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Generalised Hill–Wheeler ansatz and the eigensolutions of the one-dimensional Schrödinger equation

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Abstract. A rather powerful method, based upon the theory of distributions and the Hill-Wheeler ansatz, is introduced in order to deal with the eigensolutions of the most general one-dimensional Hamiltonian $\hat{H} = \hat{p}^2/2m + V(\hat{x})$, and illustrated with reference to two special (but important) examples.

1. Introduction

It is well known that Schrödinger's equation, even in the one-particle, one-dimensional case, rarely possesses an exact (analytical) solution. Consequently, an enormous amount of work has been devoted, over several decades, in order to develop, analyse, study and apply different approximate schemes. The eigensolutions of even the simplest (one-dimensional) Hamiltonian

$$\hat{H} = \hat{p}^2/2m + V(\hat{x}) \tag{1.1}$$

deserve careful scrutiny, in view of their relevance in many branches of physics and chemistry (for a small reference sample see, for instance, Banerjee *et al* 1978, Bender and Wu 1969, 1973, Biswas *et al* 1971, 1973, Boyd 1978, Bozzolo and Plastino 1981, Bozzolo *et al* 1982a, b, 1984, Chan *et al* 1964, Fung *et al* 1978, Gillespie 1976, Graffi *et al* 1970, 1971, Graffi and Grecchi 1973, Halpern 1973, Hioe *et al* 1976, Jaffe 1965, Kinkaid and Cohen 1975, Lu *et al* 1973, Strysewski and Giordano 1977) and efforts in the relevant fields are currently being carried out by numerous investigators.

In this work we wish to present a simple and accurate method for dealing approximately with (1.1), with no restrictions attached in respect of the functional appearance of $V(x)$. The paper is organised as follows.

In § 2 we briefly sketch the Hill-Wheeler method and discuss its generalisation in § 3. The appropriate generating functions are dealt with in § 4, two relevant examples which illustrate our proposal are given in § 5 and some conclusions are presented in § 6.

2. The Hill–Wheeler ansatz

A very powerful scheme for tackling the many-body Schrödinger equation is that proposed by Hill and Wheeler (1953) and Griffin and Wheeler (1957), based upon the

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ansatz

$$|\psi\rangle = \int d\alpha f(\alpha)|\Phi(\alpha)\rangle \tag{2.1}$$

where $|\Phi(\alpha)\rangle$, the so-called generating functions, are in general (although not necessarily) Slater determinants and the α-parameter(s) ('generating coordinate(s)') refer to specially chosen coordinates that supposedly describe the particular many-body phenomena one is interested in. The weight function $f(\alpha)$ is determined by the variational principle

$$\delta \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = 0 \tag{2.2}$$

where the expectation value of $\hat{H}$ and the normalisation factor can be written in terms of the 'Hamiltonian overlap kernel' (HOK)

$$h(\alpha, \beta) = \langle\Phi(\alpha)|\hat{H}|\Phi(\beta)\rangle \tag{2.3}$$

and the 'generator overlap kernel' (GOK)

$$n(\alpha, \beta) = \langle\Phi(\alpha)|\Phi(\beta)\rangle \tag{2.4}$$

respectively as

$$\langle\psi|H|\psi\rangle = \int d\alpha f(\alpha) \int d\beta f(\beta) h(\alpha, \beta) \tag{2.5}$$

and

$$\langle\psi|\psi\rangle = \int d\alpha f^*(\alpha) \int d\beta f(\beta) n(\alpha, \beta). \tag{2.6}$$

The variational principle (2.2) leads to the celebrated Hill-Wheeler (HW) equations

$$\int d\alpha f(\alpha)[h(\beta, \alpha) - e n(\beta, \alpha)] = 0 \tag{2.7}$$

which can be solved by recourse to well established techniques (see, for example, Faessler *et al* 1973). The Hill-Wheeler approach has been successfully applied to a wide variety of many-body problems (Ring and Schuck 1980), and it is our purpose here to take advantage of a recently proposed generalisation of this technique (Nuñez *et al* 1984) in order to find the eigensolutions of (1.1).

3. A generalised Hill–Wheeler ansatz

The idea of this generalisation is to assign to $f(a)$ the character of a distribution (Nuñez *et al* 1984)

$$f(\alpha) = \sum_{n=0}^{k} f_n(\alpha_0)(-1)^n \delta^{(n)}(\alpha - \alpha_0) \tag{3.1}$$

so that, after the introduction of the so-called 'm-states' (Nuñez *et al* 1984)

$$|m, \alpha_0\rangle = \int (-1)^m \delta^{(m)}(\alpha - \alpha_0)|\Phi(\alpha)\rangle \, d\alpha$$

$$= \frac{d^m}{d\alpha^m}|\Phi(\alpha)\rangle|_{\alpha=\alpha_0} \tag{3.2}$$

the following generalised ansatz ensues:

$$|\psi_G\rangle = \sum_{m=0}^{k} f_m(\alpha_0)|m, \alpha_0\rangle. \tag{3.3}$$

It can be shown that the m-states provide us with a basis for the so-called collective subspace S_c of the Hilbert space (Nuñez *et al* 1984), which is the smallest subspace that contains all the generating states $|\Phi(\alpha)\rangle$. Of course the limit $k \to \infty$ should be taken so as to deal with the entire subspace S_c.

Different approximations are obtained depending upon the number of terms (K-value) considered in (3.3). Considerations involving computational accuracy and capability are to be employed in the selection of K (Nuñez *et al* 1984).

The variational principle

$$\delta \frac{\langle \psi_G|H|\psi_G\rangle}{\langle \psi_G|\psi_G\rangle} = 0 \tag{3.4}$$

leads to an eigenvalue problem for the moments $f_m(\alpha_0)$ of the distribution (3.1). We obtain

$$\sum_n \{H_{mn}(\alpha_0) - e\not{k}O_{mn}(\alpha_0)\} f_n(\alpha_0) = 0 \tag{3.5}$$

with

$$H_{mn}(\alpha_0) = \langle m, \alpha_0|\hat{H}|n, \alpha_0\rangle \tag{3.6}$$

$$O_{mn}(\alpha_0) = \langle m, \alpha_0|n, \alpha_0\rangle. \tag{3.7}$$

Recourse to well known techniques provides us with a satisfactory solution to our problem. A particular aspect of our approach deserves special comment: no approximations are involved in writing down (3.5).

4. Generating functions and m-states

In order to construct m-states appropriate for the problem at hand we need first of all to avail ourselves with suitable generating functions. We start with the boson operators entering the second-quantisation expression for the harmonic oscillator Hamiltonian

$$H_0 = \hat{a}^+\hat{a} + \tfrac{1}{2} \tag{4.1}$$

and subject them to a displacement γ (a c-number)

$$\begin{aligned} \hat{b}^+ &= \hat{a}^+ - \gamma^* \\ \hat{b} &= \hat{a} - \gamma \end{aligned} \tag{4.2}$$

since a general potential well(s) $V(x)$ will not necessarily be located at the origin. The vacuum of the $\hat{b}$ operators $|0, \gamma\rangle \equiv |\gamma\rangle$

$$\hat{b}|0, \gamma\rangle = 0 \tag{4.3}$$

is an extremal state in the Fock space and thus a coherent 'ground' (or 'extremal') state (Gilmore 1974, Arecchi *et al* 1972), which in the coordinate representation will have a Gaussian shape. This Fock space is spanned by the basis

$$(\hat{b}^+)^j|0, \gamma\rangle \equiv \sqrt{j!}|j, \gamma\rangle \qquad j = 0, 1, 2 \ldots \tag{4.4}$$

in which we shall express our generating functions as

$$|\beta\rangle_e = \exp[\tfrac{1}{2}\beta(\hat{b}^\dagger)^2]|0, \gamma\rangle \tag{4.5a}$$

$$|\beta\rangle_o = \hat{b}^\dagger|\beta\rangle_e \tag{4.5b}$$

where β is a real parameter (to be presently related to the generating coordinate) and the subscript e(o) indicates that the corresponding state is even (odd). The state (4.5a) is the vacuum of the operators

$$\begin{aligned}\hat{B} &= (1-\beta^2)^{-1/2}(\hat{b} - \beta\hat{b}^\dagger)\\ \hat{B}^\dagger &= (1-\beta^2)^{-1/2}(\hat{b}^\dagger - \beta\hat{b})\end{aligned} \tag{4.6}$$

i.e.

$$\begin{aligned}\hat{B}|\beta\rangle_e &= 0\\ \hat{B}^\dagger|\beta\rangle_e &= (1-\beta^2)^{1/2}|\beta\rangle_o.\end{aligned} \tag{4.7}$$

The ket $\not{b}|\beta\rangle_e$ has a Gaussian aspect in the coordinate representation

$$\begin{aligned}\langle Q|\beta\rangle_e &= \exp(-Q^2/2)\\ \langle Q|\beta\rangle_o &= Q\exp(-Q^2/2)\end{aligned} \tag{4.8}$$

where, if we choose γ to be real, Q is the eigenvalue of the (coordinate) operator

$$\hat{Q} = \left(\frac{1-\beta}{1+\beta}\right)^{1/2}(\hat{x} - C) \tag{4.9}$$

with

$$C = \gamma(1-\beta^2). \tag{4.10}$$

If we choose as the generating coordinate the quantity

$$\omega = \left(\frac{(1-\beta)}{(1+\beta)}\right) \tag{4.11}$$

and suitably redefine (4.5) in terms of it, we immediately find as the (coordinate representation) expression for our generating functions

$$\begin{aligned}\Phi_e(\omega, x) &= \langle x|\omega\rangle_e = \exp(-\tfrac{1}{2}\omega(x-C)^2)\\ \Phi_o(\omega, x) &= \langle x|\omega\rangle_o = (x-C)\exp(-\tfrac{1}{2}\omega(x-C)^2).\end{aligned} \tag{4.12}$$

We are now in a position to write down our m-states ($[m/2]$ denotes the integer part of $m/2$) as

$$\begin{aligned}|m, \omega_0\rangle &= \frac{(-1)^{[m/2]}}{2^{[m/2]}}(x-C)^m \exp(-\tfrac{1}{2}\omega_0(x-C)^2)\\ &= \frac{d^{[m/2]}}{d\omega^{[m/2]}}|\omega_{e(o)}|_{\omega=\omega_0}\end{aligned} \tag{4.13}$$

which in more explicit form is (notice that the subindex e(o) refers to the case m even (odd))

$$\begin{aligned}|2n, \omega_0\rangle &= \sum_{i=1}^{n} S_{2i}^{(2n)}(\omega_0)(\hat{b}^\dagger)^{2i}|\omega_0\rangle\\ |2n+1, \omega_0\rangle &= \sum_{i=1}^{n} S_{2i}^{(2n)}(\omega_0)(\hat{b}^\dagger)^{2i+1}|\omega_0\rangle.\end{aligned} \tag{4.14}$$

The coefficients S arise out of the derivatives in (4.5). An alternative expression can also be given in terms of the $\hat{B}$ operators

$$|2n, \omega_0\rangle = \sum_{i=0}^{n} P_{2i}^{(2n)}(\omega_0)(\hat{B}^{+})^{2i}|\omega_0\rangle$$
$$|2n+1, \omega_0\rangle = \frac{(\hat{B}^{+}+\beta\hat{B})}{(1-\beta^2)^{1/2}}|2n, \omega_0\rangle \tag{4.15}$$

with appropriate coefficients P.

The relevant matrix elements (3.6) and (3.7) for the states defined in (4.13) are (in the case of the Hamiltonian (1.1))

$$\langle m|\hat{H}|m+2n\rangle = \langle m|m+2n\rangle\left(\frac{4m(m+2n)}{2(m+n)-1} - 2(m+n)+1\right)\frac{\omega_0}{2} + \langle m|\hat{V}|m+2n\rangle \tag{4.16}$$

$$\langle m|\hat{H}|m+2n+1\rangle = \langle m|\hat{V}|m+2n+1\rangle \tag{4.17}$$

$$\langle m|m+2n\rangle = 2(-\tfrac{1}{2})^{[m/2]+[(m+2n)/2]}\frac{(2m+2n-1)!!}{(4\omega_0)^{m+n}} \tag{4.18}$$

$$\langle m|m+2n+1\rangle = 0 \tag{4.19}$$

with

$$\langle m|\hat{V}|m+2n\rangle = \frac{(-1)^{[m/2]+[(m+2n)/2]+m+n}}{(2\sqrt{\pi})2^{[m/2]+[n/2]}}\frac{\mathrm{d}^{m+n}}{\mathrm{d}\omega_0^{m+n}}G_{+}(\omega_0) \tag{4.20}$$

$$\langle m|\hat{V}|m+2n+1\rangle = \frac{(-1)^{[m/2]+[(m+2m+1)/2]+m+n}}{(2\sqrt{\pi})2^{[n/2]+[m/2]}}\frac{\mathrm{d}^{m+n}}{\mathrm{d}\omega_0^{m+n}}G_{-}(\omega_0) \tag{4.21}$$

where G_{+}, G_{-} are appropriately constructed Laplace transforms of the potential $V(x)$

$$G_{+}(\omega_0) = L\{x^{-1/2}[V(C+x^{1/2}) + V(C-x^{1/2})]\} \tag{4.22}$$

$$G_{-}(\omega_0) = L\{V(C+x^{1/2}) - V(C-x^{1/2})\}. \tag{4.23}$$

5. Examples

We shall consider the following two examples:

$$V(x) = \tfrac{1}{2}x^2 + \lambda_1 x^3 + \lambda_2 x^4 \tag{5.1}$$

namely, a cubic plus quartic anharmonic oscillator and

$$V(x) = A(\mathrm{e}^{-2x} - 2\mathrm{e}^{-x}) \tag{5.2}$$

i.e. the Morse potential.

The selection of k in (3.1) is made according to the usual procedure one follows in facing generalised diagonalisation problems: one must be sure that the overlap matrix O of (3.5) has no zero eigenvalues. The size of k is then limited by the requirement that no such eigenvalue be smaller than a given positive constant ε (10^{-6} in this work). Of course, an *a posteriori* and rather obvious criterion is that of cutting the number of moments f_n in (3.1) when one verifies, by inspection, that 'convergence' has been achieved (Nuñez *et al* 1984).

Table 1. The cubic plus quartic anharmonic oscillator. Energies for different orders and coupling parameters.

λ_1	λ_2	Order	E_0	E_1	E_2	E_3	E_4
0.5	0.1	9	−0.255 323 790	0.464 359 331	1.248 679 381	2.346 432 789	3.782 327 465
		15	−0.255 477 028	0.452 258 771	1.196 278 554	2.192 411 618	3.332 150 666
		20	−0.255 477 259	0.452 236 430	1.196 137 185	2.191 475 677	3.328 453 666
5.0	1.0	9	−55.396 844 924	−48.302 887 939	−41.424 499 570	−34.762 664 987	−28.212 111 872
		15	−55.396 845 517	−48.302 899 053	−41.425 155 011	−34.782 041 802	−28.394 994 972
		20	−55.396 845 173	−48.302 899 063	−41.425 156 169	−34.782 102 830	−28.396 845 618
50.0	10.0	9	−640.364 516 561	−616.897 582 446	−593.620 807 341	−570.536 630 331	−574.638 583 374
		15	−640.364 516 576	−616.897 582 762	−593.620 851 062	−570.538 220 935	−574.653 798 678
		20	−640.364 516 576	−616.897 582 762	−593.620 851 064	−570.538 221 040	−574.653 802 277
100.0	10.0	9	−10 495.068 783 74	−10 447.712 304 85	−10 400.401 977 50	−10 353.137 886 74	−10 305.920 114 44
		15	−10 495.068 783 74	−10 447.712 304 85	−10 400.401 977 64	−10 353.137 912 52	−10 305.920 220 55
		20	−10 495.068 783 74	−10 447.712 304 85	−10 400.401 977 64	−10 353.137 912 52	−10 305.920 220 55

Table 2. The Morse potential. Exact and GCM energies for different values of A.

A		E_{exact}	E_{GCM}
1	E_0	−0.25	−0.249 599 1
3	E_0	−1.517 949 2	−1.517 943 5
	E_1	−0.053 847 6	0.003 400 2
10	E_0	−7.087 722 3	−7.087 722 2
	E_1	−2.763 167 0	−2.762 424 7
	E_2	−0.438 611 7	−0.264 772 3
15	E_0	−11.377 016 65	−11.377 016 63
	E_1	−5.631 050 0	−5.630 919 0
	E_2	−1.885 083 2	−1.835 176 3
	E_3	−0.139 116 6	−0.952 249 9
30	E_0	−24.772 774 42	−24.772 774 42
	E_1	−15.818 323 3	−15.818 316 9
	E_2	−8.863 872 12	−8.860 636 79
	E_3	−3.909 420 97	−3.696 008 79
	E_4	−0.954 969 824	1.135 178 18

The free parameters C and ω_0 of the preceding section are chosen so as to comply with the rather obvious requirements

$$\frac{\partial}{\partial \omega_0}\langle 0, \omega_0|\hat{H}|0, \omega_0\rangle = 0$$
$$\frac{\partial}{\partial C}\langle 0, \omega_0|\hat{H}|0, \omega_0\rangle = 0 \tag{5.3}$$

and the corresponding results are given in tables 1 and 2, for the anharmonic and Morse cases respectively. We take advantage of the theorem of separation (of eigenvalues (Pilar 1968)) in order to provide upper bounds not only for the ground state but also for the excited states. The results are quite good and faithfully exhibit the power of our formalism.

6. Conclusions

The main idea of the present work has been that of adapting a rather powerful, recently developed many-body technique (Nuñez *et al* 1984) to the study of the eigensolutions of a general one-dimensional Hamiltonian (1.1). The concomitant numerical work turns out to be very simple (just a diagonalisation of modest 'size') and the accuracy to be reached is limited only by the technical details of the computer one uses. It should be stressed that no restrictions are imposed on the form of the potential $V(x)$ contrary to other approximate treatments. From a more theoretical point of view it is also of interest to point out that in § 4 we give a concrete example of an expansion (cf (4.15)) in terms of a basis that spans the so-called 'collective subspace' (Wong 1970, de Toledo Piza *et al* 1977). This subspace appears here in a natural fashion, without recourse to any sophisticated mathematical reasoning (Wong 1970, de Toledo Piza *et al* 1977). One may assert that the present approach is flexible enough to be employed in a wide variety of related problems.

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