Position-Dependent mass FGH

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Abstract

In what follows we are going to adapt the Fourier Grid Hamiltonian Method to be applied to potentials with position-dependent masses.

1 Introduction

The Fourier-grid Hamiltonian method use a mixed position and momentum representation to describe the Hamiltonian to be applied to Schrödinger's equation.

$$\hat{H} = \hat{T} + V(\hat{x}), \tag{1}$$

where $\hat{T}$ is the kinetic energy operator and $V(\hat{x})$ is the potential energy operator. That Hamiltonian still was not put on a specific representation.

In the coordinate representation, the basis is such that

$$\hat{x}|x\rangle = x|x\rangle, \tag{2}$$

where vectors $|x\rangle$ forms an orthonormal basis

$$\langle x_s|x_j\rangle = \frac{\delta_{sj}}{\Delta x}. \tag{3}$$

The completeness relationship is

$$\sum_s |x_s\rangle \Delta x \langle x_s| = 1. \tag{4}$$

As we know in position representation potential operator is diagonal

$$\langle x_s|V(\hat{x})|x_j\rangle = V(x_s)\frac{\delta_{sj}}{\Delta x}. \tag{5}$$

The momentum representation is given by the state vectors $|k\rangle$, and the momentum operator is diagonal in such a representation

$$\hat{p}|k\rangle = \hbar k|k\rangle. \tag{6}$$

When the potential representing the system has a position-dependent mass, the Hamiltonian becomes non-hermitian. In order to rescue the hermiticity, an usual approach is to symmetrize it, by writing the kinetic energy operator as

$$\hat{K} = \frac{1}{2}\hat{p}\left[\frac{1}{m(\hat{x})}\right]\hat{p}. \tag{7}$$

The kinetic operator element of matrix becomes

$$\hat{K}_{sj} = \langle x_s|\hat{K}|x_j\rangle. \tag{8}$$

Using the completeness relationship for the momentum representation

$$\sum_q |k_q\rangle \Delta k \langle k_q| = 1, \tag{9}$$

and the one for the position representation (eq. 4),

$$\hat{K}_{sj} = \frac{1}{2}\langle x_s|\left[\hat{p}\sum_{l=-n}^{n}|k_l\rangle\Delta k\langle k_l|\left[\frac{1}{m(\hat{x})}\right]\hat{p}\sum_{q=-n}^{n}|k_q\rangle\Delta k\langle k_q|\right]|x_j\rangle. \tag{10}$$

$$\hat{K}_{sj} = \frac{1}{2}\langle x_s|\left[\hat{p}\sum_{l=-n}^{n}|k_l\rangle\Delta k\langle k_l|\sum_{r=1}^{N}\frac{1}{m(\hat{x})}|x_r\rangle\Delta x\langle x_r|\hat{p}\sum_{q=-n}^{n}|k_q\rangle\Delta k\langle k_q|\right]|x_j\rangle. \tag{11}$$

Rearranging the sums and applying the operators,

$$\hat{K}_{sj} = \frac{1}{2}\sum_{r=1}^{N}\sum_{l=-n}^{n}\sum_{q=-n}^{n}\langle x_s|\left[\hbar k_l|k_l\rangle\Delta k\langle k_l|\frac{1}{m_r}|x_r\rangle\Delta x\langle x_r|\hbar k_q|k_q\rangle\Delta k\langle k_q|\right]|x_j\rangle, \tag{12}$$

where $m_r = m(x_r)$.

$$\hat{K}_{sj} = \frac{1}{2}\sum_{r=1}^{N}\sum_{l=-n}^{n}\sum_{q=-n}^{n}\hbar k_l\langle x_s|k_l\rangle\Delta k m_r^{-1}\langle k_l|x_r\rangle\Delta x\hbar k_q\langle x_r|k_q\rangle\Delta k\langle k_q|x_j\rangle, \tag{13}$$

$$\hat{K}_{sj} = \frac{1}{2}\sum_{r=1}^{N}\sum_{l=-n}^{n}\sum_{q=-n}^{n}p_l p_q\Delta k^2\langle x_s|k_l\rangle m_r^{-1}\langle k_l|x_r\rangle\langle x_r|k_q\rangle\langle k_q|x_j\rangle\Delta x, \tag{14}$$

where $p_i = \hbar k_i = \hbar i\Delta k = 2\pi i\hbar/N\Delta x$. The transformation between representations is given by the fourier transform

$$\langle k|x\rangle = \frac{1}{\sqrt{2\pi}}e^{-ikx}. \tag{15}$$

Therefore

$$\hat{K}_{sj} = \frac{1}{2}\sum_{r=1}^{N}\sum_{l=-n}^{n}\sum_{q=-n}^{n}\frac{p_l p_q}{m_r}\Delta k^2 \frac{e^{ik_l x_s}}{\sqrt{2\pi}}\frac{e^{-ik_l x_r}}{\sqrt{2\pi}}\frac{e^{ik_q x_r}}{\sqrt{2\pi}}\frac{e^{-ik_q x_j}}{\sqrt{2\pi}}\Delta x, \qquad (16)$$

$$\hat{K}_{sj} = \frac{1}{2}\sum_{r=1}^{N}\sum_{l=-n}^{n}\sum_{q=-n}^{n}\frac{p_l p_q}{m_r}\Delta k^2 \frac{e^{ik_l(x_s-x_r)}}{2\pi}\frac{e^{ik_q(x_r-x_j)}}{2\pi}\Delta x, \qquad (17)$$

For an equally space mesh $x_i = i\Delta x$, and $k_i = i\delta k$,

$$\hat{K}_{sj} = \frac{1}{2}\sum_{r=1}^{N}\sum_{l=-n}^{n}\sum_{q=-n}^{n}\frac{p_l p_q}{m_r}\Delta k^2 \frac{e^{il\Delta k(s-r)\Delta x}}{2\pi}\frac{e^{iq\delta k(r-j)\Delta x}}{2\pi}\Delta x, \qquad (18)$$

Writing $\Delta k = 2\pi/N\Delta x$, we get

$$\hat{K}_{sj} = \frac{1}{2N^2\Delta x}\sum_{r=1}^{N}\sum_{l=-n}^{n}\sum_{q=-n}^{n}\frac{p_l p_q}{m_r} e^{2\pi i\frac{l(s-r)}{N}} e^{2\pi i\frac{q(r-j)}{N}}. \qquad (19)$$

Note that for each element of matrix we have to proceed three sums, which is quite expensive computationally. Let's try to group some terms. As we see, l and q sums are almost the same, lets examine some terms. For instance, considering $l = q$,

$$\hat{K}_{sj}^{l=q} = \frac{1}{2N^2\Delta x}\sum_{r=1}^{N} m_r^{-1}\sum_{l=-n}^{n} p_l^2 e^{2\pi i\frac{l(s-j)}{N}}. \qquad (20)$$

The sum of the mass, if its constant returns the total mass $\sum_{r=1}^{N} m_r^{-1} = N/m$, so

$$\hat{K}_{sj}^{l=q} = \frac{1}{N\Delta x}\sum_{l=-n}^{n}\frac{p_l^2}{2m} e^{2\pi i\frac{l(s-j)}{N}}, \qquad (21)$$

recovering traditional Kinetic energy element of matrix.

Considering now superior t^{th} diagonal, by setting $l = q + t$,

$$\hat{K}_{sj}^{q=l-t} = \frac{1}{2N^2\Delta x}\sum_{r=1}^{N}\sum_{l=-n}^{n}\sum_{t=l+n}^{l-n}\frac{p_l p_{l-t}}{m_r} e^{2\pi i\frac{l(s-r)}{N}} e^{2\pi i\frac{(l-t)(r-j)}{N}}. \qquad (22)$$

$$\hat{K}_{sj}^{q=l-t} = \frac{1}{2N^2\Delta x}\sum_{r=1}^{N}\sum_{l=-n}^{n}\sum_{t=l+n}^{l-n}\frac{p_l p_{l-t}}{m_r}\exp\left[2\pi i\frac{(l(s-j)+t(j-r))}{N}\right]. \qquad (23)$$

$$\hat{K}_{sj}^{q=l-t} = \frac{1}{2N^2\Delta x}\sum_{r=1}^{N}\sum_{l=-n}^{n}\sum_{t=l+n}^{l-n}\frac{p_l p_{l-t}}{m_r}\exp\left[2\pi i\frac{l(s-j)}{N}\right]\exp\left[2\pi i\frac{t(j-r)}{N}\right]. \qquad (24)$$

	l						
	-3	-2	-1	0	1	2	3
	-6	-5	-4	-3	-2	-1	0
	-5	-4	-3	-2	-1	0	1
	-4	-3	-2	-1	0	1	2
t	-3	-2	-1	0	1	2	3
	-2	-1	0	1	2	3	4
	-1	0	1	2	3	4	5
	0	1	2	3	4	5	6

$$\hat{K}_{sj}^{q=l-t} = \frac{1}{2N^2\Delta x}\sum_{r=1}^{N}\sum_{l=-n}^{n}\sum_{t=l-n}^{l+n}\frac{p_l p_{l-t}}{m_r}\exp\left[2\pi i\frac{l(s-j)}{N}\right]\exp\left[-2\pi i\frac{t(j-r)}{N}\right]. \tag{25}$$

Suppose a determined n, the second sum has three terms $-n \leq l \leq n$, and the third sum runs $l-n \leq t \leq l+n$, with a total of $2n+1$ terms for each l.

Being $[2\pi i(s-j)/N] = \beta$, and $[-2\pi i(j-r)/N] = \alpha$, we get

$$\hat{K}_{sj}^{q=l-t} = \frac{1}{2N^2\Delta x}\sum_{r=1}^{N}\sum_{l=-n}^{n}\sum_{t=l-n}^{l+n}\frac{p_l p_{l-t}}{m_r}e^{\beta l}e^{\alpha t}. \tag{26}$$

As shown in table 1, for $n = 3$, the sum over t runs from -6 to 6, depending on the l. We can use the indexes in the table to explicitly expand the product of the sums.

Rewriting only the second and third sums, for the sake of simplicity, assuming $n = 1$ (using the indexes highlighted with the box in the table 1)

$$\sum_{l=-1}^{1}\sum_{t=l-1}^{l+1} e^{\beta l}e^{\alpha t} = p_{-1}e^{-\beta}\left[p_1 e^{-2\alpha} + p_0 e^{-1\alpha} + p_{-1}e^{0\alpha}\right] + \\ p_0 e^{0\beta}\left[p_1 e^{-1\alpha} + p_0 e^{0\alpha} + p_{-1}e^{1\alpha}\right] + p_1 e^{1\beta}\left[p_1 e^{0\alpha} + p_0 e^{1\alpha} + p_{-1}e^{2\alpha}\right]. \tag{27}$$

$$\sum_{l=-1}^{1}\sum_{t=l-1}^{l+1} e^{\beta l}e^{\alpha t} = tr\begin{bmatrix} p_{-1}e^{-\beta} & p_{-1}e^{-\beta} & p_{-1}e^{-\beta} \\ p_0 e^{0\beta} & p_0 e^{0\beta} & p_0 e^{0\beta} \\ p_1 e^{\beta} & p_1 e^{\beta} & p_1 e^{\beta} \end{bmatrix}\begin{bmatrix} p_1 e^{-2\alpha} & p_1 e^{-\alpha} & p_1 e^{0\alpha} \\ p_0 e^{-\alpha} & p_0 e^{0\alpha} & p_0 e^{\alpha} \\ p_{-1}e^{0\alpha} & p_{-1}e^{\alpha} & p_{-1}e^{2\alpha} \end{bmatrix} \tag{28}$$

Therefore, the double sum could be recast as the trace of the product of two relatively simple matrices

$$\sum_{l=-1}^{1}\sum_{t=l-1}^{l+1} e^{\beta l}e^{\alpha t} = tr(\hat{A}\cdot\hat{B}). \tag{29}$$

Backing to the kinetic energy operator element of matrix,

$$\hat{K}_{sj} = \frac{1}{2N^2\Delta x}\sum_r \frac{1}{m_r} tr(\hat{A}_{s,j,r} \cdot \hat{B}_{s,j,r}). \tag{30}$$

Now we can rewrite the Hamiltonian element of matrix

$$\hat{H}_{sj} = \frac{1}{2N^2\Delta x}\sum_{r=1}^{N} \frac{1}{m_r} tr(\hat{A}_{s,j,r} \cdot \hat{B}_{s,j,r}) + V(x_s)\frac{\delta_{sj}}{\Delta x}. \tag{31}$$