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**A Numerical Bifurcation Analysis of the Ornstein-Zernike  
equation with Hypernetted Chain Closure**

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The isotropic Ornstein-Zernike (OZ) equation

$$h(r) = c(r) + \rho \int_{\mathbb{R}^3} h(\|\mathbf{x} - \mathbf{y}\|) c(\|\mathbf{y}\|) d\mathbf{y}, \quad (1)$$

that is the subject of this paper was presented almost a century ago to model the molecular structure of a fluid at varying densities. In order to form a well-posed mathematical system of equations from (1) that can be solved, at least in principle, we assume the existence of a closure relationship. This is an algebraic equation that augments (1) with a pointwise constraint that is deemed to hold throughout the fluid and it forces a relationship between the total and direct correlation functions ( $h$  and  $c$  respectively).

Some closures have a mathematically appealing structure in the sense that the total correlation function is posed as a perturbation of the *Mayer  $f$ -function* given by

$$f(r) = -1 + e^{-\beta u(r)}.$$

This perturbation depends on the potential  $u$ , temperature (essentially  $1/\beta$ ) and the indirect correlation function through a nonlinear function that we denote  $G$ :

$$h = f(r) + e^{-\beta u(r)} G(h - c), \quad (G(0) = 0), \quad (2)$$

so that (1-2) are solved together with  $\beta$  and  $\rho$  as bifurcation parameters. There are many closures in use and if we write  $\exp_1(z) = -1 + e^z$  then the hyper-netted chain (HNC) closure

$$G(\gamma) = \exp_1(\gamma) \quad (3)$$

has the form of (2) and is popular in the physics and chemistry literature.

The purpose of the talk is show that *any reasonable* discretisation method applied to (1-2) suffers from an inherent defect if the HNC closure is used that can be summarised as follows: phase transitions lead to fold bifurcations. The existence of a phase transition is characterised by the existence of a bifurcation at infinity with respect to  $h$  in an  $L^1$  norm at a certain density, such that boundedness of  $h$  is maintained in a certain  $L^p$  norm. This behaviour is difficult to mimic computationally by projecting onto a space of fixed and finite dimension and, as a result, projections of (1-2) can be shown to undergo at least one fold bifurcation if such a bifurcation at infinity is present. However, other popular closure relations do not necessarily suffer from the same defect.