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Solution of the Ornstein–Zernike Equation for a Soft-Core Yukawa Fluid. II. Numerical Results

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Numerical calculations are reported for the simplest case of the soft-core Yukawa fluid introduced in an earlier paper. Attention is given to the thermodynamic behavior, the correlation functions, and the interparticle potentials found by inverting the structural information using Percus–Yevick and hypernetted chain integration equation approximations.

KEY WORDS: Ornstein–Zernike theory; soft-core fluids; Yukawa closure; Baxter's factorization.

1. INTRODUCTION

In a recent paper[1] [hereafter referred to as I; equations from I are referred to as (I.1), etc.] a model fluid was proposed in which the direct correlation function $c(x)$ was assumed to be of Yukawa form, viz.

$$c(x) = \sum_{j=1}^{N} \frac{K_j e^{-z_j(x-1)}}{x}, \qquad x > 1 \tag{1}$$

where K_j and z_j are the Yukawa parameters and x is the interparticle separation scaled with respect to a range parameter R. On the domain $x < 1$ the effect of a soft-core potential was introduced by assuming that the total correlation function $h(x)$ could be represented by

$$h(x) = -1 + \sum_{i=1}^{M} \frac{\alpha_i \lambda_i^2}{\cosh \lambda_i} \left(\frac{\sinh \lambda_i x}{\lambda_i x} - 1 \right), \qquad 0 < x < 1 \tag{2}$$

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the parameters α_i and λ_i being arbitrary. Subject to the constraints (1) and (2) the Ornstein–Zernike (OZ) equation,[2]

$$h(|\mathbf{r}|) = c(|\mathbf{r}|) + \rho \int h(|\mathbf{r} - \mathbf{s}|)c(|\mathbf{s}|)\, d\mathbf{s} \tag{3}$$

where ρ is the number density, was solved using the Weiner–Hopf or "finite-range transformation" first derived by Baxter[3,4] with the assumption $c(x) = 0$, $x > 1$. This method was subsequently adapted by other workers for the case of the hard-core Yukawa fluid (HCYF),[5–7] which in the mean spherical approximation (MSA) yields a condition for $c(x)$ of the form given in Eq. (1), when the parameters K_j are identified as varying inversely with absolute temperature T.

In I, the OZ equation [Eq. (3)] was decoupled into two separate equations for $h(x)$ and $c(x)$, given by

$$xh(x) = -q'(x) + 12\eta \int_0^\infty (x - t)h(|x - t|)q(t)\, dt \tag{4}$$

$$xc(x) = -q'(x) + 12\eta \int_x^\infty q'(t)q(t - x)\, dt \tag{5}$$

where $\eta = \pi\rho R^3/6$ is the reduced density and the function $q(x)$ is given by

$$q(x) = q_0(x) + \sum_{j=1}^{N} \beta_j e^{-z_j(x-1)}, \qquad x > 0 \tag{6}$$

$$q_0(x) = \begin{cases} q_{sc}(x) + \displaystyle\sum_{j=1}^{M} \beta_j d_j (1 - e^{-z_j(x-1)}), & 0 < x < 1 \\ 0, & \text{otherwise} \end{cases} \tag{7}$$

and

$$q_{sc} = Q_1(x - 1) + \frac{Q_2}{2}(x^2 - 1) + \sum_{i=1}^{M} \left[Q_{i1}(\cosh\lambda_i x - \cosh\lambda_i) + Q_{i2}(\sinh\lambda_i x - \sinh\lambda_i) \right], \qquad 0 < x < 1 \tag{8}$$

The subscript "sc" indicates that part of $q(x)$ arising from the soft-core condition, Eq. (2). The parameters β_j and d_j are given by

$$\beta_j = \frac{K_j}{z_j[1 - 12\eta\tilde{q}(z_j)]} \tag{9}$$

and

$$d_j = 1 - \frac{12\eta}{z_j}\left[\tilde{g}(z_j) + \frac{\gamma - 1}{z_j^2} - \sum_{i=1}^{M} \frac{\Delta_i \lambda_i^2}{z_j^2 - \lambda_i^2} \right] \tag{10}$$

where

$$\Delta_i = \alpha_i / \cosh \lambda_i \tag{11}$$

and

$$\gamma = 1 + \sum_{i=1}^{M} \Delta_i \lambda_i^2 \tag{12}$$

The quantities $\tilde{q}(s)$ and $\tilde{g}(s)$ are the Laplace transforms of $q(x)$ and $xg(x)$, respectively. The function $g(x) = h(x) + 1$ is the radial distribution function. The details of this analysis are given in I. The $2M + 2 + N$ coefficients Q_1, Q_2, Q_{i1}, Q_{i2}, d_j are given in terms of the β_j ($j = 1, \ldots, N$) by $2M + 2$ linear equations obtained by substituting the form of $q(x)$ into Eqs. (4) and N linear equations obtained from (9) [see Eqs. (I.23)–(I.28)]. The remaining N nonlinear equations for the β_j may be obtained using the alternate expressions for $\tilde{g}(s)$ given in I [see Eqs. (I.26)–(I.35)].

In this paper we report numerical calculations for the simplest case of our model, namely, $M = N = 1$, which we refer to as the soft-core Yukawa fluid (SCYF). This case is interesting in that the results for the SCYF may be compared directly with those for the HCYF[6,7] using the same form of $c(x)$. In this way the consequences of introducing the soft core may be investigated directly. In addition, the SCYF is of interest since all solution parameters may be calculated explicitly, as we are able to derive a quartic equation for the parameter $\beta = \beta_1$ similar in form to that for the HCYF.[6,7] In Section 2 we outline the numerical procedure used to determine the solution parameters Q_1, Q_2, Q_{11}, Q_{12}, β, and d ($= d_1$), and also the scheme adopted for assigning the parameters α ($= \alpha_1$), λ ($= \lambda_1$), K ($= K_1$), and z ($= z_i$).

In Section 3 we discuss the nature of the gas–liquid transition; in Section 4 some comments are made regarding the high-density singularity in inverse compressibility. Section 5 is concerned with features of the radial distribution function. Finally in Section 6 we examine the potentials found by inverting the Percus–Yevick (PY)[8] and hypernetted chain (HNC)[9] integral equation approximations.

2. NUMERICAL PROCEDURE FOR THE SCYF

We begin by describing in outline the derivation of the quartic equation for β. From Eqs. (I.24), (I.25), (I.27), and (I.28) we may derive four linear equations for Q_1, Q_2, Q_{11}, Q_{12} in terms of β and d (which in turn depend on α, λ, K, and ξ, the SCYF parameters). This equation may be

written in the form

$$\mathbf{M}\begin{bmatrix} Q_1 \\ Q_2 \\ y \\ w \end{bmatrix} = \mathbf{L}_0 + \beta \mathbf{L}_1 + \beta d \mathbf{L}_2 \tag{13}$$

where

$$y = Q_{11}, \qquad w = e^{\lambda}(Q_{11} + Q_{12})/2 \tag{14}$$

and expressions for the matrix $\mathbf{M}$ and column vectors $\mathbf{L}_i$ ($i = 0, 1, 2$) (which do not contain terms in β for βd) are given in the Appendix. Multiplying Eq. (13) by $\mathbf{M}^{-1}$, we obtain expansion for the quantities Q_1, Q_2, y, and w, viz.

$$\begin{bmatrix} Q_1 \\ Q_2 \\ y \\ w \end{bmatrix} = \begin{bmatrix} A_{10} \\ A_{20} \\ A_{30} \\ A_{40} \end{bmatrix} + \beta \begin{bmatrix} A_{11} \\ A_{21} \\ A_{31} \\ A_{41} \end{bmatrix} + \beta d \begin{bmatrix} A_{12} \\ A_{22} \\ A_{32} \\ A_{42} \end{bmatrix} \tag{15}$$

where

$$\begin{bmatrix} A_{1i} \\ A_{2i} \\ A_{3i} \\ A_{4i} \end{bmatrix} = \mathbf{M}^{-1}\mathbf{L}_i \tag{16}$$

Using these expansions in Eq. (9), we find that

$$d = \frac{(-K + D\beta)e^{-\xi} + E\beta^2}{G\beta^2} \tag{17}$$

where the parameters D, E, and G may be expressed in terms of the parameters A_{ij}, ξ, and λ. We then note that Eqs. (9) and (10) may be written as

$$\frac{\beta z}{K} = \frac{1}{[1 - 12\eta\tilde{q}(z)]} \tag{18}$$

$$d = 1 - \frac{12\eta}{z}\left[\frac{F(z)}{[1 - 12\eta\tilde{q}(z)]} + \frac{\gamma - 1}{z^2} + \frac{\Delta\lambda^2}{z^2 - \lambda^2}\right] \tag{19}$$

where $F(z)$ is given by Eq. (I.35b). Substitution of Eq. (18) into Eq. (19), and using Eq. (17) for the parameter d in Eqs. (15) and (19), we are able to

derive a quartic equation for the parameter β whose coefficients depend only on the parameters A_{ij}, D, E, and G, which are easily calculated numerically and depend only on α, λ, K, and ξ. This quartic is analogous to that found in the case of the HCYF.[6,7]

Hence, given the parameters α, λ, K, ξ, and density η it is straightforward to find β (since there exist analytic formulas for the roots of quartic polynomials.[10] Using Eq. (17) and (15), it is then possible to find Q_1, Q_2, Q_{11}, Q_{12}, and d. It should be pointed out at this point that, using the above method, we will be able to derive a quartic for the parameter β for arbitrary M [cf. Eq. (2)], since the only difference in the above analysis is that the matrix M will be $(2 + 2M) \times (2 + 2M)$ for arbitrary M.

We now turn our attenttion to the problem of assigning values to the parameters α, λ, K, and ξ. In the MSA for the HCYF,[6,7] ξ is considered fixed, and K varies inversely with temperature. Since the MSA has not been definitely extended to soft-core fluids,[11] it is not possible to identify K as varying inversely with temperature; however, it is reasonable to suggest that increasing K corresponds in some fashion to decreasing T, the precise nature of this dependence being obscure. Some thought must also be given to the parameters α and λ. Again we find that it is not possible, within some established integral equation approximation such as PY, MSA, or HNC, to make definitive statements about the state dependence of α and λ. However, it is clear that one condition we would impose on the choice of α, λ, K, and ξ is that $h(x)$ be continuous at $x = 1$, so that the correlation functions being studied correspond to some continuous potential.

For the purposes of this paper we have chosen a rather ad hoc approach to the choice of parameters α, λ, K, and ξ. We choose λ and ξ as fixed, and determine α from the criterion that $h(r)$ be continuous. From Eqs. (4) and (7), this is equivalent to insisting that

$$q_0'(1) = 0 \tag{20}$$

We describe the behavior of the solution along lines of constant K, hence assuming a quasi-MSA approximation for $c(x)$. The results we have obtained reflect, to some extent, the artificiality of assigning the parmeters in the manner described above. On the other hand, we expect that the general features of the phase behavior of the model fluid will be retained using a more complicated assignment scheme, such as that described in I (Section 3.1). (Note that, in terms of the description given in Section 3.1 of I, we are investigating the use of the SCYF in the model sense.) Clearly such a study is a necessary precursor to understanding the difficulties in higher-order problems (which allow greater state dependence in the parameters α, λ, K, and ξ than that assumed in this paper).

3. THE GAS–LIQUID TRANSITION

The SCYF transition may be described conveniently in terms of the parameter β in the same way that the gas–liquid transition was described for the HCYF.[6,7] In Fig. 1a the SCYF parameter β is plotted against reduced density η for $\lambda = 10$, $\xi = 2$ at varying values of K. For comparison the β diagram for the HCYF is shown in Fig. 1b with the same values of K

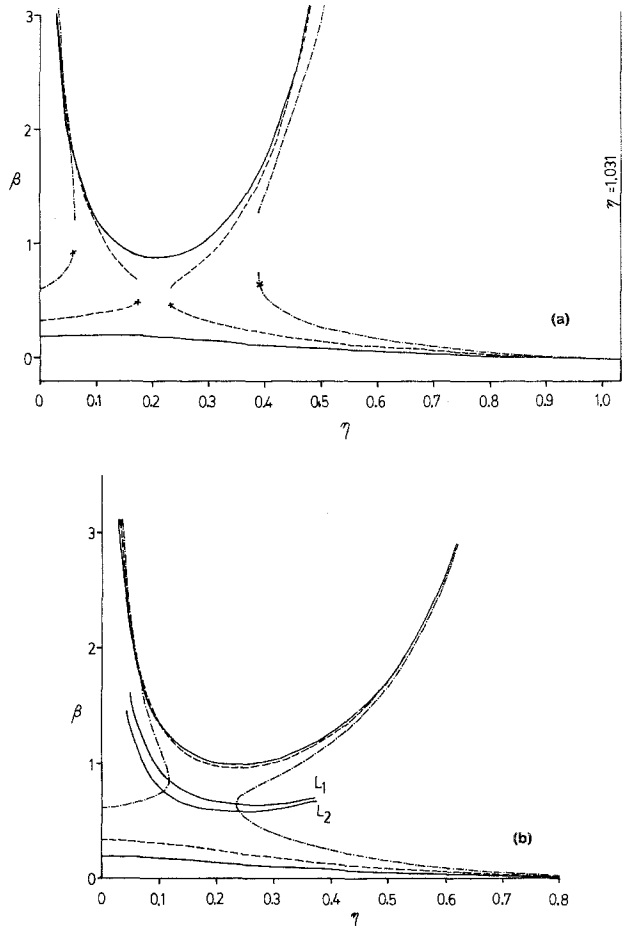

Fig. 1. (a) Behavior of the parameter β as a function of density η for the SCYF vith $\lambda = 10$, $\xi = 2$, and $K = 1.218$ (-·-), $K = 0.66$ (- - -), and $K = 0.4$ (——). The crosses represent points at which $\hat{Q}(0) = 0$. (b) Behavior of the parameter β as a function of density η for the HCYF with $\xi = 2$ and $K = 1.218$ (-·-), $K = 0.66$ (- - -), and $K = 0.4$ (——). The line L_1 represents the locus of points for which the physical and nonphysical values of β coincide. The line L_2 represents the locus of points for which $\hat{Q}(0) = 0$.

and ξ. In general the quartic for β has two real roots, as in the HCYF. In Fig. 1b the line L_1 represents the locus of points at which the two real roots are equal. The physical solutions for β are given by the lower branch of the K isotherms. The line L_2 is the locus of points at which $\hat{Q}(0) = 0$. Since the isothermal compressibility χ_T is given by (where k is Boltzmann's constant)

$$\rho kT\chi_T = 1/[\hat{Q}(0)]^2 \tag{21}$$

the line L_2 corresponds to points of infinite compressibility, and hence specifies the spinodal curve for the liquid–gas transition.[6,7]

For the SCYF we were unable to find the line corresponding to the locus L_1. Numerically, Eq. (20) corresponds to a single nonlinear equation for the parameter α, since all other parameters are calculated explicitly for a given value of α. We were unable to find values of α satisfying Eq. (20) such that the two roots of the quartic were equal. However, this is not a crucial defect since before this numerical breakdown, on any given K "isotherm" $\hat{Q}(0)$ becomes zero at accessible densities and thus we are able to specify a spinodal curve analogous to the locus L_2 in Fig. 1b. The SCYF gas–liquid transition densities are marked with crosses in Fig. 1a. As expected, the interpenetration of particles allowed by the inclusion of a soft core has the effect of widening the domain of densities lying in the gas–liquid coexistence region for a given isotherm. In addition, the $K = 0.66$ "isotherm," which is supercritical for the HCYF, has become subcritical in the SCYF as a direct result of the increased compressibility.

4. HIGH-DENSITY SINGULARITY IN $\hat{Q}(0)$

In common with the HCYF and other hard-core models of simple fluids,[4] there is a high-density singularity in the inverse compressibility $[\hat{Q}(0)^2]$ for the SCYF. In the case of the HCYF, this high-density singularity occurs at the unphysical value $\eta = 1.0$ and is independent of the parameters K and z in the Yukawa form for $c(r)$. Similarly, we find that for the SCYF, $\hat{Q}(0) \to \infty$ ($\beta \to 0$) at a density η_s which is also independent of the parameters K and z in the assignment scheme used in this paper. However, η_s is a function of λ. For $\lambda = 10$, $\eta_s = 1.031$, and this is shown in Fig. 1a. The density η_s was found to decrease with decreasing λ (See Table I).

For $\lambda < 6.5$ the numerical procedure described in Section 2 failed at a density lower than the expected η_s. That is, it was not possible to find a value of α satisfying Eq. (20) when the solution to the quartic is $\beta = 0$ $[\hat{Q}(0) \to \infty]$. This point illustrates the need for a more appropriate scheme for specifying λ as a function of K, ξ, and η.

Table I. Variation of the Density η_s with λ for Fixed $K = 1.218$ and $\xi = 2$, Together with the Corresponding Value of α

λ	η_s	α
15	1.035	0.79
10	1.031	0.6
7	0.975	0.52
6.5	0.95	0.515

5. THE RADIAL DISTRIBUTION FUNCTIONS

In Fig. 2 we have plotted the radial distribution function (rdf) for the subcritical value of $K = 1.218$, $\lambda = 10$, and $\xi = 2$ at densities covering the whole fluid range. The relevant values of β lie on the broken curve in Fig. 1a. At $\eta = 0.04$ we are below the gas–liquid transition density and $g(r)$ is typical of the gas regime, exhibiting monotonic decay. For $\eta = 0.5$ we have jumped across the gas–liquid coexistence region into the medium-density

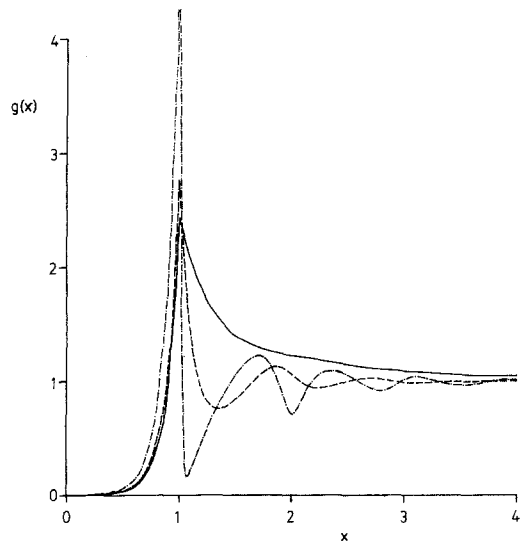

Fig. 2. Radial distribution functions for the SCYF with parameters $\lambda = 10$, $\xi = 2$, and $K = 1.218$ and densities $\eta = 0.04$ (——), $\eta = 0.5$ (- - -), and $\eta = 0.85$ (-·-).

liquid phase. The oscillations of a liquid-like rdf have a cusp at $x = 1$ due to the monotonic form we have specified for $x < 1$ in Eq. (2). A further point is that for $\eta = 0.85$ $g(r)$ is still physical, whereas the HCYF $g(r)$ at this density has become negative.

6. THE PY AND HNC POTENTIALS

Using the scheme for assigning the parameters α, λ, K, and ξ used above, it is not clear what type of potential the calculated rdf's correspond to. To obtain some information on the interaction potential we inverted the correlation function data [$g(x)$ and $c(x)$] to derive PY and HNC poten-

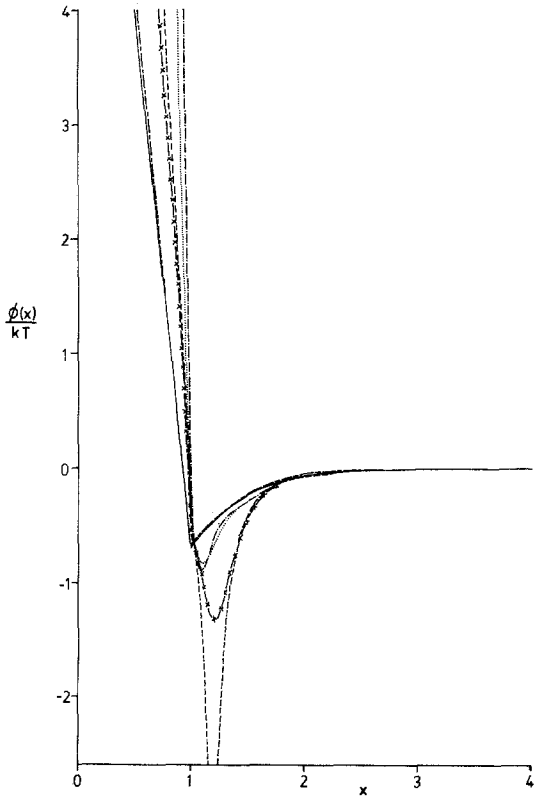

Fig. 3. Inverted potentials for the SCYF with parameters $\lambda = 10$, $\xi = 2$, $K = 1.218$ and densities $\eta = 0.041$ (PY ——, HNC - · -), $\eta = 0.5$ (PY - × -, HNC · · ·), and $\eta = 0.69$ (PY - - -, HNC - · -).

tials. That is, the functions $\phi_{PY}(x)$, $\phi_{HNC}(x)$ were calculated using the formulas[8,9]

$$\frac{\phi_{PY}(x)}{kT} = \log\left[\frac{g(x) - c(x)}{g(x)}\right] \tag{22}$$

$$\frac{\phi_{HNC}(x)}{kT} = h(x) - c(x) - \log g(x) \tag{23}$$

This procedure, known as the "inverse problem," has received considerable attention,[12,13] particularly in the study of liquid metals,[14] using $g(x)$ and $c(x)$ calculated from experimental structure factors.

These potentials are shown in Fig. 3. In general the HNC potentials are more harshly repulsive and less attractive than the PY potentials at all densities, the best agreement being at low density. For $\eta \gtrsim 0.45$ the PY well depths become very large and the potentials show a marked state dependence. When $\eta \gtrsim 0.7$ they become impossible to calculate due to the rapid falloff in $g(x)$ compared to $c(x)$ in the range $1 < x \lesssim 1.2$. By comparison the HNC potentials are far less state dependent. These observations are consistent with the known behavior of the PY and HNC theories.

The potential minima move outward with increasing density and this is again consistent with the observation that the peaks in $g(x)$, calculated from a density-independent potential such as the Lennard-Jones potential, move inward with increasing density. The former effect is a result of distance being scaled with respect to the position of the first peak in $g(r)$, whereas the usual distance scaling is with respect to the first zero of the potential.

An important feature of the intermediate- and high-density potentials is that the kink at $x = 1$ due to the cusp in $g(x)$ at $x = 1$ is imperceptible. Thus a realistic, liquid-like potential may be obtained with the use of the $M = 1$ term from Eq. (2), thus obviating the need to consider larger values of M.

7. CONCLUSION

The results for the SCYF model we have introduced suggest that further investigation is necessary, paying particular attention to establishing a more physical relationship between the parameters α, λ, K, and ξ. The work presented here may be regarded as a first step towards this goal.

APPENDIX

We give expressions for the matrix M and column vectors $\mathbf{L}_0$, $\mathbf{L}_1$, and $\mathbf{L}_2$ which appear in Eq. (13). Substituting the form of $h(x)$ given in Eq. (2) into Eq. (4) in the range $0 < x < 1$, we find that $q(x)$ is given by Eqs. (6)–(8), where

$$Q_2 = \gamma\left[1 - 12\eta\int_0^1 q_0(t)\,dt - 12\eta\sum_{j=1}^{N}\frac{\beta_j e^{\xi_j}}{\xi_j}\right] \tag{A.1}$$

$$Q_1 = 12\eta\gamma\left[\int_0^1 t q_0(t)\,dt + \sum_{j=1}^{N}\frac{\beta_j e^{\xi_j}}{\xi_j^2}\right] \tag{A.2}$$

$$Q_{i1} = \Delta_i\left[-1 + 12\eta\int_0^1 q_0(t)\cosh\lambda_i t\,dt + 12\eta\sum_{j=1}^{N}\frac{\beta_j\xi_j e^{\xi_j}}{\xi_j^2 - \lambda_i^2}\right] \tag{A.3}$$

$$Q_{i2} = -12\eta\Delta_i\left[\int_0^1 q_0(t)\sinh\lambda_i t\,dt + \left(\sum_{j=1}^{N}\frac{\beta_j e^{\xi_j}}{\xi_j^2 - \lambda_i^2}\right)\lambda_i\right] \tag{A.4}$$

Substitution of the form of $q(x)$ given in Eqs. (6)–(8) into Eqs. (A.1)–(A.4) yields four linear equations in the parameters Q_1, Q_2, Q_{i1}, and Q_{i2}. This may then be written as a matrix equation. Unfortunately this matrix is ill conditioned for large λ, in that Q_{i1} and Q_{i2} are large and opposite in sign. We are able to render this system well conditioned by making the substitution

$$y = Q_{11}, \qquad w = e^{\lambda}[\,Q_{11} + Q_{12}]/2 \tag{A.5}$$

Manipulating the linear equations in the required way, we then find that the equations may be written as

$$\mathbf{M}\begin{bmatrix} Q_2 \\ Q_1 \\ x \\ w \end{bmatrix} = \mathbf{L} \tag{A.6}$$

$$
M = \left[\begin{array}{c|c|c|c}
\frac{1}{\gamma} - 4\eta & -6\eta & \frac{12\eta}{\lambda}\left[1 - e^{-\lambda}(1+\lambda)\right] & \frac{12\eta}{\lambda}\left[1 - \lambda - e^{-\lambda} + e^{-2\lambda}(1+\lambda)\right] \\
\hline
\frac{3\eta}{2} & \frac{1}{\gamma} + 2\eta & \frac{-12\eta}{\lambda^2}\left[1 - e^{-\lambda}\left(1 + \lambda + \frac{\lambda^2}{2}\right)\right] & \frac{12\eta}{\lambda^2}\left[\left(1 - \lambda + \frac{\lambda^2}{2}\right) - e^{-2\lambda}\left(1 + \lambda + \frac{\lambda^2}{2}\right)\right] \\
\hline
6\eta\left[\frac{1}{\lambda} - \frac{2}{\lambda^3} + \frac{2e^{-\lambda}}{\lambda^2}\left(\frac{1}{\lambda} + 1\right)\right] & 12\eta\left(\frac{1}{\lambda} - \frac{1}{\lambda^2} + \frac{e^{-\lambda}}{\lambda^2}\right) & \frac{12\eta}{\lambda}\left(\frac{-1}{2} + e^{-\lambda} - \frac{e^{-2\lambda}}{2}\right) & \frac{12\eta}{\lambda} + \frac{1}{\alpha} - e^{-\lambda}6\eta\left(2 + \frac{1}{\lambda}\right) + e^{-2\lambda}\left(\frac{1}{\alpha} - \frac{12\eta}{\lambda}\right) + \frac{6\eta e^{-3\lambda}}{\lambda} \\
\hline
\frac{2}{\lambda^2}\left(\frac{1}{\lambda} - 1\right) + e^{-\lambda}\left(\frac{1}{\lambda} - \frac{2}{\lambda^3}\right) & 12\eta\left[\frac{-1}{\lambda^2} + e^{-\lambda}\left(\frac{1}{\lambda^2} + \frac{1}{\lambda}\right)\right] & \frac{-1}{\alpha} + e^{-\lambda} \cdot 12\eta\left(1 - \frac{1}{\lambda}\right) + e^{-2\lambda}\left(\frac{12\eta}{\lambda} - \frac{1}{\alpha}\right) & \frac{-6\eta}{\lambda} + e^{-\lambda}\left(\frac{12\eta}{\lambda} + \frac{1}{\alpha}\right) + e^{-2\lambda}6\eta\left(\frac{1}{\lambda} - 2\right) + e^{-3\lambda}\left(\frac{1}{\alpha} - \frac{12\eta}{\lambda}\right)
\end{array}\right] \tag{A.7}
$$

By examining **L**, we can choose the terms which have β or βd as factors and collect these together. Hence we find that

$$\mathbf{L} = \mathbf{L}_0 + \beta \mathbf{L}_1 + \beta d \mathbf{L}_2 \tag{A.8}$$

where

$$\mathbf{L}_0 = \begin{bmatrix} 1 \\ 0 \\ -1 \\ e^{-\lambda} \end{bmatrix} \tag{A.9}$$

$$\mathbf{L}_1 = 12\eta e^{\xi} \begin{bmatrix} -1/\xi \\ 1/\xi^2 \\ 1/(\xi+\lambda) \\ -e^{-\lambda}/(\xi-\lambda) \end{bmatrix} \tag{A.10}$$

$$\mathbf{L}_2 = 12\eta \begin{bmatrix} \dfrac{e^{\xi}}{\xi}\left[1 - e^{-\xi}(1+\xi)\right] \\ \dfrac{-e^{-\xi}}{\xi^2}\left[1 - e^{-\xi}\left(1 + \xi + \dfrac{\xi^2}{2}\right)\right] \\ \dfrac{-1}{\lambda} - \dfrac{e^{-\lambda}}{\lambda} + \dfrac{e^{\xi} - e^{-\lambda}}{\xi+\lambda} \\ \dfrac{-1}{\lambda} + \dfrac{e^{-\lambda}}{\lambda} + \dfrac{e^{\xi-\lambda} - 1}{\xi-\lambda} \end{bmatrix} \tag{A.11}$$

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