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Explicit solutions of the finite-element Schrödinger equation

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Abstract. Energy eigenvalues and eigenfunctions are obtained for the finite-element Schrödinger equation in the cases of linear and harmonic potentials. For the harmonic oscillator, the eigenfunctions in momentum space are related to Gegenbauer polynomials and have a simpler form than those for the usual lattice Schrödinger equation obtained using *finite differences*. In the case of linear potential the eigenfunctions are related to Whittaker functions. For each potential it is demonstrated both theoretically and numerically that the eigenvalues and eigenfunctions have the correct *continuum* limit.

1. Introduction

The lattice formulation of quantum field theories allows the non-perturbative calculation of bound state masses and decay amplitudes. However there are problems in the case of systems involving fermions where one encounters the *fermion doubling* problem, reviewed by Karsten and Smit (1981). A way of avoiding this problem is to use the method of *finite elements* to solve the field equations (Bender and Sharp 1983, Bender *et al* (1983, 1985, 1986), Moncrief 1983, Vásquez 1985, and Hands and Kenway 1986).

Unfortunately field theories such as QCD cannot be solved in closed form. However, in quantum mechanics there are two examples of potentials where the energy spectrum can be obtained explicitly on the lattice. They are the harmonic oscillator and linear potentials and these examples have been used to test numerical methods for obtaining the *continuum* limit by Jurkiewicz and Wosiek (1978a, b). These authors used the *finite-difference* form of the lattice Schrödinger equation, which we will review briefly in § 2, and we will there also introduce the corresponding *finite-element* form. The latter may also be derived using *irreducible difference* operators (Ebrahimi 1987).

The energy eigenvalues of the harmonic oscillator for the *finite-difference* case are related to the characteristic numbers of Mathieu's equation, while we will demonstrate in § 3 that, in the *finite-element* case, they are given by much simpler algebraic expressions. It will also be shown there that the corresponding eigenfunctions in momentum space are proportional to Gegenbauer polynomials. They would therefore provide, for example, a simple basis for the variational calculations of ground-state energies for more complicated systems. This section is completed by the demonstration that the eigenvalues and eigenfunctions obtained for the *finite-element* Schrödinger equation have the correct *continuum* limit in the case of harmonic oscillator potential.

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The lattice Schrödinger equation for the linear potential is considered in § 4. Using continued fractions, it is demonstrated that the eigenfunctions in the *finite-element* case are related to Whittaker functions and the corresponding eigenvalues to zeros of these functions. This is to be compared with the *finite-difference* case where eigenfunctions and eigenvalues are related to Bessel functions and their zeros (Jurkiewicz and Wosiek 1978b). Once again we will demonstrate that eigenfunctions and eigenvalues have the correct *continuum* limit.

Finally in § 5 we present numerical results comparing the two methods for latticising the Schrödinger equation and draw our conclusions.

2. Schrödinger's equation on a lattice

The Schrödinger equation for a particle of mass m moving in a potential $V(x)$ is

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x) \qquad -\infty<x<\infty. \tag{2.1}$$

We now introduce a lattice into coordinate space by setting $x=na$ with $n=0, \pm1, \pm2, \ldots$, where a is the lattice spacing.

The *finite-difference* method replaces $d\psi/dx$ by $(1/2a)\,[\psi(a(n+1))-\psi(a(n-1))]$ in (2.1) which then becomes

$$\frac{-\hbar^2}{8ma^2}[\psi(a(n+2))-2\psi(an)+\psi(a(n-2))]+V(an)\psi(an)$$
$$=E\psi(an) \qquad n=0, \pm1, \pm2, \ldots \tag{2.2}$$

It is easy to see that (2.1) may be written as the pair of coupled first-order equations:

$$\frac{-\hbar}{2m}\frac{d\psi(x)}{dx}=\phi(x) \qquad \hbar\frac{d\phi(x)}{dx}=f(x) \tag{2.3}$$

where $f(x)=[E-V(x)]\psi(x)$. In the *finite-element* method $\psi(x)$ is approximated in the intervals $[na, (n+1)a]$ by

$$\psi_A(x)=\psi(an)+[\psi(a(n+1))-\psi(an)](x-na)/a \tag{2.4}$$

and similarly for $\phi(x)$ and $f(x)$. These approximate functions are required to satisfy (2.3) at the midpoint of the above interval so that on eliminating ϕ,

$$\frac{-\hbar^2}{2ma^2}[\psi(a(n+1))-2\psi(an)+\psi(a(n-1))]$$
$$=\tfrac{1}{4}\{[E-V(a(n+1))]\psi(a(n+1))+2[E-V(an)]\psi(an)$$
$$+[E-V(a(n-1))]\psi(a(n-1))\}. \tag{2.5}$$

This is our form of the *finite-element* Schrödinger equation and it may also be constructed using *irreducible lattice difference operators* (Ebrahimi 1987).

3. The harmonic oscillator spectrum

The eigenvalue spectrum for the harmonic oscillator potential $V(x)=x^2/2$ may be found by transforming the lattice equations (2.2) and (2.5) into momentum space by

taking

$$\psi(an)=\frac{a}{2\pi}\int_{-\pi/a}^{\pi/a}\mathrm{d}p\tilde{\psi}(p)\exp(-\mathrm{i}anp) \qquad n=0,\pm1,\pm2,\ldots. \tag{3.1}$$

The *finite-element* equation is then equivalent to ($\hbar=m=1$)

$$2\sin^2(ap/2)\tilde{\psi}(p)$$
$$=\left(a^2E\cos^2(ap/2)+\tfrac{1}{2}a^2\cos^2(ap/2)\frac{\mathrm{d}^2}{\mathrm{d}p^2}\right)\tilde{\psi}(p) \qquad -\pi/a<p<\pi/a. \tag{3.2}$$

The energy spectrum is given by the following result.

Theorem 3.1. The energy eigenvalues are the set:

$$E_N^\lambda=\tfrac{1}{8}a^2[2\lambda(N+\tfrac{1}{2})+N^2] \qquad N=0,1,2,\ldots \tag{3.3}$$

with corresponding momentum space eigenfunctions:

$$\tilde{\psi}_N^\lambda(p)=A_N^\lambda[\cos(ap/2)]^\lambda C_N^\lambda(\sin(ap/2)) \qquad N=0,1,2,\ldots \tag{3.4}$$

where the normalisation constant $A_N^\lambda=2^{\lambda-1/2}\Gamma(\lambda)\{[(N+\lambda)N!]/[\Gamma(2\lambda+N)]\}^{1/2}$, C_N^λ are the usual Gegenbauer polynomials and

$$\lambda=\tfrac{1}{2}[1+(1+64/a^4)^{1/2}]. \tag{3.5}$$

Proof. We may write (3.2) in the form

$$\frac{\mathrm{d}^2\phi(\xi)}{\mathrm{d}\xi^2}-4\beta\tan^2\left(\frac{\xi}{2}\right)\phi(\xi)+\varepsilon\phi(\xi)=0 \qquad -\pi<\xi<\pi \tag{3.6}$$

with

$$\xi=ap \qquad \phi(\xi)=\tilde{\psi}(p) \qquad \beta=1/a^4 \qquad \varepsilon=2E/a^2. \tag{3.7}$$

Since the tangent square term diverges at $\xi=-\pi,\pi$ the appropriate boundary conditions are that $\phi(\pm\pi)=0$. Equation (3.6) may be transformed by the substitutions

$$\phi(\xi)=g(u)[\cos(\xi/2)]^\lambda \qquad u=\sin(\xi/2) \tag{3.8}$$

into the form

$$(1-u^2)\frac{\mathrm{d}^2g(u)}{\mathrm{d}u^2}-(1+2\lambda)u\frac{\mathrm{d}g(u)}{\mathrm{d}u}+4(\varepsilon-\tfrac{1}{4}\lambda)g(u)=0. \tag{3.9}$$

This equation has solutions which are finite at $u=\pm1(\xi=\pm\pi)$ only when

$$4\varepsilon-\lambda=N(2\lambda+N) \qquad N=0,1,2,\ldots \tag{3.10}$$

For these values of ε the solutions are the Gegenbauer polynomials $C_N^\lambda(u)$. Using (3.7) and (3.8) the corresponding eigenvalues E and eigenfunctions $\tilde{\psi}(p)$ are given by (3.3) and (3.4) with the normalisation constant A_N^λ chosen so that

$$1=\sum_{n=-\infty}^{\infty}|\psi(na)|^2=\frac{a}{\pi}\int_{-\pi/a}^{\pi/a}|\tilde{\psi}(p)|^2\,\mathrm{d}p. \tag{3.11}$$

Corollary 3.1. The lattice space wavefunction is

$$\psi_N^\lambda(an) = \sum_{m=0}^{[N/2]} B_m F(-N+2m, -n-\tfrac{1}{2}N+m-\tfrac{1}{2}\lambda; 1-n-\tfrac{1}{2}N+m+\tfrac{1}{2}\lambda; -1) \tag{3.12}$$

where

$$B_m = \frac{(-1)^{N/2}2^{-\lambda+1}\Gamma(\lambda+N-m)\lambda A_N^\lambda}{m!(N-2m)!\Gamma(1+\frac{1}{2}N-m+\frac{1}{2}\lambda+n)\Gamma(1-\frac{1}{2}N+m+\frac{1}{2}\lambda-n)}. \tag{3.13}$$

Proof. Substituting into (3.4) the polynomial expansion for $C_N^\lambda(z)$:

$$\psi_N^\lambda(an) = \sum_{m=0}^{[N/2]} \frac{(-1)^{m+n+N}2^{N-2m+1}\Gamma(\lambda+N-m)A_N^\lambda}{\pi m!(N-2m)!\Gamma(\lambda)} \times \int_0^\pi (\sin z)^\lambda (\cos z)^{N-2m} \exp(-2inz)\,dz \tag{3.14}$$

and the result follows from standard integrals (Erdelyi *et al* 1953).

We now consider the *continuum* limit ($a \to 0$ and $an \to x$) of the eigenvalues E_N^λ and eigenfunctions $\psi_N^\lambda(an)$. In this limit, $\lambda \approx 4/a^2$ so that from (3.3), $\lim_{a\to 0} E_N^\lambda = N+\frac{1}{2}$. The energy eigenvalues therefore have the correct *continuum* limit. With our chosen normalisation for the eigenfunctions, it is $\sqrt{a}\,\psi_N^\lambda(an)$ which should tend to the *continuum* wavefunction $\Psi(x)$ with normalisation $\int_{-\infty}^{\infty}|\Psi(x)|^2\,dx = 1$. That this is the case is demonstrated by the following.

Theorem 3.2. As $a \to 0$, $\lambda a^2 \to 4$ and $an \to x$,

$$\sqrt{a}\,\psi_N^\lambda(an) \to \left(\frac{1}{\pi^{1/2}2^N N!}\right)^{1/2} (-1)^{N/2}\exp(-x^2/2)H_N(x)$$
$$n = 0, \pm 1, \pm 2, \ldots; \quad N = 0, 1, 2, \ldots \tag{3.15}$$

Proof. Using Stirling's formula to approximate the gamma functions in the definition of A_N^λ and B_m given by (3.13), it may be shown that, in the limit $a \to 0$, $\lambda a^2 \to 4$ and $an \to x$,

$$B_m \approx \frac{(-1)^{N/2}\exp(-x^2/2)\lambda^{N/2-m-1/4}2^{-N/2+3/2}(N!)^{1/2}\pi^{1/4}}{m!(N-2m)!}. \tag{3.16}$$

Let us now consider the hypergeometric function appearing in the definition (3.12) of $\psi_N^\lambda(an)$. This satisfies the recurrence relation (Erdelyi *et al* 1953)

$$F(-(k+1), b; c; -1) = \frac{(3k+c+b)}{(c+k)}F(-k, b; c; -1) - \frac{2k}{(c+k)}F(-(k-1), b; c; -1) \tag{3.17}$$

where $b = -n-\frac{1}{2}N+m-\frac{1}{2}\lambda$, $c = -n-\frac{1}{2}N+m+\frac{1}{2}\lambda+1$. Inserting the limiting behaviour for n and λ in the definitions for b and c, this recurrence relation has the asymptotic form:

$$F(-(k+1), b; c; -1) \approx -\frac{2x}{\sqrt{\lambda}}F(-k, b; c; -1) - \frac{4k}{\lambda}F(-(k-1), b; c; -1). \tag{3.18}$$

Multiplying both sides by $\lambda^{(k+1)/2}/2^{(k+1)}$, we get

$$\left(\frac{\lambda^{(k+1)/2}}{2^{(k+1)}}F(-(k+1),b;c;-1)\right)$$
$$\approx x\left(\frac{-\lambda^{k/2}}{2^k}F(-k,b;c;-1)\right)-k\left(\frac{\lambda^{(k-1)/2}}{2^{(k-1)}}F(-(k-1),b;c;-1)\right). \quad (3.19)$$

Therefore the asymptotic limit of $[(-1)^k\lambda^{k/2}/2^k]F(-k,b;c;-1)$ and the Hermite polynomials $H_{e_k}(x)$ satisfy the same recurrence relations. It is straightforward to prove that

$$F(-k,b;c;-1)\approx\frac{(-2)^k}{\lambda^{k/2}}H_{e_k}(x) \quad (3.20)$$

for $k=0$ and 1 and since both sides have the same recurrence relations, (3.20) holds for all $k=0,1,2,\ldots$. Substituting from (3.16) and (3.20) in (3.12):

$$\psi_N^\lambda(an)\approx(-1)^{3N/2}(N!)^{1/2}2^{N/2+3/2}\pi^{1/4}\lambda^{1/4}$$
$$\times\exp(-x^2/2)\sum_{m=0}^{[N/2]}\frac{H_{e(N-2m)}(x)}{2^{2m}m!(N-2m)!}. \quad (3.21)$$

The result (3.15) then follows by noting that

$$\sum_{m=0}^{[N/2]}\frac{H_{e(N-2m)}(x)}{2^{2m}m!(N-2m)!}=\frac{1}{2^N N!}H_N(x) \quad (3.22)$$

where $H_N(x)=2^{N/2}H_{e_N}(x\sqrt{2})$ is an alternative definition for Hermite polynomials, as we proved by comparing coefficients of corresponding powers of x.

4. The linear potential

The *finite-element* Schrödinger equation for the linear potential $V(x)=|x|$ has the form ($\hbar=1$, $m=\frac{1}{2}$)†

$$\frac{1}{a^2}[\psi(a(n+1))-2\psi(an)+\psi(a(n-1))]$$
$$=\tfrac{1}{4}\{(E-a|n+1|)\psi(a(n+1))+2(E-a|n|)\psi(an)$$
$$+(E-a|n-1|)\psi(a(n-1))\} \qquad n=0,\pm1,\pm2,\ldots. \quad (4.1)$$

This equation has solutions $\psi(an)=C_n^+(C_n^-)$ which are symmetric (antisymmetric) in n. The recurrence relations (4.1) are equivalent to

$$[X+\lambda-(k+1)]C_{k+1}^{+(-)}-2[X-\lambda+k]C_k^{+(-)}+[X+\lambda-(k-1)]C_{k-1}^{+(-)}=0$$
$$k=1,2,3,\ldots \quad (4.2)$$

where $\lambda=E/a$ and $X=4/a^3$ with 'initial conditions'

$$[X+\lambda-1]C_1^+-[X-\lambda]C_0^+=0 \quad (4.3a)$$
$$[X+\lambda-2]C_2^--2[X-\lambda+1]C_1^-=0 \qquad C_0^-=0. \quad (4.3b)$$

† Note that the unit of mass is defined differently from that used in § 3. This is to simplify the expression for the asymptotic form of the eigenvalues and eigenfunctions given in (4.20) and (4.25), and these units were used by Jurkiewicz and Wosiek (1978b).

We see that both symmetric and antisymmetric solutions satisfy the same recurrence relations (4.2) but with different initial conditions (4.3*a*) and (4.3*b*).

It is well known that three-term recurrence relations are associated with continued fractions and we will follow a recent discussion by Masson (1988). Let $\gamma_k = (X+\lambda-k)C_k^{\pm}$; $k=0,1,2,\ldots$. Then (4.2) and (4.3) can be written in the form

$$\gamma_{k+1} - \left(\frac{z+2Gk}{1-Gk}\right)\gamma_k + \gamma_{k-1} = 0 \qquad k = 1,2,3,\ldots \tag{4.4}$$

where

$$z = 2\left(\frac{X-\lambda}{X+\lambda}\right) \qquad G = \frac{1}{X+\lambda}. \tag{4.5}$$

The 'initial conditions' are

$$\begin{aligned} &\gamma_1/\gamma_0 = z/2 \qquad \text{(symmetric case)} \\ &\gamma_0 = 0 \qquad\qquad\ \text{(antisymmetric case).} \end{aligned} \tag{4.6}$$

The three-term recurrence relation (4.4) will, in general, have two independent solutions and we require the *subdominant* solution which corresponds to the boundary condition $\psi(x)\to 0$ as $|x|\to\infty$. From (4.4) we have formally that

$$\frac{\gamma_0}{\gamma_1} = \frac{z+2G}{1-G} + \mathop{\mathrm{K}}_{k=1}^{\infty}\left(\frac{-1}{[(z+2Gk(k+1))/(1-G(k+1))]}\right) \tag{4.7}$$

where on the RHS we have used a standard notation for continued fractions (Jones and Thron, 1980).

There is a theorem by Pincherle (Gautschi 1967, Masson 1985) which states that, if the continued fraction converges, then (4.7) is satisfied by the required *subdominant* solution of (4.4). The continued fraction above may be transformed by an equivalence relation, so that

$$\frac{\gamma_0}{\gamma_1} = Z_1 + \mathop{\mathrm{K}}_{k=1}^{\infty}\left(\frac{-(A_1k^2+B_1k+C_1)}{Z_1-D_1k}\right) \tag{4.8}$$

and more generally we have

$$\frac{\gamma_{l-1}}{\gamma_l} = Z_l + \mathop{\mathrm{K}}_{k=1}^{\infty}\left(\frac{-(A_lk^2+B_lk+C_l)}{Z_l-D_lk}\right) \qquad l = 1,2,\ldots \tag{4.9}$$

where

$$\begin{aligned} &Z_l = (z+2lG)/(1-lG) && A_l = G^2/(1-lG)^2 \\ &B_l = [(2l-1)G^2-2G]/(1-lG)^2 && C_l = (1-lG+G)/(1-lG) \\ &D_l = -2G/(1-lG). \end{aligned} \tag{4.10}$$

We are now ready to prove the theorem giving the energy eigenvalues and corresponding eigenfunctions.

Theorem 4.1. The energy eigenvalue spectrum for the antisymmetric states is given by the condition

$$W_{X+\lambda,1/2}(4X) = 0 \tag{4.11a}$$

while that for the symmetric states is

$$W'_{X+\lambda,1/2}(4X)=0 \tag{4.11b}$$

where $X=4/a^3$, $\lambda=E/a$.

The corresponding eigenfunctions are

$$\psi(an)=N\zeta\left(\prod_{p=0}^{|n|-1}(X+\lambda-p)\right)W_{X+\lambda-|n|,1/2}(4X) \qquad n=\pm1,\pm2,\ldots \tag{4.12a}$$

$$=NW_{X+\lambda,1/2}(4X) \qquad n=0 \tag{4.12b}$$

where $\zeta=1$ for symmetric states and $\zeta=\operatorname{sgn} n$ for antisymmetric states. N is a normalisation constant which is independent of n but can depend on X, λ.

Proof. From relations (1.2) and (2.16) of Masson (1988) which give expressions for RHS of (4.9) in terms of confluent hypergeometric functions $\Psi(b, c; Y)$, we find

$$\frac{\gamma_{l-1}}{\gamma_l}=\left(\frac{-2}{D_l}\right)\frac{C_l\Psi(\alpha_l,\alpha_l-\beta_l+1;-2Z_l/D_l-4B_l/D_l^2-1)}{\alpha_l\beta_l\Psi(\alpha_l+1,\alpha_l-\beta_l+1;-2Z_l/D_l-4B_l/D_l^2-1)} \qquad l=1,2,3,\ldots \tag{4.13}$$

where α_l, β_l are defined by the relation

$$A_ly^2+B_ly+C_l=A_l(y+\alpha_l)(y+\beta_l).$$

Using the definition (4.5) and (4.10):

$$\alpha_l=l-X-\lambda \qquad \beta_l=\alpha_l-1. \tag{4.14}$$

The confluent hypergeometric functions are related to Whittaker's functions:

$$W_{\kappa,\mu}(Y)=\exp(-Y/2)\,Y^{\mu+1/2}\Psi(b,c;Y) \tag{4.15}$$

with

$$\kappa=\tfrac{1}{2}c-b \qquad \mu=(c-1)/2.$$

Substituting in (4.13) and using (4.14)

$$\frac{\gamma_{l-1}}{\gamma_l}=\frac{1}{(X+\lambda-l)}\frac{W_{X+\lambda+1-l,1/2}(4X)}{W_{X+\lambda-l,1/2}(4X)}. \tag{4.16}$$

For antisymmetric states, $\gamma_0=0$, so that (4.11*a*) follows from (4.16) with $l=1$. For symmetric states from (4.6) and (4.16)

$$(X+\lambda)(X+\lambda-1)W_{X+\lambda-1,1/2}(4X)-(X-\lambda)W_{X+\lambda,1/2}(4X)=0 \tag{4.17}$$

which, using identities (13.4.31) and (13.4.33) of Abramowitz and Stegun (1968), can be shown to be equivalent to (4.11*b*).

From (4.16)

$$\frac{\gamma_l}{\gamma_0}=\frac{W_{X+\lambda-l,1/2}(4X)}{W_{X+\lambda,1/2}(4X)}\left(\prod_{p=1}^{l}(X+\lambda-p)\right) \qquad l=2,3,4,\ldots. \tag{4.18}$$

The corresponding eigenfunctions are, for non-negative n,

$$\psi(an)=N\left(\prod_{p=0}^{n-1}(X+\lambda-p)\right)W_{X+\lambda-n,1/2}(4X) \tag{4.19}$$

where N is a suitable normalisation constant and the definition of γ_l in terms of C_l has been used. Equation (4.12) of the theorem then follows from the symmetry of the wavefunction.

For the case of the linear potential in the *finite-difference* Schrödinger equation (2.2), Jurkiewicz and Woseik (1978b) showed that the eigenfunctions are related to Bessel functions and eigenvalues to zeros of these functions. The asymptotic behaviour of the Bessel functions are well documented and the above authors showed that the eigenvalue spectrum had the correct *continuum* limit ($a \to 0$), related to zeros of Airy's function $\mathrm{Ai}(x)$ and its derivative, and similarly for the eigenfunctions.

The eigenvalues in the *finite-element* case are given by conditions (4.11*a*, *b*) and we are interested in the limit as $a \to 0$. The limiting behaviour of $W_{X+\lambda,1/2}(4X)$, where $\lambda = E/a$ and $X = 4/a^3$ both tend to infinity, has been discussed by Erdelyi and Swanson (1957). From their equation (10.4) the leading behaviour of the function as $a \to 0$ is

$$W_{X+\lambda,1/2}(4X) \approx (2)^{5/4}\pi^{1/2}(X+\lambda)^{X+\lambda}\exp[-(X+\lambda)](4/a^2)^{1/4}\,\mathrm{Ai}(-E). \tag{4.20}$$

This result may also be obtained using general methods for obtaining the asymptotic behaviour of special functions described in the book by Olver (1974). Theorem (3.1) in chapter 11 is particularly useful in this respect, and may also be used to obtain the corresponding leading asymptotic behaviour for the derivatives:

$$W'_{X+\lambda,1/2}(4X) \approx (2)^{-1/4}\pi^{1/2}(X+\lambda)^{X+\lambda}\exp[-(X+\lambda)](a^2/4)^{1/4}\,\mathrm{Ai}'(-E). \tag{4.21}$$

as $a \to 0$.

We are now in a position to prove the result.

Theorem 4.2. In the *continuum* limit ($a \to 0$) the energy eigenvalues and corresponding eigenfunctions for the *finite-element* Schrödinger equation with $V(x) = |x|$ tend to the corresponding *continuum* eigenvalues and eigenfunctions.

Proof. Using the asymptotic forms (4.20) and (4.21) in (4.11*a*, *b*), the eigenvalue spectrum for the antisymmetric states tends to solutions for E of

$$\mathrm{Ai}(-E) = 0 \tag{4.22a}$$

and for symmetric states to solutions of

$$\mathrm{Ai}'(-E) = 0. \tag{4.22b}$$

This is precisely the eigenvalue spectrum in the *continuum.*

To study the limit of the corresponding eigenfunctions in the symmetric case, we use (4.20) in (4.12) to give for positive $y = na$,

$$\begin{aligned}\frac{\psi(y)}{\psi(0)} &= \left(\prod_{p=0}^{n-1}(X+\lambda-p)\right)\frac{W_{X+\lambda-n,1/2}(4X)}{W_{X+\lambda,1/2}(4X)} \\ &\approx \left(\frac{(X+\lambda-n)^{X+\lambda-n}}{(X+\lambda)^{X+\lambda}}\right)\exp(n)\,\frac{\mathrm{Ai}(y-E)}{\mathrm{Ai}(-E)}\prod_{p=0}^{n-1}(X+\lambda-p) \\ &\approx \prod_{p=0}^{n-1}\left(1+\frac{(n-p)}{(X+\lambda-n)}\right)\frac{\mathrm{Ai}(y-E)}{\mathrm{Ai}(-E)} \approx \frac{\mathrm{Ai}(y-E)}{\mathrm{Ai}(-E)}.\end{aligned} \tag{4.23}$$

If we take the normalisation constant in (4.12) to be given by

$$N = \mathrm{Ai}(-E)/W_{X+\lambda,1/2}(4X) \tag{4.24}$$

we have, on combining with (4.23),

$$\psi(na) \to \mathrm{Ai}(y-E) \tag{4.25}$$

when $a \to 0$, $n \to \infty$ such that $an = y > 0$. A similar proof can be used when n, $y < 0$.

For antisymmetric states we chose the normalisation constant in (4.12) to be given by

$$N = a\ \mathrm{Ai}'(-E)/[(X+\lambda)\,W_{X+\lambda-1,1/2}(4X)] \tag{4.26}$$

which ensures that the lattice and *continuum* wavefunctions have the same slope at $y=0$, i.e $\psi(a)/a = \mathrm{Ai}'(-E)$, (we cannot use the previous normalisation (4.24) since $\psi(0) = \mathrm{Ai}(0) = 0$ in this case). From (4.12) and proceeding as previously

$$\frac{a\psi(na)}{\psi(a)} \approx \frac{\mathrm{Ai}(y-E)}{\mathrm{Ai}'(-E)} \tag{4.27}$$

and with the above normalisation we again find that $\psi(na) \to \mathrm{Ai}(y-E)$ as $a \to 0$. This completes the proof of theorem 4.2.

5. Numerical results and conclusions

The eigenvalue spectrum of the *finite-difference* Schrödinger equation (2.2) for the harmonic oscillator potential $V(x) = x^2/2$ has been given by Jurkiewicz and Wosiek (1978a). The eigenstates may be divided into two sets. For the first, the eigenfunctions are only non-zero for even values of n while for the second they are only non-zero for odd values. For the former set the energy eigenvalue spectrum is

$$E'_N = \tfrac{1}{2}a^2[a_{2N}(Y) + 2Y] \qquad N = 0, 2, 4, \ldots \tag{5.1a}$$

$$= \tfrac{1}{2}a^2[b_{2N+2}(Y) + 2Y] \qquad N = 1, 3, 5, \ldots \tag{5.1b}$$

where a_k, b_k are the characteristic values of *Mathieu's* equation, and $Y = 1/4a^4$.

We will compare here numerically rates of convergence of the E'_N to their *continuum* limit with the rates of convergence of energy eigenvalues:

$$E^{\lambda}_N = \tfrac{1}{8}a^2[2\lambda(N+\tfrac{1}{2}) + N^2] \qquad N = 0, 1, 2, \ldots$$

for the *finite-element* equation. To calculate E'_N we use asymptotic expansions for $a_{2N}(Y)$, $b_{2N+2}(Y)$ which are given by relation (20.2.30) of Abramowitz and Stegun (1968). The expansions show that E'_N have the correct *continuum* limit.

In tables 1 and 2 we give in the first column the relative error ε_N of the lattice space eigenvalue compared with its *continuum* limit, i.e. for eigenvalue $E_N = E^{\lambda}_N$ or E'_N:

$$\varepsilon_N = \left| \frac{E_N - (N+\frac{1}{2})}{(N+\frac{1}{2})} \right| . \tag{5.2}$$

Table 1. Lattice spacing for the first eigenvalue ($N = 0$) in the case of a harmonic oscillator.

Relative error	Finite-difference lattice	Finite-element lattice
0.0203	0.282	0.400
0.0167	0.256	0.364
0.0127	0.224	0.318
0.0101	0.200	0.285
0.0090	0.189	0.268
0.0066	0.168	0.231
0.0055	0.149	0.211

Table 2. Lattice spacing for the second eigenvalue ($N = 1$) in the case of a harmonic oscillator.

Relative error	Finite-difference lattice	Finite-element lattice
0.0331	0.277	0.398
0.0291	0.260	0.373
0.0222	0.228	0.326
0.0176	0.204	0.291
0.0101	0.155	0.221
0.0077	0.136	0.193
0.0055	0.115	0.163

In columns two and three we give the lattice spacing a which gives this relative error for the *finite-difference* and *finite-element* equations, respectively. Table 1 give the results for the lowest symmetric state ($N = 0$) and table 2 the results for the lowest antisymmetric state ($N = 1$).

It will be seen from these tables that the *finite-difference* eigenvalues converge more slowly to their *continuum* limit than the corresponding *finite-element* values. However, as mentioned earlier, the eigenfunctions which are solutions of the *finite-difference* eigenvalues are non-zero only on the sublattice defined by even n or odd n and the effective spacing of this sublattice is $2a$. If this spacing is used for the *finite-difference* lattice, then the numbers given in the second columns of each of the tables should be doubled. In that case the *finite-difference* eigenvalues converges more quickly than the *finite-element* eigenvalues to their *continuum* limits.

We have performed similar calculations for higher values of N and the same effect is seen. It is also observed that, as N increases, an increasingly finer lattice is needed to get the same relative error, a trend already apparent from the results in tables 1 and 2. This is to be expected since, as N increases, the *continuum* eigenfunctions become more rapidly varying functions of x.

The lattice wavefunction $\sqrt{a}\,\psi_N^{\lambda}(an)$ is compared in figures 1 and 2 with the corresponding *continuum* wavefunction $\Psi_N(x) = (1/\pi^{1/2}2^N N!)^{1/2}\exp(-x^2/2)H_N(x)$ for $N = 0$ and 1. It will seen for lattice spacing $a = 0.2$ that the lattice wavefunction is already a good approximation to the *continuum* wavefunction at the lattice points.

The eigenvalue spectrum for the *finite-difference* Schrödinger equation in the case of linear potential $V(x) = |x|$ are given by, for the symmetric case, the condition (Jurkiewicz and Woseik 1978b)

$$J'_{Y-\lambda/2}(Y) = 0 \tag{5.3a}$$

and for the antisymmetric case

$$J_{Y-\lambda/2}(Y) = 0 \tag{5.3b}$$

where $Y = X/16$, $\lambda = E/a$ and X is defined earlier. The corresponding lattice space wavefunctions are

$$\psi(an) = N' J_{Y-\lambda/2+n}(Y)$$

where N' is a suitable normalisation constant.

As in the harmonic oscillator case, we present results in tables 3 and 4 comparing numerically the rates of convergence of the two lowest energy eigenvalues in the

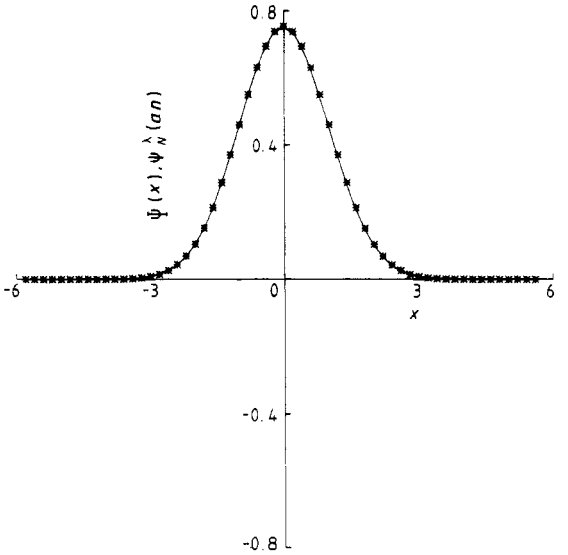

Figure 1. Lattice and continuum eigenfunctions for the ground state ($N = 0$) in the case of a harmonic oscillator. ——, continuum wavefunction; × × ×, lattice wavefunction.

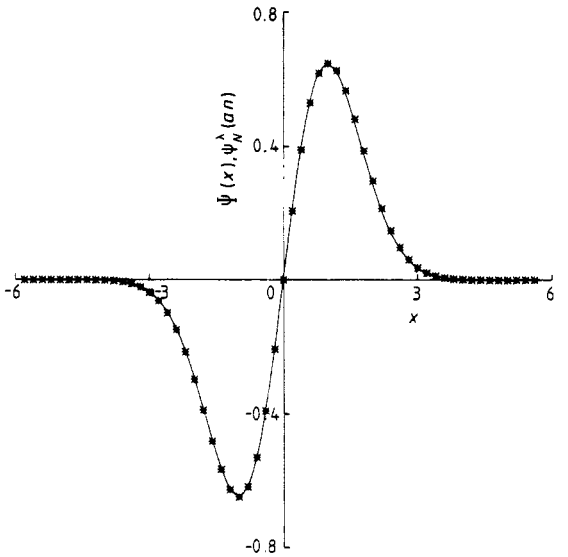

Figure 2. Lattice and continuum eigenfunctions for the first excited state ($N = 1$) in the case of a harmonic oscillator. Key as for figure 1.

finite-difference case given by (5.3) with those in the *finite-element* case given by conditions

$$W_{X+\lambda,1/2}(4X) = 0 \tag{4.11a}$$

for antisymmetric states and condition

$$W'_{X+\lambda,1/2}(4X) = 0 \tag{4.11b}$$

for symmetric states.

Table 3. Lattice spacing for the first eigenvalue ($N = 0$) in the case of a linear potential.

Relative error	Finite-difference lattice	Finite-element lattice
0.011 24	0.155 70	1.224 71
0.008 87	0.138 73	1.091 62
0.007 86	0.130 74	0.880 86
0.006 56	0.119 57	0.838 19
0.005 91	0.113 62	0.702 10
0.004 52	0.099 56	0.625 08

Table 4. Lattice spacing for the second eigenvalue ($N = 1$) in the case of a linear potential.

Relative error	Finite-difference lattice	Finite-element lattice
0.024 78	0.402 58	0.560 43
0.020 61	0.365 13	0.514 54
0.017 80	0.339 65	0.476 36
0.016 04	0.320 58	0.450 58
0.013 38	0.293 03	0.414 22
0.011 03	0.265 53	0.376 87
0.008 44	0.232 10	0.328 51

As previously, we give the lattice spacing necessary to obtain a given relative error. Once again we see that the *finite-difference* eigenvalues converge more slowly to their *continuum* values than the corresponding *finite-element* values.

Finally we compare the *finite-element* lattice wavefunction with the *continuum* wavefunction for the two lowest-energy eigenstates in figures 3 and 4. The lattice space

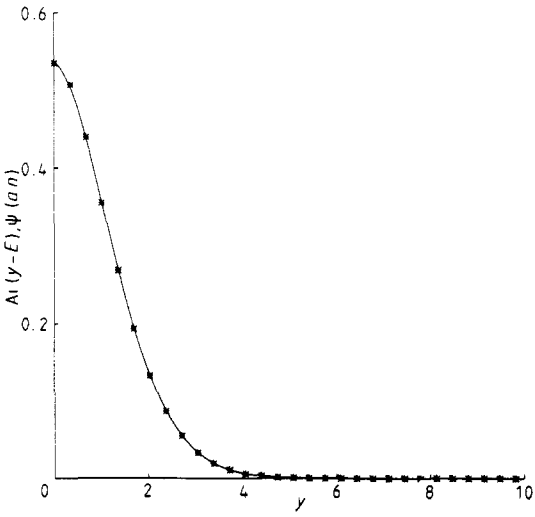

Figure 3. Lattice and continuum eigenfunctions for the ground state ($N = 0$) in the case of a linear potential. Key as for figure 1.

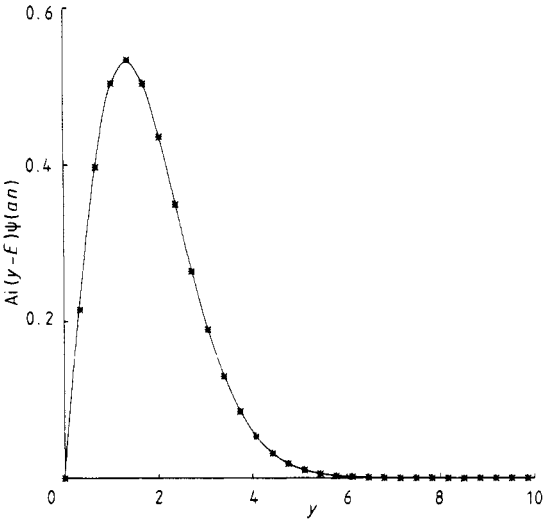

Figure 4. Lattice and continuum eigenfunctions for the first excited state ($N = 1$) in the case of a linear potential. Key as for figure 1.

wavefunction $\psi(an)$, given by (4.12*a*, *b*) and normalisation conditions (4.24) and (4.26), is plotted at the lattice points $x = na$ and compared with the *continuum* wavefunction $\mathrm{Ai}(x - E)$. We have chosen $a = 0.2$ and we see already, for this lattice spacing, $\psi(an)$, is a good approximation to the *continuum* wavefunction.

In this work we have considered the *finite-element* Schrödinger equation (2.5) which also arises from group theoretical considerations. Despite its somewhat more complicated form than the corresponding *finite-difference* expression (2.2), we have been able to find explicit solutions for the harmonic oscillator and linear potentials. Surprisingly in the harmonic oscillator case, the expression for the energy eigenvalue spectrum is much simpler for the *finite-element* case. The corresponding eigenfunctions in momentum space are proportional to Gegenbauer polynomials and could prove a useful basis for variational calculations on the lattice. Future work could involve an extension to higher dimensions and a study of properties, in particular of the harmonic oscillator eigenfunctions in lattice space such as recurrence relations.

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