

11. Numerical solutions to higher-order linear integral equations

Everything we have done to this point has dealt with integral equations in which there is a single integral, such as

$$\phi(x) = f(x) + \lambda \int_a^x N(x, y) \phi(y) dy \quad (6)$$

We have totally ignored something of the form:

$$\phi(x) = f(x) + \lambda \int_a^x \int_b^y N(x, y, z) \phi(z) dz dy \quad (56)$$

How do we deal with these?

We'll consider what we did with higher-order ODEs and PDEs. The first thing we did was convert nth order ODEs to a system of n first order ODEs. We do that because we already know how to solve systems and the conversion process is easy and requires no intuition. In dealing with IEs, it would serve us well to first see if we could do the same thing.

Let's define

$$\phi_1(x) = \phi(x) \quad (57)$$

$$\phi_2(x, y) = \int_b^y N(x, y, z) \phi(z) dz \quad (58)$$

With these definitions, we see that we have two first-order integral equations,

$$\phi_1(x) = f(x) + \lambda \int_a^x \phi_2(x, y) dy \quad (59)$$

$$\phi_2(x, y) = \int_b^y N(x, y, z) \phi_1(z) dz \quad (60)$$

Very nice. We have effectively reduced the second-order IE to a system of two first-order IEs. However, there is a problem and it is a nontrivial problem. In our transformation, we have introduced partial IEs. Previously, we had only encountered ordinary IEs, whose solutions were a function of a single variable, $\phi(x)$. But in equation (6), we have a partial IE, with a solution which is a function of two variables, $\phi(x, y)$, so we will need to know how to solve them in order to can handle single higher-order ODEs.

There is no way to get around the computational intensity of multidimensional integrals. When we had an integral in one dimension, we were forced to discretize it along y into n intervals and evaluate it at each of those intervals for every value of x. If x is also discretized in n intervals, then we have n^2 function evaluations.

When we have integrals in 2 dimensions, we are forced to discretize it along y and z into n^2 intervals and evaluate it at each of those intervals for every value of x. If x is also discretized in n intervals, then we have n^3 function evaluations.

In general, when we have integrals in m dimensions, we are forced to discretize it into n^m intervals and evaluate it at each of those intervals for every value of x . If x is also discretized in n intervals, then we have n^{m+1} function evaluations.

The trick we used in integrating the single linear integral problem in Section 8. was to use the same discretization for x and y . That allowed us to simultaneously perform the integration along y and the evaluation of ϕ along x , so that instead of n^2 function evaluations, we only had n function evaluations.

In this higher-order IE case, we still want to eliminate one exponent of our evaluations. In the following linear example, we will see that we have to discretize x and z in the same way to eliminate one term from the exponent. However, we cannot use the same trick to collapse the y evaluations onto the x and z evaluations. We are forced to perform n^2 function evaluations.

$$\phi_1(x) = f(x) + \lambda \int_{y_o}^{y_f=x} \phi_2(x, y) dy \quad (61)$$

$$\phi_2(x, y) = \int_{z_o}^{z_f=y} N(x, y, z) \phi_1(z) dz \quad (62)$$

In this linear problem, we have $(n_x + 1)[1 + (n_y + 1)]$ unknowns. $(n_x + 1)$ of these unknowns are $\phi_1(x_i)$ and $(n_x + 1)(n_y + 1)$ of these unknowns are $\phi_2(x_i, y_j)$.

We can rewrite equation (61) using the 1-D trapezoidal rule as:

$$\phi_1(x) = f(x) + \lambda \frac{h_y}{2} \left[\phi_2(x, y_o) + \phi_2(x, y_f(x)) + 2 \sum_{i=2}^{n_y(x)} \phi_2(x, y_i(x)) \right] \quad (63)$$

$$\phi_2(x, y) = \frac{h_z}{2} \left[N(x, y, z_o) \phi_1(z_o) + N(x, y, z_f(y)) \phi_1(z_f(y)) + 2 \sum_{i=2}^{n_z(y)} N(x, y, z_i) \phi_1(z_i) \right] \quad (64)$$

If we have $(n_x + 1)[1 + (n_y + 1)]$ unknowns, then we need $(n_x + 1)$ equations.

We have $(n_x + 1)$ equation of the form of equation (63) where we increment k from 0 to n_x .

$$\phi_1(x_k) = f(x_k) + \lambda \frac{h_y}{2} \left[\phi_2(x_k, y_o) + \phi_2(x_k, y_f(x_k)) + 2 \sum_{i=2}^{n_y(x)} \phi_2(x_k, y_i(x_k)) \right] \quad (65)$$

Remember though that the integral will be zero if $k=0$ because then we are only integrating over a point and not the entire range (This is because the upper limit of integration is variable). Another way of saying that is that if $n_y(x) = 1$, then there is no integral contribution.

We have $(n_x + 1)(n_y + 1)$ equation of the form of equation (64) where we increment k from 0 to n_x and we increment j from 0 to n_y .

$$\phi_2(x_k, y_j) = \frac{h_z}{2} \left[N(x_k, y_j, z_0) \phi_1(z_0) + N(x_k, y_j, z_f(y_j)) \phi_1(z_f(y_j)) + 2 \sum_{i=2}^{n_z(y)} N(x_k, y_j, z_i) \phi_1(z_i) \right] \quad (66)$$

Example. If we divide x in 2 intervals and y into 2 intervals then we will have $(n_x + 1)[1 + (n_y + 1)] = 12$

unknowns and 12 equations. This will be a set of linear algebraic equations which we can solve using the rules of linear algebra.

$$\underline{\underline{A}} \underline{\phi} = \underline{b} \quad (67)$$

where our vector of 12 unknown variables is

$$\underline{\phi} = \begin{bmatrix} \phi_1(x_0) \phi_1(x_1) \phi_1(x_2) \phi_2(x_0, y_0) \phi_2(x_0, y_1) \phi_2(x_0, y_2) \dots \\ \phi_2(x_1, y_0) \phi_2(x_1, y_1) \phi_2(x_1, y_2) \phi_2(x_2, y_0) \phi_2(x_2, y_1) \phi_2(x_2, y_2) \end{bmatrix}^T \quad (68)$$

and where the constant matrix is

$$\underline{b} = [f(x_0) f(x_1) f(x_2) 0 0 0 0 0 0 0 0]^T \quad (69)$$

and where the matrix of constants is

$$\underline{\underline{A}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & a & a & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & a & 2a & a \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ b_{010} & b_{011} & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ b_{020} & 2b_{021} & b_{022} & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ b_{110} & b_{111} & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ b_{120} & 2b_{121} & b_{122} & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ b_{210} & b_{211} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ b_{220} & 2b_{221} & b_{222} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \quad (70)$$

where

$$a = -\lambda \frac{h_y}{2} \quad \text{and} \quad b_{kji} = -\lambda \frac{h_z}{2} N(x_k, y_j, z_i) \quad (71)$$

At this point, it should be clear why we had to use the same discretization for z and x . In the first three equations, the first three unknowns are $\phi_1(x_0) \phi_1(x_1) \phi_1(x_2)$. But in the last nine equations, the first three unknowns are $\phi_1(z_0) \phi_1(z_1) \phi_1(z_2)$. Therefore the discretization of x and z must be identical.

Had the limits of integration been constant rather than functions of x or y (as they were in this example, the only difference would have been that the matrix would have had a slightly different form.

$$\underline{\underline{A}} = \begin{bmatrix} 1 & 0 & 0 & a & 2a & a & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & a & 2a & a & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & a & 2a & a \\ b_{000} & 2b_{001} & b_{002} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ b_{010} & 2b_{011} & b_{012} & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ b_{020} & 2b_{021} & b_{022} & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ b_{100} & 2b_{101} & b_{102} & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ b_{110} & 2b_{111} & b_{112} & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ b_{120} & 2b_{121} & b_{122} & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ b_{200} & 2b_{201} & b_{202} & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ b_{210} & 2b_{211} & b_{212} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ b_{220} & 2b_{221} & b_{222} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \quad (72)$$

12. Numerical solutions to higher-order nonlinear integral equations

As in the linear case, we reduce the nth-order IE to a system of first-order IEs.

$$\phi(x) = f(x) + \lambda \int_a^x \int_b^y F[x, y, z, \phi(z)] dz dy \quad (12.1)$$

How do we deal with these?

We'll consider what we did with higher-order ODEs and PDEs. The first thing we did was convert nth order ODEs to a system of n first order ODEs. We do that because we already know how to solve systems and the conversion process is easy and requires no intuition. In dealing with IEs, it would serve us well to first see if we could do the same thing.

Let's define

$$\phi^{(1)}(x) = \phi(x) \quad (12.2)$$

$$\phi^{(2)}(x, y) = \int_b^y F[x, y, z, \phi(z)] dz \quad (12.3)$$

With these definitions, we see that we have two first-order integral equations,

$$\phi^{(1)}(x) = f(x) + \lambda \int_a^x \phi^{(2)}(x, y) dy \quad (12.4)$$

$$\phi^{(2)}(x, y) = \int_b^y F[x, y, z, \phi^{(1)}(z)] dz \quad (12.5)$$

At this point we have a system of first-order IEs, but again, just as in the linear case, the second IE (equation (12.5)) is not of the usual form since $\phi^{(2)}(x, y)$ is a function of two variables.

Just as was the case in Section 9. when we had a single first-order IE, where we had two choices for solving the IE, so too when we have a system of nonlinear IEs, do we still have two choices. The first choice is to use the trapezoidal approximation as was done in the linear case and solve the resulting system of nonlinear algebraic equations using some technique for solving systems of nonlinear algebraic equations, like the multivariate Newton-Raphson method. The derivation of this method follows that outlined in Section 11.

The second method for solving a nonlinear integral equation is the method of successive approximations. Again, referring to Pogorzelski [page 192], we see that equation (4)

$$\phi(x) = f(x) + \lambda \int_a^x F[x, y, \phi(y)] dy \quad (4)$$

can be solved using the recursive relation

$$\phi_i(x) = f(x) + \lambda \int_a^x F[x, y, \phi_{i-1}(y)] dy \quad (52)$$

You repeat this procedure until $|\phi_{i+1}(x) - \phi_i(x)|$ is acceptably small. The only additional information needed for this method is the starting point

$$\phi_0(x) = f(x) \quad (53)$$

We know that we can apply this technique if we just had a system with unknowns $\{\phi^{(i)}(x)\}$. What we have above is a system with unknowns $\{\phi^{(i)}(x, y)\}$.

At this point, the solution is to discretize in x and y and z, using the same discretization for x and z.

We use initial estimates for $\{\phi^{(i)}(x, y)\}$

$$\phi^{(1)}_0(x) = f(x) \quad (12.6)$$

Then, repeated, alternating applications of

$$\phi^{(2)}_i(x, y) = \int_b^y F[x, y, z, \phi^{(1)}_i(z)] dz \quad (12.7)$$

and

$$\phi^{(1)}_{i+1}(x) = f(x) + \lambda \int_a^x \phi^{(2)}_i(x, y) dy \quad (12.8)$$

will eventually converge to the solution for $\{\phi^{(i)}(x, y)\}$.

The storage matrix for $\phi^{(1)}_{i+1}(x)$ must be the size of the discretization of x, namely, $n_x + 1$. The storage matrix for the discretization of $\phi^{(2)}_i(x, y)$ must be of size $(n_x + 1)(n_y + 1)$.

13. Numerical solutions to multivariate integral equations

Everything we have done to this point has dealt with ordinary or single-variable integral equations, where the solution was, $\phi(x)$. When we encountered higher-order OIEs, we were forced to create a system of first-order IEs, some of which turned out to have unknowns of the form $\phi(x, y)$.

This fact of integral equations should be contrasted with that of differential equations. When we have an nth-order ODE, we can reduce it to a system of n first-order ODEs. PDEs do not appear in the transformation. However, when we have an nth-order OIE, we end up reducing it to a system of n first-order OIEs and PIEs, as shown in sections 11 and 12. Now, PIEs appear on there own as well, and not just as a result of the reductive transformation of a higher order OIE.

Here is an example of a linear PIE first order in both x and y:

$$\phi(x, y) = f(x, y) + \lambda_1 \int_b^y N_1(x, y, z) \phi(x, z) dz + \lambda_2 \int_a^x N_2(x, y, w) \phi(w, y) dw \quad (13.1)$$

Here are two examples of nonlinear PIEs, first order in both x and y:

$$\phi(x, y) = f(x, y) + \lambda_1 \int_b^y F_1[x, y, z, \phi(x, z)] dz + \lambda_2 \int_a^x F_2[x, y, w, \phi(w, y)] dw \quad (13.2)$$

$$\phi(x, y) = f(x, y) + \frac{\lambda \int_b^y F_1[x, y, z, \phi(x, z)] dz}{\lambda_2 \int_a^x F_2[x, y, w, \phi(w, y)] dw} \quad (13.3)$$

We already know how to solve both of these situations from Section 11. and Section 12. If we have a linear equation, we discretize along x and y. We choose the same discretization along y and z because they are both the second arguments in $\phi(x, y)$ or $\phi(x, z)$. That way, we don't have to evaluate these functions more than once. Similarly, we choose the same discretization along x and w because they are both the first arguments in $\phi(x, y)$ or $\phi(w, y)$. Then, still for the linear case, we can substitute into equation (13.1) using the trapezoidal rule, as was done in Section 11. This results in $(n_x + 1)(n_y + 1)$ linear algebraic equations which we can solve as we did in Section 11.

If the PIE is nonlinear as is the case in equations (13.2) and (13.3) then we can solve it as we did in Section 12, using successive approximations in two dimensions. We begin with

$$\phi_0(x, y) = f(x, y) \quad (13.4)$$

And we keep plugging into equation (13.2) until $\phi(x, y)$ no longer changes. The discretization again results in $(n_x + 1)(n_y + 1)$ points.

14. Applications of integral equations

In Moiseiwitsch's book, a concise history of integral equations is given.

Integral equations have uncountable applications. In my mind, these applications come under two categories. Linz cites two reasons for the interest in integral equations: "In some cases, as in the work of Abel on tautochrone curves, integral equations are the natural mathematical model for representing a physically interesting system. The second and perhaps more common reason is that integral operators, transforms, and equations, are convenient tools for studying differential equations." These, then, are my two categories. The first category includes systems which are naturally and exclusively described by integral equations. Under this category are applications like:

- pair correlation functions of an inhomogeneous fluid (the Ornstein-Zernike closure)
- density distributions of an inhomogeneous fluid (the Yvon-Born-Green hierarchy)
- the renewal equation (history dependent problems in component failure analysis)
- population dynamics (Volterra integral equation)
- systems theory (circuits, feedback, process control, computer systems; convolution integrals)
- problems of experimental inference (obtaining data profiles from noisy external measurements)
- tautochrone curves (Abel's integral equation)
- viscoelasticity
- epidemics
- superfluidity
- damped vibrations

The second category of applications includes systems which can be described by either differential equations (ODEs or PDEs) or by integral equations. As engineers, we are not so interested in these latter types of problems since we already know how to solve ODEs and PDEs. We are not out looking for more trouble.

Many (but not all) ODEs and PDEs can be reframed as IEs. Both initial-value and boundary-value ODEs can be converted into IEs. Elliptic, parabolic, and hyperbolic PDEs can all be converted into integral equations. Given this fact, one can see that just about everything in the universe can be represented by an integral equation. The heat equation and the diffusion (parabolic PDEs) can be solved as integral equations. The wave equation (a hyperbolic PDE) can be solved as an integral equation. Poisson's equation (an elliptic PDE) can be solved as an integral equation. To make a list of them all is pointless. All I would like to do is reiterate that we already know how to solve these problems when they are formulated as differential equations. We should do alright by that.

If you want to see the heat equation reframed as an integral equation, check out Linz, Chapter 2. It's nasty. All of the physical intuition an engineer has about the individual terms in the heat and diffusion PDEs are not apparent in the integral equation formulation.

Example #1: The Ornstein-Zernike closure

Our goal is to determine the density distribution of a fluid in the influence of an arbitrary external potential. The Ornstein-Zernike closure for open, isothermal systems formulates the equations as

$$g^{(2)}(\underline{r}, \underline{r}') - 1 = C^{(2)}(\underline{r}, \underline{r}') + \int C^{(2)}(\underline{r}, \underline{r}'') n^{(1)}(\underline{r}'') [g^{(2)}(\underline{r}'', \underline{r}') - 1] d^3 \underline{r}'' \quad (13.1)$$

where

$$g^{(2)}(\underline{r}, \underline{r}') = \frac{n^{(2)}(\underline{r}, \underline{r}')}{n^{(1)}(\underline{r}) n^{(1)}(\underline{r}')} \text{ is the pair correlation function}$$

$$C^{(2)}(\underline{r}, \underline{r}') \text{ is the direct correlation function}$$

$$n^{(1)}(\underline{r}) \text{ is the singlet density distribution}$$

Unfortunately in equation (13.1), we have 1 equation and 3 unknowns $g^{(2)}(\underline{r}, \underline{r}')$, $n^{(1)}(\underline{r})$, and $C^{(2)}(\underline{r}, \underline{r}')$. Some external constitutive information must be provided. One such approximation is called the Percus-Yevick approximation, namely that the direct correlation function is given by

$$C^{(2)}(\underline{r}, \underline{r}') = \left[1 - e^{\frac{u(\underline{r})}{kT}} \right] g^{(2)}(\underline{r}, \underline{r}') \quad (13.2)$$

and that the fluid is homogeneous (which is equivalent to saying that the singlet density is constant)

$$n^{(1)} = \rho \cdot MW = \text{constant} \quad (13.3)$$

With these substitutions, equation (13.1) becomes

$$g^{(2)}(\underline{r}, \underline{r}') - 1 = \left[1 - e^{\frac{u(\underline{r})}{kT}} \right] g^{(2)}(\underline{r}, \underline{r}') + \int \left[1 - e^{\frac{u(\underline{r})}{kT}} \right] g^{(2)}(\underline{r}, \underline{r}'') n^{(1)} [g^{(2)}(\underline{r}'', \underline{r}') - 1] d^3 \underline{r}'' \quad (13.4)$$

If we make the change of variable,

$$\underline{R} = \underline{r} - \underline{r}' \text{ and } \underline{R}' = \underline{r} - \underline{r}'' \text{ then we can rewrite equation (13.4) as}$$

$$g^{(2)}(\underline{R}) = e^{-\frac{u(\underline{R})}{kT}} + n^{(1)} e^{-\frac{u(\underline{R})}{kT}} \int \left[1 - e^{\frac{u(\underline{R})}{kT}} \right] g^{(2)}(\underline{R}') [g^{(2)}(\underline{R} - \underline{R}') - 1] d^3 \underline{R}' \quad (13.5)$$

Equation (13.5) is a nonlinear third-order ordinary integral equation. It is third-order because we have three integrals. It is ordinary because our unknown, $g^{(2)}(\underline{R})$, is a function of only one variable, $\underline{R}$. We should know how to solve this. First we identify what type of equation we have. A Fredholm integral equation, in which the limits of integration are fixed, of the second kind, has the form:

$$\phi(x) = f(x) + \lambda \int_a^b N(x, y) \phi(y) dy \quad (7)$$

If we make the identifications

$$\begin{aligned} x &= \underline{R} & y &= \underline{R}' & f(x) &= e^{-\frac{u(\underline{R})}{kT}} & \lambda(x) &= n^{(1)} e^{-\frac{u(\underline{R})}{kT}} \\ N(x, y) &= \left[1 - e^{-\frac{u(\underline{R})}{kT}} \right] \left[g^{(2)}(|\underline{R} - \underline{R}'|) - 1 \right] & \phi(x) &= g^{(2)}(\underline{R}) \end{aligned}$$

then we can rewrite equation (13.5) as

$$g^{(2)}(\underline{R}) = e^{-\frac{u(\underline{R})}{kT}} + n^{(1)} e^{-\frac{u(\underline{R})}{kT}} \int \left[1 - e^{-\frac{u(\underline{R})}{kT}} \right] g^{(2)}(\underline{R}') \left[g^{(2)}(|\underline{R} - \underline{R}'|) - 1 \right] d^3 \underline{R}' \quad (13.5)$$

$$\phi(x) = f(x) + \lambda(x) \int_a^b N(x, y, \phi) \phi(y) dy \quad (13.6)$$

which is a Fredholm equation of the second kind with two differences. First $\lambda(x)$ is not a constant but a function of x . [Does this invalidate the analytical solution?] This doesn't really affect the numerical solution except that it makes the elements of the matrix A in equations (44) and (45) functions of x . The other difference is that the kernel is now a function of the unknown, $N(x, y, \phi)$ instead of $N(x, y)$. This presents a problem for an analytical solution but again doesn't affect the problem for the numerical solution.

If we consider that we neglect the angular components of the problem and reduce our dimensionality to a one-dimension system described by the radius vector, then we can rewrite equation (13.6) as a nonlinear first-order ordinary integral equation:

$$\phi(x) = f(x) + 4\pi\lambda(x) \int_a^b N(x, y, \phi) \phi(y) y^2 dy \quad (13.7)$$

or

$$\phi(x) = f(x) + \lambda'(x) \int_a^b N'(x, y, \phi) \phi(y) dy \quad (13.8)$$

where

$$\lambda'(x) = 4\pi\lambda(x) \quad \text{and} \quad N'(x, y, \phi) = N(x, y, \phi) y^2$$

Equation (13.8) we should be able to solve numerically, in a straightforward manner.

Example #2: The Yvon-Born-Green (YBG) Hierarchy for open, isothermal systems

Our goal is to determine the density distribution of a fluid in the influence of an arbitrary external potential. The Yvon-Born-Green (YBG) Hierarchy for open, isothermal systems formulates the equations as

$$-kT\nabla_{r_i} n^{(s)} = \left[\nabla_{r_i} u^e(\underline{r}_i) + \sum_{j \neq i}^s \nabla_{r_i} u(r_{ij}) \right] n^{(s)} + \int \nabla_{r_i} u(r_{i,s+1}) n^{(s+1)} d^3 r_{s+1} \quad (13.9)$$

where

k is Boltzmann's constant

T is the temperature

S is the number of atoms for which we want the density distribution

$n^{(s)}$ is the density distribution of s atoms

$\underline{r}_i$ is the position of the i th atom in 3-D real space

$r_{ij} = |\underline{r}_i - \underline{r}_j|$ is the magnitude of the separation between the i th and j th atom

$u^e(\underline{r}_i)$ is the external potential experienced by the i th atom

$u(r_{ij})$ is the pairwise interaction potential between atoms

Equation (13.1) can be written for $s = 1, 2, 3, \dots, N$ so that it forms a system of N integrodifferential equations, where N is the number of atoms and is usually on the order of Avogadro's number. The system of equations is called a hierarchy because it gives $n^{(s)}$ as a function of $n^{(s+1)}$, so that the singlet density distribution is a function of the doublet density distribution, which is a function of the triplet density distribution, etc. We are forced to use some approximation to end the system of equations somewhere. Various approximations have been developed and are still being developed. One of the earliest approximations is called the superposition principle, which says that the triplet density distribution, $n^{(s=3)}$, can be expressed as a product of the 3 doublet density distributions, $n^{(s=2)}$, normalized by the singlet density distributions:

$$n^{(3)}(\underline{r}, \underline{r}', \underline{r}'') = \frac{n^{(2)}(\underline{r}, \underline{r}') n^{(2)}(\underline{r}', \underline{r}'') n^{(2)}(\underline{r}, \underline{r}'')}{n^{(1)}(\underline{r}) n^{(1)}(\underline{r}') n^{(1)}(\underline{r}'')} \quad (13.10)$$

If we explicitly write equation (13.1) for $s=1$ and $s=2$, we have

$$-kT\nabla_{r_i} n^{(1)}(\underline{r}) = \nabla_{r_i} u^e(\underline{r}) n^{(1)}(\underline{r}) + \int \nabla_{r_i} u(|\underline{r} - \underline{r}'|) n^{(2)}(\underline{r}, \underline{r}') d^3 \underline{r}' \quad (13.11)$$

$$-kT\nabla_{r_i} n^{(2)}(\underline{r}, \underline{r}') = \left[\nabla_{r_i} u^e(\underline{r}) + \nabla_{r_i} u(|\underline{r} - \underline{r}'|) \right] n^{(2)}(\underline{r}, \underline{r}') + \int \nabla_{r_i} u(|\underline{r} - \underline{r}''|) n^{(3)}(\underline{r}, \underline{r}', \underline{r}'') d^3 \underline{r}'' \quad (13.12)$$

Equations (13.2)-(13.4) form a closed set of three integrodifferential equations which can be solved for the three unknowns, the singlet, doublet, and triplet density distributions. Frequently, people just substitute 13.2 into 13.4 so that there is a system of 2 integrodifferential equations which can be solved for the two unknowns, the singlet and doublet density distributions.

$$\begin{aligned} -kT\nabla_{r_i} n^{(2)}(\underline{r}, \underline{r}') &= \left[\nabla_{r_i} u^e(\underline{r}) + \nabla_{r_i} u(|\underline{r} - \underline{r}'|) \right] n^{(2)}(\underline{r}, \underline{r}') \\ &+ \int \nabla_{r_i} u(|\underline{r} - \underline{r}''|) \frac{n^{(2)}(\underline{r}, \underline{r}') n^{(2)}(\underline{r}', \underline{r}'') n^{(2)}(\underline{r}, \underline{r}'')}{n^{(1)}(\underline{r}) n^{(1)}(\underline{r}') n^{(1)}(\underline{r}'')} d^3 \underline{r}'' \end{aligned} \quad (13.13)$$

So that the system of integrodifferential equations formed by (13.3) and (13.5) is closed.

This system of equations was solved the case where $u^e(r_i) = 0$, $u(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma^{12}}{r^{12}} \right) - \left(\frac{\sigma^6}{r^6} \right) \right]$, and

$n^{(1)} = \rho \cdot MW = \text{constant}$ for gaseous argon by Kirkwood et al. (1952) and later by many others including Kerins et al. (1986) who used a finite element method.

In this class, we have not developed specific tools to solve this problem. We have developed the tools which would be modified to solve the problem. As the problems get this complex, people are forced to develop their own tools to solve the problem. Part of earning a Ph.D. in a field like this is the development of a numerical method which can solve the problem.

15. Sources for more information on integral equations

Where can I find out more about integral equations?

The University Library has shelves and shelves of books on integral equations. Unfortunately, many of those books have two faults. First, the books are not textbooks but reference books. Therefore, they are not written to teach someone about integral equations, who has no previous knowledge of them. These books lack introductions and begin somewhere in the middle of integral equation analysis, pursuing details which are interesting to the various authors. The second shortcoming of these books is that most of them are written by mathematicians in what I perceive as mathematical jargon. We have all taken courses in calculus and differential equations. We have all the tools we need to handle integral equations. However, when you start reading these books, a lot of the texts are difficult or impossible to understand because they abandon the “jargon” we learned for calculus and ODEs and invent new jargon.

Much of the purpose in my retyping this material is simply to translate the key ideas of integral equations into language that the graduate level engineer is already familiar with and can easily digest. The discussion presented here is a summary of discussions in several texts.

For the best, most easily understandable to the non-mathematician introduction, consult:

Pogorzelski, W., “Integral Equations and their Applications”, Volume I, Polish Scientific Publishers/Pergamon Press, Warsaw/Oxford, 1966.

Also relatively clear texts are

Moiseiwitsch, B.L., “Integral Equations”, Longman Mathematical Texts, London, 1977.

Lovitt, William V., “Linear Integral Equations”, McGraw-Hill, New York, 1924.

For numerical solution techniques to integral equations, consult

Linz, Peter, “Analytical and Numerical Methods for Volterra Equations”, SIAM, Philadelphia, 1985.

Atkinson, Kendall E., “The Numerical Solution of Integral Equations of the Second Kind”, Cambridge University Press, Cambridge, 1997.

These books have numerous references to other texts.