# USE OF WAVELETS IN POTENTIAL SCATTERING PROBLEMS

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Daubechies compact support wavelets are applied for solving integral Lippmann-Schwinger equation describing particle scattering on a spherically symmetric potential. Structure of wavelet representations of physical operators is discussed. It is shown that for fast decaying potentials wavelets enable a sparse approximation of the Lippmann-Schwinger equation kernel. Constraints for such potentials are derived.

Wavelet analysis was originally developed in the field of signal processing, since then the number of applications has increasingly grown. Due to more effective treatment of local phenomena at different levels of detail it seems to be more appropriate than Fourier analysis in various problems, such as data and image compression, seismology, nonlinear dynamics and many others.

Wavelets have also been found useful to construct an orthogonal basis set in separable Hilbert spaces, namely $L^2(\mathbf{R})$. These bases provide reasonable compromise between analyticity and the compact support of the basis functions. Several attempts at using these bases for variational calculus in the quantum mechanics, concentrating mostly on solving the Schrödinger equation, already appeared, see [4,6]. However, the results being less satisfactory than expected because of long-range behaviour of physical systems.

## Orthogonal wavelet bases

The present mathematical theory of wavelets is much more evolved than needs to be considered to our purposes. Therefore we briefly describe here only the essential ideas of constructing compactly supported wavelets in $L^2(\mathbf{R})$, based on multiresolution analysis. More detailed discussion can be found in many places, see e.g. [3].

A sequence of subspaces $V_m$ in $L^2(\mathbf{R})$ constitutes the multiresolution analysis, if for all $m \in \mathbf{Z}$ following conditions hold

$$V_{m+1} \subset V_m,$$
$$f(x) \in V_{m+1} \Leftrightarrow f(2x) \in V_m,$$
$$f(x) \in V_m \Rightarrow f(x-1) \in V_m,$$
$$\bigcap_{m\in\mathbf{Z}} V_m = \{0\}, \quad \overline{\bigcup_{m\in\mathbf{Z}} V_m} = L^2(\mathbf{R})$$

and there must exists a *scaling* function $\varphi(x) \in V_0$ such that its translated copies $\varphi(x-k)$, $k \in \mathbf{Z}$ form an orthogonal basis for $V_0$. The meaning of the sequence is that projecting a given function onto a subspace $V_m$ gives a finer approximation than projecting it onto $V_{m+1}$. Defining complementary subspaces $W_m = V_{m-1} \ominus V_m$ it is obvious that $W_m$ keeps details from $V_{m-1}$ which are missing at the coarser level $V_m$. The translation and dilation properties of the mutually orthogonal spaces $W_m$ are dictated by those of $V_m$. The theory then ensures the existence of a *wavelet* function $\psi(x) \in W_0$ such that its integer translations $\psi(x-k)$, $k \in \mathbf{Z}$ form an orthogonal basis for $W_0$. Thus, following decomposition of the whole $L^2(\mathbf{R})$ space is possible

$$L^2(\mathbf{R}) = V_M \oplus \bigoplus_{m=-\infty}^{M} W_m. \qquad (1)$$

The definition of $W_m$ and the orthogonality conditions strongly couple the scaling function and the mother wavelet at different levels

$$\varphi(x) = \sqrt{2}\sum_k h_k \varphi(2x-k),$$

$$\psi(x) = (-1)^k \sqrt{2} \sum_k \overline{h}_{\lambda-k} \varphi(2x-k),$$

see [3]. These equations are extremely useful especially for numerical computations [1], they state that properties of any scaling function and corresponding wavelets are fully determined by a unique, possibly small, set of coefficients $h_k$.

If the sequence $\{h_k\}$ consist only of a finite (even) number $2P$ of constituents, the orthogonality relations do not determine $h_k$ uniquely. They give just $P+1$ conditions to $2P$ independent coefficients $h_k$ and we are allowed to introduce another $P-1$ restrictions to $h_k$. Substantial simplifications appear when a special choice, first proposed by Daubechies, is taken into account

$$\int x^p \psi(x)\, dx = 0, \quad 1 \le p \le P-1.$$

The idea underlying such a suggestion is that all polynomials up to $P-1$ -st power belong to subspace $V_m$ at *any* level and thus can be *exactly* written as a linear combination including *only* translates of the scaling function at an arbitrary level $m$. These wavelets possess remarkable attributes: differentiability increasing with the parameter $P$ or compact support of length $2P-1$.

Representations of operators in particular bases are of great importance in the quantum mechanics. From the point of view of compactly supported Daubechies wavelets, there are two distinct classes of operators acting in $L^2(\mathbf{R})$, whose representations in wavelet bases exhibit rather different patterns.

Firstly, we consider *local* operators such as the free particle Hamiltonian $\frac{\hat{P}^2}{2M}$ or a local potential $\hat{V}$ . Evidently, projecting a given operator $\hat{K}$ to $V_n$, matrix elements including scaling functions which are distant from each other vanish due to the compact support of $\varphi(x)$. In practice, only a finite number $N$ of base vectors $|\varphi_k^n\rangle \in V_n$ is taken into account and the operator $\hat{K}$ is hence approximated by $N \times N$ matrix with a band of the width $4P-3$ around the diagonal.

However, a slight complication appears when converting $V_m$ to the equivalent decomposition (1). While the amount of nonzero elements in the representation matrix pertaining to $V_m$ is in the order of $N$, the latter form requires $\mathcal{O}(N \log N)$ elements and the matrix possess particular "fingerbanded" structure as shown in Fig. 1a. To get rid of redundancy, it is convenient to deal with a certain set of elements (note there's no mixing between different levels)

$$\alpha_{k,l}^m = \langle \psi_k^m | \hat{K} | \psi_l^m \rangle, \quad \beta_{k,l}^m = \langle \psi_k^m | \hat{K} | \varphi_l^m \rangle,$$
$$\gamma_{k,l}^m = \langle \varphi_k^m | \hat{K} | \psi_l^m \rangle, \quad t_{k,l}^M = \langle \varphi_k^M | \hat{K} | \varphi_l^M \rangle,$$

$M \ge m$, with no loss of information. Coefficients $\alpha$, $\beta$, $\gamma$, $t$ may be arranged in a table as depicted in Fig. 1b.

Obviously, the above defined set, called non-standard form[1], does not constitute a representation, so the table should not be treated as a matrix. On the contrary, multiplication of two non-standard forms of operators can be easily computed, just introducing some additional terms, in $\mathcal{O}(N)$ operations. For detailed information about the non-standard form we refer to [2].

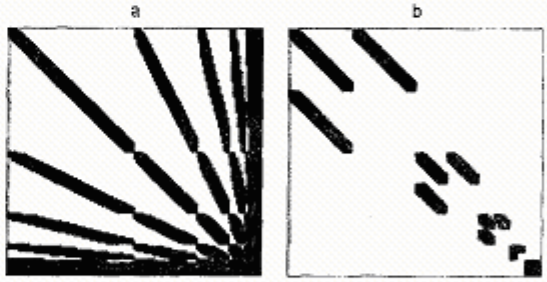


Figure 1. Structure of (a) standard form and (b) non-standard form (half sized) of local operators.

Secondly, we pay attention to operators which are *nonlocal*. The Green operator $(E-\hat{H}+i\epsilon)^{-1}$ can serve as a physical example. In general, even matrix elements between wavelets with non-overlapping supports are nonzero: this leads to dealing with large dense matrices which is very difficult in practise. Though, considering some special classes of operators, we are

[1]Since the representation associated with resolution (1) is sometimes called "standard form".

facing more favourable situation. As shown in [1], if the following conditions hold

$$\begin{aligned} |K(x,x')| &\leq \frac{1}{|x-x'|}, \qquad (2)\\ |\partial_x^P K(x,x')| &\leq \frac{C}{|x-x'|^{P+1}},\\ |\partial_{x'}^P K(x,x')| &\leq \frac{C'}{|x-x'|^{P+1}}, \end{aligned}$$

then, taking the basis of Daubechies wavelets with $P$ vanishing moments, the non-standard form matrices $\alpha, \beta, \gamma$ exhibit fast decaying off the diagonal

$$\begin{aligned} |\alpha_{k,l}^m| + |\beta_{k,l}^m| + |\gamma_{k,l}^m| &\leq \frac{C_P}{(1+|k-l|)^{P+1}},\\ \forall |k-l| &\geq 2P. \qquad (3) \end{aligned}$$

In practical computations, the precision is always limited and thence the representation matrices can be made sparse, showing the same structure as in Fig. 1. Matrices satisfying the estimate (3) also form an algebra, it means that the product and the inverse of them retain the same structure.

Considerable consequences to quantum mechanical computations with respect to potential scattering problems are discussed in the next section.

### Lippmann-Schwinger equation

Solving the Lippmann-Schwinger equation is of primary interest when taking the time independent approach to one-particle potential scattering

$$|\chi\rangle = |\chi_0\rangle + (E - \hat{H}_0 + i\epsilon)^{-1}\hat{H}_I|\chi\rangle,$$

introducing the free particle Hamiltonian $\hat{H}_0$ and the interaction $\hat{H}_I$. Vector $|\chi\rangle$ then contains the whole information about scattering and measurable quantities, like differential cross sections, can be expressed in terms of $\langle\chi_0|\hat{H}_I|\chi\rangle$.

Suppose now that the interaction is presented by a spherically symmetric potential $V(r)$ and $\vec{p}$ is the initial momentum of the particle, then the solution $|\chi\rangle$ can be decomposed into its angular and radial part and we obtain following equation for the radial part $\chi_l(r)$

$$\chi_l(r) = prj_l(pr) + \int_0^\infty g_l(r,r')V(r')\chi_l(r')\,dr',$$

$$g_l(p,r,r') = p\,rr' j_l(pr_<)n_l(pr_>). \qquad (4)$$

Mathematically, this is an integral equation of Fredholm type with the kernel given by $g_l(p,r,r')\,V(r')$.

To solve (4) we need to calculate the inverse of the nonlocal operator $\hat{K} = \hat{I} - \hat{G}_0(E)\hat{V}$. As we already mentioned, if a nonlocal operator satisfies additional conditions, its representation in some bases of Daubechies wavelets can be well approximated by a sparse matrix. To see whether $\hat{K}$ obeys such restrictions, behaviour of the Green function $g_l(p,r,r')$ and its derivatives must be investigated. Here we outline only the basic results: $g_l(p,r,r')$ is symmetric and continuous in spatial variables $r$, $r'$, stays finite for any fixed $r$ and $r' \to \infty$ and the same holds for its derivatives, partial derivatives with respect to both $r$ and $r'$ possess singularity at $r = r'$ – the higher order of derivatives taken the stronger the singularity is.

However, recalling (2, 3), complications arise from the oscillations as $r \to \infty$ and not from the existence of a singularity at $r = r'$. Therefore we employ symmetrised version of the Lippmann-Schwinger equation

$$\hat{V}|\chi\rangle = \hat{V}|\chi_0\rangle + \hat{V}\hat{G}_0(E)\hat{V}|\chi\rangle.$$

Because the behaviour of the corresponding kernel $V(r)\,g_l(p,r,r')\,V(r')$ at large distances $r$ and $r'$ strongly depends on the form of the potential $V(r)$, it is reasonable to expect that estimates (2) hold for fast decaying potentials. Then we want to know how fast they must decay.

Requirements to a local potential $V(r)$ written in terms of $|r-r'|$ immediately follow from (2), however, they are not very transparent. To that purpose, we deduced alternative conditions for $V(r)$ which are easier to verify, but which are more restrictive. Derivation of such conditions is rather lengthy, so we state here only the

final result: if derivatives up to P-th order of a spherically symmetric potential $V(r)$ are continuous in $\langle 0, \infty)$ and obey

$$\left|\frac{d^n}{dr^n}V(r)\right| \leq \frac{D_n}{r^{P+1}}, \quad n = 0 \ldots P,$$

then the non-standard form matrices of the operator $\hat{V}\hat{G}_0(E)\hat{V}$ satisfy the previously appointed inequality (3). Clearly, potentials that are smooth enough and decay exponentially can serve as an illustrative example, but this is rarely the case we are encountering in physics (remind Coulomb or dipole interaction).

## Discussion

In practice, we are always dealing with a finite subset of basis functions and hence approximating wavelet representations of operators by $N \times N$ matrices. An integral equation can then be solved by a standard direct method in $\mathcal{O}(N^3)$ operations. Using wavelet bases, the representation matrices are large in dimension, but we may choose noindent only such basis functions that approximate the solution well. This was done in [4,6], however, it requires some preliminary information about the solution which is not always available.

When the representation matrices are sparse, retaining all the basis functions and applying an iterative method seems to be more suitable. Considering a Daubechies wavelet basis, the number of iterations $M$ does not depend on $N$ and the solution of the Lippmann-Schwinger equation can be obtained, in case of fast decaying potentials, in $\mathcal{O}(MN\log^2 N)$ or even (using the non-standard form) $\mathcal{O}(MN)$ operations.

In the end, we would like to point out that it is mainly the translation invariance property that complicates numerical treatment of Daubechies wavelets in two ways. Due to the compact support of $|\psi_k^n\rangle$ we must take a large number $N$ of basis functions to get a reasonable approximation of a function. Secondly, restriction of wavelet bases to a finite interval is highly nontrivial and in fact we lose the translation invariance then. An efficient method of restriction, presented in [5], consist in changing the scaling functions and the wavelets near the boundary preserving some properties (vanishing moments of the wavelets at least). Consequently, the matrix elements corresponding to wavelets near the ends of the interval are modified, fortunately, the amount of such elements does not depend on $N$. On the contrary, the idea of scaling invariance, decomposition into an average and a detail, is very understandable and useful.

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# ВИКОРИСТАННЯ ЕЛЕМЕНТАРНИХ ХВИЛЬ У ЗАДАЧАХ ПОТЕНЦІАЛІВ РОЗСІЮВАННЯ


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Для розв'язання інтегрального рівняння Ліпмана-Швінгера, що описує розсіювання частинок на сферично симетричному потенціалі, використовуються компактні елементарні хвилі Добеш'є. Обговорюється структура представлення фізичних операторів елементарними хвилями. Показано, що для потенціалів зі швидким розпадом елементарні хвилі дають змогу апроксимувати ядро рівняння Ліпмана-Швінгера. Виведено обмеження для таких потенціалів.