Fourier Grid Hamiltonian

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1 Theory

Fourier Grid Hamiltonian (FGH) is a numerical technique used to solve the Schrodinger equation for bound states. Instead of using basis functions (like harmonic oscillators or plane waves), the method discretizes the coordinate space into a grid and constructs the Hamiltonian. The kinetic energy matrix is computed using Fourier transformation, which efficiently connects the momentum space and coordinate space representations. More simply, the total Hamiltonian is devided into two parts, one is kinetic energy part and another one is potential energy part. Finally to get the full energy of the system, kinetic energy part is solved in momentum space and potential energy part in coordinate space. A simple derivation of FGH is given below:

For a single particle of mass m, the Hmiltonian will be,

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

$$\hat{H} = \frac{\hat{p^2}}{2m} + V(\hat{x}) \tag{2}$$

Now for the potential energy operator, the coordinate space is chosen as the basis function and from the concept of orthogonality and completeness relation one can write,

$$\langle x|x'\rangle = \delta(x - x') \tag{3}$$

and

$$\hat{I}_x = \int_{-\infty}^{+\infty} |x\rangle \langle x| \, dx \tag{4}$$

so,

$$\langle x'| V(\hat{x}) |x\rangle = V(x)\delta(x - x') \tag{5}$$

Similarly for the momentum operator,

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

and from the orthogonality and completeness concept one can again write,

$$\langle k|k'\rangle = \delta(x - x') \tag{7}$$

and

$$\hat{I}_k = \int_{-\infty}^{+\infty} |k\rangle \langle k| \, dk \tag{8}$$

So,

$$\langle k'| \hat{T} |k\rangle = T_k \delta(k-k') \tag{9}$$

$$\langle k'| \hat{T} |k\rangle = \frac{p^2}{2m}\delta(k-k') \tag{10}$$

$$\langle k'| \hat{T} |k\rangle = \frac{\hbar^2 k^2}{2m}\delta(k-k') \tag{11}$$

Now to transform coordinate space to momentum space, one can use Fourier transformation.

$$\langle k|x\rangle = \frac{1}{\sqrt{2\pi}} \exp^{-ikx} \tag{12}$$

So, the total hamiltonian will be,

$$\begin{aligned}
\langle x| \hat{H} |x'\rangle &= \langle x| \hat{T} |x'\rangle + \langle x| V(\hat{x}) |x'\rangle \\
&= \langle x| \hat{T} |x'\rangle + V(x) \langle x|x'\rangle \\
&= \langle x| \hat{T}_x \hat{I}_k |x'\rangle + V(x) \langle x|x'\rangle \\
&= \langle x| \hat{T} (\int_{-\infty}^{+\infty} |k\rangle \langle k|) |x'\rangle \, dk + V(x) \langle x|x'\rangle \, , from (9) \\
&= \int_{-\infty}^{+\infty} ((\langle x|k\rangle \hat{T} \langle k|x'\rangle) dk + V(x) \langle x|x'\rangle \\
&= \frac{1}{\sqrt{2\pi}} [\int_{-\infty}^{+\infty} (\exp^{ikx} T_x \langle k|x'\rangle) dk] + V(x) \langle x|x'\rangle \, , from (13) \\
&= \frac{1}{2\pi} [\int_{-\infty}^{+\infty} (\exp^{ikx} \exp^{-ikx'} T_x) dk] + V(x) \langle x|x'\rangle \, , from (13) \\
&= \frac{1}{2\pi} [\int_{-\infty}^{+\infty} (\exp^{ik(x-x')} T_x) dk] + V(x) \langle x|x'\rangle
\end{aligned} \tag{13}$$

Finally the hamiltonian equation become,

$$\langle x| \hat{H} |x'\rangle = \frac{1}{2\pi} [\int_{-\infty}^{+\infty} (\exp^{ik(x-x')} T_x) dk] + V(x) \langle x|x'\rangle \tag{14}$$

Now, for solving the equation (15), the continuous range of coordinate values x is replaced by discrete grid value x_i.
x_i = iΔx, where i = no. of grid and Δx = uniform spacing between the grids.
From the normalization for continuous range one can write,

$$\int_{-\infty}^{+\infty} \psi^*(x)\psi(x) dx = 1 \tag{15}$$

So, in discrete grid system equation (16) become,

$$\sum_{i=1}^{N} \psi^*(x)\psi(x)\Delta x = 1 \tag{16}$$

If the uniform spacing between the grids is Δx and i goes from 1 to N, then the total length will be NΔx and the largest wavelength (λ_{max}) is fitted inside this length, means,

$$\lambda_{max} = N\Delta x \tag{17}$$

So, the frequency will be the reciprocal of λ_{max}. Means, for the grid system of momentum space, the uniform spacing between the momentum grids will be the reciprocal of total length.

$$\Delta k = \frac{2\pi}{\lambda_{max}} \tag{18}$$

$$\Delta k = \frac{2\pi}{N\Delta x} \tag{19}$$

The Fourier transform decomposes any wavefunction into plane waves (e.g., ψ(x) = $\sum_j c_j$ e^{ik_jx}). A positive k means oscillation to the right (increasing phase with x) and a negative k means oscillation to left (decreasing phase with x). So for the full wave, the final boundary vales (negative to positive) should be considered. Here, the central point in the momentum space grid is taken as k=0, and the grid points are evenly distributed about zero. So, the relation between highest number of grid in coordinate space (N) and momentum space (n) will be,

$$2n = (N-1) \tag{20}$$

Here, N is odd no. of grid and the total no. of momentum grid will be l, where l goes from -n to +n.

For the grid system, equation (9) becomes,

$$\hat{I}_k = \sum_{l=-n}^{n} |k_i\rangle \, \Delta k \, \langle k_i| \tag{21}$$

And the orthogonality becomes,

$$\Delta x \, \langle x_i|x_j\rangle = \delta_{ij} \tag{22}$$

and

$$T_l = \frac{\hbar^2}{2m}(l\Delta k)^2 \tag{23}$$

So, equation (15) becomes,

$$
\begin{aligned}
\hat{H}_{ij} &= \langle x_i|\,\hat{H}\,|x_j\rangle \\
&= \frac{1}{2\pi}[\sum_{l=-n}^{n}(\exp^{il\Delta k(x_i-x_j)}\ \frac{\hbar^2}{2m}(l\Delta k)^2)\Delta k] + \frac{V(x_i)\delta_{ij}}{\Delta x}, from(23) \\
&= \frac{1}{2\pi}\Delta k[\sum_{l=-n}^{n}(\exp^{il\frac{2\pi}{N\Delta x}(i-j)\Delta x}\ \frac{\hbar^2}{2m}(l\Delta k)^2)] + \frac{V(x_i)\delta_{ij}}{\Delta x}, from(20) \\
&= \frac{1}{2\pi}\frac{2\pi}{N\Delta x}[\sum_{l=-n}^{n}(\exp^{\frac{il2\pi(i-j)}{N}}\ \frac{\hbar^2}{2m}(l\Delta k)^2)] + \frac{V(x_i)\delta_{ij}}{\Delta x}, from(20) \\
&= \frac{1}{\Delta x}[\sum_{l=-n}^{n}(\frac{1}{N}\exp^{\frac{il2\pi(i-j)}{N}}\ \frac{\hbar^2}{2m}(l\Delta k)^2) + V(x_i)\delta_{ij}]
\end{aligned} \tag{24}
$$

using Euler formula (2cos(x) = $\exp^{ix}$ - $\exp^{-ix}$), one can write,

$$
\hat{H}_{ij} = \frac{1}{\Delta x}[\sum_{l=1}^{n}(\frac{1}{N}2cos(\frac{l2\pi(i-j)}{N})\frac{\hbar^2}{2m}(l\Delta k)^2) + V(x_i)\delta_{ij}] \tag{25}
$$

So, upon renormalized the Hamiltonian matrix, equation (26) becomes,

$$
\hat{H}^0_{ij} = \frac{2}{N}\sum_{l=1}^{n}(cos(\frac{l2\pi(i-j)}{N})\frac{\hbar^2}{2m}(l\Delta k)^2) + V(x_i)\delta_{ij} \tag{26}
$$

And this Hamiltonian form of equation (27) will be used further to solve the 1D Schrodinger equation.

[**For more details:** *J. Chem. Phys.* (1989) **91**:3571-3576]