

## “Free energy of the Square-Well fluid by Singular Value Decomposition”

Prof Dr Fernando del Río Haza  
Profesor Emérito y Distinguido  
Universidad Autónoma Metropolitana, Iztapalapa  
Departamento de Física  
Laboratorio de Termodinámica [fdri@xanum.uam.mx](mailto:fdri@xanum.uam.mx)  
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The thermodynamics of Square-Well fluids of variable range has been a subject of interest for decades. The free-energy of these systems is nowadays known from molecular simulations by various authors, following the high-temperature perturbation theory of Barker and Henderson. Nevertheless, appropriate analytic expressions to the terms in the perturbation expansion, which are functions of density and temperature, have not been found previously. Here, we propose a procedure, based on the technique of Singular Value Decomposition, that renders separate components depending on density and temperature, and which admits a simple rendering in terms of orthonormal polynomials. The whole interval of SW ranges is covered, from those very short to the van der Waals limit. The method should be useful in other 2-variable problems of statistical thermodynamics.