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ON INEFFICIENCY OF REPULSIVE δ-POTENTIALS IN MULTIDIMENSIONAL SPACES

A complete account of correlations has been shown to make δ-like repulsive interaction potentials inefficient for any N-particle quantum system in the D-dimensional space with $D \geq 2$.

Keywords: N-particle system, D-dimensional space, δ-like interaction potential, energy spectrum, wave function.

1. Introduction

Since the works by Fermi and Göppert-Mayer, simplified versions of potentials in the form of δ-like interaction potentials have been used in various fields of theoretical physics. In one time, a discussion of the role of relativistic correction terms in the form of δ-potentials to the Coulomb interaction in the QED was problematic when considering the quasi-relativistic Breit potentials [1]. Modern studies of Bose condensation effects are based on using the self-consistent Gross–Pitaevskii field [2,3] and the idea of δ-like interaction potentials (see works [4,5]). In general, various D-dimensional nonlinear evolution equations like the nonlinear Schrödinger one are often considered as associated with certain many-body systems characterized by δ-like interaction potentials. Some versions of effective Skyrme forces [6] (see also works [7,8]) in the form of a superposition of two- and three-particle δ-like potentials remain still popular in nuclear physics as a model of interaction between nucleons, which is used to describe the structure characteristics of atomic nuclei, from light and intermediate ones up to the most heavy nuclei, within the simplest one-particle self-consistent mean-field approximation.

It should be noted that a consideration of the problems containing δ-potentials is very often restricted to calculations in the first-order approximation of perturbation theory (which are convenient to be done just with such potentials) and assuming that the exact solution of the problem does not change the result from the qualitative point of view. However, such an assumption has not been substantiated. In this work, we study the issue of whether δ-potentials are applicable and effective in the case of many-body systems in a D-dimensional space, as well as the role of the consistent account of pair correlation effects in such problems.

2. Formulation and Preliminary Analysis of the Problem

Consider a quantum-mechanical system of N particles in a D-dimensional space. In addition to some usual potentials, $U(r_{ij})$, the interaction between particles also includes δ-like potentials. Moreover, the system can be located in an external potential field $V(\mathbf{r})$. As a result, the Hamiltonian of the system looks like

$$\hat{H} = \sum_{i=1}^{N} \left(\frac{\mathbf{p}_i^2}{2m} + V(\mathbf{r}_i) \right) + \sum_{j>i=1}^{N} U(r_{ij}) + \\ + g \sum_{j>i=1}^{N} \delta_\varepsilon(\mathbf{r}_{ij}). \quad (1)$$

Hereafter, the δ-functions are defined by means of a sequence of δ_ε-like functions, in particular, in the form

$$\delta_\varepsilon(\mathbf{x}) = \frac{1}{(\sqrt{\pi}\,\varepsilon)^D}\, e^{-\mathbf{x}^2/\varepsilon^2}, \quad \delta_\varepsilon(\mathbf{x}) \underset{\varepsilon\to 0}{\longrightarrow} \delta(\mathbf{x}), \tag{2}$$

where $\mathbf{x}^2 \equiv \sum_{k=1}^{D} x_k^2$ is the squared interval in the D-dimensional space. Generally speaking, the specific profile of δ_ε is not too important, and it is chosen in form (2) for convenience. It is important that the limit $\varepsilon \to 0$ should be understood as the one carried out in the final solutions obtained for a given ε.

Let us firstly consider, for simplicity, a model consisting of two particles interacting via the oscillator and repulsive δ-like potentials (in the center-of-mass frame, with the unit reduced mass and the unit circular oscillation frequency):

$$\left(-\frac{1}{2}\triangle + \frac{1}{2}\mathbf{r}^2 + g\delta(\mathbf{r})\right)\psi(\mathbf{r}) = E\psi(\mathbf{r}). \tag{3}$$

Which physical consequences follow from the presence of the δ-potential in Eq. (3) in the D-dimensional space? In the one-dimensional case, one can find that, due to the repulsive δ-potential, all even-parity oscillator levels would shift upward, and they would approach the neighbor odd-parity oscillator levels as $g \to \infty$. At the same time, the odd-parity oscillator levels would not be shifted by the δ-potential, which turns out inefficient for them (because the corresponding wave functions equal zero just at the point, where the δ-function is located).

Let us consider a nontrivial three-dimensional case for Eq. (3) and a spherically symmetric state of the system (since the δ-potential is not efficient for the states with non-zero angular momenta owing to the factor $\sim r^l$ in the wave function). Expanding the solution of the Schrödinger equation (3) into a series of oscillator eigen-functions for the zero-order (unperturbed by the δ-potential) problem,

$$\psi(r) = \sum_k c_k \psi_k(r), \tag{4}$$

we obtain the explicit solution

$$\psi(r) = \frac{1}{\sqrt{\sum\limits_{i=0}^{K} \frac{|\psi_i(0)|^2}{(E-E_i)^2}}} \sum_{k=0}^{K} \frac{\psi_k^*(0)}{E-E_k}\psi_k(r), \tag{5}$$

which approaches the exact one, as K grows. As $K \to \infty$, series (5) would have been an exact solution, if it is convergent. The energy levels in the D-dimensional problem (5) are determined from the secular equation

$$\frac{1}{g} = \sum_{k=0}^{K} \frac{|\psi_k(0)|^2}{E-E_k} = \frac{1}{\pi^{D/2}\Gamma(D/2)} \sum_{k=0}^{K} \frac{1}{\Delta - 2k} \frac{\Gamma(k+D/2)}{\Gamma(k+1)}, \tag{6}$$

where $\Delta \equiv E - D/2$ is the energy shift, and $\Gamma(z)$ is the Euler gamma function. At a fixed K, the transcendental equation (6) has a solution Δ_0 describing the upward shift of the ground-state energy, which obviously falls within the interval $0 < \Delta_0 < 2$. The shift Δ_1 of the first excited state lies within the interval $2 < \Delta_1 < 4$; the shift of the next level, Δ_2, within the interval $4 < \Delta_2 < 6$; and so on. The terms

$$b_k = \frac{1}{\Delta - 2k} \frac{\Gamma(k+D/2)}{\Gamma(k+1)}$$

in series (6) have the following asymptotic behavior at large k:

$$b_k \approx C\, k^{D/2-2}. \tag{7}$$

Therefore, in the case $D \geq 2$, sum (6) diverges if the set of basis functions is extended ($K \to \infty$). In the limiting two-dimensional case, series (6) is logarithmically divergent; at higher dimensions, it is power-like divergent. One can verify that, in the case $D \geq 2$, the resulting energy levels of the ground and excited states become closer and closer to the corresponding oscillator levels, as $K \to \infty$; i.e. the level shifts vanish. In particular, the ground-state energy tends to the unperturbed energy level as follows:

$$\begin{aligned} &E_0 \underset{K\to\infty}{\longrightarrow} \frac{D}{2} + \frac{(D-2)\,\Gamma(D/2)}{(K+D/2)^{(D-2)/2}}, \quad D \geq 2; \\ &E_0 \underset{K\to\infty}{\longrightarrow} 1 + \frac{2}{\ln K + \gamma}, \quad D = 2, \end{aligned} \tag{8}$$

where $\gamma = 0.5772\ldots$ is the Euler constant. At the same time, the wave function tends to the unperturbed oscillator one at all distances but the point $r = 0$, where it vanishes: $\psi(0) = 0$.

In Figure, in order to illustrate what happens to the wave function (5) when the basis is expanded, we show successive approximations for the ground-state wave function calculated for various K's in the three-dimensional case (for definiteness, we took $g = 1$). Similar results could be demonstrated for various $D \geq 2$ and coupling constants g. The larger is K, the smaller is the value of wave function at the point $r = 0$, and that is why the role of the repulsive δ-potential becomes less important (the integral of its product with the squared absolute value of wave function tends to zero). In the limit $K \to \infty$, the contribution of the repulsive δ-potential exactly equals zero (for $D \geq 2$). Note also that, at other points, the successive approximations tend to the unperturbed function, though non-uniformly.

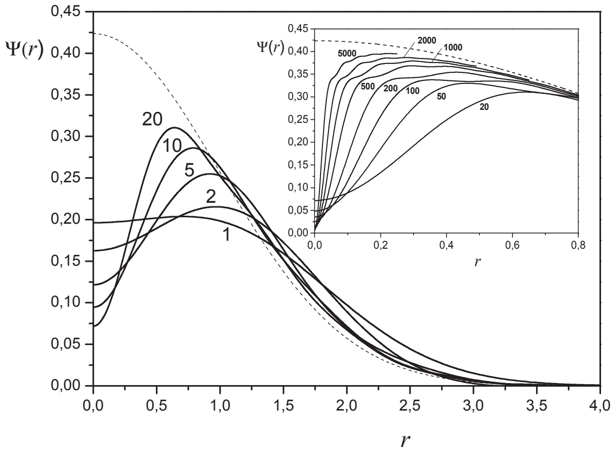
Thus, the repulsive δ-potential with an arbitrary coupling constant g does not shift the energy levels and does not change the wave functions of the unperturbed problem almost everywhere, except the discontinuity point at the coordinate origin, i.e. it is not efficient in the case $D \geq 2$.

It should be emphasized once again that the consideration of problem (3) in the first approximation of perturbation theory with respect to the δ-potential has no sense at $D \geq 2$. In particular, in the first-order approximation for the energy levels $E_n^{(1)}$, one has

$$E_n^{(1)} = 2n + \frac{D}{2} + g \left|\psi_n(0)\right|^2, \qquad (9)$$

whereas higher-order correction terms form a divergent series. At the same time, the exact energy shift equals zero; in other words, the repulsive δ-potential is not efficient at $D \geq 2$. This fact can be confirmed reliably only in the framework of non-perturbative analysis. In the next section, we give the proof of this fact on the basis of the variational principle, without use of perturbation theory.

To confirm the general conclusions about the role of δ-like potentials, let us demonstrate similar results obtained at $D = 3$ for another profile of an external field (instead of the oscillator in Eq. (3)): for a spherical rectangular well of radius R, where $V(r) = 0$ if $r < R$, and $V(r) \to \infty$ if $r > R$. In addition, instead of the sequence of functions δ_ε in form (2), we take the potential δ_ε as a repulsive spherical barrier of radius ε; i.e. the potential is nonzero only at $r < \varepsilon$, where it is constant: $\delta_\varepsilon = \frac{3}{4\pi\varepsilon^3} g$. The passage to the limit $\varepsilon \to 0$ is done in the solutions that are obtained in the explicit form. It can be shown directly that, at $\varepsilon \to 0$, the ground-state energy of this system approaches the value $E_0 = \frac{\pi^2}{R^2}$ for the unperturbed problem with the spherical potential



Successive approximations of the ground-state wave function (5) of problem (3) in the three-dimensional case. The numbers near the curves denote the number K of basis functions that were taken into account. In the insert, the region of small distances is shown for large K. The dotted line depicts the wave function of the unperturbed problem

well as $E_\varepsilon \equiv k^2 \xrightarrow[\varepsilon \to 0]{} \frac{\pi^2}{(R-\varepsilon)^2}\left(1 - 2\sqrt{\frac{4\pi\varepsilon}{3g}}\frac{\varepsilon}{R} + ...\right)$. The corresponding wave function at $\varepsilon < r < R$ also approaches the unperturbed one: $\psi_\varepsilon(r) \xrightarrow[\varepsilon \to 0]{} \psi_0(r) = \frac{\sin(k_0 r)}{r}$, where $k_0 = \pi/R$. Only within the internal region of the repulsive potential, the wave function rapidly decreases near the coordinate origin according to the law $\psi_\varepsilon(r) = c\,\frac{\sinh(\lambda r)}{r}$, where $\lambda = \sqrt{\frac{3g}{4\pi\varepsilon^3} - k^2}$, being exponentially small at $r = 0$: $\psi_\varepsilon(0) = c\lambda \xrightarrow[\varepsilon \to 0]{} \frac{2\pi}{R}\exp\left(-\sqrt{\frac{3g}{4\pi\varepsilon}}\right)$. Even in the case $g \to \infty$ (the hard core), both the ground-state energy $E_\varepsilon = k^2 = \frac{\pi^2}{(R-\varepsilon)^2}$ and the wave function $\psi_\varepsilon(r) = \frac{1}{r}\sin\left(\pi\frac{(R-r)}{(R-\varepsilon)}\right)$ approach the corresponding unperturbed values (in the region $r > \varepsilon$) as $\varepsilon \to 0$. If this conclusion is correct even for the repulsive hard core, it is all the more correct for a weaker repulsive potential with a finite radius and an arbitrary profile. Note that, for rapidly decreasing repulsive potentials (in particular, like formula (2)), all main conclusions remain valid irrespective of the specific potential profile.

Note that, in the case $D < 2$, the sum in Eq. (6) converges for both repulsive and attractive δ-potentials. Hence, in this case (in particular, in the often used one-dimensional space), the shifts of energy levels are finite (upward for the repulsive δ-potential), and the wave functions change substantially. For the attractive δ-potential, the ground-state energy decreases ($\Delta_0 < 0$). The same is observed for excited states, but the corresponding shifts remain within the intervals $2(n-1) < \Delta_n < 2n$. Thus, the attractive δ-potential can stimulate the appearance of only one bound state with a negative energy in the system with Hamiltonian (3) in accordance with the fact that the δ-potential is the first-rank operator.

A specific role is played by the attractive δ-potentials in the case $D \geq 2$ where problem (3) is known to have no sense, since the system collapses. Generally speaking, the sum of the standard Hamiltonian, which has the ordinary interaction potential distributed in the space, and an attractive δ-potential becomes an operator that is not bounded below, and the ground state of the system becomes undefined. In this case, there is no sense to use expansions of type (5), (6), because they also become undefined. At the same time, the consideration of this problem in the first order of perturbation theory has no sense as well, because it brings us to solution (9) that has no relation to the final result. Note also the well-known important example: the three-particle problem in the limit of zero force range [8]. This limit can be interpreted as the attraction between particles described by a δ-like interaction potential of type (2), but the attraction intensity also tends to zero as $\varepsilon \to 0$ following a law that allows a finite (given *a priori*) energy of the two-particle bound state to be fixed. However, even in the case of such a "weaker" δ-like attraction potential, the system of three and more particles will collapse. The collapse in the system of three particles in the three-dimensional case and in the limit of zero force range was studied in works [9, 10] in detail. The cited authors even found the law describing how the energy levels, the number of which becomes infinitely large, tend to minus infinity and predicted the main relations for the phenomenon, which is now known as the Efimov effect.

Conclusions drawn for problem (3), irrespective of whether the δ-potential is repulsive or attractive, are completely confirmed by other examples of similar problems. In particular, besides the example of interaction in an external area in the form of a spherical potential well, which was mentioned above, we could take other exactly solvable problems, e.g., a D-dimensional cubic box with infinitely high walls or the Coulomb potential. In all those cases, the divergence of (6)-type series at $D \geq 2$ leads to results similar to Eq. (8). The main conclusion concerning the inefficiency of the repulsive δ-potential in the case $D \geq 2$ remains valid. Note that, for problems with external potentials that generate a finite number of discrete levels and a continuous spectrum, while considering a generalized expression of type (6) with an additional (besides the summation over the discrete spectrum) integration over the continuum spectrum, all the principal conclusions concerning the inefficiency of the δ-potential remain in force.

In the next section, we prove the statements made above with the help of the variational principle used in the framework of rather general assumptions concerning the Hamiltonian that contains a repulsion in the form of the δ-potential.

3. Proof on the Basis of the Variational Principle

First, let us consider the case $D = 2$ in detail, which is the most delicate for proof. This is a "critical" case, because the repulsive δ-potential becomes efficient at $D < 2$: it affects the physical observable quantities and changes the wave functions. We accept the most general assumptions for the Hamiltonian unperturbed by the δ-potential: the only requirement is that the wave functions of the unperturbed problem should be finite at $r = 0$, which is reasonable for a wide class of commonly used potentials $V(r)$. Let the ground state of the unperturbed system have the energy E_0 and be described by the wave function $\psi_0(r)$. In order to variationally estimate the ground-state energy, keeping in mind the preliminary consideration of the possible influence of the δ-potential on the system and understanding that the account of the wave function behavior at small distances is crucially important, we construct the trial wave function $\psi(r)$ in the form

$$\psi(r) = f(r)\,\psi_0(r)\,. \qquad (10)$$

The correlation factor is chosen to equal $f(r) \equiv 1 - \exp\left(-(\beta r)^{1/\alpha}\right)$, where the parameter $\alpha = \alpha(\beta)$ is an infinitely increasing function of β, i.e. $\alpha(\beta) \xrightarrow[\beta\to\infty]{} \infty$. Omitting the general analysis of allowable functions $\alpha = \alpha(\beta)$, we restrict ourselves to the example $\alpha \equiv \ln(\ln\beta)$, which is sufficient for the proof of our statement. The ground-state energy is denoted by E_0, and the corresponding wave function of the unperturbed (by the δ-potential) problem by $\psi_0(r)$. The variational estimate of the ground-state energy corresponding to the Hamiltonian with an additional repulsive δ-potential with the use of the wave functions (10) can be presented in the form

$$E \leq \frac{\int \psi^*(r)\left(-\frac{1}{2}\triangle + V(r) + g\delta(\mathbf{r})\right)\psi(r)\,d\mathbf{r}}{\int |\psi(r)|^2\,d\mathbf{r}} \equiv$$

$$\equiv E_0 + \frac{\frac{1}{2}\int |\psi_0(r)|^2 (\nabla f(r))^2\,d\mathbf{r}}{\int |\psi_0(r)|^2 f^2(r)\,d\mathbf{r}}, \tag{11}$$

where the integration is carried out over the two-dimentional space. Note that the δ-potential itself makes no contribution to the numerator in Eq. (11) because of the correlation factor property $f(0) = 0$. However, owing to the same correlation factor, there arises another, additional to E_0, term in Eq. (10), which follows from the kinetic energy operator. If the normalized wave function of the unperturbed problem is finite, i.e. $|\psi_0(r)|^2 \leq C_0$ (which is valid for an arbitrary non-singular Hamiltonian), the normalization integral in the denominator of Eq. (11) tends to 1 as $\beta \to \infty$,

$$\int |\psi(r)|^2\,d\mathbf{r} \underset{\beta\to\infty}{\longrightarrow} 1 + \mathcal{O}\left(\frac{\alpha\Gamma(2\alpha)}{\beta^2}\right) \underset{\beta\to\infty}{\longrightarrow} 1, \tag{12}$$

since $\alpha = \ln(\ln\beta)$ and due to the asymptotic properties of the gamma function $\Gamma(z)$. Let us consider now the integral in the numerator of Eq. (10),

$$\frac{1}{2}\int |\psi_0(r)|^2 (\nabla f(r))^2\,d\mathbf{r} \leq \frac{1}{2}C_0 \int (\nabla f(r))^2\,d\mathbf{r} =$$

$$= \frac{\pi C_0}{4\alpha}. \tag{13}$$

Hence, we have $E \leq E_0 + \frac{\pi C_0}{4\alpha} \underset{\beta\to\infty}{\longrightarrow} E_0$. Since the repulsive δ-potential can shift the energy only upward, i.e. $E \geq E_0$, we ultimately obtain that $E = E_0$ in the two-dimensional case.

The proof becomes essentially simpler for spaces of higher dimensionalities, because the larger is D, the more important role is played by the r^{D-1} factor in the integration at small distances. Already for $D > 2$, it is sufficient to choose a simpler correlation factor in the trial function (10), e.g.,

$$f(r) = 1 - \exp\left(-(r/b)^2\right), \tag{14}$$

and pass to the limit $b \to 0$ in final expressions. Using the correlation factor (14), let us consider the problem of δ-potential efficiency for the systems of N particles in the case $D > 2$. To carry out the variational estimation of the ground-state energy, we use a trial variational function in the form

$$\Psi = \Psi_0 F(r_{12}, r_{13}, ...) = \Psi_0 \prod_{i>j=1}^{N} f(r_{ij}), \tag{15}$$

where the pair correlation factors $f(r_{ij})$ have form (14), and Ψ_0 is the wave function of the ground state for the Hamiltonian H_0 that differs from Hamiltonian (1) by the absence of the term $\delta V = g\sum_{i>j=1}^{N}\delta(\mathbf{r}_{ij})$. For the ground-state energy of problem (1), we obtain the following variational estimate (similar to Eq. (11)):

$$E \leq E_0 + \frac{\frac{1}{2m}\sum\limits_{i=1}^{N}\int (d\mathbf{r})^N |\Psi_0|^2 \left((\nabla_i F)^2 + \delta V F^2\right)}{\int (d\mathbf{r})^N |\Psi_0|^2 F^2} =$$

$$= E_0 + \frac{\frac{1}{2m}\sum\limits_{i=1}^{N}\int (d\mathbf{r})^N |\Psi_0|^2 (\nabla_i F)^2}{\int (d\mathbf{r})^N |\Psi_0|^2 F^2}. \tag{16}$$

The potential δV disappears from the numerator of Eq. (16) due to the following correlation factor property: $F = 0$ if any of the pair distances $r_{ij} = 0$. We emphasize once more that the term additional to E_0 in Eq. (16) originates from the kinetic energy operator action on the correlation factors. We omit the straightforward but cumbersome calculations of the derivatives of F, as well as the estimation of the integrals in Eq. (16) as $b \to 0$, and give the ultimate estimate for the energy (under the natural assumption that the squared wave function is finite, $|\Psi_0|^2 \leq C_0$):

$$E \leq E_0 + \mathcal{O}\left(b^{D-2}\right). \tag{17}$$

The higher the dimension D of the space, the more rapidly tends this value of energy to the unperturbed value, thus $E \leq E_0$ as $b \to 0$. It is clear *a priori* that any repulsive potential δV can result only in $E \geq E_0$. Therefore, we ultimately obtain that $E = E_0$.

We point out that, in the case $D = 2$, the correlation factor may be taken in the form used in Eq. (10) for the two-particle problem, and the above-mentioned arguments can be repeated for a system of N particles. But instead of formula (17), we will obtain an estimation of type (13).

Note that the obtained results concerning the inefficiency of a repulsive δ-potential in spaces with $D \geq 2$ dimensions can be directly generalized to the excited energy levels. To this end, it is sufficient to take into account that the trial variational wave functions of the n-th excited state should be orthogonal to the functions corresponding to the lower levels. This requirement is satisfied automatically for the functions of type (10) or (15) (where Ψ_0 is to be substituted by Ψ_n) in the limit of zero correlation radius, due to the orthogonality of the wave functions in the unperturbed problem.

It is important to understand that the repulsive δ-potential does not affect other physical observable quantities. In particular, it was shown in work [11] that the repulsive δ-potential does not change the phase shifts in the two-dimensional case, which is the most delicate for the proof. This means that, if $D > 2$, the obtained result is even more valid (unfortunately, this fact was not emphasized in work [11]). In any case, if a repulsive δ-potential affects neither the spectrum nor the phase shifts, it is inefficient at $D \geq 2$.

4. Conclusions

To summarize, it has been shown that a repulsive δ-potential is inefficient for a quantum system of particles with an interaction containing δ-potentials, if the space dimensionality $D \geq 2$. The consideration of such problems in the first order of perturbation theory leads to incorrect results. The consistent account of short-range correlations demonstrates that such potentials make no influence on the energy spectrum and other physical observable quantities. On the other hand, in the case $D \geq 2$, attractive δ-potentials are known to produce the collapse of a system. So, the δ-potentials are efficient only for one-dimensional problems. But for a system in a D-dimensional space with $D \geq 2$ and in the framework of the accurate problem formulation, there is no sense to use such interaction potentials at all.

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ПРО НЕЕФЕКТИВНІСТЬ
ВІДШТОВХУВАЛЬНИХ δ-ПОТЕНЦІАЛІВ
У БАГАТОВИМІРНИХ ПРОСТОРАХ

Р е з ю м е

Показано, що δ-подібні відштовхувальні потенціали взаємодії при повному врахуванні кореляцій є неефективними для будь-якої N-частинкової квантової системи у D-вимірному просторі при $D \geq 2$.