Sketch of proof: For simplicity we consider here only the case of one pure state. With this assumption one obtains the Φ_j as critical points of the functional

$$J(\Phi) = \int_Q \{|\nabla\Phi|^2 + B(\Phi^2 - m(\Phi^2))\,(\Phi^2 - m(\Phi^2))\}\,\mathrm{d}x\,,$$

where $m(f) = \int_Q f(x)\,\mathrm{d}x$, and $B: L_0^2(Q) \to H^1_{\mathrm{per},0}(Q)$ is the solution operator $u = Bf$ of the Poisson problem $-\Delta u = f$ on Q with $m(u) = 0$; the index zero on a function space means 'mean value zero'. It can be shown that B is a compact injection of $L_0^2(Q)$ into itself. Then the main point is to show that J satisfies a Palais-Smale condition on the set $\{\Phi \in H^1_{\mathrm{per}}(Q) \mid m(\Phi^2) = 1\}$; this is done by using again compact and continuous Sobolev embeddings.

Remarks:

1) By the same method as used in the proof of Theorem 1 one can show the existence of weak X^1-solutions of (SP) under the assumption $\Phi = (\varphi_m) \in X^1$, but we are not able to prove uniqueness of weak solutions.

2) Actually, under the assumptions of Theorem 1, the whole Galerkin sequence (and not only a subsequence) is converging in various topologies to the unique strong solution of (SP) which is stated in

Corollary 1: *Under the assumptions of Theorem 1 there exists for any* $T > 0$ *a constant* $C(T)$ *depending only on* T *(and on* $\|\Phi\|_{X^2}$*) sucht that for all* $N \in \mathbb{N}$, $t \in S_T = [0, T]$,

$$\|\Psi(.,t) - \Psi^{(N)}(.,t)\|_{X^0} \leqq C(T)/N\,.$$

3) All results stated for (SP) transfer by using the Wigner transform (1) to similar results for (WP) which we do not formulate here.

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Critical-Type Fluctuations of Metastable Water at the Negative Pressure Instability

MSC (1991): 76B15, 76Y05, 76N10

A classical van der Waals-fluid can exist in a metastable state at pressures lower than its vapor pressure, even at negative pressures. With increasing tension a mechanical stability limit, associated with critical-type fluctuations, is approached. This stability limit is located on a continuous spinodal line, which starts at the critical point and runs towards infinite negative pressures, when the temperature is decreased.

It has been conjectured that the van der Waals-behavior is drastically altered in the case of water [1]. Starting from the critical point as the spinodal of a superheated fluid, instead of diverging to increasingly negative pressures with

decreasing temperatures, the spinodal bends back towards positive pressures and finally passes into the singularity line extracted from the behavior of supercooled water. The molecular basis of this unusual phenomenon has been studied only little so far.

Therefore, we have investigated water under tension in a series of molecular dynamics simulation runs. The long range density fluctuations are studied by calculating the structure factor $S(Q)$ for low scattering vectors Q.

Molecular dynamics simulation runs consist of integrating Newton's equations of motion to obtain the trajectories of N interacting molecules in an energetically isolated (microcanonical) ensemble with fixed volume. The numerical integration was accomplished for 216 water molecules, interacting via the so-called ST2 effective pair potential. Periodic boundary conditions were imposed to simulate an infinite bulk. This prevents the occurrence of inhomogeneities which are longer than the side of the box L. A more detailed description of the simulation can be found in [2, 3]. The results which are discussed in the following refer to a simulation series, performed at various densities (from $\varrho = 1.0$ to 0.7 g/cm^3) at constant temperature ($T \approx 273$ K).

The limit of mechanical stability, which is equivalent to the loss of tensile strength, is characterised by $(\partial p/\partial v)_T = 0$. This corresponds to a diverging isothermal compressibility $\chi_T = \varrho^{-1}(\partial\varrho/\partial p)_T \to \infty$. χ_T is a measure for the density fluctuations in the system: $\chi_T \sim \langle(\delta\varrho^2)\rangle$. Accordingly, on approaching the spinodal, increasing density fluctuations are occurring. A quantity which can easily be derived from computer experiments to characterize density fluctuations is the static structure factor

$$S(|\boldsymbol{Q}|) = \frac{1}{N}\left\langle \sum_{i,j}^{N} \exp\left(i\boldsymbol{Q}\cdot\boldsymbol{R}_{ij}\right)\right\rangle .$$

$\boldsymbol{R}_{ij}$ is the oxygen distance vector between molecules i and j and $\boldsymbol{Q}$ the scattering vector. In the limit of a vanishing scattering vector

$$S(\boldsymbol{Q}=0) = \varrho k T \chi_T ,$$

$S(Q)$ has been calculated for $|\boldsymbol{Q}| \geqq 1.2$ Å^{-1} by Fourier transforming the oxygen pair correlation function $g_\infty(r)$. For smaller Q-values $S(Q)$ is calculated directly from the sum in the equation above. The smallest accessible wave vector is $Q_1 = 2\pi/L$, where L is the simulation box size, which varies between 18.6 and 21.0 Å for the different densities and the given number of molecules.

As one can see from Fig. 1b, for densities below 0.8 g/cm^3 (the density at the spinodal, predicted by SPEEDY), a strong increase at small Q-values indicates the presence of large scale density fluctuations.

On a microscopic scale the molecules aggregate into denser patches, thus creating large holes in the system: the homogeneous phase is decomposing. A graphical description of the local density fluctuations in water at different global densities ϱ is given in Fig. 1a. To get these pictures, the simulation box is cross-sectioned by an arbitrarily positioned, finely meshed plane. Then, each mesh point, which is closer than 2.5 Å to any water oxygen in the system is marked by

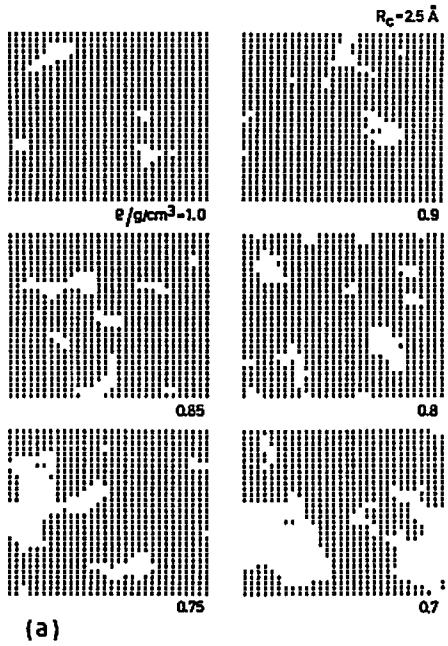

Fig. 1a. Picture of the density fluctuations in low density water

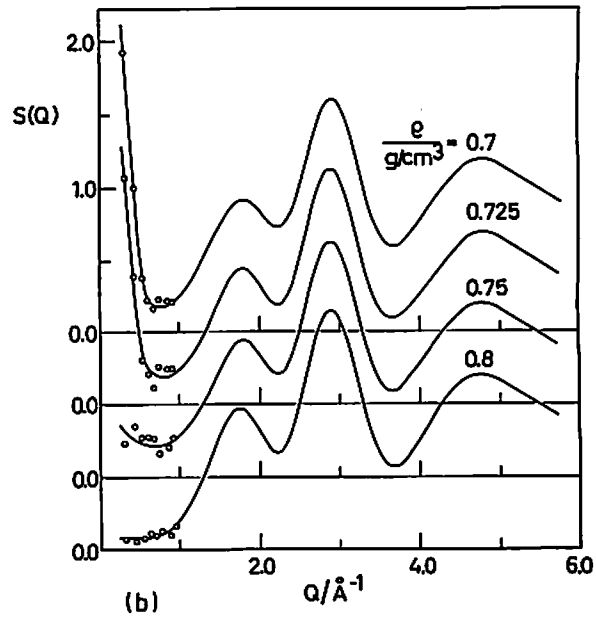

Fig. 1b. Structure factor $S(Q)$ for different densities

a cross. Thus the empty white areas in Fig. 1a indicate cavities in the water. As one can see, between 1.0 and 0.8 g/cm^3 the decreasing global density produces more, but not larger cavities. But below 0.8 g/cm^3 very large cavities occur, indicating the onset of loss of tensile strength.

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Reissel, M.

Über die Äquivalenz zweier Transmissionsrandwertprobleme aus der elektromagnetischen Streutheorie

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1. Einleitung

Die hier beschriebenen Untersuchungen entstanden im Rahmen eines gemeinsamen Projektes mit einem Unternehmen der elektrotechnischen Industrie, welches auf die Herstellung von Kraftwerksgeneratoren spezialisiert ist. Da beim Kraftwerksbau die Tendenz zu immer größeren Einheiten geht, werden keine Standardprodukte eingesetzt, sondern jeder Generator wird individuell auf seine Umgebung abgestimmt. Dadurch entfällt die Möglichkeit der stufenweisen Verbesserung der Maschine, wie sie bei Serienfertigung üblich ist.

Um nun vorab Informationen über die projektierte Maschine zu erhalten, wird versucht, durch numerische Berechnungen die zu erwartenden Leistungsdaten (insbesondere die Verteilungen der elektromagnetischen Felder) zu ermitteln. Ein vom Hersteller entwickeltes Softwarepaket lieferte (wie auch zahlreiche andere Pakete) unbefriedigende Ergebnisse. Die Ursache dieses Versagens soll hier geklärt werden.

2. Aufgabenstellung

Das Verhalten elektromagnetischer Felder wird durch die Maxwellgleichungen beschrieben. Da Generatoren bei konstanter Drehfrequenz arbeiten, können wir einen zeitlich periodischen Verlauf der Felder annehmen. Weiterhin vereinfachen wir die Geometrie unseres Problems, indem wir den Generator als ein beschränktes, offenes Gebiet D_- leitfähigen Materials idealisieren. Im zusammenhängenden Gebiet $D_+ = R^3 \setminus \bar{D}_-$ befinde sich ein Isolator (Luft) sowie eine gegebene Stromdichte J, die Felder in D_- induziert. Uns interessiert nun, wie diese Felder aussehen.

Definieren wir Γ als $\Gamma := \partial D_+ = \partial D_-$, so erhalten wir für homogene, lineare, isotrope Medien das klassische Transmissionsproblem

$$\begin{array}{l} \operatorname{rot} H_+ = J - i\omega\varepsilon_+ E_+ \\ \operatorname{rot} E_+ = i\omega\mu_+ H_+ \end{array} \text{ in } D_+, \qquad \begin{array}{l} \operatorname{rot} H_- = (\sigma_- - i\omega\varepsilon_-) E_- \\ \operatorname{rot} E_- = i\omega\mu_- H_- \end{array} \text{ in } D_-, \qquad \begin{array}{l} n \times H_+ = n \times H_- \\ n \times E_+ = n \times E_- \end{array} \text{ auf } \Gamma \tag{1}$$

mit Silver-Müller-Ausstrahlbedingung $H_+ \times (x/|x|) - E_+ = o(1/|x|)$, $|x| \to \infty$. Falls Γ und J gewissen Regularitätsanforderungen genügen, besitzt (1) eine eindeutige, starke Lösung [2].

Zur Beschreibung von Generatoren wird (1) weiter vereinfacht. Da Generatoren bei sehr niedrigen Frequenzen ω arbeiten, ist $\omega\varepsilon_\pm$ sehr klein. Deshalb werden die Terme in (1), in denen diese Ausdrücke auftreten, gleich Null gesetzt, d. h. die Verschiebungsströme werden vernachlässigt. Berücksichtigen wir noch, daß für alle Lösungen von (1) mit $\varepsilon_\pm > 0$ auch