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On the limit of approximate solutions of generator coordinate integral equations

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Abstract. By formulating the generator coordinate method for bound states as a super-eigenvalue problem and using a Weyl theorem we provide a mathematical background for the commonly used approximation schemes to solve the Hill–Wheeler integral equation.

1. Introduction: the Hill–Wheeler eigenvalue problem†

In the generator coordinate method (GCM) (Hill and Wheeler 1953, Wheeler 1955, Griffin and Wheeler 1957) one starts out from a trial function

$$\psi(x)=\int f(\alpha)\phi(x|\alpha)\,\mathrm{d}\alpha \tag{1.1}$$

which is a superposition of continuously labelled basis functions $\phi(x|\alpha)$ each having a weight $f(\alpha)$. The labels α, known as generator coordinates (GC), are parameters which play an intermediate role since they do not appear in the final wavefunction. The variational principle, applied to the above trial function, yields an integral equation, the Hill–Wheeler equation (HW equation), for the unknown weights $f(\alpha)$

$$\int (H(\alpha,\beta)-E\Delta(\alpha,\beta))f(\beta)\,\mathrm{d}\beta=0. \tag{1.2}$$

The Hamiltonian kernel $H(\alpha,\beta)$ and the overlap kernel $\Delta(\alpha,\beta)$ defined by

$$H(\alpha,\beta)=\int\phi^*(x|\alpha)H\phi(x|\beta)\,\mathrm{d}x \qquad \Delta(\alpha,\beta)=\int\phi^*(x|\alpha)\phi(x|\beta)\,\mathrm{d}x \tag{1.3}$$

are clearly Hermitian

$$H^*(\alpha,\beta)=H(\alpha,\beta) \qquad \Delta^*(\alpha,\beta)=\Delta(\beta,\alpha). \tag{1.4}$$

Supplemented with a boundary condition the HW equation defines an eigenvalue problem. The GCM has been applied extensively in nuclear physics to both bound states and scattering problems (Lathouwers 1974‡). Whereas in scattering applications one requires $\psi(x)$ to have a certain asymptotic behaviour, the boundary condition for bound

† It is assumed throughout that both $f(\alpha)$ and $\phi(x|\alpha)$ satisfy the necessary conditions for interchanging integrations.

‡ Available on request at SCK–CEN Boeretang 200, 2400 Mol, Belgium.

state problems is simply that $f(\alpha)$ should generate square integrable ($\mathscr{L}^2$) trial functions, i.e.,

$$\|\psi\| = \left(\int f^*(\alpha)\Delta(\alpha, \beta)f(\beta)\,d\alpha\,d\beta\right)^{1/2} = \|f\|_\Delta < +\infty. \tag{1.5}$$

Thus $\mathscr{L}^2$ wavefunctions correspond to weights having a finite norm in the non-diagonal metric $\Delta(\alpha, \beta)$.

In general, the analytical solution of the eigenvalue problem (1.2)+(1.5) is impossible. One must therefore rely upon approximation schemes, the most simple one being to replace the integral (1.2) by a finite sum:

$$\sum_{j=1}^{N} (H(\alpha_i, \alpha_j) - E\Delta(\alpha_i, \alpha_j))f(\alpha_j) = 0. \tag{1.6}$$

Using this discretization technique one can run into two kinds of problems as one increases the number of mesh points. The first one is due to the non-orthogonality of the functions $\phi(x|\alpha_i)$ and is known as approximate linear dependence. It can, to a certain degree, be eliminated by applying canonical orthonormalization (Lowdin 1956, Lathouwers 1976a). Whereas the first problem is a technical one, caused essentially by a limited machine accuracy, the second one throws serious doubts upon the validity of the discretization procedure. Numerical experience tells us that sometimes, as N increases, the coefficients $f(\alpha_j)$ oscillate more and more violently instead of converging to a regular weight function. When one studies the properties of the $f(\alpha)$ theoretically (Lathouwers 1976b) one finds that they can behave in a variety of ways ranging from $\mathscr{L}^2$ functions over non-$\mathscr{L}^2$ functions to divergent series expansions and tempered distributions. In the latter cases the above oscillation phenomenon occurs. It is the aim of this paper to prove that, no matter how the eigenvectors of (1.6) behave, the eigenvalues of the discretized HW equation converge to the true solutions of the HW eigenvalue problem as $N \to \infty$. The theorem to be proved will be more general and applicable to any procedure based on a finite expansion of the kernels in some suitable set of functions:

$$H(\alpha, \beta) \cong \sum_{i=1}^{N}\sum_{j=1}^{N} \chi_i(\alpha)H_{ij}\chi_j^*(\beta) \tag{1.7}$$

$$\Delta(\alpha, \beta) \cong \sum_{i=1}^{N}\sum_{j=1}^{N} \chi_i(\alpha)\Delta_{ij}\chi_j^*(\beta). \tag{1.8}$$

The discretization technique then corresponds to using the stepfunctions, associated with the chosen mesh, for the above expansions.

We will thus provide the necessary mathematical background for the commonly used approximation schemes to solve the HW eigenvalue problem.

2. A super-eigenvalue problem

The HW equation is not a classical type of integral equation for two reasons. Firstly, it involves two kernels instead of one, and secondly, these kernels are not of the Hilbert–Schmidt type, i.e., they are not $\mathscr{L}^2$. These two drawbacks can be removed by choosing an appropriate normalization for $\phi(x|\alpha)$ (Lathouwers 1976c). The Hilbert–Schmidt theory of Fredholm integral equations (Tricomi 1957) is therefore at our disposal. For completeness we will give a short summary of the results obtained by Lathouwers (1976c).

It is a general strategy to choose $\phi(x|\alpha)\mathscr{L}^2$ in x and situated in the domain of H for all values of α. One can then introduce a renormalization factor

$$R(\alpha) = r(\alpha)/\max(\|\phi(\alpha)\|, \|H\phi(\alpha)\|) \tag{2.1}$$

where $r(\alpha)$ is an arbitrary $\mathscr{L}^2$ function in α, non-zero almost everywhere. The renormalized function $R(\alpha)\phi(x|\alpha)$ yields a $\mathscr{L}^2$ Hamiltonian and overlap kernel, i.e., there exist two constants C_H and C_Δ such that

$$\int |H(\alpha, \beta)|^2 \, \mathrm{d}\alpha \, \mathrm{d}\beta = C_H < +\infty \tag{2.2}$$

$$\int |\Delta(\alpha, \beta)|^2 \, \mathrm{d}\alpha \, \mathrm{d}\beta = C_\Delta < +\infty. \tag{2.3}$$

It follows that the kernel $K(\alpha, \beta|E) = H(\alpha, \beta) - E\Delta(\alpha, \beta)$ is $\mathscr{L}^2$ for all values of E since one readily verifies that

$$\int |K(\alpha, \beta|E)|^2 \, \mathrm{d}\alpha \, \mathrm{d}\beta \leqslant C_H + 2|E|(C_H C_\Delta)^{1/2} + E^2 C_\Delta. \tag{2.4}$$

The eigenvalue problem

$$\begin{aligned} &\int K(\alpha, \beta|E) g(\beta|E) \, \mathrm{d}\beta = \lambda(E) g(\alpha|E) \\ &\int |g(\alpha|E)|^2 \, \mathrm{d}\alpha < +\infty \end{aligned} \tag{2.5}$$

is therefore a homogeneous Fredholm equation of the second kind with a $\mathscr{L}^2$ kernel. Its eigenvalues and eigenfunctions depend upon energy as a parameter. The above procedure, which eliminates the non-orthogonal metric $\Delta(\alpha, \beta)$, was introduced by Löwdin for matrix equations (Löwdin 1967). He replaced the secular equation for a finite non-orthogonal basis by the so called super-secular equation which is the matrix analogue of (2.5). Taking over Lödwin's terminology (2.5) will be referred to as the super-HW equation.

In order to study the HW equation by the super-HW equation one must establish the connection between the eigenvalues and eigenfunctions of these two equations. As for the super-eigenvalues $\lambda(E)$ one can show (Lathouwers 1976c) that

$$\begin{aligned} &\mathrm{d}\lambda(E)/\mathrm{d}E = -(\|g(E)\|_\Delta/\|g(E)\|)^2 \leqslant 0 \\ &\lim_{E \to \pm\infty} \lambda(E) = \pm\infty. \end{aligned} \tag{2.6}$$

Thus the $\lambda(E)$ are monotonically decreasing functions having a single zero point. At E_i, the zero point of $\lambda_i(E)$, the super-HW equation can be written as

$$\int (H(\alpha, \beta) - E_i \Delta(\alpha, \beta)) g(\beta|E_i) \, \mathrm{d}\beta = 0. \tag{2.7}$$

Hence the HW eigenvalues E_i are the zeros of the super-eigenvalues $\lambda_i(E)$ while the weights $f_i(\alpha)$ are to be identified with the $g_i(\alpha|E_i)$. We have thus formulated the HW eigenvalue problem in terms of a classical Fredholm eigenvalue problem depending parametrically upon energy.

3. Weyl's theorem and the limit of approximate eigenvalues

In order to prove that approximate eigenvalues converge to the true solutions one needs some tool to compare the eigenvalues of the equations involved. For eigenvalue problems of self-adjoint, completely continuous operators there exists an important theorem, due to Weyl (1912), which allows one to compare eigenvalues of equal order without any previous knowledge concerning their eigenvectors. Weyl's theorem implies that, if A_1 and A_2 are two self-adjoint completely continuous operators and a_n^1 respectively a_n^2 their nth eigenvalue, then

$$|a_n^1 - a_n^2| \leqslant \|A_1 - A_2\| \tag{3.1}$$

where the norm of an operator is defined as

$$\|A\| = \operatorname{supr}(\|Af\|/\|f\|). \tag{3.2}$$

For a $\mathscr{L}^2$ kernel, being a completely continuous operator on the space of $\mathscr{L}^2$ functions, one readily verifies, using Schwarz's inequality, that

$$\|A\| \leqslant ((A)) = \left(\int |A(\alpha, \beta)|^2 \, d\alpha \, d\beta\right)^{1/2}. \tag{3.3}$$

Here $((A))$ is the norm of $A(\alpha, \beta)$ considered as a $\mathscr{L}^2$ function in α and β. As such the kernel $A(\alpha, \beta)$ can be expanded in a double Fourier series

$$A(\alpha, \beta) = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \psi_m(\alpha) a_{mn} \psi_n^*(\beta) \tag{3.4}$$

where $\{\psi_n(\alpha)\}$ is a complete set of functions. The equality sign in (3.4) stands for convergence in the mean, i.e., convergence in the (( )) norm. From this property of (3.4), the inequality (3.3) and Weyl's theorem, it follows that, for an arbitrary $\epsilon > 0$, there exists a number N such that

$$|a_n - a_n^{(N)}| \leqslant \|A - A_N\| \leqslant ((A - A_N)) < \epsilon \tag{3.5}$$

where $A_N(\alpha, \beta)$ is the truncation of (3.4) after N terms in m and n.

Since $K(\alpha, \beta|E)$ is $\mathscr{L}^2$, everything stated above applies to it. Truncating the expansions

$$\begin{aligned}
K(\alpha, \beta|E) &= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \psi_m(\alpha) k_{mn}(E) \psi_n^*(\beta) \\
H(\alpha, \beta) &= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \psi_m(\alpha) h_{mn} \psi_n^*(\beta) \\
\Delta(\alpha, \beta) &= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \psi_m(\alpha) \Delta_{mn} \psi_n^*(\beta) \\
k_{mn}(E) &= h_{mn} - E\Delta_{mn}
\end{aligned} \tag{3.6}$$

after N terms one obtains a secular and a super-secular equation

$$\sum_{n=1}^{N} (h_{mn} - E^{(N)} \Delta_{mn}) c_n = 0 \tag{3.7a}$$

$$\sum_{n=1}^{N} k_{mn}(E) d_n(E) = \lambda^{(N)}(E) d_m(E) \tag{3.7b}$$

which are equivalent to the finite rank integral equations

$$\int (H_N(\alpha, \beta) - E^{(N)}\Delta_N(\alpha, \beta)) f^{(N)}(\beta)\, d\beta = 0 \tag{3.8a}$$

$$\int K_N(\alpha, \beta|E) g^{(N)}(\beta|E) = \lambda^{(N)}(E) g^{(N)}(\alpha|E). \tag{3.8b}$$

The eigenvalues $E_i^{(N)}$ of (3.7a) and (3.8a) are the zeros of the super-eigenvalues $\lambda_i^{(N)}(E)$ of (3.7b) and (3.8b).

It is clear that the number of terms needed to make the quadratic deviation between $K(\alpha, \beta|E)$ and $K_N(\alpha, \beta|E)$ smaller than ϵ will be a function of E. Let E_i be an eigenvalue of the HW equation and $I_i = [E_i^-, E_i^+]$ a finite interval containing E_i. Then putting

$$N = \sup_{E \in I_i} N(E) \tag{3.9}$$

it follows from (3.5) that

$$|\lambda_i(E) - \lambda_i^{(N)}(E)| < \epsilon \tag{3.10}$$

for all E in I_i and consequently

$$\lim_{N\to\infty} \lambda_i^{(N)}(E) = \lambda_i(E). \tag{3.11}$$

Since the curve $\lambda_i^{(N)}(E)$ converges to $\lambda_i(E)$ its zero point $E_i^{(N)}$ goes to E_i, i.e.,

$$\lim_{N\to\infty} E_i^{(N)} = E_i \tag{3.12}$$

which completes the proof of our theorem. The limiting process is illustrated in figure 1.

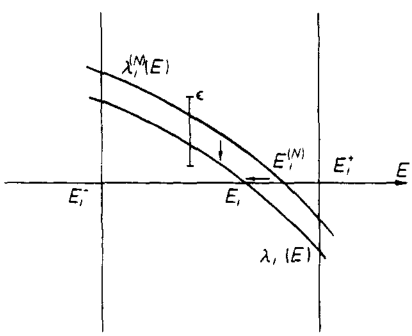

Figure 1.

4. Conclusion

It should be noticed that, although the above theorem is completely satisfactory from the mathematical point of view, it is of little practical use. Indeed, it gives us no information about the precise way in which the $E_i^{(N)}$ converge to the HW eigenvalues E_i. This results from the fact that we had to make a detour via the super-HW equation in order to apply Weyl's theorem. The latter theorem is much more powerful since it provides error bounds for the approximate eigenvalues. For real symmetric kernels and specific rules for numerical integration explicit error bounds have been given by Wielandt (1956). It would be extremely useful if one could generalize Weyl's theorem directly to integral equations of the HW type.

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