Chapter 3

The quantum one-body problem

3.1 The time-independent 1D Schrödinger equation

We start the numerical solution of quantum problems with the time-indepent one-dimensional Schrödinger equation for a particle with mass m in a Potential $V(x)$. In one dimension the Schrödinger equation is just an ordinary differential equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi(x) = E\psi(x). \tag{3.1}$$

We start with simple finite-difference schemes and discretize space into intervals of length Δx and denote the space points by

$$x_n = n\Delta x \tag{3.2}$$

and the wave function at these points by

$$\psi_n = \psi(x_n). \tag{3.3}$$

3.1.1 The Numerov algorithm

After rewriting the second order differential equation to a coupled system of two first order differential equations, any ODE solver such as the Runge-Kutta method could be applied, but there exist better methods. For the special form

$$\psi''(x) + k(x)\psi(x) = 0, \tag{3.4}$$

of the Schrödinger equation, with $k(x) = 2m(E - V(x))/\hbar^2$ we can derive the Numerov algorithm by starting from the Taylor expansion of ψ_n:

$$\psi_{n\pm1} = \psi_n \pm \Delta x\psi'_n + \frac{\Delta x^2}{2}\psi''_n \pm \frac{\Delta x^3}{6}\psi^{(3)}_n + \frac{\Delta x^4}{24}\psi^{(4)}_n \pm \frac{\Delta x^5}{120}\psi^{(5)}_n + \mathrm{O}(\Delta x^6) \tag{3.5}$$

Adding ψ_{n+1} and ψ_{n-1} we obtain

$$\psi_{n+1} + \psi_{n-1} = 2\psi_n + (\Delta x)^2\psi''_n + \frac{(\Delta x)^4}{12}\psi^{(4)}_n. \tag{3.6}$$

Replacing the fourth derivatives by a finite difference second derivative of the second derivatives

$$\psi_n^{(4)} = \frac{\psi''_{n+1} + \psi''_{n-1} - 2\psi''_n}{\Delta x^2} \tag{3.7}$$

and substituting $-k(x)\psi(x)$ for $\psi''(x)$ we obtain the Numerov algorithm

$$\begin{aligned}\left(1 + \frac{(\Delta x)^2}{12} k_{n+1}\right)\psi_{n+1} = \quad & 2\left(1 - \frac{5(\Delta x)^2}{12} k_n\right)\psi_n \\ & - \left(1 + \frac{(\Delta x)^2}{12} k_{n-1}\right)\psi_{n-1} + \mathrm{O}(\Delta x^6),\end{aligned} \tag{3.8}$$

which is locally of sixth order!

Initial values

To start the Numerov algorithm we need the wave function not just at one but at two initial values and will now present several ways to obtain these.

For potentials $V(x)$ with reflection symmetry $V(x) = V(-x)$ the wave functions need to be either even $\psi(x) = \psi(-x)$ or odd $\psi(x) = -\psi(-x)$ under reflection, which can be used to find initial values:

- For the even solution we use a half-integer mesh with mesh points $x_{n+1/2} = (n + 1/2)\Delta x$ and pick initial values $\psi_(x_{-1/2}) = \psi(x_{1/2}) = 1$.
- For the odd solution we know that $\psi(0) = -\psi(0)$ and hence $\psi(0) = 0$, specifying the first starting value. Using an integer mesh with mesh points $x_n = n\Delta x$ we pick $\psi(x_1) = 1$ as the second starting value.

In general potentials we need to use other approaches. If the potentials vanishes for large distances: $V(x) = 0$ for $|x| \geq a$ we can use the exact solution of the Schrödinger equation at large distances to define starting points, e.g.

$$\psi(-a) = 1 \tag{3.9}$$

$$\psi(-a - \Delta x) = \exp(-\Delta x\sqrt{2mE/\hbar}). \tag{3.10}$$

Finally, if the potential never vanishes we need to begin with a single starting value $\psi(x_0)$ and obtain the second starting value $\psi(x_1)$ by performing an integration over the first time step $\Delta\tau$ with an Euler or Runge-Kutta algorithm.

3.1.2 The one-dimensional scattering problem

The scattering problem is the numerically easiest quantum problem since solutions exist for all energies $E > 0$, if the potential vanishes at large distances ($V(x) \to 0$ for $|x| \to \infty$). The solution becomes particularly simple if the potential is nonzero only on a finite interval $[0, a]$. For a particle approaching the potential barrier from the left ($x < 0$) we can make the following ansatz for the free propagation when $x < 0$:

$$\psi_L(x) = A\exp(-iqx) + B\exp(iqx) \tag{3.11}$$

where A is the amplitude of the incoming wave and B the amplitude of the reflected wave. On the right hand side, once the particle has left the region of finite potential ($x > a$), we can again make a free propagation ansatz,

$$\psi_R(x) = C \exp(-iqx) \tag{3.12}$$

The coefficients A, B and C have to be determined self-consistently by matching to a numerical solution of the Schrödinger equation in the interval $[0, a]$. This is best done in the following way:

- Set $C = 1$ and use the two points a and $a + \Delta x$ as starting points for a Numerov integration.
- Integrate the Schrödinger equation numerically – backwards in space, from a to 0 – using the Numerov algorithm.
- Match the numerical solution of the Schrödinger equation for $x < 0$ to the free propagation ansatz (3.11) to determine A and B.

Once A and B have been determined the reflection and transmission probabilities R and T are given by

$$R = |B|^2/|A|^2 \tag{3.13}$$
$$T = 1/|A|^2 \tag{3.14}$$

3.1.3 Bound states and solution of the eigenvalue problem

While there exist scattering states for all energies $E > 0$, bound states solutions of the Schrödinger equation with $E < 0$ exist only for discrete energy eigenvalues. Integrating the Schrödinger equation from $-\infty$ to $+\infty$ the solution will diverge to $\pm\infty$ as $x \to \infty$ for almost all values. These functions cannot be normalized and thus do not constitute solutions to the Schrödinger equation. Only for some special eigenvalues E, will the solution go to zero as $x \to \infty$.

A simple eigensolver can be implemented using the following shooting method, where we again will assume that the potential is zero outside an interval $[0, a]$:

- Start with an initial guess E
- Integrate the Schrödinger equation for $\psi_E(x)$ from $x = 0$ to $x_f \gg a$ and determine the value $\psi_E(x_f)$
- use a root solver, such as a bisection method (see appendix A.1), to look for an energy E with $\psi_E(x_f) \approx 0$

This algorithm is not ideal since the divergence of the wave function for $x \pm \infty$ will cause roundoff error to proliferate.

A better solution is to integrate the Schrödinger equation from both sides towards the center:

- We pick a starting point b and choose as energy $E = V(b)$

- Starting from $x = 0$ we integrate the left hand side solution $\psi_L(x)$ to a chosen point b and obtain $\psi_L(b)$ and a numerical estimate for $\psi'_L(b) = (\psi_L(b) - \psi_L(b - \Delta x))/\Delta x$.

- Starting from $x = a$ we integrate the right hand solution $\psi_R(x)$ down to the same point b and obtain $\psi_R(b)$ and a numerical estimate for $\psi'_R(b) = (\psi_R(b + \Delta x) - \psi_R(b))/\Delta x$.

- At the point b the wave functions and their first two derivatives have to match, since solutions to the Schrödinger equation have to be twice continuously differentiable. Keeping in mind that we can multiply the wave functions by an arbitrary factor we obtain the conditions

$$\begin{aligned} \psi_L(b) &= \alpha\psi_R(b) && (3.15)\\ \psi'_L(b) &= \alpha\psi'_R(b) && (3.16)\\ \psi''_L(b) &= \alpha\psi''_R(b) && (3.17) \end{aligned}$$

  The last condition is automatically fulfilled since by the choice $V(b) = E$ the Schrödinger equation at b reduces to $\psi''(b) = 0$. The first two conditions can be combined to the condition that the logarithmic derivatives vanish:

$$\frac{d\log\psi_L}{dx}|_{x=b} = \frac{\psi'_L(b)}{\psi_L(b)} = \frac{\psi'_R(b)}{\psi_R(b)} = \frac{d\log\psi_R}{dx}|_{x=b} \qquad (3.18)$$

- This last equation has to be solved for in a shooting method, e.g. using a bisection algorithm

Finally, at the end of the calculation, normalize the wave function.

3.2 The time-independent Schrödinger equation in higher dimensions

The time independent Schrödinger equation in more than one dimension is a partial differential equation and cannot, in general, be solved by a simple ODE solver such as the Numerov algorithm. Before employing a PDE solver we should thus always first try to reduce the problem to a one-dimensional problem. This can be done if the problem factorizes.

3.2.1 Factorization along coordinate axis

A first example is a three-dimensional Schrödinger equation in a cubic box with potential $V(\vec{r}) = V(x)V(y)V(z)$ with $\vec{r} = (x, y, z)$. Using the product ansatz

$$\psi(\vec{r}) = \psi_x(x)\psi_y(y)\psi_z(z) \qquad (3.19)$$

the PDE factorizes into three ODEs which can be solved as above.

3.2.2 Potential with spherical symmetry

Another famous trick is possible for spherically symmetric potentials with $V(\vec{r}) = V(|\vec{r}|)$ where an ansatz using spherical harmonics

$$\psi_{l,m}(\vec{r}) = \psi_{l,m}(r, \theta, \phi) = \frac{u(r)}{r} Y_{lm}(\theta, \phi) \tag{3.20}$$

can be used to reduce the three-dimensional Schrödinger equation to a one-dimensional one for the radial wave function $u(r)$:

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r) \right] u(r) = E u(r) \tag{3.21}$$

in the interval $[0, \infty[$. Given the singular character of the potential for $r \to 0$, a numerical integration should start at large distances r and integrate towards $r = 0$, so that the largest errors are accumulated only at the last steps of the integration.

In the exercises we will solve a three-dimensional scattering problem and calculate the scattering length for two atoms.

3.2.3 Finite difference methods

The simplest solvers for partial differential equations, the finite difference solvers can also be used for the Schrödinger equation. Replacing differentials by differences we convert the Schrödinger equation to a system of coupled inear equations. Starting from the three-dimensional Schrödinger equation (we set $\hbar = 1$ from now on)

$$\nabla^2 \psi(\vec{x}) + 2m(V - E(\vec{x}))\psi(\vec{x}) = 0, \tag{3.22}$$

we discretize space and obtain the system of linear equations

$$\begin{aligned} \frac{1}{\Delta x^2} & [\psi(x_{n+1}, y_n, z_n) + \psi(x_{n-1}, y_n, z_n) \\ & + \psi(x_n, y_{n+1}, z_n) + \psi(x_n, y_{n-1}, z_n) \\ & + \psi(x_n, y_n, z_{n+1}) + \psi(x_n, y_n, z_{n-1})] \\ + & \left[2m(V(\vec{x}) - E) - \frac{6}{\Delta x^2} \right] \psi(x_n, y_n, z_n) \quad = \quad 0. \end{aligned} \tag{3.23}$$

For the scattering problem a linear equation solver can now be used to solve the system of equations. For small linear problems Mathematica can be used, or the `dsysv` function of the LAPACK library. For larger problems it is essential to realize that the matrices produced by the discretization of the Schrödinger equation are usually very sparse, meaning that only $O(N)$ of the N^2 matrix elements are nonzero. For these sparse systems of equations, optimized iterative numerical algorithms exist[1] and are implemented in numerical libraries such as in the ITL library.[2]

[1] R. Barret, M. Berry, T.F. Chan, J. Demmel, J. Donato, J. Dongarra, V. Eijkhout, R. Pozo, C. Romine, and H. van der Vorst, *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods* (SIAM, 1993)

[2] J.G. Siek, A. Lumsdaine and Lie-Quan Lee, *Generic Programming for High Performance Numerical Linear Algebra* in *Proceedings of the SIAM Workshop on Object Oriented Methods for Inter-operable Scientific and Engineering Computing (OO'98)* (SIAM, 1998); the library is availavle on the web at: `http://www.osl.iu.edu/research/itl/`

To calculate bound states, an eigenvalue problem has to be solved. For small problems, where the full matrix can be stored in memory, Mathematica or the `dsyev` eigensolver in the LAPACK library can be used. For bigger systems, sparse solvers such as the Lanczos algorithm (see appendix A.2) are best. Again there exist efficient implementations[3] of iterative algorithms for sparse matrices.[4]

3.2.4 Variational solutions using a finite basis set

In the case of general potentials, or for more than two particles, it will not be possible to reduce the Schrödinger equation to a one-dimensional problem and we need to employ a PDE solver. One approach will again be to discretize the Schrödinger equation on a discrete mesh using a finite difference approximation. A better solution is to expand the wave functions in terms of a finite set of basis functions

$$|\phi\rangle = \sum_{i=1}^{N} a_i |u_i\rangle. \tag{3.24}$$

To estimate the ground state energy we want to minimize the energy of the variational wave function

$$E^* = \frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle}. \tag{3.25}$$

Keep in mind that, since we only chose a finite basis set $\{|u_i\rangle\}$ the variational estimate E^* will always be larger than the true ground state energy E_0, but will converge towards E_0 as the size of the basis set is increased, e.g. by reducing the mesh size in a finite element basis.

To perform the minimization we denote by

$$H_{ij} = \langle u_i|H|u_j\rangle = \int d\vec{r} u_i(\vec{r})^* \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right) u_j(\vec{r}) \tag{3.26}$$

the matrix elements of the Hamilton operator H and by

$$S_{ij} = \langle u_i|u_j\rangle = \int d\vec{r} u_i(\vec{r})^* u_j(\vec{r}) \tag{3.27}$$

the overlap matrix. Note that for an orthogonal basis set, S_{ij} is the identity matrix δ_{ij}. Minimizing equation (3.25) we obtain a generalized eigenvalue problem

$$\sum_j H_{ij} a_j = E \sum_k S_{ik} a_k. \tag{3.28}$$

or in a compact notation with $\vec{a} = (a_1, \ldots, a_N)$

$$H\vec{a} = ES\vec{a}. \tag{3.29}$$

[3] http://www.comp-phys.org/software/ietl/

[4] Z. Bai, J. Demmel and J. Dongarra (Eds.), *Templates for the Solution of Algebraic Eigenvalue Problems: A Practical Guide* (SIAM, 2000).

If the basis set is orthogonal this reduces to an ordinary eigenvalue problem and we can use the Lanczos algorithm.

In the general case we have to find orthogonal matrices U such that $U^T S U$ is the identity matrix. Introducing a new vector $\vec{b} = U^{-1}\vec{a}$. we can then rearrange the problem into

$$\begin{aligned} H\vec{a} &= ES\vec{a} \\ HU\vec{b} &= ESU\vec{b} \\ U^T HU\vec{b} &= EU^T SU\vec{b} = E\vec{b} \end{aligned} \tag{3.30}$$

and we end up with a standard eigenvalue problem for $U^T H U$. Mathematica and LAPACK both contain eigensolvers for such generalized eigenvalue problems.

Example: the anharmonic oscillator

The final issue is the choice of basis functions. It is advantageous to make use of known solutions to a similar problem as we will illustrate in the case of an anharmonic oscillator with Hamilton operator

$$\begin{aligned} H &= H_0 + \lambda q^4 \\ H_0 &= \frac{1}{2}(p^2 + q^2), \end{aligned} \tag{3.31}$$

where the harmonic oscillator H_0 was already discussed in section 2.4.1. It makes sense to use the N lowest harmonic oscillator eigenvectors $|n\rangle$ as basis states of a finite basis and write the Hamiltonian as

$$H = \frac{1}{2} + \hat{n} + \lambda \hat{q}^4 = \frac{1}{2} + \hat{n} + \frac{\lambda}{4}(a^\dagger + a)^4 \tag{3.32}$$

Since the operators a and $a^\dagger$ are nonzero only in the first sub or superdiagonal, the resulting matrix is a banded matrix of bandwidth 9. A sparse eigensolver such as the Lanczos algorithm can again be used to calculate the spectrum. Note that since we use the orthonormal eigenstates of H_0 as basis elements, the overlap matrix S here is the identity matrix and we have to deal only with a standard eigenvalue problem.

The finite element method

In cases where we have irregular geometries or want higher precision than the lowest order finite difference method, and do not know a suitable set of basis function, the finite element method (FEM) should be chosen over the finite difference method. Since explaining the FEM can take a full semester in itself, we refer interested students to classes on solving partial differential equations.

3.3 The time-dependent Schrödinger equation

Finally we will reintroduce the time dependence to study dynamics in non-stationary quantum systems.

3.3.1 Spectral methods

By introducing a basis and solving for the complete spectrum of energy eigenstates we can directly solve the time-dependent problem in the case of a stationary Hamiltonian. This is a consequence of the linearity of the Schrödinger equation.

To calculate the time evolution of a state $|\psi(t_0)\rangle$ from time t_0 to t we first solve the stationary eigenvalue problem $H|\phi\rangle = E|\phi\rangle$ and calculate the eigenvectors $|\phi_n\rangle$ and eigenvalues ϵ_n. Next we represent the initial wave function $|\psi\rangle$ by a spectral decomposition

$$|\psi(t_0)\rangle = \sum_n c_n |\phi_n\rangle. \tag{3.33}$$

Since each of the $|\phi_n\rangle$ is an eigenvector of H, the time evolution $e^{-i\hbar H(t-t_0)}$ is trivial and we obtain at time t:

$$|\psi(t)\rangle = \sum_n c_n e^{-i\hbar\epsilon_n(t-t_0)} |\phi_n\rangle. \tag{3.34}$$

3.3.2 Direct numerical integration

If the number of basis states is too large to perform a complete diagonalization of the Hamiltonian, or if the Hamiltonian changes over time we need to perform a direct integration of the Schrödinger equation. Like other initial value problems of partial differential equations the Schrödinger equation can be solved by the method of lines. After choosing a set of basis functions or discretizing the spatial derivatives we obtain a set of coupled ordinary differential equations which can be evolved for each point along the time line (hence the name) by standard ODE solvers.

In the remainder of this chapter we use the symbol H to refer the representation of the Hamiltonian in the chosen finite basis set. A forward Euler scheme

$$|\psi(t_{n+1})\rangle = |\psi(t_n)\rangle - i\hbar\Delta_t H|\psi(t_n)\rangle \tag{3.35}$$

is not only numerically unstable. It also violates the conservation of the norm of the wave function $\langle\psi|\psi\rangle = 1$. Since the exact quantum evolution

$$\psi(x, t+\Delta_t) = e^{-i\hbar H\Delta_t}\psi(x,t). \tag{3.36}$$

is unitary and thus conserves the norm, we want to look for a unitary approximant as integrator. Instead of using the forward Euler method (3.35) which is just a first order Taylor expansion of the exact time evolution

$$e^{-i\hbar H\Delta_t} = 1 - i\hbar H\Delta_t + \mathrm{O}(\Delta_t^2), \tag{3.37}$$

we reformulate the time evolution operator as

$$e^{-i\hbar H\Delta_t} = \left(e^{i\hbar H\Delta_t/2}\right)^{-1} e^{-i\hbar H\Delta_t/2} = \left(1 + i\hbar H\frac{\Delta_t}{2}\right)^{-1}\left(1 - i\hbar H\frac{\Delta_t}{2}\right) + \mathrm{O}(\Delta_t^3), \tag{3.38}$$

which is unitary!

This gives the simplest stable and unitary integrator algorithm

$$\psi(x,t+\Delta_t) = \left(1 + i\hbar H\frac{\Delta_t}{2}\right)^{-1}\left(1 - i\hbar H\frac{\Delta_t}{2}\right)\psi(x,t) \tag{3.39}$$

or equivalently

$$\left(1 + i\hbar H\frac{\Delta_t}{2}\right)\psi(x,t+\Delta_t) = \left(1 - i\hbar H\frac{\Delta_t}{2}\right)\psi(x,t). \tag{3.40}$$

Unfortunately this is an implicit integrator. At each time step, after evaluating the right hand side a linear system of equations needs to be solved. For one-dimensional problems the matrix representation of H is often tridiagonal and a tridiagonal solver can be used. In higher dimensions the matrix H will no longer be simply tridiagonal but still very sparse and we can use iterative algorithms, similar to the Lanczos algorithm for the eigenvalue problem. For details about these algorithms we refer to the nice summary at `http://mathworld.wolfram.com/topics/Templates.html` and especially the biconjugate gradient (BiCG) algorithm. Implementations of this algorithm are available, e.g. in the Iterative Template Library (ITL).

3.3.3 The split operator method

A simpler and explicit method is possible for a quantum particle in the real space picture with the "standard" Schrödinger equation (2.52). Writing the Hamilton operator as

$$H = \hat{T} + \hat{V} \tag{3.41}$$

with

$$\hat{T} = \frac{1}{2m}\hat{p}^2 \tag{3.42}$$

$$\hat{V} = V(\vec{x}) \tag{3.43}$$

it is easy to see that $\hat{V}$ is diagonal in position space while $\hat{T}$ is diagonal in momentum space. If we split the time evolution as

$$e^{-i\hbar\Delta_t H} = e^{-i\hbar\Delta_t\hat{V}/2}e^{-i\hbar\Delta_t\hat{T}}e^{-i\hbar\Delta_t\hat{V}/2} + \mathrm{O}(\Delta_t^3) \tag{3.44}$$

we can perform the individual time evolutions $e^{-i\hbar\Delta_t\hat{V}/2}$ and $e^{-i\hbar\Delta_t\hat{T}}$ exactly:

$$\left[e^{-i\hbar\Delta_t\hat{V}/2}|\psi\rangle\right](\vec{x}) = e^{-i\hbar\Delta_t V(\vec{x})/2}\psi(\vec{x}) \tag{3.45}$$

$$\left[e^{-i\hbar\Delta_t\hat{T}/2}|\psi\rangle\right](\vec{k}) = e^{-i\hbar\Delta_t||\vec{k}||^2/2m}\psi(\vec{k}) \tag{3.46}$$

in real space for the first term and momentum space for the second term. This requires a basis change from real to momentum space, which is efficiently performed using a Fast Fourier Transform (FFT) algorithm. Propagating for a time $t = N\Delta_t$, two consecutive

applications of $e^{-i\hbar\Delta_t\hat{V}/2}$ can easily be combined into a propagation by a full time step $e^{-i\hbar\Delta_t\hat{V}}$, resulting in the propagation:

$$\begin{aligned} e^{-i\hbar\Delta_t H} &= \left(e^{-i\hbar\Delta_t\hat{V}/2}e^{-i\hbar\Delta_t\hat{T}}e^{-i\hbar\Delta_t\hat{V}/2}\right)^N + \mathrm{O}(\Delta_t^2) \\ &= e^{-i\hbar\Delta_t\hat{V}/2}\left[e^{-i\hbar\Delta_t\hat{T}}e^{-i\hbar\Delta_t\hat{V}}\right]^{N-1} e^{-i\hbar\Delta_t\hat{T}}e^{-i\hbar\Delta_t\hat{V}/2} \end{aligned} \tag{3.47}$$

and the discretized algorithm starts as

$$\psi_1(\vec{x}) = e^{-i\hbar\Delta_t V(\vec{x})/2}\psi_0(\vec{x}) \tag{3.48}$$

$$\psi_1(\vec{k}) = \mathcal{F}\psi_1(\vec{x}) \tag{3.49}$$

where $\mathcal{F}$ denotes the Fourier transform and $\mathcal{F}^{-1}$ will denote the inverse Fourier transform. Next we propagate in time using full time steps:

$$\psi_{2n}(\vec{k}) = e^{-i\hbar\Delta_t||\vec{k}||^2/2m}\psi_{2n-1}(\vec{k}) \tag{3.50}$$

$$\psi_{2n}(\vec{x}) = \mathcal{F}^{-1}\psi_{2n}(\vec{k}) \tag{3.51}$$

$$\psi_{2n+1}(\vec{x}) = e^{-i\hbar\Delta_t V(\vec{x})}\psi_{2n}(\vec{x}) \tag{3.52}$$

$$\psi_{2n+1}(\vec{k}) = \mathcal{F}\psi_{2n+1}(\vec{x}) \tag{3.53}$$

except that in the last step we finish with another half time step in real space:

$$\psi_{2N+1}(\vec{x}) = e^{-i\hbar\Delta_t V(\vec{x})/2}\psi_{2N}(\vec{x}) \tag{3.54}$$

This is a fast and unitary integrator for the Schrödinger equation in real space. It could be improved by replacing the locally third order splitting (3.44) by a fifth-order version involving five instead of three terms.