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Discrete wavelets and perturbation theory

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Abstract

We show with the help of examples that discrete wavelets can be a useful tool in perturbation theory of finite-dimensional quantum Hamilton systems.

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In perturbation theory the Hamilton operator $\hat{H}$ is given by $\hat{H} = \hat{H}_0 + \hat{H}_1$ where $\hat{H}_0$ and $\hat{H}_1$ are self-adjoint operators in a Hilbert space [1]. It is assumed that the perturbation $\hat{H}_1$ is relatively 'small' in comparison to the soluble part $\hat{H}_0$. Quite often $\hat{H}_0$ is the diagonal term. We also quite often have the problem that (for example after a Fourier transform) $\hat{H}_1$ is the soluble part and $\hat{H}_0$ is the perturbation. A typical example is the Hubbard model. Thus it would be quite useful to have a transformation such that $\hat{H}_0$ is always the dominant term independent of the parameters. We assume that the Hamilton operator acts in a finite-dimensional Hilbert space. For Hamilton operators acting in a finite-dimensional vector space the discrete wavelet transform [2, 3] can play such a role.

In our first example we consider the Hubbard model. For the sake of simplicity we consider the two-point Hubbard model. In Wannier representation we have

$$\hat{H} = t\left(c^\dagger_{1\uparrow}c_{2\uparrow} + c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\uparrow}c_{1\uparrow} + c^\dagger_{2\downarrow}c_{1\downarrow}\right) + U\sum_{j=1}^{2} c^\dagger_{j\uparrow}c_{j\uparrow}c^\dagger_{j\downarrow}c_{j\downarrow} \qquad (1)$$

where the parameters $t > 0$ and $U > 0$. After a discrete Fourier transform we find the Bloch representation

$$\hat{H}_B = \sum_{k\sigma}\epsilon(k)c^\dagger_{k\sigma}c_{k\sigma} + U\sum_{k_1,k_2,k_3,k_4}\delta(k_1 - k_2 + k_3 - k_4)c^\dagger_{k_1\uparrow}c_{k_2\uparrow}c^\dagger_{k_3\downarrow}c_{k_4\downarrow} \qquad (2)$$

where

$$\epsilon(k) = t\cos(k) \qquad k = 0, \pi \bmod 2\pi. \qquad (3)$$

Thus we would like to consider the cases $U \gg t$ and $t \gg U$ under one approach. The Hubbard operator commutes with the total number operator $\hat{N}$ and the total spin operator in the z-direction $\hat{S}_z$. We consider the case with two particles and $S_z = 0$. Then a basis in Wannier representation is given by

$$c^\dagger_{1\uparrow}c^\dagger_{1\downarrow}|0\rangle \quad c^\dagger_{1\uparrow}c^\dagger_{1\downarrow}|0\rangle \quad c^\dagger_{2\uparrow}c^\dagger_{1\downarrow}|0\rangle \quad c^\dagger_{2\uparrow}c^\dagger_{2\downarrow}|0\rangle. \tag{4}$$

Thus we find the Hubbard Hamilton operator in Wannier representation has the matrix representation

$$\hat{H}_W = \begin{pmatrix} U & t & t & 0 \\ t & 0 & 0 & t \\ t & 0 & 0 & t \\ 0 & t & t & U \end{pmatrix}. \tag{5}$$

We see that if $t \gg U$ the non-diagonal elements are dominant. In Bloch representation we have the basis

$$c^\dagger_{0\uparrow}c^\dagger_{0\downarrow}|0\rangle \quad c^\dagger_{\pi\uparrow}c^\dagger_{\pi\downarrow}|0\rangle \quad c^\dagger_{0\uparrow}c^\dagger_{\pi\downarrow}|0\rangle \quad c^\dagger_{\pi\uparrow}c^\dagger_{0\downarrow}|0\rangle \tag{6}$$

and the matrix representation

$$\hat{H}_B = \begin{pmatrix} U/2+2t & U/2 & 0 & 0 \\ U/2 & U/2-2t & 0 & 0 \\ 0 & 0 & U/2 & U/2 \\ 0 & 0 & U/2 & U/2 \end{pmatrix}. \tag{7}$$

The matrices given by (5) and (7) are related by the unitary transformation $\hat{H}_B = V\hat{H}_W V^*$, where the unitary matrix V is given by

$$V = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \end{pmatrix}. \tag{8}$$

Now we apply the discrete wavelet transform. The Haar matrices [2] are given by

$$K(k+1) = \begin{pmatrix} K(k) \otimes (1 \quad 1) \\ 2^{k/2} I_{2^k} \otimes (1 \quad -1) \end{pmatrix} \qquad k > 1 \tag{9}$$

using the Kronecker product and recursion [2], where

$$K(1) = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{10}$$

Thus the 4×4 Haar matrix K (after normalizing the columns) is given by

$$K = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ \sqrt{2} & -\sqrt{2} & 0 & 0 \\ 0 & 0 & \sqrt{2} & -\sqrt{2} \end{pmatrix}. \tag{11}$$

Then we find that

$$\tilde{H}_W = K\hat{H}_W K^T = \frac{1}{4}\begin{pmatrix} 2U+8t & 0 & \sqrt{2}U & -\sqrt{2}U \\ 0 & 2U & \sqrt{2}U & \sqrt{2}U \\ \sqrt{2}U & \sqrt{2}U & 2U-4t & 4t \\ -\sqrt{2}U & \sqrt{2}U & 4t & 2U-4t \end{pmatrix}. \tag{12}$$

Thus we find that the largest term $(2U + 8t)/4$ is on the diagonal.

By a Walsh–Hadamard matrix of order n, W_n, is meant a matrix whose elements are either +1 or −1 and for which $W_n W_n^T = W_n^T W_n = nI_n$, where I_n is the $n \times n$ unit matrix. Thus $n^{-1/2} W_n$ is an orthogonal matrix. We call this Walsh–Hadamard matrix normalized. For example, the matrix given by equation (8) is a normalized Walsh–Hadamard matrix. Another 4×4 Walsh–Hadamard matrix is given by

$$W = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ -1 & -1 & 1 & 1 \\ -1 & 1 & 1 & -1 \\ 1 & -1 & 1 & -1 \end{pmatrix} \tag{13}$$

where we have normalized the matrix. Then the Hamilton matrix (5) takes the form

$$\tilde{H}_W = W\hat{H}_W W^T = \frac{1}{4}\begin{pmatrix} 2U+8t & 0 & -2U & 0 \\ 0 & 2U & 0 & -2U \\ -2U & 0 & 2U-8t & 0 \\ 0 & -2U & 0 & 2U \end{pmatrix}. \tag{14}$$

Thus we find again that the dominant term is on the diagonal. A subset of the Walsh–Hadamard matrices can be extended to higher dimensions as follows using the Kronecker product

$$W_1 = (1) \qquad W_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{15}$$

and

$$W_{2^{n+1}} = W_{2^n} \otimes W_2. \tag{16}$$

As a higher dimensional example we consider the spin Hamilton operator [4]

$$\hat{H} = a\sum_{j=1}^{3} \sigma_3(j)\sigma_3(j+1) + b\sum_{j=1}^{3}\sigma_1(j) \tag{17}$$

with cyclic boundary conditions, i.e. $\sigma_3(4) \equiv \sigma_3(1)$. Here a, b are real constants and σ_1, σ_2 and σ_3 are the Pauli matrices. Since

$$\sigma_k(1) = \sigma_k \otimes I \otimes I \qquad \sigma_k(2) = I \otimes \sigma_k \otimes I \qquad \sigma_k(3) = I \otimes I \otimes \sigma_k \tag{18}$$

$(k = 1, 2, 3)$ we obtain an 8×8 matrix. For the first term in the spin Hamilton operator (17) we find a diagonal matrix. The second term leads to non-diagonal terms. Using (18) we find the symmetric 8×8 matrix for $\hat{H}$

$$\begin{pmatrix} 3a & b & b & 0 & b & 0 & 0 & 0 \\ b & a & 0 & b & 0 & b & 0 & 0 \\ b & 0 & a & b & 0 & 0 & b & 0 \\ 0 & b & b & -a & 0 & 0 & 0 & b \\ b & 0 & 0 & 0 & a & b & b & 0 \\ 0 & b & 0 & 0 & b & -a & 0 & b \\ 0 & 0 & b & 0 & b & 0 & -a & b \\ 0 & 0 & 0 & b & 0 & b & b & -3a \end{pmatrix}. \tag{19}$$

Applying the 8×8 Haar matrix constructed from equation (9) we find that

$$K\hat{H}K^{-1} = \begin{pmatrix} 3b & a & a/\sqrt{2} & a/\sqrt{2} & a/2 & a/2 & a/2 & a/2 \\ a & b & a/\sqrt{2} & -a/\sqrt{2} & a/2 & a/2 & -a/2 & -a/2 \\ a/\sqrt{2} & a/\sqrt{2} & a & b & a/\sqrt{2} & -a/\sqrt{2} & 0 & 0 \\ a/\sqrt{2} & -a/\sqrt{2} & b & -a & 0 & 0 & a/\sqrt{2} & -a/\sqrt{2} \\ a/2 & a/2 & a/\sqrt{2} & 0 & 2a-b & b & b & 0 \\ a/2 & a/2 & -a/\sqrt{2} & 0 & b & -b & 0 & b \\ a/2 & -a/2 & 0 & a/\sqrt{2} & b & 0 & -b & b \\ a/2 & -a/2 & 0 & -a/\sqrt{2} & 0 & b & b & -2a-b \end{pmatrix}. \tag{20}$$

We see again that the dominant terms are on the diagonal. If we apply the Hadamard matrix $W := W_2 \otimes W_2 \otimes W_2$ we find that $W\hat{H}W^T$ takes the same form as equation (19) but with constants a and b interchanged. This is due to the fact that $\sigma_1 = W_2\sigma_3W_2^T$ and $\sigma_3 = W_2\sigma_1W_2^T$. Thus the subgroup of Hadamard matrices constructed from the Kronecker product of the 2×2 Hadamard matrix does not rotate a and b on the diagonal for the Hamilton operator (17). The operator $W_2 \otimes W_2 \otimes \cdots \otimes W_2$ plays a central role in quantum computing [5]. It generates a linear combination of the integers from 0 to $2^n - 1$.

In the examples given above we have shown that the Haar and Walsh–Hadamard transforms yield a Hamilton operator with dominant terms on the diagonal of the matrix representation. The standard Rayleigh–Schrödinger perturbation expansion [6] for systems with a discrete spectrum $\hat{H} = \hat{H}_0 + \lambda\hat{V}$ and bounded from below yields up to second-order approximation

$$E_n(\lambda) \approx E_n(0) + \lambda\langle\psi_n(0)|\hat{V}|\psi_n(0)\rangle + \lambda^2 \sum_{m\neq n} \frac{|V_{mn}(0)|^2}{E_n(0) - E_m(0)}.$$

This approximation follows as a special case of the solution of the initial value problem of the autonomous system of ordinary differential equations [1, 7]

$$\frac{\mathrm{d}E_n}{\mathrm{d}\lambda} = p_n \qquad \frac{\mathrm{d}p_n}{\mathrm{d}\lambda} = 2\sum_{m\neq n} \frac{V_{mn}V_{nm}}{E_n - E_m}$$

$$\frac{\mathrm{d}V_{mn}}{\mathrm{d}\lambda} = \sum_{k(\neq m,n)} \left(V_{mk}V_{kn}\left(\frac{1}{E_m - E_k} + \frac{1}{E_n - E_k}\right)\right) + \frac{V_{mn}(p_n - p_m)}{E_m - E_n}$$

using a Lie series expansion of the vector field of the autonomous system up to second order [1]. Here $p_n(\lambda) := \langle\psi_n(\lambda)|\hat{V}|\psi_n(\lambda)\rangle$ and $V_{mn}(\lambda) := \langle\psi_m(\lambda)|\hat{V}|\psi_n(\lambda)\rangle$ $(m \neq n)$. This system has to be solved with the initial values $E_n(0) = \langle\psi_n(0)|\hat{H}_0|\psi_n(0)\rangle$ etc. The approach described above provides a new $\hat{H}_0$ and $\hat{V}$ so that we can deal with two parameters using one expansion. This system of differential equations also allows the study of the Riemann sheet structure of the energy levels $E_n(\lambda)$ (λ complex) and of exceptional points [8, 9].

References

[1] Steeb W-H 1998 *Hilbert Spaces, Wavelets, Generalized Functions, and Modern Quantum Mechanics* (Dordrecht: Kluwer)

[2] Steeb W-H 1997 *Matrix Calculus and Kronecker Product with Applications and C++ Programs* (Singapore: World Scientific)

[3] Steeb W-H 2002 *The Nonlinear Workbook: Chaos, Fractals, Cellular Automata, Neural Networks, Genetic Algorithms, Gene Expression Programming, Wavelets, Fuzzy Logic with C++, Java and Symbolic C++ Programs* 2nd edn (Singapore: World Scientific)

[4] Steeb W-H 2003 *Problems and Solutions in Theoretical and Mathematical Physics volume II, Advanced Level* 2nd edn (Singapore: World Scientific)

[5] Hardy Y and Steeb W-H 2001 *Classical and Quantum Computing with C++ and Java Simulations* (Basel: Birkhäuser Verlag)

[6] Bohm A 1994 *Quantum Mechanics* 3rd edn (New York: Springer)

[7] Yukawa T 1986 *Phys. Lett.* **54** 227

[8] Heiss W D and Steeb W-H 1991 *J. Math. Phys.* **32** 3003

[9] Steeb W-H and Heiss W D 1993 *Phys. Scr.* **47** 321