Wavelets in the Hamiltonian

Aidan Macdonald (amacdona@ucsd.edu)

September 19, 2015

Abstract

Here a standard Hamiltonian is simplified and made diagonal in the momentum domain by using a Wavelet frame to approximate the potential.

1 Introduction

Throughout this document, $\hbar = 1$, as it should be. (q, p) are generalized position and momentum respectively.

We take Hamiltonians of the form,

$$\hat{H} = \frac{\hat{P}^2}{2m} + \hat{V}$$

where $\hat{V}$ is diagonal in q-space. Thus we can write $\langle q|\hat{V}|q\rangle = V(q)\langle q|q\rangle$.

2 Diagonalization

We wish to find the eigenvalues of the time-independent Schrodinger equations,

$$\hat{H}|E\rangle = E|E\rangle$$

so that we can take the time dependent eigenvector as $e^{-iEt}|E\rangle$.

Expanding the equation in p space and letting $|E\rangle = |p\rangle$,

$$\begin{aligned} \frac{1}{2m}\langle p|\hat{P}^2|E\rangle + \langle p|\hat{V}|E\rangle &= E\langle p|E\rangle \\ \frac{p^2}{2m} + \langle p|\hat{V}|p\rangle &= E \end{aligned}$$

The $\hat{V}$ is not naturally diagonal in p-space, but we can use discrete Wavelet frames to solve this. Take a "snug" wavelet frame [1],

3 Wavelet Frames

Let a "snug" wavelet frame be defined by,

$$\sum_{\alpha} |\psi_\alpha\rangle\langle\psi_\alpha| \approx A\hat{\mathbf{1}}$$

for $|\psi_\alpha\rangle = \hat{U}(\alpha)|\psi_0\rangle$ where $\hat{U}$ is the unitary representation of a group and $\|\psi_0\|^2 = 1$.

We can use these frames to further reduce the Hamiltonian. Looking at the potential part,

$$\begin{aligned}\langle p|\hat{V}|p\rangle &\approx \frac{1}{A^2}\sum_{\alpha,\beta}\langle p|\psi_\alpha\rangle\langle\psi_\alpha|\hat{V}|\psi_\beta\rangle\langle\psi_\beta|p\rangle \\ &= \frac{1}{A^2}\sum_{\alpha,\beta}\psi_\alpha(p)\overline{\psi_\beta(p)}V_{\alpha\beta}\end{aligned}$$

where $V_{\alpha\beta} = \langle\psi_\alpha|\hat{V}|\psi_\beta\rangle$ follows the reasonably obvious notation.

We can write this as a matrix vector product,

$$\langle p|\hat{V}|p\rangle = \vec{\psi}(p)^T\mathbf{V}\vec{\psi}(p)$$

4 Finite Frames

We can get excellent approximations of the potential with just finitely many frame vectors. This has to do with the redundancy and space-momentum localization of the wavelet vectors [1].

This is done case by case and heuristically if the $V_{\alpha\beta}$ is computed numerically. Closed form solutions could just simply look at the way the closed form falls off and pick termination point based on that.

5 Simple Example

Take the step rectangle function as the potential,

$$V(x) = V_0\mathbf{1}_{|x|\in(-x_0,x_0)}$$

We use the Mexican Hat Wavelet,

$$\begin{aligned}\langle p|\psi_0\rangle &= \frac{2}{\sqrt{3}\sqrt[4]{\pi}}\langle p|\hat{P}^2|g\rangle \\ &= \frac{2}{\sqrt{3}\sqrt[4]{\pi}}p^2e^{-p^2/2} \\ \langle q|\psi_0\rangle &= -\frac{2}{\sqrt{3}\sqrt[4]{\pi}}\partial_q^2 e^{-q^2/2} \\ &= \frac{2}{\sqrt{3}\sqrt[4]{\pi}}(1-q^2)e^{-q^2/2}\end{aligned}$$

which is unit length.

We use the affine group, with representation,

$$\langle q|\hat{U}(a,b)|f\rangle = f(\frac{q-b}{a})/\sqrt{|a|}$$
$$\langle p|\hat{U}(a,b)|f\rangle = \tilde{f}(ap)e^{-ibp}\sqrt{|a|}$$

References

[1] Ingrid Daubechies et al. *Ten lectures on wavelets*, volume 61. SIAM, 1992.