMO University, St. Petersburg, Russian Federation (9–11 September 2015). It is with great gratitude that we acknowledge his scientific legacy and dedicate this work to his memory.

References

[1] Albeverio S., Fassari S., Rinaldi F. Spectral properties of a symmetric three-dimensional quantum dot with a pair of identical attractive δ-impurities symmetrically situated around the origin. *Nanosystems: Physics, Chemistry, Mathematics*, 2016, **7** (2), P. 268–289.

[2] Schmidtke H.-H. *Quantenchemie*. Weinheim: VCH, 1987 (in German).

[3] Byers Brown W., Steiner E. On the electronic energy of a one-electron diatomic molecule near the united atom. *Journal of Chemical Physics*, 1966, **44**, P. 3934.

[4] Klaus M. On H_2^+ for small internuclear separation. *Journal of Physics A: Mathematical and General*, 1983, **16**, P. 2709–2720.

[5] Albeverio S., Fassari S., Rinaldi F. The discrete spectrum of the spinless Salpeter Hamiltonian perturbed by δ-interactions. *Journal of Physics A: Mathematical and Theoretical*, 2015, **48** (18), P. 185301.

[6] Albeverio S., Gesztesy F., Høegh-Krohn R., Holden H. *Solvable models in Quantum Mechanics*. AMS (Chelsea Series) second edition, 2004.

[7] Albeverio S., Kurasov P. *Singular Perturbations of Differential Operators: Solvable Type Operators*. Cambridge University Press, 2000.

[8] Albeverio S., Fassari S., Rinaldi F. A remarkable spectral feature of the Schrödinger Hamiltonian of the harmonic oscillator perturbed by an attractive δ'-interaction centred at the origin: double degeneracy and level crossing. *Journal of Physics A: Mathematical and Theoretical*, 2013, **46** (38), P. 385305.

[9] Fassari S., Inglese G. Spectroscopy of a three-dimensional isotropic harmonic oscillator with a δ-type perturbation. *Helvetica Physica Acta*, 1996, **69**, P. 130–140.

[10] Fassari S., Rinaldi F. On the spectrum of the Schrödinger Hamiltonian of the one-dimensional harmonic oscillator perturbed by two identical attractive point interactions. *Reports on Mathematical Physics*, 2012, **69** (3), P. 353–370.

[11] Reed M., Simon B. *Fourier Analysis, Self-adjointness – Methods of Modern Mathematical Physics II*, Academic Press NY, 1975.

[12] Exner P., Neidhardt H., Zagrebnov V.A. Potential approximations to δ': an inverse Klauder phenomenon with norm resolvent convergence. *Communications in Mathematical Physics*, 2001, **22**, P. 4593–4612.

[13] Fassari S., Rinaldi F. On the spectrum of the Schrödinger Hamiltonian with a particular configuration of three point interactions. *Reports on Mathematical Physics*, 2009, **64** (3), P. 367–393.

[14] Albeverio S., Fassari S., Rinaldi F. The Hamiltonian of the harmonic oscillator with an attractive δ'-interaction centred at the origin as approximated by the one with a triple of attractive δ-interactions. *Journal of Physics A: Mathematical and Theoretical*, 2016, **49** (2), P. 025302.

[15] Fassari S., Inglese G. On the spectrum of the harmonic oscillator with a δ-type perturbation. *Helvetica Physica Acta*, 1994, **67**, P. 650–659.

[16] Fassari S., Inglese G. On the spectrum of the harmonic oscillator with a δ-type perturbation II. *Helvetica Physica Acta*, 1997, **70**, P. 858–865.

[17] Combescure M., Khare A., et al. Level rearrangement in exotic atoms and quantum dots. *International Journal of Modern Physics B*, 2006, **21** (22), P. 3765.

[18] Zeldovich Ya.B. Energy levels in a distorted Coulomb field. *Soviet Journal Solid State*, 1960, **1**, P. 1497.

[19] Farrell A., MacDonald Z., van Zyl B. The Zeldovich effect in harmonically trapped, ultra-cold quantum gases. *Journal of Physics A: Mathematical and Theoretical*, 2012, **45**, P. 045303.

[20] Brüning J., Geyler V., Lobanov I. Spectral properties of a short-range impurity in a quantum dot. *Journal of Mathematical Physics*, 2004, **45**, P. 1267–1290.

[21] Plancherel M., Rotach W. Sur les valeurs asymptotiques des polynomes d'Hermite. *Commentarii Mathematici Helvetici*, 1929, **1** (1), P. 227–254.

[22] Reed M., Simon B. *Functional Analysis – Methods of Modern Mathematical Physics I*. Academic Press, NY, 1972.

[23] Mityagin B., Siegl P. Root system of singular perturbations of the harmonic oscillator type operators. *Letters in Mathematical Physics*, 2016, **106** (2), P. 147–167.