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On the accuracy of wavefunctions obtained by the Fourier grid Hamiltonian method

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Abstract. The quality of wavefunctions obtained by the Fourier grid Hamiltonian (FGH) method is analyzed. The criteria used for judging the quality are the extent to which virial, hypervirial and Hellmann-Feynman theorems are satisfied by the numerically computed FGH-wavefunction. The quality of the FGH-wavefunction is also examined from the point of view of local error in the wavefunction. It is shown that high quality wavefunctions can be obtained from the FGH recipe if the grid length (L) and grid spacings are chosen after properly examining the range of the potential and its nature.

Keywords. Fourier grid Hamiltonian (FGH); discrete variable representation; accurate quantum mechanical methods for bound states; accuracy of FGH wavefunction; Fourier transform methods.

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1. Introduction

The Fourier transform method [1–2] has emerged as a very powerful tool in solving both time-dependent and time-independent quantum mechanical problems. The idea has been to use different representations to treat the kinetic and potential energy terms in evaluating the quantity $H\psi$ which is central to the time propagation, and use fast Fourier transform technique to move back and forth from one representation to the other. In a couple of recent papers, Marston and Balint-Kurti [3–4] have beautifully demonstrated that the matrix representation of the Hamiltonian ($\hat{H}$) in the vector space generated by the values of ψ and $H\psi$ on a grid of points in the coordinate space is extremely simple, requiring only the evaluation of the potential at the grid points and applications of forward and inverse Fourier transforms which analytically reduce to a finite sum over cosine functions. Once the H matrix is formed in this space, straightforward diagonalization of the Hamiltonian matrix (H matrix is symmetric in this representation as opposed to the unsymmetric H matrix encountered in the collocation method [5]), provides the bound state eigenvalues, the eigenvectors directly providing the amplitudes of the eigenfunctions of H on the grid points chosen. It may be noted that the Fourier grid Hamiltonian (FGH) method as Marston and Balint-Kurti calls it, is variational in the same sense as most other methods for calculating eigenvalues and eigenfunctions of Hamiltonian operator. In fact the FGH method is a special case of the socalled discrete variable representation (DVR) method extensively developed by Light *et al* [6–7], following

the earlier work of Harris *et al* [8]. DVR has been shown to be related to the gaussian quadrature method by Dickinson and Certain [9]. Viewed from a variational point of view, the FGH method works with two crucial parameters, the grid length (L) and grid density (N/L). It is therefore important to understand how the choice of these parameters affect the accuracy of the FGH eigenfunctions and eigenvalues. Marston and Balint-Kurti [3] showed that the FGH-wavefunction for a Morse oscillator nicely coincides with the corresponding analytical solution at the grid points and that the convergence of eigenvalues with respect to the number of grid points is fast. The level of accuracy of FGH wavefunctions is of paramount importance since energy eigenvalues are always estimated one order better than the corresponding eigenfunctions. How does one check the accuracy of the computed eigenfunctions which directly affects values of other non-commuting observables? One obvious solution is to compare the FGH-wavefunction with the corresponding exact wavefunction, if known. But the FGH method is expected to be of value in cases where analytical solutions are not easily obtained or are unavailable. An alternative strategy therefore would be to check whether FGH wavefunctions obey certain theorems which the exact wavefunctions would satisfy; for example, we may think of virial and hypervirial theorems, Hellmann-Feynman theorem, Frost's local energy criterion, etc.

It may be noted in this context that the DVR is isomorphic with an approximate finite basis set representation in which some matrix elements of the Hamiltonian are determined by numerical quadrature over the DVR points. Light *et al* [6] have shown that in one dimensional problems DVR may be truncated just as in the finite basis set representation with comparable loss of accuracy in the eigenvalues. However, impact of truncation on the quality of the eigenfunctions and other non-commuting observables was not analyzed. The present paper focuses on this central question; how does the truncation affect the quality of the FGH wavefunctions? The yardstick for quality of ψ employed by us is conformability of FGH-wavefunction with certain theorems obeyed by exact wavefunctions. The analysis has special significance in the context of many dimensional extension of the FGH method [10] which leads to a rapid escalation of the dimensionality of the space in which the Hamiltonian has to be diagonalized. Alternatively, some mean-field approximations must be used. Truncation is thus inevitable in multidimensional problems. One must therefore know in advance the impact of truncation on the FGH-wavefunction at least in one-dimensional problems where the parameters of crucial importance as noted already, are the grid length and grid spacing. In what follows we attempt to achieve this objective.

2. Results and discussion

i) *FGH-wavefunction and virial theorem*

Although satisfaction of the virial theorem does not guarantee the exactness of the wave function, it is a necessary condition that accurate wavefunctions obey the virial theorem [11]. To investigate the extent to which the FGH-wavefunction conforms to this necessary condition we have solved the one-dimensional Schrödinger equation for i) harmonic and ii) quartic anharmonic oscillators by the FGH method. The wavefunctions thus obtained for different bound states have been used to calculate the expectation values required to compute the virial ratio. The vth eigenstate of the

oscillator $|\psi_v\rangle$ obtained by FGH method is represented as follows:

$$|\psi_v\rangle = \sum_{i=1}^{N} \omega_i^v \Delta x |x_i\rangle \tag{1}$$

where, N is the number of grid points, ω_i^vs are the values of the vth bound state wavefunction at the grid points. The expectation value of a quantum mechanical operator A corresponding to the normalized state function $|\psi\rangle$ is

$$\langle A\rangle_\psi = \langle\psi|\hat{A}|\psi\rangle/\langle\psi|\psi\rangle = \sum_{ij} \omega_i^* \omega_j A_{ij} \Big/ \sum_i |\omega_i|^2 \tag{2}$$

where

$$A_{ij} = \langle x_i|\hat{A}|x_j\rangle.$$

Virial theorem for a potential V which is homogeneous in coordinate x_i and of degree n leads to the equation

$$2\langle T\rangle = \langle \Sigma x_i \partial V/\partial x_i\rangle = n\langle V\rangle \tag{3}$$

where $\langle T\rangle$ and $\langle V\rangle$ are the expectation values corresponding to kinetic and potential energy operators, respectively. The virial equation for a harmonic oscillator potential $[V(x) = (1/2)kx^2]$ therefore takes the form

$$2\langle T\rangle_v = 2\langle V\rangle_v \quad \text{or} \quad \langle T\rangle_v/\langle V\rangle_v - 1 = 0. \tag{4}$$

For an anharmonic quartic potential $[V(x) = (1/2)kx^2 + \lambda x^4]$ the corresponding virial equation is as follows:

$$2\langle T\rangle = \langle x\partial V/\partial x\rangle = 2\langle V\rangle + 2\lambda\langle x^4\rangle \quad \text{i.e.}$$

$$\langle T\rangle_v = \langle V\rangle_v + \lambda\langle x^4\rangle_v. \tag{5}$$

Table 1. Required expectation values have been calculated using the FGH wavefunctions for the first few vibrational states of a harmonic and quartic oscillator to demonstrate that the FGH wavefunctions satisfy virial theorem.

	Harmonic oscillator*	Quartic oscillator#	
v	$[\langle T\rangle/\langle V\rangle - 1]_v$	$\langle T\rangle_v$	$[\langle V\rangle + \lambda\langle x^4\rangle]_v$
0	0·000 000 00	0·253 656 42	0·253 656 42
1	0·000 000 00	0·768 032 06	0·768 032 06
2	0·000 000 00	1·296 143 24	1·296 143 24
3	0·000 000 00	1·837 256 76	1·837 256 76
4	0·000 000 00	2·390 725 30	2·390 725 30
5	0·000 000 00	2·955 972 88	2·955 972 88
6	0·000 000 00	3·532 483 48	3·532 483 48
7	0·000 000 00	4·119 791 93	4·119 791 93
8	0·000 000 00	4·717 476 60	4·717 476 60

*see text, eq. (4) #see text, eq. (5)

The angular brackets denote expectation values of the operators in the FGH representation enclosed within [equation 2]. These expectation values [$\langle T\rangle$, $\langle V\rangle$ and $\langle x^4\rangle$] for different bound states have been calculated with the FGH-wavefunction obtained by solving the corresponding Schrödinger equation by the FGH method. The grid length ($L = 13$ a.u) and the number of grid points ($N = 69$) used in our calculations for both the cases were found to be adequate (the appropriate choices of these parameters are discussed in detail in § 3). The results corresponding to (4) and (5) [$\lambda = 0{\cdot}005$] are displayed in table 1 which confirm that the FGH-wavefunction fulfils the necessary condition of complying with the virial theorem when a sufficient number of grid points (N) are taken. The point to note is that N is not large at all. Since the representation used is discrete, scale-optimization and virial satisfaction need not be explored in the present context, as the effect of coordinate scaling can be effectively mimicked by making Δx small enough.

ii) *FGH-wavefunction and Hellmann–Feynman theorem*

The variational version of the Hellmann–Feynman (H–F) theorem [12] is often written as

$$\partial E/\partial\sigma = \langle \partial H/\partial\sigma\rangle \tag{6}$$

where, σ is a real parameter in the Hamiltonian (H) of the system under study. Here, we have dealt with three different types of one-dimensional oscillators.

a) *Harmonic oscillator*: The system of harmonic oscillator is represented by the Hamiltonian H which is a function of the force constant (k) of the oscillator as follows:

$$H(k) = T + (1/2)kx^2.$$

Differentiation of H with respect to k gives,

$$\langle \partial H/\partial k\rangle = (1/2)\langle x^2\rangle. \tag{7}$$

Since the analytical values of energy (E) as well as ($\partial E/\partial k$) as functions of k are available for the harmonic oscillator, one can measure what may be called the "deviation from the HF theorem" ($\delta_{\text{H-F}}$) by comparing the analytical $\partial E/\partial k$ value with that on the right hand side of (7) computed with the FGH-wavefunction for a specific vibrational state. The comparison is made in table 2 for a grid of 69 points. Compliance with HF theorem is easily noticeable.

b) *Quartic oscillator*: The Hamiltonian H representing the anharmonic quartic oscillator is of the form:

$$H(\lambda) = T + (1/2)x^2 + \lambda x^4. \tag{8}$$

Differentiating both sides of (8) with respect to λ we get

$$\langle \partial H/\partial\lambda\rangle = \langle x^4\rangle. \tag{9}$$

The quantity $\langle x^4\rangle$ in (9) has been calculated using the FGH wavefunctions for different bound states obtained by solving the Schrödinger equation for the quartic

Table 2. Results computed with the FGH wavefunctions have been reported to demonstrate the compatibility of the FGH wavefunctions with the Hellmann–Feynman theorem.

	Harmonic*	Quartic#		Morse&	
v	δ_{H-F}	$\langle\partial H/\partial\lambda\rangle_v$	$\langle\partial E/\partial\lambda\rangle_v$	$\langle\partial H/\partial\beta\rangle_v$	$\langle\partial E/\partial\beta\rangle_v$
0	0·000 000 00	0·664 281	0·664 282	0·007 693	0·007 693
1	0·000 000 00	3·131 412	3·131 410	0·022 048	0·022 048
2	0·000 000 00	7·637 511	7·637 502	0·035 026	0·035 026
3	0·000 000 00	13·790 941	13·790 910	0·046 627	0·046 627
4	0·000 000 00	21·331 281	21·331 203	0·056 851	0·056 851

*see text, eq. (7) #see text, eq. (9) &see text, eqs (12, 13).

oscillator by the FGH method using $L = 13$ a.u. and $N = 69$. Since the analytical energy (E) and ($\partial E/\partial\lambda$) values are not available in this case, we have computed ($\partial E/\partial\lambda$), numerically. The close agreement between $\langle\partial H/\partial\lambda\rangle$ obtained from (9) and $\partial E/\partial\lambda$ (obtained numerically) as shown in table 2 again shows that the FGH wavefunctions are quite accurate if L and N are carefully chosen.

c) *Morse oscillator*: In the case of a Morse oscillator the Hamiltonian (H) is a function of the real parameter β as defined below:

$$\hat{H} = \hat{T} + D_e[1 - \exp\{-\beta(\hat{x} - x_{eq})\}]^2. \tag{10}$$

The problem at hand is analytically solvable and the analytical energy eigenvalues are given by

$$E_v = \beta\sqrt{2D_e/\mu}(v + 0{\cdot}5) - (\beta^2/2\mu)(v + 0{\cdot}5)^2 \tag{11}$$

where, D_e is dissociation energy, μ is the reduced mass of the system and β is the non-linear parameter in the potential. Differentiating both sides of (10) with respect to β followed by quantum mechanical averaging over the state (ψ_v) [equation (2)] gives

$$\langle\partial H/\partial\beta\rangle_v = 2D_e\langle(x - x_{eq})[1 - \exp\{-\beta(x - x_{eq})\}][\exp\{-\beta(x - x_{eq})\}]\rangle \tag{12}$$

Differentiation of (11) with respect to β on the other hand gives

$$(\partial E/\partial\beta)_v = [(v + 0{\cdot}5)\sqrt{2D/\mu} - (\beta/\mu)(v + 0{\cdot}5)^2] \tag{13}$$

The computed results displayed in table 2 are the quantities corresponding to (12) and (13) for the first few vibrational states ($v = 0 - 4$) and are just as the exact wavefunctions are supposed to give.

iii) *Hypervirial theorems and FGH eigenfunctions*

If $\hat{A}$ is a hermitian operator such that the set of trial function is invariant under the continuous family of unitary transformations $U(\alpha) = e^{i\alpha A}$ (α real parameter), then a

Table 3. Results computed with the FGH wavefunctions for the first few states of a Morse oscillator [see eq. (14)] have been reported to demonstrate the compatibility of the FGH wavefunctions with the diagonal hypervirial theorem.

v	$\langle e^{-\beta u}\rangle_v$	$\langle e^{-2\beta u}\rangle_v$
0	0·978 2011	0·978 2011
1	0·934 6037	0·934 6037
2	0·891 0072	0·891 0072
3	0·847 4115	0·847 4115
4	0·803 8113	0·803 8113
5	0·760 2138	0·760 2138
6	0·716 6163	0·716 6163
7	0·673 0188	0·673 0188

variationaly selected ψ will satisfy the condition

$$\langle\psi|[\hat{H},\hat{A}]|\psi\rangle = 0$$

for any state ψ. The condition has been known as the diagonal hypervirial theorem [13–14]. The condition is obviously obeyed by an exact wavefunction. For a Morse oscillator $[V(x)]$, one can show [15] that the diagonal hypervirial theorem leads to the following relation:

$$\langle e^{-\beta u} - e^{-2\beta u}\rangle_v = 0$$

i.e.

$$\langle e^{-\beta u}\rangle_v = \langle e^{-2\beta u}\rangle_v \tag{14}$$

where the potential $V(x)$ is represented as follows:

$$V(x) = D[e^{-2\beta u} - 2e^{-\beta u}], \quad u = (x - x_{eq}).$$

We have reported in table 3 the expectation values on the left and right hand side of (14) computed with FGH wavefunctions for the first few states of a Morse oscillator. A reasonable choice of grid ensures compatibility of FGH wavefunctions with the diagonal hypervirial theorem.

iv) *FGH-wavefunctions and local error*

As demonstrated in [3] and to be discussed further in §3, the FGH method with adequate grid length (L) and number of grid points (N) can provide highly accurate value of global energy or energy eigenvalues (E)

$$E = \langle\psi|H|\psi\rangle/\langle\psi|\psi\rangle. \tag{15}$$

But one may ask whether the FGH wavefunctions are equally good from a local point of view. Needless to mention that an exact wavefunction is expected to satisfy

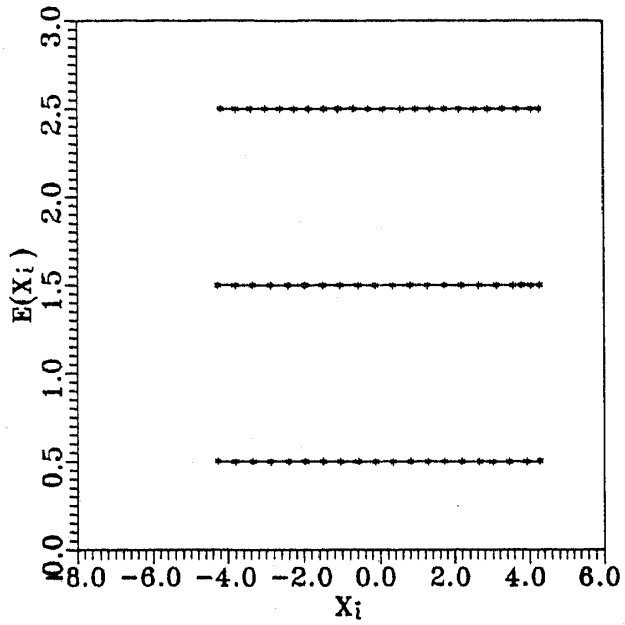

Figure 1. Energy values $E_v(x_i)$ (represented as $***$) at all the grid points $\{x_i\}$ obtained by the FGH method are the same and equal to the corresponding energy eigenvalue (denoted by solid line) [$v = 0, 1$ and 2].

certain local criteria as well [16]. The Schrödinger equation at a coordinate point (x_i) is

$$H\psi(x_i) = E(x_i)\psi(x_i),$$
$$E(x_i) = H\psi(x_i)/\psi(x_i). \tag{16}$$

In general, the local energy $E(x_i)$ in (16) is coordinate dependent for an approximate wavefunction while the exact wavefunction provides local energy values $(E(x_i))$ independent of x_i and equal to the global E of (15). As the eigenvectors obtained by FGH method directly gives the amplitudes or values of the wavefunction at the grid points, the question now turns out to be whether the $E(x_i)$ calculated (eq. 16) at each grid point (x_i) are the same and is equal to the value E in (15)?

To answer this question we have employed the FGH method for a harmonic oscillator and obtained both the energy eigenvalues (E_v) (eq. 15) and the wavefunctions $[\psi_v(x)]$. The $E_v(x_i)$ values at all the grid points $\{x_i\}$ have been calculated by invoking a suitable numerical differentiation scheme to compute the $H[\psi(x_i)]$ part in (16). The results, as is clear from figure 1 which displays the profiles of $E_v(x_i)$ for $v = 0, 1$ and 2 at the grid points $\{x_i\}$, answer the question in the affirmative.

3. Convergence properties

As far as the success of any numerical method for solving Schrödinger equation is concerned, the computational cost that the method involves is no less important than the accuracy of the energy eigenvalues provided by the method. As the method requires matrices of order $(N \times N)$ to be diagonalized, where N is the number of grid points, the convergence property of the method with respect to N plays a key role in its success. Another important parameter, the total length (L) of the grid also needs to be optimized to provide results of desired accuracy. In [3] Marston and Balint-

Kurti have used $L = 1{\cdot}5$ times the outer classical turning point of the highest bound state in the case of a Morse oscillator. We think that it would be worthwhile to have a closer look into the convergence properties of the method with respect to both L and N. In a way these two parameters together conform to what may be analogous to a measure of completeness of the basis set in a finite basis set representation. For the purpose at hand, we have done two sets of calculations for two types of exactly solvable potential (harmonic and Morse):

i) Keeping N fixed and sufficiently high ($N = 99$) the grid length (L) has been varied from a small value (7·5 a.u) to an appreciably high value for solving the Schrödinger equation by the FGH method.
ii) The same course of calculations have been done by varying the number of grid points (N) keeping L fixed at an adequately high value ($L = 13$ a.u).

To demonstrate the convergence properties, one obvious choice is to check the convergence of energy with respect to N or L or both. In addition to that one can enquire about the convergence of FGH-wavefunctions in the context of satisfaction of the virial and Hellmann–Feynman theorems. For this purpose, let us define three terms δ_E, δ_{VT} and $\delta_{H\text{-}F}$. δ_E measures the deviation of computed energy obtained by using particular values of N and L, from the exact or converged energy, whichever is available, i.e.

$$\delta_E = E(\text{computed}) - E(\text{exact or converged})$$

δ_{VT} stands for deviation from the virial theorem and $\delta_{H\text{-}F}$ for deviation from the Hellmann–Feynman theorem. For harmonic potential they are measured by

$$\delta_{VT} = \{\langle T\rangle/\langle V\rangle - 1\} \quad \text{and} \quad \delta_{H\text{-}F} = \{\langle \partial H/\partial k\rangle - (1/2)\langle x^2\rangle\}. \tag{17}$$

Both δ_{VT} and $\delta_{H\text{-}F}$ are zero for exact wavefunctions [eqs (4) and (7)]. In figure 2 the profiles of δ_E, δ_{VT} and δ_{HF} values for $v = 9$ have been displayed against L (grid length) while figure 3 shows the convergence of δ_E, δ_{VT} and δ_{HF} for different N values for $v = 9$. In each case, the convergence is near exponential so that highly accurate wavefunctions can be obtained at a low computational cost.

Now the question arises whether the *adequate* values of N and L are system (potential) and state dependent? If so, how sensitive are these values? To answer these questions we have done a series of calculations to see the convergence of energy of ground as well as of higher energy states of the quartic anharmonic oscillator (eq. 8) for different values of the coupling strength (λ varies from 0·01 to 5·0). Figure 4 displays the variation of *adequate* N i.e. the minimum N value required to get the converged energies (E_v, $v = 0, 4, 9$) as a function of the coupling strength (λ) for a fixed value of $L = 13$. The variation of *adequate* L (using fixed and high value of $N = 99$) for three different states ($v = 0, 4$ and 9) as a function of λ is demonstrated in figure 5. Both the figures show that the variation in N or L is sharp initially but saturates quickly as λ increases. The convergence profiles for three different states are different but the trend of variation is the same in each case. It is to be noted that the difference in adequate N or L values for different states is not much which suggests that the method can be used for providing good wavefunctions even for higher states at reasonably low computational cost. However, for certain long range potentials with singularity at the origin (e.g. $-1/x$, $-1/x^2$, $-1/|x|$, etc.), our experience so far indicates that for an appropriately large length L, the energy eigenvalues do not show

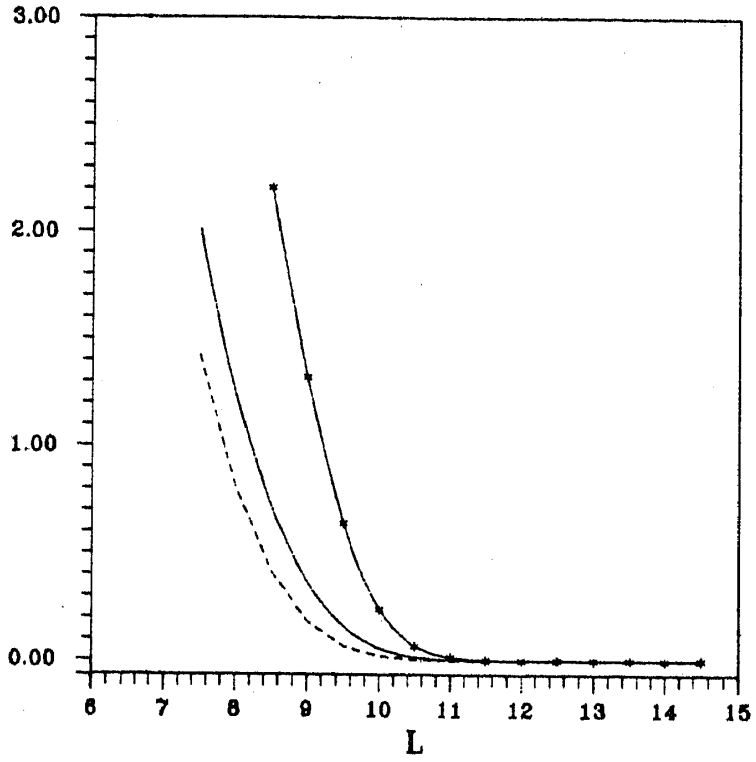

Figure 2. Profiles δ_{VT}(—— line), δ_{HF}(–––– line) and δ_E(–∗–∗–∗–) for the 10th vibrational state ($v = 9$) of harmonic oscillator [see text, eq. 17] as a function of the grid length (L).

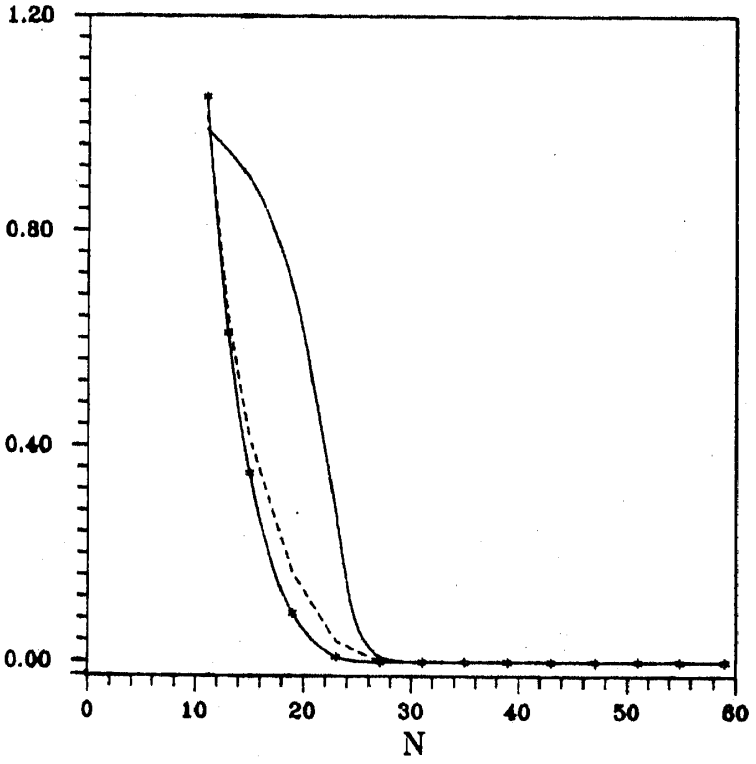

Figure 3. Convergence of δ_{VT}(—— line) and δ_{HF}(–––– line) and δ_E(–∗–∗–∗–) for the 10th vibrational state ($v = 9$) of harmonic oscillator [see text, eq. 17] for different number of grid points (N) used.

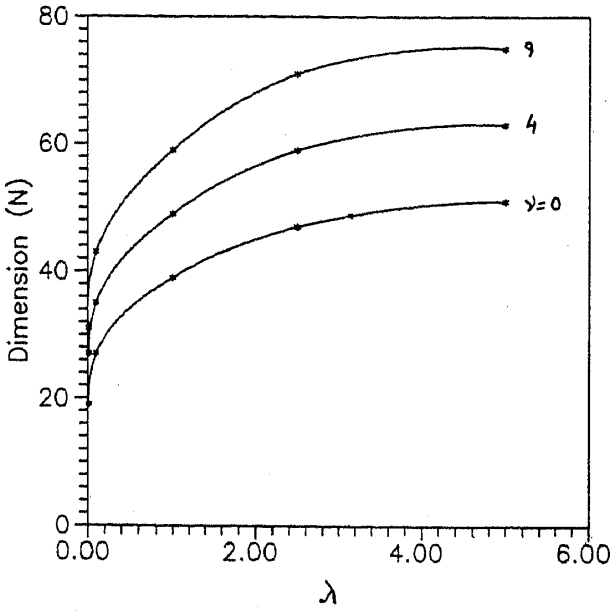

Figure 4. The variation of adequate N for $v = 0, 4, 9$ as a function of oscillator strength (λ) of a quartic anharmonic oscillator (see eq. 8), for $L = 13$ a.u.

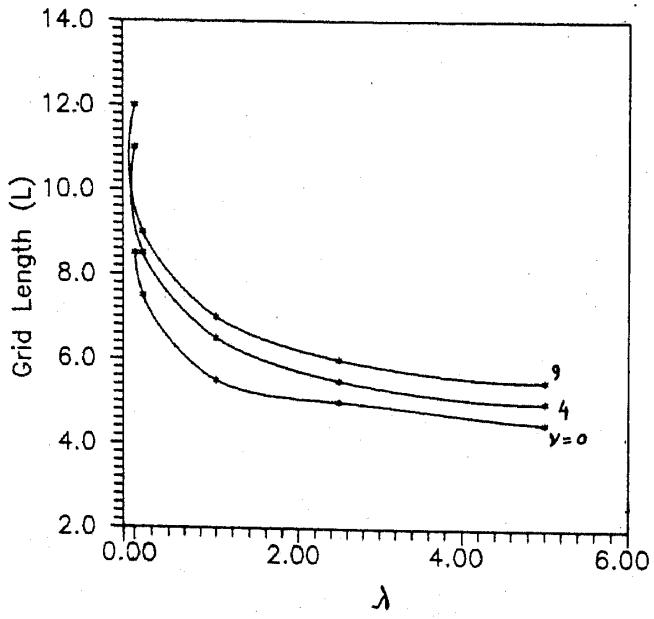

Figure 5. The variation of adequate L (using $N = 99$) for three different states ($v = 0, 4$ and 9) as a function of λ for the same system as in figure 4.

monotonic convergence with respect to the number of grid points (N) or grid density (L/N). For a given L, there appears to be an optimum grid density for which best eigenvalues are obtained. The reason for this non-monotonicity of the convergence is intimately related with the problem of representing a state on the discretized co-ordinate or momentum space. Further analysis is on the way at present.

4. Conclusion

The FGH method has been shown to provide very accurate wavefunction as well as energy eigenvalues. Both the local and global properties of FGH wavefunctions are generally satisfactory if sufficient number of grid points and an appropriate grid length are chosen. Convergence with respect to grid length (L) and number of points (N) is nearly exponential. In a many-dimensional application therefore, effective dimensionality of the problem can be kept within limits with suitable truncation along each axis. A detailed analysis of the accuracy of the wavefunctions for the many-dimensional cases will be reported in due course.

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