Fourier grid Hamiltonian method and Lagrange-mesh calculations

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Bound state eigenvalues and eigenfunctions of a Schrödinger equation or a spinless Salpeter equation can be simply and accurately computed by the Fourier grid Hamiltonian (FGH) method. It requires only the evaluation of the potential at equally spaced grid points, and yields the eigenfunctions at the same grid points. The Lagrange-mesh (LM) method is another simple procedure to solve a Schrödinger equation on a mesh. It is shown that the FGH method is a special case of a LM calculation in which the kinetic energy operator is treated by a discrete Fourier transformation. This gives a firm basis for the FGH method and makes possible the evaluation of the eigenfunctions obtained with this method at any arbitrary values.

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I. INTRODUCTION

The Fourier grid Hamiltonian (FGH) method [1,2] is a very accurate and simple procedure to compute eigenvalues and eigenfunctions of a Schrödinger equation. This method requires only the evaluation of the potential at equally spaced grid points, and yields directly the amplitude of the eigenfunctions at the same grid points. It relies on the fact that the kinetic energy operator is best represented in momentum space, while the potential energy is generally given in coordinate space. This method has been generalized to treat semirelativistic operators in the three-dimensional space for bound states [3]. The accuracy of the method depends on the number of grid points and on the maximal radial distance considered to integrate the eigenvalue equation. An ansatz to evaluate at best this last parameter is given in Ref. [3]. The FGH method has also been applied to the study of scattering equations [4].

The Lagrange-mesh (LM) method is another simple procedure to solve with a great precision a Schrödinger equation on a mesh [5]. Actually, trial eigenstates are developed in a basis of well chosen functions and Hamiltonian matrix elements are obtained with a Gauss approximate quadrature. No numerical evaluation of matrix elements is required, only the computation of the potential at grid points. With this method, the spacings between grid points depend on the basis chosen and are not necessarily equal. As a consequence, a Schrödinger equation can be solved with the same accuracy with fewer points in the LM method than in the FGH method. The LM method can be extended to treat three-body systems very accurately [6] as well in nuclear physics as in atomic physics. Recently, a general procedure for deriving an infinity of new Lagrange meshes related to orthogonal or nonorthogonal bases has been developed [7].

In this paper, it is shown that the FGH method is equivalent to a LM calculation in which the matrix elements of the kinetic energy operator are computed by a discrete Fourier transformation. This makes possible the computation of bound states for semirelativistic kinematics. The FGH method can then be reinterpreted in terms of firm theoretical bases. As a result, it appears that this method is not fully variational but that the eigenfunctions stemming from FGH computations can be obtained at arbitrary values and not only at grid points. It is worth noting that both FGH and LM techniques can be applied if the potential is nonlocal, or if couplings exist between different channels.

The connection between the FGH method and the LM method for one-dimensional problems is outlined in Sec. II, while the three-dimensional case is treated in Sec. III. A brief summary is given in Sec. IV.

II. ONE-DIMENSIONAL FGH METHOD

Within the one-dimensional FGH method, the eigenfunctions are assumed to be defined within a finite range of values [1]. So we will present the main ingredients of the LM method on a finite domain of values. Let us assume the existence of a set of M dimensionless functions $g_i(y)$ and M values y_i in the range [0,1] such that

$$g_i(y_j)=\delta_{ij}\,,\qquad \int_0^1 g_i^*(y)g_j(y)dy=\lambda_i\delta_{ij}\,. \tag{1}$$

With these functions, we can build M new functions $f_i(x)$ depending on the dimensioned variable x on the interval $[a,b]$,

$$f_i(x)=g_i\left(\frac{x-a}{h}\right)\quad \text{with}\quad h=b-a\quad \text{and}\quad x=hy+a. \tag{2}$$

These functions $f_i(x)$ have then the following properties:

$$f_i(x_j)=\delta_{ij}\,,\qquad \int_a^b f_i^*(x)f_j(x)dx=h\lambda_i\delta_{ij}\,. \tag{3}$$

With the numbers $\{\lambda_i\}$ and $\{x_i\}$, we can define an approximate Gauss quadrature formula

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$$\int_a^b F(x)dx \approx h\sum_{i=1}^{M} \lambda_i F(x_i). \tag{4}$$

With the properties (3), one verifies that Eq. (4) is exact for any product $f_i^* f_j$.

Now, let us introduce a set of trial basis states $|f_i\rangle$ whose representation in the position variable x is given by

$$\langle x|f_i\rangle = f_i(x), \tag{5}$$

the identity operator $\mathbb{1}_{[a,b]}$ on the interval $[a,b]$ being written

$$\mathbb{1}_{[a,b]} = \int_a^b |x\rangle dx\langle x|. \tag{6}$$

The orthogonality properties of these basis states are

$$\langle f_j|f_i\rangle = \int_a^b \langle f_j|x\rangle\langle x|f_i\rangle dx = \int_a^b f_j^*(x) f_i(x)dx = h\lambda_i \delta_{ij}. \tag{7}$$

A trial state $|\phi\rangle$ can be developed within this basis,

$$|\phi\rangle = \sum_{i=1}^{M} c_i |f_i\rangle. \tag{8}$$

From Eqs. (3), it follows immediately that $c_i = \phi(x_i)$ with $\phi(x) = \langle x|\phi\rangle$.

We can now search for a variational solution of an eigenvalue equation. In the restricted space of trial states, the closure relation is written

$$|\phi\rangle = \left[\sum_{i=1}^{M} |f_i\rangle \frac{1}{h\lambda_i}\langle f_i|\right]|\phi\rangle. \tag{9}$$

The eigenvalue equation for a Hamiltonian H is then given by

$$\sum_{j=1}^{M} H_{ij}\sqrt{\lambda_j}\phi(x_j) = E\sqrt{\lambda_i}\phi(x_i) \quad \text{with} \quad H_{ij} = \frac{\langle f_i|H|f_j\rangle}{h\sqrt{\lambda_i\lambda_j}}, \tag{10}$$

where E is an upper bound of an eigenvalue of H. We can see that the M components of the eigenvector are directly the values of the trial states at the M mesh points $\{x_i\}$.

Let us consider a general Hamiltonian H with a kinetic part T, a local potential V, and a nonlocal interaction W,

$$\langle x'|H|x\rangle = T(x,x') + V(x)\delta(x-x') + W(x,x'). \tag{11}$$

In the following, we will work with natural units ($\hbar = c = 1$). The matrix elements of the potentials are very easy to compute within the approximate quadrature rule (4). One finds

$$\begin{aligned} V_{ij} &= V(x_i)\delta_{ij}, \\ W_{ij} &= h\sqrt{\lambda_i\lambda_j}W(x_i,x_j). \end{aligned} \tag{12}$$

It is necessary to compute the potential only at the mesh points. It is worth noting that, when matrix elements (12) are used, the variational character of the method cannot be guaranteed. This is only possible if an exact quadrature is performed. In practice, for a sufficiently high number of basis states, the method is often variational. But this is not always the case. We will show an example below.

If the kinetic operator is the nonrelativistic one, then its matrix elements can easily be obtained [5],

$$T(x',x) = C\,\delta(x-x')\frac{d^2}{dx^2} \quad \Rightarrow \quad T_{ij} = C\sqrt{\frac{\lambda_j}{\lambda_i}}f_i''(x_j). \tag{13}$$

Note that the Hamiltonian matrix can be nonsymmetrical.

For semirelativistic systems, the kinetic energy operator has no simple form in the configuration space. It is best represented in the momentum space. As the eigenvalue equation is solved on a finite interval of length h, there exists a minimal possible momentum $\Delta k = 2\pi/h$, and all the values of the momenta are quantified $k_n = n\Delta k$, where n is an integer. Expressed in terms of the eigenstates $|k_n\rangle$ of the square relative impulsion operator $\hat{k}^2$, the identity operator can be written

$$\mathbb{1}_{[a,b]} = \sum_{n=-\infty}^{+\infty} |k_n\rangle \frac{2\pi}{h}\langle k_n|, \tag{14}$$

where the states $|k_n\rangle$ are given in configuration space ($x \in [a,b]$) by

$$\langle x|k_n\rangle = \frac{1}{\sqrt{2\pi}}\exp\left(i\frac{2\pi n}{h}(x-a)\right) \quad \text{with} \quad k_n = \frac{2\pi n}{h}. \tag{15}$$

From Eq. (15), the orthogonality relation of these states is

$$\langle k_m|k_n\rangle = \frac{h}{2\pi}\delta_{mn}. \tag{16}$$

Insertion of expression (14) in the scalar product $\langle x|\psi\rangle$ gives the Fourier decomposition of $\psi(x)$ in the interval $[a,b]$.

The computation of a matrix element of a general kinetic energy operator $T(\hat{k}^2)$ gives

$$\begin{aligned} \langle f_i|T|f_j\rangle = \int_a^b dx \int_a^b dx' \sum_{n=-\infty}^{+\infty}\sum_{m=-\infty}^{+\infty} \left(\frac{2\pi}{h}\right)^2 \langle f_i|x\rangle\langle x|k_n\rangle \\ \times\langle k_n|T|k_m\rangle\langle k_m|x'\rangle\langle x'|f_j\rangle, \end{aligned} \tag{17}$$

in which

$$\langle k_n|T|k_m\rangle = T(k_n^2)\frac{h}{2\pi}\delta_{nm} \quad \text{with} \quad k_n = \frac{2\pi}{h}n. \tag{18}$$

Using relation (5), we obtain

$$\begin{aligned} \langle f_i|T|f_j\rangle = \frac{1}{h}\int_a^b dx \int_a^b dx' f_i^*(x) f_j(x') \\ \times \sum_{n=-\infty}^{+\infty} \exp\left(i\frac{2\pi n}{h}(x-x')\right) T(k_n^2). \end{aligned} \tag{19}$$

Now we replace the integrations on position variables by the approximate quadrature formula (4). But in this case the variables x and x' cannot be arbitrarily close to each other, since there is always a finite spacing between two mesh points. This implies that the momentum cannot be arbitrarily large. Consequently, we cut the infinite sum on momenta and consider only momenta below $K\Delta k$. We will compute the value of K below. This procedure gives

$$\langle f_i|T|f_j\rangle \approx \frac{1}{h}\sum_{r=1}^{M}\sum_{s=1}^{M} h^2\lambda_r\lambda_s f_i^*(x_r)f_j(x_s) \times \sum_{n=-K}^{K}\exp\left(i\frac{2\pi n}{h}(x_r-x_s)\right)T(k_n^2). \quad (20)$$

Finally, we obtain the real matrix elements

$$T_{ij}=\frac{\langle f_i|T|f_j\rangle}{h\sqrt{\lambda_i\lambda_j}}=\sqrt{\lambda_i\lambda_j}\left[\sum_{n=1}^{K}2\cos\left(\frac{2\pi n}{h}(x_i-x_j)\right)\times T(k_n^2)+T(0)\right]. \quad (21)$$

To compute the value of K, we replace the kinetic energy operator T by the identity operator. The expression (21) must then reduce to

$$\delta_{ij}=\sqrt{\lambda_i\lambda_j}\left[\sum_{n=1}^{K}2\cos\left(\frac{2\pi n}{h}(x_i-x_j)\right)+1\right]. \quad (22)$$

In particular, for $i=j$, we must verify the equality

$$1=\lambda_i(2K+1). \quad (23)$$

Consequently, all factors λ_i must be equal. But they are used to define a quadrature rule, approximate for arbitrary functions and exact for the basis functions $f_i(x)$. Moreover, for physical problems, one can expect that these basis functions vanish at both boundaries of the interval $[a,b]$ in order to match the asymptotic behavior of a real eigenfunction. The simple way to satisfy all these conditions is to use the second sine basis functions defined in Ref. [8]. They are given in the appendix.

With the $N-1$ basis functions (A1), $\lambda_i=1/N$, $K=(N-1)/2$, and $y_i=i/N$, Eq. (21) is then written

$$\delta_{ij}=\frac{1}{N}\left[\sum_{n=1}^{(N-1)/2}2\cos\left(\frac{2\pi n}{N}(i-j)\right)+1\right], \quad (24)$$

which is a well-known identity. A matrix element of the kinetic energy operator $T(\hat{k}^2)$ is then

$$T_{ij}=\frac{1}{N}\left[\sum_{n=1}^{(N-1)/2}2\cos\left(\frac{2\pi n}{N}(i-j)\right)T(k_n^2)+T(0)\right] \quad \text{with} \quad i,j=1,\ldots,N-1. \quad (25)$$

This is exactly the expression obtained in Ref. [1] adapted for a more general operator than the nonrelativistic one. Let us remark that $T_{ij}=T_{ji}$.

III. THREE-DIMENSIONAL FGH METHOD

In the following, we will assume that a wave function $|\Psi\rangle$ can be decomposed into its central and orbital parts,

$$\langle r,\hat{r}|\Psi\rangle=R_l(r)Y_{l,m}(\hat{r}) \quad \text{with} \quad \hat{r}=\vec{r}/r. \quad (26)$$

Within the three-dimensional FGH method, it is assumed that the regularized radial part of the wave function $u_l(r)=rR_l(r)$ vanishes at the origin and at a distance R sufficiently large. An ansatz to evaluate at best this distance is given in Ref. [3]. As the wave function exists in a ball of radius R, we will consider the identity operator $\mathbb{1}_{B_R}$ for this domain,

$$\mathbb{1}_{B_R}=\int_0^R r^2dr\int_S d\hat{r}|r,\hat{r}\rangle\langle r,\hat{r}|. \quad (27)$$

Expressed in term of states $|k_n,\lambda,\nu\rangle$ characterized by good orbital quantum numbers (λ,ν), and eigenstates of the square relative impulsion operator $\hat{k}^2$, the identity operator is written

$$\mathbb{1}_{B_R}=\sum_{n=1}^{\infty}\sum_{\lambda=0}^{\infty}\sum_{\nu=-\lambda}^{\lambda}|k_n,\lambda,\nu\rangle\langle k_n,\lambda,\nu|. \quad (28)$$

The representation of these states in the configuration space $(r\in[0,R])$ is given by

$$\langle r,\hat{r}|k_n,\lambda,\nu\rangle=\sqrt{\frac{2}{[j_{\lambda+1}(q_n)]^2R^3}}j_\lambda\left(q_n\frac{r}{R}\right)Y_{\lambda,\nu}(\hat{r}) \quad \text{with} \quad k_n=\frac{q_n}{R}, \quad (29)$$

where j_μ is a spherical Bessel function and q_n is a positive zero of this function. The orthogonality properties of these states come from the following relation [9]:

$$\int_0^1 xJ_{\lambda+1/2}(q_mx)J_{\lambda+1/2}(q_nx)dx=\delta_{nm}\frac{1}{2}[J'_{\lambda+1/2}(q_n)]^2, \quad (30)$$

where J_μ is a Bessel function of the first kind (a positive zero of j_μ is also a positive zero of $J_{\mu+1/2}$).

The basis for the LM method can be built with the functions f_i defined in the previous section. In the three-dimensional space, the basis states are then given by

$$\langle\vec{r}|f_i\rangle=\frac{f_i(r)}{r}Y_{l,m}(\hat{r}) \quad \text{with} \quad r\in[0,R]. \quad (31)$$

With the previous notations, we take $a=0$ and $b=h=R$. The computation of potential (local or nonlocal) matrix elements does not differ from the one-dimensional case and gives the result (12) (in which x_i must be replaced by r_i, and

h by R). Let us focus on the calculation of the matrix element of a general kinetic energy operator $T(\hat{k}^2)$,

$$\langle f_i|T|f_j\rangle = \int d\vec{r}' \int d\vec{r} \sum_{\{n',\lambda',\nu'\}} \sum_{\{n,\lambda,\nu\}} \langle f_i|\vec{r}'\rangle\langle\vec{r}'|k_{n'},\lambda',\nu'\rangle \times\langle k_{n'},\lambda',\nu'|T|k_n,\lambda,\nu\rangle\langle k_n,\lambda,\nu|\vec{r}\rangle\langle\vec{r}|f_j\rangle. \quad (32)$$

Since we have

$$\langle k_{n'},\lambda',\nu'|T|k_n,\lambda,\nu\rangle = T(k_n^2)\delta_{nn'}\delta_{\lambda\lambda'}\delta_{\nu\nu'} \quad \text{with} \quad k_n=\frac{q_n}{R}, \quad (33)$$

the matrix element (32) can be written

$$\langle f_i|T|f_j\rangle = \int_0^R dr \int_0^R dr' rr' f_i(r') f_j(r) T(r,r'), \quad (34)$$

in which

$$T(r,r') = \frac{2}{R^3}\sum_{n=1}^{\infty} \frac{1}{[j_{l+1}(q_n)]^2} j_l\left(q_n\frac{r'}{R}\right) j_l\left(q_n\frac{r}{R}\right) T\left(\frac{q_n^2}{R^2}\right). \quad (35)$$

Now we replace the integrations on radial variables by the approximate quadrature formula (4). As in the one-dimensional case, the variables r and r' cannot be arbitrarily close to each other, since there is always a finite spacing between two mesh points. This implies that the momentum cannot be arbitrarily large and that we have to cut the infinite summation on momenta. This procedure gives

$$T_{ij} = \frac{\langle f_i|T|f_j\rangle}{R\sqrt{\lambda_i\lambda_j}} \approx R\sqrt{\lambda_i\lambda_j} r_i r_j T(r_i,r_j). \quad (36)$$

To find where to cut the infinite summation in $T(r_i,r_j)$, we replace the kinetic energy operator by the identity. In this case the matrix element (36) must reduce to

$$\delta_{ij} = 2\sqrt{\lambda_i\lambda_j} y_i y_j \sum_{n=1}^{K} \frac{1}{[j_{l+1}(q_n)]^2} j_l(q_n y_i) j_l(q_n y_j) \quad \text{with} \quad y_i \in [0,1]. \quad (37)$$

To simplify more, let us consider the case $l=0$, for which $q_n = n\pi$ and $[j_1(n\pi)]^2 = 1/(n\pi)^2$. Equation (37) is then written

$$\delta_{ij} = 2\pi^2\sqrt{\lambda_i\lambda_j} y_i y_j \sum_{n=1}^{K} n^2 j_0(n\pi y_i) j_0(n\pi y_j). \quad (38)$$

This equation is true [see Eq. (A1) of Ref. [3]] if we have $\lambda_i = 1/N$, $K = N-1$ or N, and $y_i = i/N$, that is to say, if the f_i functions are built with the sine basis functions used in the previous section [the term $n=N$ in the summation has a vanishing contribution since $j_0(i\pi)=0$].

With this choice of Lagrange functions, Eq. (37) is written

TABLE I. Error on δ_{ij} for formula (39) as a function of N and K in the case $l=1$.

N	K	i	j	Error on δ_{ij}	i	j	Error on δ_{ij}
100	N	1	1	0.020	1	2	0.020
		50	50	0.0099	50	51	0.0097
	$N-1$	1	1	3.6×10^{-6}	1	2	3.6×10^{-6}
		50	50	2.9×10^{-6}	1	2	2.9×10^{-6}
10	$N-1$	1	1	3.6×10^{-4}	1	2	3.5×10^{-4}
100		1	1	3.6×10^{-6}	1	2	3.6×10^{-6}
1000		1	1	3.6×10^{-8}	1	2	3.6×10^{-8}

$$\delta_{ij} \approx \frac{2}{N^3} ij \sum_{n=1}^{K} \frac{1}{[j_{l+1}(q_n)]^2} j_l\left(q_n\frac{i}{N}\right) j_l\left(q_n\frac{j}{N}\right). \quad (39)$$

An exact equality occurs only in the case $l=0$ with $K=N-1$ or N. For $l=1$, a strict equality is no longer possible. We have numerically verified that it is preferable to take $K=N-1$ instead of N or any other values, and that the equality (39) is true in the limit $N\to\infty$ (see Table I). For $l\geqslant 2$, the situation is similar but formula (39) cannot be satisfied for small values of i and j, even for large values of N. Consequently, the accuracy of this method becomes poorer when l increases; nevertheless, for large enough number of grid points, very good results can be obtained. Finally, the matrix elements of the kinetic energy operator are given by

$$T_{ij} = \frac{2}{N^3} ij \sum_{n=1}^{N-1} \frac{1}{[j_{l+1}(q_n)]^2} j_l\left(q_n\frac{i}{N}\right) j_l\left(q_n\frac{j}{N}\right) T\left(\frac{q_n^2}{R^2}\right) \quad \text{with} \quad i,j=1,\ldots,N-1. \quad (40)$$

Actually, Eq. (40) is equivalent to Eq. (18) of Ref. [3] only when $l=0$. Indeed, for $l\neq 0$, we have $q_n \neq n\pi$ and $1/[j_{l+1}(n\pi)]^2 \neq (n\pi)^2$. In Ref. [3], the discretization of the eigenvalue equation was performed on the basis of physical arguments, which led to a form different from the one found here. Surprisingly, the results from the two forms are not very different. In Table II, binding energies of two hydrogen atom states obtained with Eq. (40) are compared with the ones obtained with Eq. (18) of Ref. [3]. Differences between values given by both equations are small with respect to the gaps from the exact value. These differences tend to vanish when the number of points increases. As there is no analytical form known for the zeros of spherical Bessel functions, it is preferable to use the simplest form of Ref. [3]. With Table II, it can be seen that the exact values can be reached from above ($l=2$) or from below ($l=1$), which clearly shows that the method is not variational.

It could be interesting to have an estimation of the convergence speed of eigenvalues as a function of the number of grid points. Unfortunately, this speed depends strongly on the potential. For instance, 50 grid points are sufficient to obtain five exact digits for the ground state of a Schrödinger equation with a linear potential. The same accuracy is obtained with about 1000 grid points for the Coulomb potential. Some extrapolation methods to compute an estimation of the exact eigenvalues knowing some successive approxi-

TABLE II. Binding energies in eV for the P and D ground states of the hydrogen atom calculated with the FGH method, as a function of the number N of mesh intervals, using formula (40) or formula (18) of Ref. [3]. The exact binding energy is the value obtained with the analytical expression for the energy with the parameters of the Hamiltonian used.

l	N	Formula (40)	Ref. [3]
1	25	−3.4056204	−3.4062227
	50	−3.4003916	−3.4004032
	100	−3.3996396	−3.3996398
	200	−3.3995777	−3.3995777
	Exact	−3.3995731	
2	25	−1.5029362	−1.5030474
	50	−1.5107195	−1.5107219
	100	−1.5109177	−1.5109177
	200	−1.5109213	−1.5109213
	Exact	−1.5109214	

mations have been tested (see Ref. [10] for instance). But they cannot give reliable results. A good procedure to reach a high precision is to calculate the optimal value of the integration radius R with a small number of grid points. Then, with R fixed, the number of grid points can be increased until the required accuracy is reached. It is worth noting that the calculation time increases, in good approximation, with the cube of the numbers of grid points.

IV. CONCLUDING REMARKS

In this paper, we have shown that the Fourier grid Hamiltonian method is equivalent to a Lagrange-mesh calculation in which the matrix elements of the kinetic energy operator are computed by a discrete Fourier transformation. Consequently, any kinetic energy operator that depends only on the square relative impulsion can be considered. Moreover, the Hamiltonian matrix is always symmetrical, which makes diagonalizations easier.

The FGH method is reinterpreted in terms of firm theoretical bases. As a first result, it appears that this method is not fully variational. Secondly, the eigenfunctions stemming from FGH computations can be obtained in an analytical form and not only as a set of values at grid points, since each eigenvector can be considered as the set of coefficients of an expansion in a basis. Any operation on the eigenfunctions (derivation, integration) can then be performed more reliably.

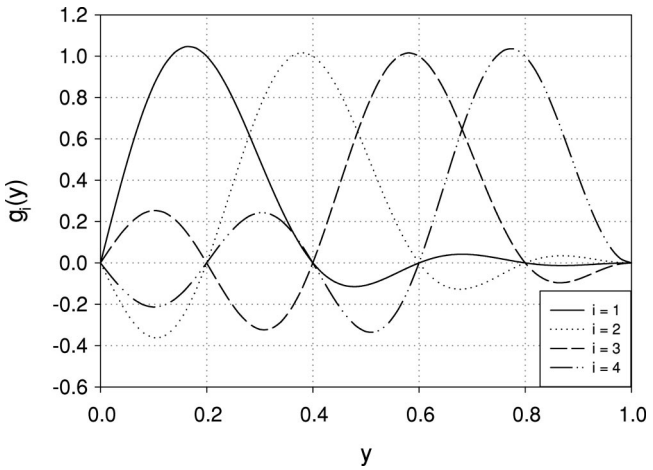

FIG. 1. The four sine basis functions (A1) for $N=5$ are given between 0 and 1.

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APPENDIX: SINE BASIS

The $N-1$ basis functions $f_i(x)$ suitable for the FGH method are built with the $N-1$ dimensionless functions $g_i(y)$ defined on the interval [0,1] by the following relation [8]:

$$g_i(y)=\frac{1}{2N}\left[\frac{\sin N\pi(y-y_i)}{\sin(\pi/2)(y-y_i)}-\frac{\sin N\pi(y+y_i)}{\sin(\pi/2)(y+y_i)}\right]. \tag{A1}$$

They satisfy conditions (1) with

$$\lambda_i=\frac{1}{N} \quad \text{and} \quad y_i=\frac{i}{N} \quad \text{for} \quad i=1,\ldots,N-1. \tag{A2}$$

Their boundary values are

$$g_i(0)=g_i(1)=0 \quad \Rightarrow \quad f_i(a)=f_i(b)=0 \quad \text{for} \quad i=1,\ldots,N-1. \tag{A3}$$

The four functions $g_i(y)$ are represented in Fig. 1 in the case $N=5$.

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