A BIFURCATION ANALYSIS OF THE ORNSTEIN-ZERNIKE EQUATION WITH HYPERNETTED CHAIN CLOSURE

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Abstract. Motivated by the large number of solutions obtained when applying bifurcation algorithms to the Ornstein-Zernike (OZ) equation with the hyper-netted chain (HNC) closure from liquid state theory, we provide existence and bifurcation results for a computationally-motivated version of the problem.

We first establish the natural result that if the potential satisfies a short-range condition then a low-density branch of smooth solutions exists. We then consider the so-called *truncated–OZ HNC* equation that is obtained when truncating the region occupied by the fluid in the original OZ equation to a finite ball, as is often done in the physics literature before applying a numerical technique.

On physical grounds one expects to find one or two solution branches corresponding to vapour and liquid phases of the fluid. However, we are able to demonstrate the existence of infinitely many solution branches and bifurcation points at very low temperatures for the truncated one-dimensional problem provided that the potential is purely repulsive and homogeneous.

1. Introduction. The Ornstein-Zernike (OZ) equation [11] is a renewal equation introduced in 1914 as a model for the molecular structure of a fluid with mean particle density ρ:

$$h(r) = c(r) + \rho \int_{\mathbb{R}^d} h(\|x-y\|)c(\|y\|)dy, \tag{1.1}$$

where $x, y \in \mathbb{R}^d$ and $d \leq 3$. Here and throughout, $r = \|x\|$ is the spatial coordinate where the norm is Euclidean and the structure of the fluid can be deduced from h, the pair correlation function, where c is the direct correlation function. Finally, we also define the indirect correlation function $\gamma := h - c$.

If the direct correlation function were known for a given fluid, one could in principle deduce the total correlation function via a contraction mapping argument. However, if this information is not known *a-priori* both correlation functions have to be found from (1.1). Clearly this is not possible and a closure relation must be supplemented in order to allow one to determine the structure of the fluid.

The closure relation that augments (1.1) depends on both the intermolecular potential u and the Boltzmann factor $\beta = 1/(Tk_B)$, where T is the temperature of the fluid. While there are many closures in the physics and chemistry literature, we only consider the hyper-netted chain (HNC) closure:

$$h(r) = -1 + e^{-\beta u(r)} \cdot \exp(h(r) - c(r)) \qquad (\forall r \geq 0). \tag{1.2}$$

We shall often write (1.2) in the following form

$$h(r) = f(r) + e^{-\beta u(r)} \cdot \exp_1(h(r) - c(r)), \tag{1.3}$$

where $f := -1 + e^{-\beta u(r)}$ is the so-called *Mayer f-function* which, for fixed $\beta > 0$ is always extended to be equal to -1 at $r = 0$. Moreover, $\exp_1(x) := -1 + e^x$ for all $x \in \mathbb{R}$ and this of course coincides with the sum $\sum_{n=1}^{\infty} \frac{x^n}{n!}$.

For any set Ω and a suitably defined function $a : \Omega \to \mathbb{R}$, we define a Nemitskii operator $M_\beta(a)$ via

$$M_\beta(a)(r) := f(r) + e^{-\beta u(r)} \cdot \exp_1(a(r)), \tag{1.4}$$

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the domain of which will be a space of radial functions on $\mathbb{R}^d$ that will be specified in due course. Note that when this domain is specified, all elements of the system of equations that result from (1.1-1.2) will be C^∞-smooth and so we refrain from stipulating precise smoothness properties of the systems of equations that appear in this article.

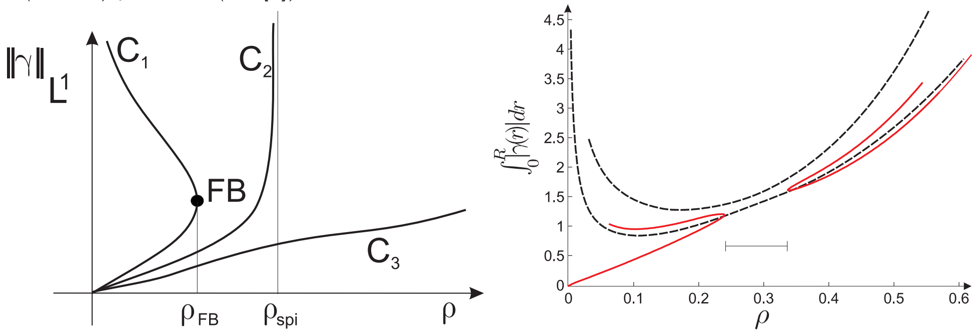


Fig. 1.1. *(left) Three schematic solution branches: FB denotes a fold bifurcation and* C_2 *possesses a* spinodal *at* $\rho = \rho_{\mathsf{spi}}$*. (right) Four solution branches obtained at a fixed temperature for a Lennard-Jones fluid computed using a numerical continuation code developed in Matlab and applied to (1.1-1.2) for* $d = 3$ *(see [2]).*

1.1. The Problem. Two diagrams are shown in Figure 1.1 and in the left-hand of the two we have depicted the kind of bifurcation structure one may expect to find in (1.1-1.2). In the curve marked C_3 there corresponds a single *vapour* correlation function γ at each density ρ. However, in the curve marked C_2 there is a value of density ρ_{spi} beyond which the solution branch will not pass and a bifurcation at infinity occurs: this is a so-called *spinodal* that is associated with a phase-transition from liquid to vapour, or *vice-versa*. Let us make this a little more precise with a definition.

Definition 1. *There is a* spinodal *of (1.1-1.2) at* ρ_{spi} *if there is a sequence* (h_n, c_n, ρ_n) *of solutions such that* $\lim_{n\to\infty} \rho_n = \rho_{\mathsf{spi}} > 0$ *and* $\lim_{n\to\infty} \int_{\mathbb{R}^d} h_n = \infty$.

However, the curve marked C_1 from Figure 1.1(left) is more typical of what is often computed in practice using continuation algorithms [2]. In this case there is a maximal density supported by the solution branch, but this behaviour is not associated with a spinodal, but rather with a fold bifurcation. We can see this in the right-hand diagram of Figure 1.1 where the Lennard-Jones potential with collision distance and well-depth both unity have been used, so that

$$u(r) = 4\,(r^{-12} - r^{-6}),$$

and we have taken $\beta = 0.73$. There is not only a single vapour branch, nor even just a vapour-liquid pair of solution branches, but in fact four solution branches have been located and many of the solutions contained on these branches are not physically relevant.

The purpose of this paper is to demonstrate that the apparently large number of computed solution branches is not simply an artefact of the numerical method applied to (1.1-1.2), but that when (1.1) is modified to form an integral over a finite ball, the resulting equation supports a large number of solutions in certain regions of parameter space. Despite the advancements in the numerical treatment of problems over unbounded domains, this replacement remains standard practise in the physics and chemistry literature and has been undertaken in all of the papers we have cited that include computational results, even if the authors have not explicitly stated this; see any of [17, 3, 15, 14, 12, 4, 9, 8, 7] for example.

We only treat the case of *repulsive* intermolecular potentials, our analysis does not yet extend to potentials with regions of attraction such as the Lennard-Jones potential given above. Moreover, we only cover the details of the one-dimensional or $d = 1$ case of (1.1) although results for the $d \geq 2$ cases follow from similar arguments.

In Figure 1.1(right) a horizontal line marks a region of density values that lies between two fold bifurcations on the solution branches plotted with full lines (not dashed lines); it is thought that the existence of such a region may relate to the existence of spinodals and phase transitions in the Ornstein-Zernike equation. A series of discussions regarding the meaning of bifurcations in the Ornstein-Zernike equation can be found in [15, 14, 12, 7, 17, 4, 9, 3, 1].

1.2. Notation. For clarity we continue with a brief synopsis of our notation. If X and Y are Banach spaces then $BL(Y, X)$ denotes the space of continuous linear mappings from Y to X and $BL(X) = BL(X, X)$. If $J \subseteq \mathbb{R}$ is an open interval, $L^p(J)$ is the space of measurable *functions* $u : J \to \mathbb{R}$ such that $\int_J |u(r)|^p dr < \infty$. By $C^k(\overline{J})$ we mean the space of k-times continuously differentiable maps and then $W^{k,p}(J)$ can be identified with the space of functions in $C^{k-1}(\overline{J})$ whose k-th weak derivative lies in $L^p(J)$, where $p \in \mathbb{N} \cup \{\infty\}$. By $Y \hookrightarrow X$ we mean that the first space is compactly embedded in the second. To ensure no ambiguity arises when using a particular norm, the notation $\|x\|_X$ may be used for $x \in X$ and $\|y\|_Y$ for $y \in Y$ and we shall use $\langle \cdot, \cdot \rangle$ for the usual L^2-inner product.

If $\mathbb{R}_+ = [0, \infty)$ then $BC(\mathbb{R}_+)$ denotes the space of bounded, continuous maps from $\mathbb{R}_+$ to $\mathbb{R}$ and $BC(\mathbb{R}^d)$ is defined to be the space of continuous and bounded, radially symmetric functions mapping into $\mathbb{R}$ if $d \in \{1, 2, 3\}$. Thus, $BC(\mathbb{R}^1)$ is the space of continuous and bounded even functions mapping into $\mathbb{R}$ that can be identified with $BC(\mathbb{R}_+)$. By X^d we mean the Banach space $BC(\mathbb{R}^d) \cap L^1(\mathbb{R}^d)$ that can be identified with the weighted space

$$\{u : \mathbb{R}_+ \to \mathbb{R} \text{ continuous} : r^{d-1}u(r) \in L^1(\mathbb{R}_+)\} \cap BC(\mathbb{R}_+),$$

with norm $\|u\|_{X^d} = \max(\|u\|_{L^1(\mathbb{R}^d)}, \|u\|_{BC(\mathbb{R}^d)})$.

Now suppose that a, b are suitably defined radially symmetric functions defined on $\mathbb{R}^d$ and mapping into $\mathbb{R}$. Any element $a \in X^d$ satisfies the inequality

$$\|a\|_{L^p(\mathbb{R}^d)} \leq (\|a\|^{p-1}_{BC(\mathbb{R}^d)} \|a\|_{L^1(\mathbb{R}^d)})^{1/p} \leq \|a\|_{X^d}$$

and so lies in $L^p(\mathbb{R}^d)$ for each $p \geq 1$. From standard properties of convolution on $\mathbb{R}^d$, $a * b$ is a radially symmetric function and $\|a * b\|_{L^1(\mathbb{R}^d)} \leq \|a\|_{L^1(\mathbb{R}^d)} \|b\|_{L^1(\mathbb{R}^d)}$ and $\|a * b\|_{BC(\mathbb{R}^d)} \leq \|a\|_{L^1(\mathbb{R}^d)} \|b\|_{BC(\mathbb{R}^d)}$, so that $*$ provides X^d with the structure of a Banach algebra. We note that the bilinear form $B : X^d \times X^d \to X^d$ given by $B(a, b) = a * b$ is continuously Fréchet differentiable. Moreover, for $a, b \in X^d$ there results

$$\|ab\|_{L^1} \leq \|a\|_{L^1} \|b\|_{BC} \text{ and } \|ab\|_{BC} \leq \|a\|_{BC} \|b\|_{BC},$$

so that pointwise multiplication also provides an algebra structure on X^d.

Let $R > 0$ be a real parameter. If $a : \mathbb{R}^d \to \mathbb{R}$ then $\mathcal{E}_R(a)(r)$ denotes the restricted function given by $\mathcal{E}_R(a)(r) = a(\|x\|)$ for $0 \leq \|x\| < R$ and $\mathcal{E}_R(a)(r) = 0$ otherwise. We shall also use the natural restriction or embedding operator $\mathcal{R}_R : X^d \to C^0(\overline{B_R(\mathbf{0})})$ where $B_R(\mathbf{x})$ denotes the open Euclidean ball of radius R about x in $\mathbb{R}^d$ and an overbar denotes closure.

2. A Fixed-Point Problem for the Indirect Correlation Function. A single convolution equation for γ in the form of a fixed-point problem can be obtained from (1.1-1.2), namely

$$\gamma = \rho[-\gamma + M_\beta(\gamma)] * M_\beta(\gamma), \tag{2.1}$$

and as a result it is convenient to define the nonlinear operator

$$N_\beta(\gamma) := [-\gamma + M_\beta(\gamma)] * M_\beta(\gamma). \tag{2.2}$$

We will need the potential u to be sufficiently *short-range* that $f \in X^d$, so that the condition given in [13] applies:

$$\int_0^\infty r^{d-1} | \overbrace{\exp_1(-\beta u(r))}^{f(r)} | dr < \infty. \tag{2.3}$$

Condition (2.3) is satisfied by the Mayer f-function if u satisfies

(U1) $\lim_{r \to 0} u(r) = +\infty$,

(U2) u is continuous on $(0, \infty)$ and

(U3) $\int_1^\infty r^{d-1} u(r) dr < \infty$.

The Mayer f-function associated with the Lennard-Jones potential is therefore short-range for any value of d. However, for the potential $u(r) = \mathsf{Const}/r$ the associated Mayer f-function is *long-range* in any dimension and $u(r) = \mathsf{Const}/r^2$ is long-range in two or more dimensions, but is short range in one-dimension. A potential of the form $u(r) = e^{-\mathsf{k}r}/r$ is short-ranged in any dimension where the parameter k takes any positive value.

2.1. Existence of a Small-Density Vapour Solution Branch. The following basic theorem shows that (1.1-1.2) possesses a branch of small-density solutions under reasonable assumptions.

THEOREM 1 (Existence of a vapour solution branch). *Suppose that* (**U1**-**U3**) *hold,* $d \in \{1, 2, 3\}$ *and* $\beta > 0$*, then there is a* $\rho_0 > 0$ *and a mapping* $S : [0, \rho_0) \to X^d$ *such that if* $\gamma = S(\rho)$ *then* γ *satisfies (2.1). Thus (1.1-1.2) has a locally unique, small-density solution branch.*

Theorem 1 is a direct consequence of the implicit function theorem applied to (2.1). Such an argument works thanks to the following proposition.

PROPOSITION 1. *Suppose that* $d \in \{1, 2, 3\}, \beta > 0$ *and that* (**U1**-**U3**) *apply. Then* $M_\beta : X^d \to X^d$ *is a* C^1 *mapping and since* X^d *is a convolution algebra,* N_β *is also a* C^1 *mapping on* X^d.

Proof. Fixing $\beta > 0$, we omit the dependence of M_β on β and simply write M in the proof. We show first that $M : X^d \to X^d$ is well-defined. Using a subscript L^1 to denote the **one-dimensional** L^1-norm of a function a so that $\|a\|_{L^1} = \int_0^\infty |a(r)| dr$, we have

$$\|r^{d-1} M(\gamma)\|_{L^1} \le \|r^{d-1} \exp_1(-\beta u(r))\|_{L^1} + \|e^{-\beta u(r)}\|_{BC} \int_0^\infty r^{d-1} |\exp_1(\gamma(r))| dr.$$

The first term in this expression is finite by assumption and the last term can be bounded as follows:

$$\int_0^\infty r^{d-1} |\exp_1(\gamma(r))| dr = \int_0^\infty r^{d-1} \left| \sum_{n=1}^\infty \frac{1}{n!} \gamma(r)^n \right| dr$$

$$
\begin{aligned}
&\le \int_0^\infty r^{d-1} \sum_{n=1}^\infty \frac{1}{n\,!} \, |\gamma(r)|^n \, dr \\
&\le \int_0^\infty r^{d-1} \sum_{n=1}^\infty \frac{1}{n\,!} |\gamma(r)| \|\gamma\|_{BC}^{n-1} dr \\
&\le \sum_{n=0}^\infty \frac{1}{(n+1)\,!} \|\gamma\|_{BC}^n \int_0^\infty r^{d-1} |\gamma(r)| dr \\
&\le e^{\|\gamma\|_{BC}} \|r^{d-1}\gamma\|_{L^1},
\end{aligned}
$$

which is finite. There remains to consider $\|M(\gamma)\|_{BC}$, but this is clearly bounded by $\|\exp_1(-\beta u(r))\|_{BC} + \|e^{-\beta u(r)}\|_{BC} \|(e^{\|\gamma\|_{BC}} + 1)$ which is finite, so M is well-defined on X^d.

Now we claim that M is Fréchet differentiable on X^d with derivative $dM \in C^0(X, BL(X))$ given by $dM(\gamma)[h] = L(\gamma)[h]$, for $\gamma, h \in X^d$, where L is the multiplication operator acting on h given by

$$
L(\gamma)[h] = e^{-\beta u(r)} \exp(\gamma) h. \tag{2.4}
$$

Let $\gamma, \gamma_1, \gamma_2, h \in X^d$ and note that $\|L(\gamma)[h]\|_{BC} \le \|h\|_{BC} \|e^{-\beta u(r)} \exp(\gamma)\|_{BC}$ is clearly finite, but also $\|r^{d-1} L(\gamma)[h]\|_{L^1} \le \|r^{d-1}h\|_{L^1} \|e^{-\beta u(r)} \exp(\gamma)\|_{BC}$, whence $L : X^d \to BL(X^d)$ with

$$
\|L(\gamma)\|_{BL(X^d)} \le \|e^{-\beta u(r)} \exp(\gamma)\|_{BC}.
$$

Now,

$$
\begin{aligned}
\|r^{d-1}L(\gamma_1)[h] - r^{d-1}L(\gamma_2)[h]\|_{L^1} &\le \int_0^\infty r^{d-1} e^{-\beta u(r)} |\exp(\gamma_1) - \exp(\gamma_2)| \cdot |h| dr \\
&\le \int_0^\infty r^{d-1} e^{-\beta u(r)} \left| \sum_{n=1}^\infty \frac{1}{n\ !} (\gamma_1^n - \gamma_2^n) \right| \cdot |h| dr \\
&\le \int_0^\infty r^{d-1} e^{-\beta u(r)} \sum_{n=1}^\infty \left[\frac{1}{n\ !} |\gamma_1 - \gamma_2| \sum_{i=0}^{n-1} |\gamma_1|^i |\gamma_2|^{n-(i+1)} \right] |h| dr \\
&\le \|\gamma_1 - \gamma_2\|_{BC} \|r^{d-1}h\|_{L^1} \|e^{-\beta u(r)}\|_{BC} \Sigma(\gamma_1, \gamma_2),
\end{aligned}
$$

and also

$$
\begin{aligned}
\|L(\gamma_1)[h] - L(\gamma_2)[h]\|_{BC} &\le \|e^{-\beta u(r)}\|_{BC} \|(\exp(\gamma_1) - \exp(\gamma_2))h\|_{BC} \\
&\le \|\gamma_1 - \gamma_2\|_{BC} \|h\|_{BC} \|e^{-\beta u(r)}\|_{BC} \Sigma(\gamma_1, \gamma_2),
\end{aligned}
$$

where

$$
\Sigma(\gamma_1, \gamma_2) = \sum_{n=1}^\infty \sum_{i=0}^{n-1} \frac{\|\gamma_1\|_{BC}^i \|\gamma_2\|_{BC}^{n-(i+1)}}{n\,!} \le e^{\max(\|\gamma_1\|_{BC}, \|\gamma_2\|_{BC})} < \infty.
$$

These inequalities demonstrate that

$$
\|L(\gamma_1) - L(\gamma_2)\|_{BL(X^d)} \le \left(e^{\max(\|\gamma_1\|_{BC}, \|\gamma_2\|_{BC})} \|e^{-\beta u(r)}\|_{BC} \right) \|\gamma_1 - \gamma_2\|_{X^d},
$$

so that $L : X^d \to BL(X^d)$ is locally Lipschitz continuous.

To show that M is differentiable with L as its derivative, consider

$$\begin{aligned}
&\|M(\gamma+h) - M(\gamma) - L(\gamma)[h]\|_{X^d} \\
&\qquad = \|e^{-\beta u(r)}(\exp_1(\gamma+h) - \exp_1(\gamma) - \exp(\gamma)h)\|_{X^d} \\
&\qquad = \|e^{-\beta u(r)}\exp(\gamma)(\exp_1(h) - h)\|_{X^d} \\
&\qquad \le \|e^{-\beta u(r)}\exp(\gamma)\|_{BC}\|\exp_1(h) - h\|_{X^d}.
\end{aligned}$$

Since

$$|\exp_1(z) - z| = \left|\sum_{n=2}^{\infty}\frac{z^n}{n\,!}\right| \le |z|^2\sum_{n=0}^{\infty}\frac{|z|^n}{(n+2)\,!} \le |z|^2 e^{|z|} \qquad (z\in\mathbb{R}),$$

we find $\|\exp_1(h) - h\|_{BC} \le \|h\|_{BC}^2 e^{\|h\|_{BC}}$ and

$$\int_0^\infty r^{d-1}|\exp_1(h) - h|dr \le \int_0^\infty r^{d-1}|h|^2 e^{\|h\|_{BC}}dr \le \|r^{d-1}h\|_{L^1}\|h\|_{BC}e^{\|h\|_{BC}},$$

so that

$$\|\exp_1(h) - h\|_{X^d} \le \|h\|_{X^d}^2 e^{\|h\|_{X^d}}.$$

Since this quantity is $O(\|h\|_{X^d}^2)$ as $h \to 0$ in X^d, we conclude that M is differentiable, and since dM was shown to be Lipschitz, M is C^1. As a result, N_β is the composition of C^1 mappings on X^d and so is also C^1 with

$$dN_\beta(\gamma)[h] = (dM(\gamma)[h] - h) * M(\gamma) + (M(\gamma) - \gamma) * dM(\gamma)[h].$$

□

Theorem 1 carries through with minor modifications to the case whereby $BC(\mathbb{R}^d)$ is replaced with $L^\infty(\mathbb{R}^d)$ and (**U2**) is suitably modified to the condition that $e^{-\beta u(r)} \in L^\infty(\mathbb{R}_+)$. This is an important alteration as potentials are often *truncated* or redefined in the far-field, resulting in non-smooth potentials [16]. For instance, one can obtain an extension of Theorem 1 to cover the cases of the modified Lennard-Jones potentials

$$\underline{u}(r) = \begin{cases} 4(r^{-12} - r^{-6}) & : \quad 0 \le r \le R_0, \\ 0 & : \quad\quad r > R_0. \end{cases}$$

and

$$\overline{u}(r) = \begin{cases} 4(r^{-12} - r^{-6}) & : \quad 0 \le r \le R_0, \\ \infty & : \quad\quad r > R_0. \end{cases}$$

3. The Truncated OZ-HNC Equation. The numerical computations that have been performed and reported in the liquid state literature for the Ornstein-Zernike equation are not undertaken for the *infinite domain* problem (1.1-1.2) itself. Instead computations are performed for a truncated version of the problem that has the effect of reducing the convolution operator to a finite region of integration.

This has obvious computational advantages, but may change the character of the equations considerably. We now develop some bifurcation results for the integral equation that arises from performing such a truncation operation and we demonstrate that this problem possesses an intricate bifurcation structure when using either density or temperature (in the guise of β) as a bifurcation parameter.

Let $\mathcal{H}$ denote the Hankel transform that is normalised to be idempotent in the space of radially symmetric functions in $L^2(\mathbb{R}^3)$, so that

$$\mathcal{H}(a(r))(s) = \left(\frac{2}{\pi}\right)^{1/2} \int_0^\infty \operatorname{sinc}(rs)a(r)r^2 dr.$$

Now apply the convolution theorem to write (1.1) in the form

$$h(r) = c(r) + \rho \cdot \mathcal{H}(\mathcal{H}h \cdot \mathcal{H}c)(r). \tag{3.1}$$

There are different choices of how to truncate the fluid and in [8] the authors undertake the following operation: introduce a large *finite section* parameter R and approximate h and c by their near-field truncations $h_{_R} = \mathcal{E}_{_R}(h)$ and $c_{_R} = \mathcal{E}_{_R}(c)$. One now studies (1.2) restricted to $[0, R]$ coupled to the integral equation

$$h_{_R}(r) = c_{_R}(r) + \rho\mathcal{R}_{_R}\mathcal{H}\mathcal{E}_{_R}[\mathcal{H}(h_{_R}) \cdot \mathcal{H}(c_{_R})] \tag{3.2}$$

that corresponds to (3.1).

Another feasible way of approximating (1.1) for the purposes of numerical discretisation is could be to replace that equation with

$$h(r) = c(r) + \rho\mathcal{R}_{_R}\left[\int_{\|y\|\le R} (\mathcal{E}_{_R}h)(\|x-y\|)(\mathcal{E}_{_R}c)(\|y\|)dy\right]. \tag{3.3}$$

Taking our motivation from (3.3) the equation that is the subject of the remainder of the paper is the following system of integro-algebraic equations:

$$h(r) = c(r) + \rho\mathcal{R}_{_R}\left[\int_{-R}^{R} (\mathcal{E}_{_R}h)(|r-s|)(\mathcal{E}_{_R}c)(|s|)ds\right], \tag{3.4}$$

$$h(r) = f(r) + e^{-\beta u(r)} \exp_1(h(r) - c(r)), \tag{3.5}$$

that holds for all r such that $0 \le r \le R$. The truncated convolution operator in (3.4-3.5) arises when applying an analogous truncation procedure to the one-dimensional convolution operator

$$(h * c)(r) = \int_{\mathbb{R}} h(|r-s|)c(|s|)ds.$$

The following lemma shows that we can obtain simple compactness and regularity properties for the windowed convolution operator $B_{_R}$ defined by

$$B_{_R}(a, b) = \int_{-R}^{R} (\mathcal{E}_{_R}a)(|r-s|)(\mathcal{E}_{_R}b)(|s|)ds \tag{3.6}$$

for suitable functions $a, b : [0, R] \to \mathbb{R}$.

LEMMA 1. *The symmetric, bilinear form $B_{_R}$ has the following smoothing properties:*

1. $B_{_R} : X \times X \to X$ *where X is either* $L^\infty(0, R)$ *or* $C^0[0, R]$,
2. $B_{_R} : C^0[0, R] \times W^{1,p}(0, R) \to W^{1,\infty}(0, R), \qquad (1 \le p \le \infty)$,
3. $B_{_R} : W^{1,\infty}(0, R) \times W^{1,\infty}(0, R) \to W^{2,\infty}(0, R)$ *and*
4. $B_{_R} : C^k[0, R] \times C^k[0, R] \to C^{k+1}[0, R], \qquad (k \in \{1, 2, 3, ...\})$.

Proof. Property (1) of the lemma is immediate from $\|B_R(a,b)\|_X \leq 2R\|a\|_X\|b\|_X$. Now let $a, b \in C^\infty[0,R], t \in [0,R]$ and write

$$\begin{aligned}
B_R(a,b)(t) &= \int_{\mathbb{R}} (\mathcal{E}_R a)(|t-s|)(\mathcal{E}_R b)(|s|)ds = \int_{-R}^{R} (\mathcal{E}_R a)(|t-s|)b(|s|)ds, \\
(s \mapsto t-s) &= \int_{t-R}^{t+R} (\mathcal{E}_R a)(|s|)b(|t-s|)ds, \\
&= \left(\int_{t-R}^{0} + \int_{0}^{t+R} \right) (\mathcal{E}_R a)(|s|)b(|t-s|)ds, \\
(s \mapsto -s) &= \int_0^{R-t} a(s)b(t+s)ds + \int_0^R a(s)b(|t-s|)ds, \\
&= \int_0^t a(s)b(t-s)ds + \int_t^R a(s)b(s-t)ds + \int_0^{R-t} a(s)b(t+s)ds, \\
&= \int_0^t a(t-s)b(s)ds + \int_t^R a(s-t)b(s)ds + \int_0^{R-t} a(s+t)b(s)ds,
\end{aligned}$$

which clearly illustrates the symmetry of B_R. Properties 2-4 of the lemma are established by the formulae

$$\begin{aligned}
\frac{d}{dt} B_R(a,b)(t) &= \int_0^t a(s)b'(t-s)ds + \int_t^R a(s)b'(s-t)ds + \int_0^{R-t} a(s)b'(t+s)ds \\
&\quad -a(R-t)b(R) \\
&= \int_0^t a(t-s)b'(s)ds + \int_t^R a(s-t)b'(s)ds + \int_0^{R-t} a(s+t)b'(s)ds \\
&\quad -a(R-t)b(R)
\end{aligned}$$

and

$$\begin{aligned}
\frac{d^2}{dt^2} B_R(a,b)(t) &= \int_0^t a'(t-s)b'(s)ds - \int_t^R a'(s-t)b'(s)ds + \int_0^{R-t} a'(t+s)b'(s)ds \\
&\quad -a'(R-t)b(R) - a(R)b'(R-t),
\end{aligned}$$

that can be extended to the chosen spaces by a density argument. $\square$

3.1. The One-Dimensional, Truncated OZ-HNC Equation. In a truncated domain no short-range decay requirements are required in order to obtain a small-density solution branch of (3.4-3.5). This allows one to work, for instance, with the Dirichlet potential $u(r) = \mathsf{Const}/r$ which is long-range for the infinite-domain problem (1.1-1.2).

With this comment in mind, the remainder of the section is dedicated to the integral equation

$$\gamma = \rho \overbrace{B_R(M_\beta(\gamma) - \gamma, M_\beta(\gamma))}^{N_{\beta,R}(\gamma)}, \tag{3.7}$$

where, just as in the infinite-domain case, $M_\beta : X \to X$ is given by

$$M_\beta(\gamma) = \exp_1(-\beta u(r)) + e^{-\beta u(r)} \exp_1(\gamma), \qquad 0 \leq r \leq R,$$

where we have in mind $X = C^0[0,R]$ or $X = L^\infty(0,R)$. We continue with the following theorem that is the analogy of Theorem 1 for (3.7).

Theorem 2. *Suppose that $\beta > 0, u$ satisfies* (**U1**)*,* $\exp(-\beta u) \in X$ *where X is either $L^\infty(0,R)$ or $X = C^0[0,R]$ and $d = 1$. Then there is a $\rho_0 > 0$ and a mapping $S : [0,\rho_0) \to X$ such that if $\gamma = S(\rho)$ then, γ satisfies the one-dimensional, truncated Ornstein-Zernike equation (3.7).*

Proof. This follows immediately from the fact that the operator $N_{\beta,R}$ defined in (3.7) is smooth in either candidate space X. ◻

Throughout the following section the derivatives of $N_{\beta,R}$ and M_β will be needed on several occasions, so we list them now for convenience (dropping the reference to R and β temporarily for clarity):

(D1) $M'(\gamma)h := d_\gamma M(\gamma)[h] = e^{-\beta u(r)} \cdot e^\gamma h$,
(D2) $M''(\gamma)[h,k] := d^2_{\gamma\gamma} M(\gamma)[h,k] = e^{-\beta u(r)} \cdot e^\gamma hk$,
(D3) $d_\gamma N(\gamma)[h] = B_R(M(\gamma), (M'(\gamma) - 1)h) + B_R(M'(\gamma)h, M(\gamma) - \gamma)$,
(D4) and

$$\begin{aligned} d^2_{\gamma\gamma} N(\gamma)[h,k] = B_R(M'(\gamma)k, (M'(\gamma) - 1)h) + B_R(M(\gamma), M''(\gamma)hk) + \\ B_R(M''(\gamma)hk, M(\gamma) - \gamma) + B_R(M'(\gamma)h, (M'(\gamma) - 1)k). \end{aligned}$$

These derivatives are only formally defined without the specification of suitable domains for the underlying operators, but these shall be made in due course that render (D1-D4) rigorous.

3.2. Global Bifurcation Structure. We now show that by placing some differentiability properties on the Meyer f-function associated with the potential u, one can obtain global information regarding the vapour solution branch associated with (3.7).

Theorem 3. *Suppose that X denotes the space $W^{1,p}(0,R)$ and $\beta > 0, u$ satisfies* (**U1**) *and $\exp_1(-\beta u) \in X$ for some $p \in \{1,2,3,...\}$, then there is a $\rho_0 > 0$ and a mapping $S : [0,\rho_0) \to X$ such that if $\gamma = S(\rho)$ then γ satisfies (3.7).*

1. *If we define the set $\Sigma = \{(\gamma,\rho) \in X \times [0,\infty) : \gamma = \rho N_{\beta,R}(\gamma), \rho \geq 0\}$, then there is a connected, unbounded set $\mathsf{C} \subset \Sigma$ that contains the graph of S.*
2. *If there is a sequence $(\gamma_n,\rho_n) \in \mathsf{C}$ such that $\lim_{n\to\infty} \rho_n = 0$, then either (i) $\lim_{n\to\infty} \gamma_n = 0$ uniformly or (ii) $\lim_{n\to\infty} \|\gamma_n\|_X = \infty$.*
3. *If the Mayer f-function associated with the potential u lies in $C^\infty[0,R]$, then $\gamma \in C^\infty[0,R]$.*

Proof. The small-density existence result in X follows from the implicit function theorem because the mapping M_β satisfies $M_\beta : X \to X$, which follows from the fact that $\gamma \mapsto \exp_1(\gamma)$ is C^1 on $W^{1,p}(0,R)$. From Lemma 1 the map $N_{\beta,R}(\gamma) = B_R(M_\beta(\gamma) - \gamma, M_\beta(\gamma))$ satisfies $N_{\beta,R} : X \to W^{1,\infty}(0,R) \hookrightarrow X$ and so is compact. The Leray-Schauder continuation principle [18] applies and the first two conclusions in the statement of the theorem follow.

The last part of the theorem comes from the bootstrapping properties of the map $N_{\beta,R}$ from properties (1-4) of Lemma 1 that apply when the Mayer f-function is C^∞-smooth. These imply that if $\gamma = \rho N_{\beta,R}(\gamma)$ and $\gamma \in W^{1,p}(0,R)$ then $\gamma \in W^{1,\infty}(0,R)$ by property (2) of Lemma 1, but then $N_{\beta,R} : W^{1,\infty}(0,R) \to W^{2,\infty}(0,R)$ by property (3) of Lemma 1 so that $\gamma \in C^1[0,R]$. Hence, by property (4) of Lemma 1, $\gamma \in C^2[0,R]$ and the statement of the theorem follows by a similar inductive argument. ◻

From Theorem 3 we argue that the Mayer f-function $\exp_1(-\beta u)$ can be non-smooth to a certain degree and yet one still may obtain global solution existence for solutions of (3.7); f must however be continuous, but it may have cusps and corners. However, Theorem 3 does not cover the case whereby u has jump discontinuities in which case we still only have a small density existence result.

The smoothness requirement on the potential in Theorem 3 stipulates that the weak derivative of $\exp_1(-\beta u)$, namely the function $-\beta \cdot u' e^{-\beta u}$, has integrable p-th power on $(0, R)$, where u' denotes the weak derivative of u on $(0, R)$. This condition holds for many potentials, including the potentials $u(r) = 4\epsilon(\sigma/r)^n$, for $n \in \{1, 2, 3, ...\}$, and for the Lennard-Jones potential.

In the case of a purely repulsive potential of the form

$$u(r) = \mathsf{Const}\, r^{-q}$$

for a positive power q, the following result may be established.

THEOREM 4. *Suppose that u satisfies* (**U1**)*, is strictly positive (that is, repulsive) and positively homogeneous:*

$$u(r) > 0,\ u(\lambda r) = \lambda^{\alpha} u(r), \qquad (\text{for some } \alpha < 0, \forall \lambda > 0, r \in (0, R]).$$

Suppose also that $\exp_1(-u) \in C^1[0, R]$, then there a discrete set $\mathsf{R} \subset (0, \infty)$ such that for each positive $\rho \notin \mathsf{R}$ there is an unbounded, one-dimensional Cartesian curve $\mathsf{C}_\rho \subset C^0[0, R] \times [0, \infty)$ such that each $(\gamma, \beta) \in \mathsf{C}_\rho$ is a solution of the truncated Ornstein-Zernike equation (3.7) for this value of ρ.

Proof. First note that the positive homogeneity of u implies that the relationship $u(\delta r) = \beta u(r)$ holds identically in r when $\delta = \beta^{1/\alpha}$. Now, the extended function

$$\hat{f}(r) = \begin{cases} e^{-u(r)} & : \quad r \in [0, R] \\ 0 & : \quad r \in [-R, 0] \end{cases}$$

is C^1 smooth by assumption and by (**U1**) with $\hat{f}(0) = 0$. Therefore, the family of extended Mayer f-functions, $\upsilon(r, \delta) = \exp_1(\hat{f}(\delta r))$ is also C^1 on $[0, R] \times (-\Delta, \Delta)$ as it is a composition of C^1 functions, here $\Delta \in (0, 1)$ is a sufficiently small real constant.

Now consider

$$M(\gamma, \delta) := \exp_1(-u(r\delta)) + e^{-u(r\delta)} \exp_1(\gamma)$$

as a one-parameter family of maps $M : C^0[0, R] \times (-\Delta, \Delta) \to C^0[0, R]$. In fact, this is a C^1-smooth one parameter family that satisfies $M(\gamma, 0) = -1$ because $\lim_{\delta \to 0} e^{-u(r\delta)} = 0$. We now seek solutions to the following version of the Ornstein-Zernike equation with HNC closure,

$$\gamma = \rho \cdot B_R(M(\gamma, \delta) - \gamma, M(\gamma, \delta)) \qquad (=: \rho \cdot N_R(\gamma, \delta)) \tag{3.8}$$

for $\gamma \in C^0[0, R]$ and small δ. Note that (3.8) is directly related to (3.7) via the replacement $\delta = \beta^{1/\alpha}$.

We first consider the equation for γ_0 that is obtained by setting $\delta = 0$ in (3.8), namely

$$\gamma_0 = \rho N_R(\gamma_0, 0),$$

which is the affine equation

$$\gamma_0 = \rho B_R(1 + \gamma_0, 1). \tag{3.9}$$

For $a \in C^0[0, R]$, we define a linear operator K by *convolution with unity*:

$$(Ka)(t) := B_R(a, 1) = \int_0^R a(s) ds + \int_0^{R-t} a(s) ds,$$

which can be written

$$(Ka)(t) = \int_0^R k(t,s)a(s)ds,$$

where the kernel k is strictly positive:

$$k(t,s) = 1 + \begin{cases} 1 & : \quad 0 \le s \le R-t, \\ 0 & : \quad \textit{otherwise}. \end{cases}$$

Clearly K is a compact and self-adjoint integral operator on $L^2(0,R)$ and in fact $K : L^2(0,R) \to C^{1/2}(0,R) \hookrightarrow C^0[0,R]$ so that the non-zero elements of the spectrum of K as an operator on $L^2(0,R)$ and $C^0[0,R]$ are the same, but then K is injective on $L^2(0,R)$ so 0 is not an element of the point spectrum of K. Thus K only has point spectrum, apart from the zero element in its essential spectrum.

We now define the set R by

$$\mathsf{R} := \sigma(K)^{-1} \cap (0,\infty).$$

Noting that K is strongly positive on $C^0[0,R]$:

$$a \ge 0 \Rightarrow Ka \ge 0, \qquad a > 0 \Rightarrow Ka \gg 0,$$

by the Krein-Rutman theorem K has an algebraically simple, positive eigenvalue given by its spectral radius with associated strictly positive eigenfunction. Hence R is non-empty and discrete.

Returning to equation (3.9), this can now be written

$$(I - \rho K)\gamma_0 = \rho(2R - t), \tag{3.10}$$

and $I - \rho K \in BL(C^0[0,R])$ is an isomorphism on $C^0[0,R]$ for $\rho \notin \sigma(K)$. Therefore (3.10) and hence (3.9) has a unique solution γ_0 for $\rho \notin \mathsf{R}$ as ρ was assumed to be positive in the statement of the theorem.

Now, the derivative of $\gamma - \rho N(\gamma,\delta)$ at $(\gamma_0, 0)$ is the mapping $I - \rho d_\gamma N(\gamma_0, 0)$ and from (D1) $d_\gamma M(\gamma,\delta)[h] = e^{-u(r\delta)}e^\gamma \cdot h$ so that $d_\gamma M(\gamma_0,0) = 0$. By (D3) and the fact that $M(\gamma,0) = -1$

$$d_\gamma N(\gamma_0,0)[h] = B_{_R}(M(\gamma,0) - \gamma, 0) + B_{_R}(-h, M(\gamma,0)) = B_{_R}(h,1) = Kh.$$

Hence, for positive $\rho \notin \mathsf{R}$, $I - \rho d_\gamma N(\gamma_0,0) = I - \rho K$ and as this is an isomorphism on $C^0[0,R]$ and $2R - t \in C^0[0,R]$, we can solve (3.8) by the implicit function theorem for functions $\gamma = \gamma(\delta)$ in a neighbourhood of $\gamma = \gamma_0$ and $\delta = 0$ such that $\gamma(0) = \gamma_0$. As a result, a solution curve of (3.8) exists on which $\gamma = \gamma(\beta^{1/\alpha})$ for all β sufficiently large and positive. □

We would like to have a global version of Theorem 4. However, the dependence on δ of the function $e^{-u(r\delta)}$ is not analytic and it seems that we cannot apply the global theory of analytic nonlinear problems from [5].

If we inspect the proof of Theorem 4 it becomes apparent that the result actually shows that one can solve for an unbounded two-dimensional surface of solutions of (3.7) as a Cartesian graph on which $\gamma = \gamma(\rho,\delta)$ near to $\delta = 0$ and in a neighbourhood of any positive value of $\rho \notin \mathsf{R}$; we have included the statement of this result as a separate result below for completeness (see Theorem 5).

Theorem 5. *Suppose that u satisfies* **(U1)***, is strictly positive and positively homogeneous and that* $\exp_1(-u) \in C^1[0,R]$. *Then there a discrete set* $\mathsf{R} \subset (0,\infty)$

such that for each positive $\rho_0 \notin \mathsf{R}$ there is an unbounded, smooth two-dimensional surface $\mathsf{C}_2 \subset C^0[0,R] \times \mathbb{R}^2_+$ depending on ρ_0 such that each $(\gamma, \rho, \beta) \in \mathsf{C}_2$ is a solution of (3.7) for this value of (ρ, β). Moreover, there are sequences $(\gamma_n, \rho_n, \beta_n)_{n \geq 1} \subset \mathsf{C}_2$ such that $\rho_n \to \rho_0$ and $\beta_n \to \infty$ as $n \to \infty$.

Proof. This follows the proof of Theorem 4. The final part follows as we can graph γ as a function $\gamma = \gamma(\rho, \delta)$ near to $(\rho, \delta) = (\rho_0, 0)$ on which $\beta = \delta^\alpha$ and $\alpha < 0$, whence any sequence $\delta_n \to 0$ provides a sequence $\beta_n \to 0$ as claimed. □

The question remains regarding what happens to the geometry of the surface C_2 from Theorem 5 near to a value of $\rho \in \mathsf{R}$, so we first give a precise description of the set R.

LEMMA 2. *The set of reciprocals of eigenvalues of K from Theorem 4 (whose positive elements form R) consists of two divergent sequences: the Dirichlet values $(\pm\rho_k^D)_{k\geq 2}$ and the non-local values $(\pm\rho_k^N)_{k\in\mathbb{Z}}$ where $\rho_k^D > 0$ and $\rho_k^N > 0$. These are given as follows:*

- *(Dirichlet boundary conditions) Each value $\rho = \rho_k^D$ satisfies*

$$\varphi'' + \rho^2 \varphi = 0,$$

  subject to Dirichlet boundary conditions

$$\varphi(0) = \varphi(R) = 0, \quad \left(\textit{when} \quad \int_0^R \varphi(s) ds = 0 \right),$$

  and we shall denote these solutions φ_k^D.
- *(Non-local boundary conditions) Each value $\rho = \rho_k^N$ satisfies*

$$\varphi'' + \rho^2 \varphi = 0,$$

  subject to non-local boundary conditions

$$\varphi(0) = 2\rho \int_0^R \varphi(s) ds, \quad \varphi(R) = \rho \int_0^R \varphi(s) ds \;\left(\textit{when} \quad \int_0^R \varphi(s) ds \neq 0 \right),$$

  and we shall denote these solutions φ_k^N.

Hence $\rho_k^D = \frac{k\pi}{R}$ for all even $k \geq 2$ and ρ_k^N satisfies the equation

$$\operatorname{sinc}(\rho_k^N \cdot R) = (\cos(\rho_k^N \cdot R) + 1)/R,$$

whence $\rho_k^N \sim \frac{k\pi}{R}$ as $k \to \infty$ for odd and positive k.

Proof. If $\rho K \varphi = \varphi$ is satisfied for $\varphi \in L^2(0,R)$ and $\rho \neq 0$, then $\varphi \in C^2[0,R]$ follows. Now,

$$\varphi(t) = \rho \left(\int_0^R \varphi(s) ds + \int_0^{R-t} \varphi(s) ds \right), \tag{3.11}$$

yields

$$\varphi'(t) = -\rho \varphi(R-t) \qquad \text{and} \qquad \varphi''(t) = \rho \varphi'(R-t).$$

As a result, $\varphi'(R-t) = -\rho\varphi(t)$ and therefore $\varphi'' + \rho^2 \varphi = 0$. As the latter equation is symmetric in ρ and has no non-trivial solutions for $\rho = 0$ since K is injective, we may restrict attention to $\rho > 0$. The boundary conditions that φ satisfies are obtained from setting $t = 0$ and $t = R$ in equation (3.11) giving

$$\varphi(0) = \rho \left(\int_0^R \varphi(s)ds + \int_0^R \varphi(s)ds \right) \text{ and } \varphi(R) = \rho \left(\int_0^R \varphi(s)ds \right). \tag{3.12}$$

The Dirichlet values ρ_k^D coincide with the square root of the eigenvalues of the sign-changing eigenfunctions of the Dirichlet problem (meaning $\varphi(0) = \varphi(R) = 0$) on the interval $[0, R]$, so that the eigenfunctions are given by $\varphi_k^D(t) = \sin(k\pi t/R)$ and these satisfy $\int_0^R \varphi_k^D(t)dt = 0$. It follows that k must be even and non-zero and the eigenvalues satisfy $\rho^2 = (k\pi/R)^2$.

The non-local values ρ_k^N come from setting $\varphi(t) = A\cos(\rho t) + B\sin(\rho t)$ for $A, B \in \mathbb{R}$ and enforcing the non-local boundary conditions (3.12). This requires that the two-by-two matrix

$$\begin{bmatrix} 1 - 2\cos(\rho R) & -2\sin(\rho R) \\ \cos(\rho R) - \rho\sin(\rho R) & \rho\cos(\rho R) + \rho + \sin(\rho R) \end{bmatrix}$$

be singular, the determinant of this matrix being $\sin(\rho R) - \rho(\cos(\rho R) + 1)$. The remainder of the lemma follows because $\cos(\rho R) + 1$ must be close to zero for large $\rho > 0$ so there must be an integer ℓ such that $\rho R \sim (2\ell + 1)\pi$ as ρ increases. □

Remark 1. *Let us reiterate the eigenvalue-eigenfunction pairs*

$$(\rho_{2k+1}^N, \varphi_{2k+1}^N) \text{ and } (\rho_{2k}^D, \varphi_{2k}^D) \in \mathbb{R} \times C^\infty[0, R]$$

that are defined in Lemma 2 provide the complete eigenstructure of the operator K. We shall use these objects routinely throughout the remainder of the article but we shall write ρ_k^N rather than ρ_{2k+1}^N, invoking the tacit assumption that k is odd, or even if we are using the Dirichlet eigenvalues ρ_k^D.

We continue with a definition.

Definition 2. *A parameterised, nonlinear mapping of Banach spaces $G : X \times \mathbb{R}^p \to Y$ is said to have a bifurcation from infinity relative to $Z(\supset X)$ at $\lambda_\infty \in \mathbb{R}^p$ if there are sequences $(x_n) \subset X$ and $(\lambda_n) \subset \mathbb{R}^p$ such that $G(x_n, \lambda_n) \equiv 0$ and $\lambda_n \to \lambda_\infty$ yet $\|x_n\|_Z \to \infty$ as $n \to \infty$. A bifurcation from infinity relative to X is simply called a bifurcation from infinity.*

Let us note that because the Mayer f-function is sufficiently smooth, Theorem 4 still holds if we replace the ambient function space $C^0[0, R]$ in which we seek solutions of (3.7) with the smoother space $C^1[0, R]$ and seek solutions there; the same comment applies to Theorem 5. However, any C^1 solution of (3.7) immediately lies in C^2 by Lemma 1 and with this observation have the following lemma.

Lemma 3. *Suppose* (**U1**) *holds and that* $\exp(-u) \in C^1[0, R]$. *Now write $\lambda := (\delta, \rho) \in \mathbb{R}^2$ and*

$$G(\gamma, \lambda) := -\gamma + \rho N_{\beta,R}(\gamma, \delta)$$

where $G : C^1[0, R] \times \mathbb{R}^2 \to C^1[0, R]$. Then G has a bifurcation from infinity relative to $W^{1,p}(0, R)$ at $\lambda = (0, \rho_k^N)$ for all $k \geq 1$ and any $p \geq 1$.

Proof. From Theorem 5 we may suppose that the following sequences exist: (ρ_n) and $(\delta_n) \subset (0, \infty)$ and $(\gamma_n) \subset C^1[0, R]$ (which in fact lies in $C^2[0, R]$ by Lemma 1) such that

$$\gamma_n = \rho_n B_R(M(\gamma_n, \delta_n) - \gamma_n, M(\gamma_n, \delta_n))$$

for all n where $\delta_n \to 0$ but $\rho_n \to \rho_k^N$ for some $k \geq 1$ as $n \to \infty$.

Now suppose that $\|\gamma_n\|_{W^{1,p}}$ is bounded. It follows that there is a γ^N such that $\gamma_n \rightharpoonup \gamma^N$ in $W^{1,p}(0,R)$ as $n \to \infty$ and as a result we may assume that $\gamma_n \to \gamma^N$ in $C^0[0,R]$. Since $M(\gamma_n(r),\delta_n) \to -1$ in $C^0[0,R]$, there results $\gamma^N = \rho_k^N B_{\scriptscriptstyle R}(1+\gamma^N,1)$, that is $(-I+\rho_k^N K)\gamma^N + \rho_k^N \cdot K\ 1 = 0$. Hence, if φ_k^N is the eigenfunction of K associated with eigenvalue $1/\rho_k^N$ then

$$\begin{aligned} 0 &= \left\langle \varphi_k^N, (-I+\rho_k^N K)\gamma^N + \rho_k^N \cdot K\ 1\right\rangle = \left\langle (I-\rho_k^N K)\varphi_k^N, \gamma^N\right\rangle + \rho_k^N \cdot \left\langle K\varphi_k^N, 1\right\rangle \\ &= \left\langle \varphi_k^N, 1\right\rangle = \int_0^R \varphi_k^N(s)ds \neq 0. \end{aligned}$$

This is a contradiction from where $\|\gamma_n\|_{W^{1,p}}$ cannot be bounded and the lemma follows. □

Motivated by Lemma 3, we now consider the structure of the set of solutions of the low-temperature problem $\gamma = \rho N(\gamma,\delta)$ obtained on setting $\delta = 0$. Then $N(\gamma,0) = B_{\scriptscriptstyle R}(M(\gamma,0)-\gamma, M(\gamma,0)) = B_{\scriptscriptstyle R}(-1-\gamma,-1) = B_{\scriptscriptstyle R}(1+\gamma,1) = K(1+\gamma)$, leading to the affine equation (3.9) that we reiterate here:

$$\gamma_0 = \rho K\gamma_0 + \rho K[1], \tag{3.13}$$

where 1 is the function that is identically one.

Clearly, for ρ such that $1/\rho \notin \sigma(K)$, which includes the set R, the unique solution of (3.13) is given by

$$\gamma_0(\rho) = \rho(I-\rho K)^{-1}K[1].$$

Now suppose that $\rho_n \to \rho_k^N$ for some $k \geq 1$ as $n \to \infty$ and that $\|\gamma_0(\rho_n)\|_{L^2}$ is bounded. There then exists a subsequence of $\gamma_0(\rho_n)$, call it (γ_n), and a function $\Gamma \in L^2(0,R)$ such that $\gamma_n \rightharpoonup \Gamma$ in L^2 as $n \to \infty$. Clearly, the mapping $N(\gamma,0) = -\gamma + \rho K\gamma + \rho K[1]$ is weakly sequentially continuous on $L^2(0,R)$ and so $N(\gamma_n,0) \rightharpoonup N(\Gamma,0)$, whence

$$\Gamma = \rho_k^N K\Gamma + \rho_k^N K[1].$$

But then $\varphi = \rho_k^N K\varphi$ for some $\varphi \in L^2(0,T)$ such that $\int_0^R \varphi(s)ds \neq 0$ and as a result

$$\begin{aligned} 0 &= \left\langle \varphi, -\Gamma + \rho_k^N K\Gamma + \rho_k^N K[1]\right\rangle = \left\langle (-I+\rho_k^N K)\varphi, \Gamma\right\rangle + \left\langle \varphi, \rho_k^N K[1]\right\rangle, \\ &= \rho_k^N \left\langle K\varphi, 1\right\rangle = \left\langle \varphi, 1\right\rangle = \int_0^R \varphi(s)ds. \end{aligned}$$

This contradiction ensures that each element of the sequence $(\rho_k^N)_{k\geq 1}$ is a singularity of the function $\gamma_0(\rho)$ as a mapping $\gamma_0 : \mathbb{R} \to L^2(0,R)$; this is the cause of the bifurcations from infinity in Lemma 3.

So what of elements in the set $(\rho_k^D)_{k\geq 2}$? If we define the space

$$X_D := \bigoplus_{k=1}^{\infty} \left\langle \varphi_k^D \right\rangle,$$

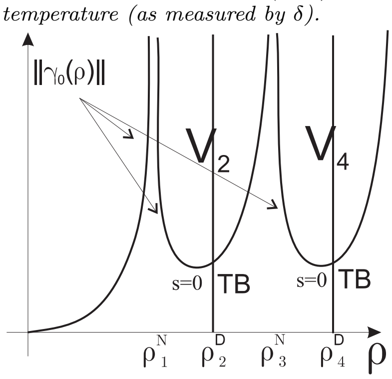
then because K is self-adjoint and $K : X_D \to X_D$, $L^2(0,R) = X_D \oplus X_D^\perp$ forms an orthogonal decomposition of $L^2(0,R)$ into K-invariant subspaces. Now, if $\rho \notin \{\rho_k^D\}_{k\geq 1}$ but ρ is close to some ρ_k^D, then $(I-\rho K)^{-1}$ exists as an element of $BL(X_D^\perp)$. Since $1 \in X_D^\perp, K1 \in X_D^\perp$ also and we find that $\gamma(\rho) \in X_D^\perp \subset L^2(0,R)$ and $(\rho_k^D)_{k\geq 2}$ are *removable singularities* of the mapping $\gamma_0(\rho)$ and so we may consider $\gamma_0(\rho_k^D)$ to be a well-defined member of $X_D^\perp$. This can also be seen by constructing the eigenfunction expansion of $I - \rho K$ via eigenfunctions of K.

Finally, there is an unbounded *vertical* solution branch of (3.13) that exists when $\rho = \rho_k^D$ that has the form

$$\gamma = \gamma_0(\rho_k^D) + s \cdot \varphi_k^D \in X_D \oplus X_D^\perp$$

for any value of the real parameter $s \in \mathbb{R}$. So we define $V_k = \bigcup_{s\in\mathbb{R}} \gamma_0(\rho_k^D) + s\varphi_k^D$ for even $k \geq 2$.

FIG. 3.1. *A schematic of the bifurcation diagram of (3.13): TB denotes a transcritical bifurcation that persists to non-zero temperature (as measured by δ).*



The purpose of the remainder of the paper is to show that Figure 3.1, the bifurcation diagram associated with (3.13), persists if temperature (the reciprocal of β) is taken to be small but non-zero. So, we now give an existence result for (3.7) near the *vertical* branches V_k described above, extending Theorem 5 to cover the cases whereby ρ is contained in a neighbourhood of some point on the set $\{\rho_k^D\}_{k\geq 1}$.

THEOREM 6. *Suppose that u satisfies* (**U1**)*, is strictly positive and positively homogeneous,* $\exp_1(-u) \in C^1[0, R]$ *and that* $\rho_0 \in \{\rho_k^D\}_{k\geq 2}$*. Then there is an unbounded, smooth two-dimensional manifold* $\mathsf{C}_2 \subset C^0[0, R] \times \mathbb{R}_+^2$ *such that each* $(\gamma, \rho, \beta) \in \mathsf{C}_2$ *is a solution of the one-dimensional, truncated Ornstein-Zernike equation (3.7). Moreover, there are sequences* $(\gamma_n, \rho_n, \beta_n)_{n\geq 1} \subset \mathsf{C}_2$ *such that* $\rho_n \to \rho_0$ *and* $\beta_n \to \infty$ *as* $n \to \infty$.

Proof. In order to solve (3.8) and hence (3.7) for small δ, let us write

$$\gamma = s\varphi_0 + \gamma_0 + \Gamma,$$

where $s \in \mathbb{R}$ and γ_0 is the unique function in $L^2(0, R)$ that satisfies

$$\gamma_0 = \rho_0 K\gamma_0 + \rho_0 K[1], \qquad \int_0^R \gamma_0(r)\varphi_0(r)dr = 0,$$

where $\rho_0 \in \{\rho_k^D\}_{k\geq 2}$ is non-zero and

$$\varphi_0 = \rho_0 K\varphi_0, \qquad \int_0^R \varphi_0(r)dr = 0, \int_0^R \varphi_0(r)^2 dr = 1.$$

We also assume that $\Gamma \in X_0$ where $X_0 = \langle\varphi_0\rangle^\perp \cap C^0[0, R]$. As a result, if we define the projection mapping

$$Q : L^2(0, R) \to \langle\varphi_0\rangle^\perp ; u \mapsto u - \varphi \int_0^R u(r)\varphi_0(r)dr \tag{3.14}$$

then (3.8) becomes the system

$$s\varphi_0 + \gamma_0 + \Gamma = \rho N(s\varphi_0 + \gamma_0 + \Gamma, \delta)$$

that can be projected onto X_0 and its orthogonal complement in $L^2(0, R)$ to yield the problem

$$-(\gamma_0 + \Gamma) + \rho Q \cdot N(s\varphi_0 + \gamma_0 + \Gamma, \delta) = 0, \tag{3.15}$$

$$-s + \rho \int_0^R \varphi_0 N(s\varphi_0 + \gamma_0 + \Gamma, \delta) dr = 0, \tag{3.16}$$

as $\langle \varphi_0, \Gamma \rangle = 0$.

The system (3.15-3.16) defines a smooth map $G(= G(\Gamma, \rho, s, \delta)) : X_0 \times \mathbb{R}^3 \to X_0 \times \mathbb{R}$ that satisfies

$$\begin{aligned}
G(0, \rho_0, s, 0) &= \begin{pmatrix} -\gamma_0 + \rho_0 Q N(\gamma_0 + s\varphi_0, 0) \\ -s + \rho_0 \int_0^R \varphi_0 N(s\varphi_0 + \gamma_0, 0) \end{pmatrix} \\
&= \begin{pmatrix} -\gamma_0 + \rho_0 Q K[1 + \gamma_0 + s\varphi_0] \\ -s + \rho_0 \int_0^R \varphi_0 K[1 + s\varphi_0 + \gamma_0] dr \end{pmatrix} \\
&= \begin{pmatrix} -\gamma_0 + \rho_0 K \gamma_0 + \rho_0 K[1] \\ -s + \int_0^R \varphi_0 (1 + s\varphi_0 + \gamma_0) dr \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}
\end{aligned}$$

for all $s \in \mathbb{R}$ using $Q(K1) = K1$ and $Q(K\varphi_0) = 0$. Thus $G(\Gamma, \rho, s, \delta) = 0$ has a trivial solution branch parameterised by s; this is the set V_k.

Now, the derivative $d_{\Gamma,\rho} G(0, \rho_0, s, 0)$ acting on a vector $[h, \alpha] \in X_0 \times \mathbb{R}$ can be found from

$$d_{\Gamma,\rho} G(\Gamma, \rho, s, \delta)[h, \alpha] =$$
$$\begin{pmatrix} -h + \rho Q d_\gamma N(\gamma_0 + s\varphi_0 + \Gamma, \delta)[h] + \alpha Q N(\gamma_0 + s\varphi_0 + \Gamma, \delta) \\ \rho \int_0^R \varphi_0 d_\gamma N(s\varphi_0 + \gamma_0 + \Gamma, \delta)[h] dr + \alpha \int_0^R \varphi_0 N(s\varphi_0 + \gamma_0 + \Gamma, \delta) dr \end{pmatrix}$$

and using (D3), $d_\gamma N(\gamma_0 + s\varphi_0, 0)[h] = B_R(-1, -h) = K[h]$ so that

$$\begin{aligned}
d_{\Gamma,\rho} G(0, \rho_0, s, 0)[h, \alpha] &= \begin{pmatrix} -h + \rho_0 Q K h + \alpha Q K(1 + \gamma_0 + s\varphi_0) \\ \rho_0 \int_0^R \varphi_0 K h dr + \alpha \int_0^R \varphi_0 K(1 + s\varphi_0 + \gamma_0) dr \end{pmatrix} \\
&= \begin{pmatrix} (-I + \rho_0 K) h + \alpha K(1 + \gamma_0) \\ s\alpha/\rho_0 \end{pmatrix}.
\end{aligned}$$

Now, seeking a bifurcation we suppose that $d_{\Gamma,\rho} G(0, \rho_0, s, 0)[h, \alpha] = [0, 0]$, then $s\alpha/\rho_0 = 0$ and so $\alpha = 0$ must hold if $s \neq 0$, so we assume the latter condition. Then $(-I + \rho_0 K) h = 0$ and so h lies in the span of φ_0, but the fact that $h \in X_0$ yields $h = 0$.

It follows that $d_{\Gamma,\rho} G(0, \rho_0, s, 0) \in GL(X_0 \times \mathbb{R})$ is an injective, Fredholm mapping and hence an isomorphism provided $s \neq 0$ and, as a result, the equation $G(\Gamma, \rho, s, \delta) = 0$ can be solved near to any point (at which $s = s_0$ say) on the given trivial branch parameterised by s for two smooth functions $\Gamma = \Gamma(s, \delta)$ and $\rho = \rho(s, \delta)$, where $\Gamma(s_0, 0) = 0$ and $\rho(s_0, 0) = \rho_0$, using the implicit function theorem. □

The following extension of Theorem 6 shows that equation (3.7) can possess transcritical bifurcations at low temperatures that are stable to changes in temperature.

THEOREM 7. *Suppose that u satisfies* (**U1**), *is strictly positive and positively homogeneous,* $\exp_1(-u) \in C^1[0, R]$ *and that* $\rho_0 \in \{\rho_k^D\}_{k \geq 2}$. *For each even* $k \in \mathbb{N}$

there are two unbounded, smooth two-dimensional manifolds $\mathsf{M}_1, \mathsf{M}_2 \subset C^0[0,R] \times \mathbb{R}^2_+$ *(depending on k) such that each* $(\gamma, \rho, \beta) \in \mathsf{M}_i$ *(for* $i = 1, 2$*) is a solution of (3.7). Moreover, the set* $\mathsf{M}_1 \cap \mathsf{M}_2$ *is a smooth, unbounded, one-dimensional curve representing transcritical bifurcations of (3.7).*

Proof. As in Theorem 6, we seek solutions of (3.8) for small δ and again set

$$\gamma = s\varphi_0 + \gamma_0 + \Gamma,$$

where s is now assumed to lie in some neighbourhood of 0 (see the penultimate paragraph of Theorem 6 where that proof breaks down if $s = 0$). We again consider equations (3.15) and (3.16) in a neighbourhood of $(\Gamma, s, \rho, \delta) = (0, 0, \rho_0, 0)$, noting that (3.15) can be solved in a neighbourhood of this point for a smooth function $\Gamma = \Gamma(s, \rho, \delta)$ by the implicit function theorem where $\Gamma(s, \rho, \delta) \in \langle \varphi_0 \rangle^{\perp}$.

This is a Lyapunov-Schmidt procedure that reduces (3.7) to a local, smooth system of low dimension obtained on substituting $\Gamma = \Gamma(s, \rho, \delta)$ into (3.16). The remainder of the proof therefore establishes the local nature of the bifurcation equation given by (3.16) on the graph of Γ.

This results in one equation with three unknowns, viz:

$$-s + \rho \int_0^R \varphi_0 N(s\varphi_0 + \gamma_0 + \Gamma(s, \rho, \delta), \delta) dr = 0, \tag{3.17}$$

and accordingly we define the function

$$b(s, \rho, \delta) := \int_0^R \varphi_0 N(s\varphi_0 + \gamma_0 + \Gamma(s, \rho, \delta), \delta) dr.$$

We shall now establish the existence of an expansion of b in the form

$$b(s, \rho, \delta) = \frac{s}{\rho_0} + h(s, \rho - \rho_0, \delta), \tag{3.18}$$

where h is a smooth function that vanishes at least to second order at zero.

From (3.15), using subscripts to denote derivatives with respect to the subscripted variable, we find that

$$-\Gamma_s + \rho Q \cdot d_\gamma N(s\varphi_0 + \gamma_0 + \Gamma, \delta)[\varphi_0 + \Gamma_s] = 0, \tag{3.19}$$

and

$$-\Gamma_\rho + \rho Q \cdot d_\gamma N(s\varphi_0 + \gamma_0 + \Gamma, \delta)[\varphi_0 + \Gamma_\rho] + QN(s\varphi_0 + \gamma_0 + \Gamma, \delta) = 0, \tag{3.20}$$

where Q is the projection operator defined in (3.14).

We recall that upon setting $\delta = 0$ we obtain $M(\gamma, 0) = -1 + e^{-u(r\delta)} e^{\gamma} \big|_{\delta=0} = -1$, for any $\gamma \in C^0[0,R]$ and so $d_\gamma N(\gamma, 0) = K$ and $d^2_{\gamma\gamma} N(\gamma, 0) = 0$ from (D1-D4). Thus, setting $(s, \rho, \delta) = (0, \rho_0, 0)$ and using a superscript 0 to denote the evaluation of a function or operator at this point, equation (3.19) yields

$$-\Gamma^0_s + \rho_0 Q \cdot K[\varphi_0 + \Gamma^0_s] = 0 \Longrightarrow -\Gamma^0_s + \rho_0 Q \cdot K\Gamma^0_s = 0,$$

and therefore $\Gamma^0_s = 0$ because $\Gamma(s, \rho, \delta) \in \langle \varphi_0 \rangle^{\perp}$. Also, (3.20) becomes

$$-\Gamma^0_\rho + \rho_0 Q \cdot K[\varphi_0 + \Gamma^0_\rho] + QB(-1, -1 - \gamma_0) = 0,$$

and using the defining properties of γ_0, namely $\gamma_0/\rho_0 = B_{R}(1, 1+\gamma_0) = K[\gamma_0+1]$, we find

$$(-I+\rho_0 Q\,K)\Gamma^0_\rho + \gamma_0/\rho_0 = 0, \tag{3.21}$$

using in both cases the fact that $Q(K\varphi_0) = 0$. Equation (3.21) tells us that $\Gamma^0_\rho \neq 0$ because $\gamma_0 \in \langle\varphi_0\rangle^\perp$.

Now for the second derivatives. Using

$$\begin{aligned} -\Gamma_{ss} + \rho Q \cdot d^2_{\gamma\gamma} N(s\varphi_0+\gamma_0+\Gamma,\delta)[\varphi_0+\Gamma_s, \varphi_0+\Gamma_s] \\ + \ \rho Q\cdot d_\gamma N(s\varphi_0+\gamma_0+\Gamma,\delta)[\Gamma_{ss}] = 0, \end{aligned}$$

we find from (D4) that the $d^2_{\gamma\gamma}N$ terms is zero and so

$$-\Gamma^0_{ss} + \rho_0 Q\cdot K[\Gamma^0_{ss}] = 0 \Longrightarrow \Gamma^0_{ss} = 0.$$

Also,

$$\begin{aligned} -\Gamma_{\rho\rho} + \rho Q\cdot d^2_{\gamma\gamma}N(s\varphi_0+\gamma_0+\Gamma,\delta)[\Gamma_\rho,\Gamma_\rho] + \rho Q\cdot d_\gamma N(s\varphi_0+\gamma_0+\Gamma,\delta)[\Gamma_{\rho\rho}] \\ +2Q d_\gamma N(s\varphi_0+\gamma_0+\Gamma,\delta)[\Gamma_\rho] = 0, \end{aligned}$$

and therefore

$$(-I+\rho_0 Q\cdot K)\Gamma^0_{\rho\rho} + 2QK[\Gamma^0_\rho] = 0,$$

whence $\Gamma^0_{\rho\rho\neq 0}$ as $\Gamma^0_\rho \in \langle\varphi_0\rangle^\perp$ and K is injective. Now

$$b(0,\rho_0,0) = \langle\varphi_0, B(-1,-1-\gamma_0)\rangle = \langle\varphi_0, K(1+\gamma_0)\rangle = \langle K\varphi_0, 1+\gamma_0\rangle = 0$$

and

$$b_s = \langle\varphi_0, d_\gamma N(s\varphi_0+\gamma_0+\Gamma,\delta)[\varphi_0+\Gamma_s]\rangle,$$

so that upon setting $(s,\rho,\delta) = (0,\rho_0,0)$

$$b^0_s = \langle\varphi_0, K\varphi_0\rangle = \rho_0^{-1}\langle\varphi_0,\varphi_0\rangle = \rho_0^{-1}.$$

Also, because $\langle\varphi_0, \Gamma^0_\rho\rangle = 0$ we have

$$b_\rho = \langle\varphi_0, d_\gamma N(s\varphi_0+\gamma_0+\Gamma,\delta)[\Gamma_\rho]\rangle \Longrightarrow b^0_\rho = \langle\varphi_0, K\Gamma^0_\rho\rangle = \langle K\varphi_0,\Gamma^0_\rho\rangle = 0.$$

In order to evaluate b_δ we need the derivatives of N and M with respect to δ: if $0 \leq r \leq R$ then

(M1) $d_\delta M(\gamma,\delta) = -ru'(r\delta)e^{-u(r\delta)}e^\gamma$,
(M2) $d^2_{\gamma\delta}M(\gamma,\delta)[h,1] = -ru'(r\delta)e^{-u(r\delta)}e^\gamma\cdot h$,
(M3) $d^2_{\delta\delta}M(\gamma,\delta) = r^2 e^{-u(r\delta)}\left(u'(r\delta)^2 - u''(r\delta)\right)e^\gamma$,
(M4) $d_\delta N(\gamma,\delta) = B_{R}(d_\delta M, M(\gamma)) + B_{R}(d_\delta M, M(\gamma)-\gamma)$,
(M5) $d^2_{\delta\delta}N(\gamma,\delta) = B_{R}(d^2_{\delta\delta}M, M(\gamma)) + 2B_{R}(d_\delta M, d_\delta M) + B_{R}(d_{\delta\delta}M, M(\gamma)-\gamma)$,
(M6)

$$\begin{aligned} d^2_{\gamma\delta}N(\gamma,\delta)[h,1] = B_{R}(d_\delta M'[h], M(\gamma)) + B_{R}(d_\delta M, M'[h]) + \\ B_{R}(d_\delta M'[h], M(\gamma)-\gamma) + B_{R}(d_\delta M, M'[h]-h), \end{aligned}$$

where $d_\delta M'[h] = d^2_{\gamma\delta} M(\gamma, \delta)[h, 1]$. When taking the low temperature limit $\delta \to 0$, the exponential terms dominate in (M1) and (M2) above and we obtain

$$d_\delta M(\gamma, 0) = 0, d^2_{\gamma\delta} M(\gamma, 0)[h, 1] = 0 \text{ and } d^2_{\delta\delta} M(\gamma, 0) = 0,$$

but also

$$d^2_{\gamma\delta} N(\gamma, 0)[h, 1] = 0.$$

As a result,

$$-\Gamma_\delta + \rho Q \cdot d_\gamma N(s\varphi_0 + \gamma_0 + \Gamma, \delta)[\Gamma_\delta] + \rho Q \cdot d_\delta N(s\varphi_0 + \gamma_0 + \Gamma, \delta) = 0,$$

whence

$$-\Gamma^0_\delta + \rho_0 Q \cdot K[\Gamma^0_\delta] = 0 \Longrightarrow \Gamma^0_\delta = 0.$$

In addition,

$$\begin{aligned} -\Gamma_{\delta\delta} + \rho Q \cdot d_\gamma N(s\varphi_0 + \gamma_0 + \Gamma, \delta)[\Gamma_{\delta\delta}] + 2\rho Q \cdot d^2_{\delta\gamma} N(s\varphi_0 + \gamma_0 + \Gamma, \delta)[1, \Gamma_\delta] \\ + \rho Q \cdot d^2_{\delta\delta} N(s\varphi_0 + \gamma_0 + \Gamma, \delta) = 0, \end{aligned}$$

from where $\Gamma^0_{\delta\delta} + \rho_0 Q \cdot K\Gamma^0_{\delta\delta} = 0$ and therefore $\Gamma^0_{\delta\delta} = 0$.
Similarly,

$$b_\delta = \langle \varphi_0, d_\gamma N(s\varphi_0 + \gamma_0 + \Gamma, \delta)[\Gamma_\delta] + d_\delta N(s\varphi_0 + \gamma_0 + \Gamma, \delta) \rangle,$$

and so, on setting $\delta = 0$ we obtain

$$b^0_\delta = \langle \varphi_0, K[\Gamma_\delta] \rangle = \langle K\varphi_0, \Gamma_\delta \rangle = 0.$$

Continuing in the same vein using properties (D1-D4) established previously, we obtain

$$\begin{aligned} b^0_{ss} &= \left\langle \varphi_0, d^2_{\gamma\gamma} N(\gamma_0, 0)[\varphi_0 + \Gamma^0_s, \varphi_0 + \Gamma^0_s] + d_\gamma N(\gamma_0, 0)[\Gamma^0_{ss}] \right\rangle \\ &= 0, \\ b^0_{\rho\rho} &= \left\langle \varphi_0, d^2_{\gamma\gamma} N(\gamma_0, 0)[\Gamma^0_\rho, \Gamma^0_\rho] + d_\gamma N(\gamma_0, 0)[\Gamma^0_{\rho\rho}] \right\rangle = \left\langle \varphi_0, K\Gamma^0_{\rho\rho} \right\rangle \\ &= 0, \\ b^0_{\delta\delta} &= \left\langle \varphi_0, d^2_{\delta\delta} N(\gamma_0, 0) + d^2_{\gamma\gamma} N(\gamma_0, 0)[\Gamma^0_\delta, \Gamma^0_\delta] + d_\gamma N(\gamma_0, 0)[\Gamma^0_\delta] \right\rangle \\ &\quad + \left\langle \varphi_0, 2d_{\gamma\delta} N(\gamma_0, 0)[\Gamma^0_\delta, 1] \right\rangle \\ &= 0. \end{aligned}$$

This establishes the validity of (3.18) for b up to terms of second order and therefore the bifurcation equation for (3.8) near $(\Gamma, s, \rho, \delta) = (0, 0, \rho_0, 0)$ is given by $-s + \rho \cdot b(s, \rho - \rho_0, \delta) = 0$, or

$$(\rho - \rho_0) \cdot s + \rho\rho_0 h(s, \rho - \rho_0, s) = 0. \tag{3.22}$$

If we introduce a desingularising set of coordinates (t, σ_0, Δ) in (3.22) given by

$$\rho - \rho_0 = t, s = \sigma_0 t, \delta = \Delta t,$$

equation (3.22) then yields

$$\sigma_0 = \rho_0(\rho_0 + t) \cdot t^{-2} h(\sigma_0 t, t, \Delta t)$$

and as h only contains terms of order three and higher this is a smooth equation that can be solved near $(t, \sigma_0, \Delta) = (0, 0, 0)$ by the implicit function theorem for $\sigma_0 = \sigma_0(t, \Delta)$. The graph of σ_0 gives the manifold M_1 in the statement of the theorem.

If we introduce a different set of coordinates (t, σ_1, Δ) in (3.22) now given by

$$\rho - \rho_0 = \sigma_1 t, s = t, \delta = \Delta t,$$

equation (3.22) becomes

$$\sigma_1 = \rho_0(\rho_0 + \sigma_1 t) \cdot t^{-2} h(t, \sigma_1 t, \Delta t). \tag{3.23}$$

Equation (3.23) is also a smooth equation that can be solved near $(t, \sigma_1, \Delta) = (0, 0, 0)$ by the implicit function theorem for $\sigma_1 = \sigma_1(t, \Delta)$ and the graph of σ_1 gives the manifold M_2 in the statement of the theorem.

If $(\rho, s, \delta) \in \mathsf{M}_1 \cap \mathsf{M}_2$ then there are parameter values t and t' such that

$$(\rho, s, \delta) = (\rho_0 + t, t\sigma_0(t, \Delta), t\Delta) = (\rho_0 + t'\sigma_1(t', \Delta'), t', t'\Delta'),$$

so that

$$t = t'\sigma_1(t', \Delta'), t' = t\sigma_0(t, \Delta), t'\Delta' = t\Delta.$$

Hence $t\Delta = t\sigma_0(t, \Delta)\Delta'$ and so we may desingularise the problem by dividing through by t provided $t \neq 0$, we thus obtain a system of equations that describes $\mathsf{M}_1 \cap \mathsf{M}_2$ locally:

$$t = t'\sigma_1(t', \Delta'), \tag{3.24}$$
$$t' = t\sigma_0(t, \Delta), \tag{3.25}$$
$$\Delta = \Delta'\sigma_0(t, \Delta). \tag{3.26}$$

The system of equations (3.24-3.26) can be solved for (t, t', Δ) as a function of Δ' near to the solution $(t, t', \Delta, \Delta') = (0, 0, 0, 0)$ using the implicit function theorem and the existence of a smooth curve in $\mathsf{M}_1 \cap \mathsf{M}_2$ is established. $\square$

4. Discussion. The purpose of this article is to locate regions in the (ρ, β)-plane containing solutions and bifurcations of the Ornstein-Zernike equation with no intrinsic physical meaning. This is motivated by recent computations that are depicted in Figure 1.1(right) (obtained using the numerical approach of [2]) which demonstrate that the three-dimensional problem has more than the expected two solution branches. In a sense, this article is analogous to [10] which tackles the problem of finding unique minimisers for a variational problem from density functional theory.

The rationale that we have used in this paper can be described as follows. Using the fact that $e^{-\beta u(r)}$ converges in the zero-temperature limit $\beta \to \infty$ to the zero function, provided that u is strictly positive, the singularity of the potential at $r = 0$ allows us to collapse (3.7) to an affine equation that has spectral parameter ρ. If u is homogeneous of degree $-\alpha$ then $e^{-\beta u(r)} = e^{-u(\delta r)}$ holds for all $r \geq 0$, as seen by making the substitution $\beta = \delta^{-\alpha}$. One may now use δ as the bifurcation parameter because the resulting problem, where δ is a bifurcation parameter and not β, is smooth as a function of δ near $\delta = 0$. In order to demonstrate that this procedure yields physically relevant solutions, one would have to study how the solution branches behave as β is reduced using global bifurcation theory; undoubtedly this is a very difficult problem.

The results in this paper extend in several directions. For example, consider an abstract formulation of (2.1):

$$\gamma = \rho B(M_\delta(\gamma) - \gamma, M_\delta(\gamma)), \tag{4.1}$$

on a space X that is a Banach algebra under multiplication with unit element $1 \in X$. If

(1) B is a symmetric bilinear form on X,
(2) M is a smooth family of Nemitskii operators on X such that $M_0(\gamma) \equiv -1$ and
(3) $K[\cdot] := B(1, \cdot)$,

then upon setting $\delta = 0$, (4.1) reduces to

$$\gamma = \rho K\gamma + \rho B(1, 1). \tag{4.2}$$

One can study (4.2) and its perturbation (4.1) using the same methods in this article.

For example, in the case whereby convolution over the two or three-dimensional ball $B_R(\mathbf{0})$ is used for the convolution operator that defines B in (4.1), K becomes the operator

$$(Ku)(\mathbf{x}) = \int_{\|\mathbf{x}-\mathbf{y}\|<R} u(\|\mathbf{x} - \mathbf{y}\|)d\mathbf{y}.$$

If X is spanned by finitely many basis functions and B is a projection of the convolution of, say, continuous functions onto this span, then (4.1) corresponds to a finite element dicretisation of (2.1). If $M_\delta(\gamma) = -1+e^{-u(r\delta)}(-1+\gamma)$ and B is a convolution operator, then (4.1) is the Ornstein-Zernike equation with Percus-Yevick closure, as defined in [6]. In all of these cases, many of the results of this paper carry through with the necessary modifications.

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