Fourier Quadrature

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I. INTRODUCTION

The purpose of this write-up is to gain insight into Fourier quadrature, Fourier expansions and the rectangular integration method. We should find that Fourier quadrature points are equivalent to a uniform mesh, rectangular integration is identical to Fourier quadrature, and the leading coefficient in a Fourier expansion of a function has the exact same value as the integral of the function obtained with rectangular integration or Fourier quadrature.

II. BACKGROUND

This write-up was motivated by special points methods found in the literature of Brillouin zone integration. In plane-wave DFT codes, such as VASP [1–4] the band energy is calculated by numerical integration. Since evaluating the electron energy states, the multivalued function being integrated, is computationally expensive, one typically wants the greatest accuracy with the lowest number of sampling points possible. For this purpose were special point methods created, such as the mean value point[5], Chadi and Cohen points[6], and Monkhorst-Pack points[7].

As Froyen points out, all of these methods for calculating sampling points fall under the umbrella of Fourier quadrature[8]. In fact, each method generates a uniform grid. Today sampling points generated from the Monkhorst-Pack scheme are among the most popular in DFT calculations.

III. FOURIER QUADRATURE POINTS

In order to gain a better understanding of special point methods or Fourier quadrature, I'll first show that Fourier quadrature is the same as rectangular integration. Derivations will be performed in 1D but the results should generalize to higher dimensions.

We begin by expanding a function $f(x)$

$$f(x) \approx \sum_{i=0}^{N-1} a_i b_i(x) \tag{1}$$

where N is the number of basis functions kept in the expansion, a_i are expansion coefficients, and $b_i(x)$ are the basis functions. Next we sample our function on a mesh $\{x_0, x_1, \ldots, x_{N-1}\}$

to obtain the system of equations

$$f(x_j) \approx \sum_{i=0}^{N-1} a_i b_i(x_j), \quad \text{for } j = 0, 1, 2, \ldots, N-1. \tag{2}$$

These can be written in matrix form as $\mathbf{f} = B\mathbf{A}$ where

$$\mathbf{f} = \begin{pmatrix} f(x_0) \\ f(x_1) \\ \vdots \\ f(x_{N-1}) \end{pmatrix}, \tag{3}$$

$$B = \begin{pmatrix} b_0(x_0) & b_1(x_0) & \cdots & b_{N-1}(x_0) \\ b_0(x_1) & b_1(x_1) & \cdots & b_{N-1}(x_1) \\ & \vdots & & \\ b_0(x_{N-1}) & b_1(x_{N-1}) & \cdots & b_{N-1}(x_{N-1}) \end{pmatrix}, \tag{4}$$

and

$$\mathbf{a} = \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{N-1} \end{pmatrix} \tag{5}$$

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