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COMMENT

Soliton dynamics of hydrogen-bonded systems

B Dey† and M Daniel‡

† Institute for Plasma Research, Bhat, Gandhinagar-382424, India

‡ Department of Physics, Bharathidasan University, Tiruchirapalli-620024, India

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Abstract. Soliton dynamics in hydrogen-bonded systems are usually modelled by considering the system to consist of two interacting sublattices: one of protons with a non-linear on-site potential and the other of coupled heavy ions. Using the potential recently proposed by Pnevmatikos but with a linear interaction between the sublattices, we propose an alternative model which explains the formation and propagation of ionic and Bjerrum defects in ice and other hydrogen-bonded systems.

Recently, there have been many attempts (Zolotariuk *et al* 1984, Laedke *et al* 1985, Pnevmatikos 1987, Yomosa 1983) to describe the mechanism of proton conductivity in hydrogen-bonded systems. The common features in all these theories is that one can model the dynamics of protons in hydrogen-bonded networks by a characteristic non-linear substrate potential with two degenerate equilibrium positions. The model usually consists of two interacting sublattices: one of harmonically coupled light ions (protons) with a doubly degenerate non-linear on-site potential and the other of harmonically coupled heavy ions. The theories differ in choosing the form of interaction between the two sublattices. Usually a non-linear (in light-ion displacement) coupling (Zolotariuk *et al* 1984, Laedke *et al* 1985) between the two sublattices are considered, although there are models (Pnevmatikos 1987, Yomosa 1983) which consider a linear coupling. The two-component soliton (kink) propagation (which occurs in all these theories) is proposed as a possible mechanism for proton conductivity in these hydrogen-bonded systems. In a recent letter, Pnevmatikos (1988) proposed a new model for describing 'simultaneously' both ionic and Bjerrum defect formation and propagation in ice and other related hydrogen-bonded semiconductors. In that model, a non-linear on-site potential of double sine–Gordon type (instead of the usual $\lambda\varphi^4$ type) is considered for the light ions (protons) with a non-linear coupling between the two sublattices.

In this communication, we propose an alternative model for proton conductivity in hydrogen-bonded systems, which consists of the same non-linear on-site potential as in the letter by Pnevmatikos (1988), but with only a 'linear' interaction between the two sublattices. We show that the two-component soliton in this model is also able to explain the formation and propagation of ionic and Bjerrum defects in ice and other related hydrogen-bonded systems. The interaction term satisfies the condition (Pnevmatikos 1988) that it vanishes when one of the two sublattices is at rest.

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The Lagrangian which describes our model can be written in the continuum limit as

$$\mathcal{L} = (m/2)[(\partial u/\partial t)^2 - c_0^2(\partial u/\partial x)^2] - \gamma V(u) + (M/2)[(\partial v/\partial t)^2 - v_0^2(\partial v/\partial x)^2] - g(\partial u/\partial x)(\partial v/\partial x) \quad (1)$$

where the fields $u(x, t)$ and $v(x, t)$ describe the displacements of light ions (protons of mass m) and heavy ions (mass M) respectively, $V(u)$ is the non-linear on-site potential which is taken to be of the same form as that used by Pnevmatikos (1988) (equation (3)), g and γ are the coupling constants, and c_0 and v_0 are the characteristic velocities of the light- and heavy-ion lattices respectively with $c_0 > v_0$. In the travelling-wave frame $\xi = x - ct$, the equations of motions can be written as

$$m(c^2 - c_0^2)u_{\xi\xi} - gv_{\xi\xi} + \gamma(\mathrm{d}V/\mathrm{d}u) = 0 \quad (2)$$

$$M(c^2 - v_0^2)v_{\xi\xi} - gu_{\xi\xi} = 0. \quad (3)$$

Equation (3) can be integrated once to give

$$-v_\xi = [g/M(v_0^2 - c^2)]u_\xi + I \quad (4)$$

where the integration constant I can be taken to be zero if we assume that $u_\xi, v_\xi \rightarrow 0$ as $\xi \rightarrow \pm\infty$. Using equation (4) in equation (2) we obtain

$$[m(c^2 - c_0^2) + g^2/M(v_0^2 - c^2)]u_{\xi\xi} + \gamma(\mathrm{d}V/\mathrm{d}u) = 0. \quad (5)$$

Now, if we use the same non-linear on-site potential $V(u)$ as considered by Pnevmatikos (1988), then equations (4) and (5) reduce to the same form as equations (6) and (7) respectively of the letter by Pnevmatikos. Thus, the displacement fields of the light and heavy ions in our model will be of the same form as those used by Pnevmatikos (1988) and consequently the four defects (kinks and anti-kinks) should also show the same behaviour in the presence of an externally applied DC field.

Thus we see that even a linear coupling between the two sublattices produces displacement field patterns which can effectively explain the ionic and Bjerrum defects in ice and related hydrogen-bonded systems. The displacement field patterns are shown to be of the same form as those obtained by Pnevmatikos (1988) in which a non-linear coupling between the two sublattices is considered.

In conclusion, we would like to note the following observations: as has been mentioned above, various theories for describing the dynamics of proton in hydrogen-bonded systems differ mainly in choosing the form of interaction between the sublattices. When one examines these current 'solvable' models for hydrogen-bonded systems, one finds that their solvability originates from the chosen form of interaction term between the sublattices. The 'trick' is to choose the interaction term in such a way that, after it is eliminated from the equation for $u(\xi)$, the resultant equation reduces to one of the well known soliton equations. For example, in the models used by Laedke *et al* (1985) and Pnevmatikos (1988), the interaction term depends on $u(x)$ through a function $\Phi(u)$ which is chosen such that $\Phi^2(u) \propto V(u)$. As a result of this assumed form of interaction, the coupling term only modifies the coefficient of $\mathrm{d}V/\mathrm{d}u$ term in the equation for $u(x)$, which in turn becomes solvable. On the other hand, in our case, the coupling term modifies the coefficient of the $u_{\xi\xi}$ term (equation (2)) and here also the theory becomes solvable. However, a better model is one which not only is solvable but also provides more information about the system, which may be experimentally tested. Apart from the common features (such as soliton excitation) between the Pnevmatikos and the present model, we feel that our model is more suitable in this context, for the following two reasons.

(i) It is expected that energetically a linear coupling between the two sublattices would be preferable to a non-linear coupling.

(ii) Because of the structure of the theory, two modes of soliton excitation, i.e. fast-mode and slow-mode solitons (Yomosa 1983) are possible here.

The fast-mode soliton is an interesting type of soliton, which cannot be found in the Pnevmatikos (1988) model. This is because in our case the soliton velocity modulates the characteristic velocity of the light-ion sublattice as a direct implication of the two-sublattice coupling. The slow- and fast-mode solitons contribute to the negative and positive energies respectively of the interaction between two sublattices (Yomosa 1983). In the Pnevmatikos (1988) model, the implication of the sublattice coupling is only to modify the coefficient of the $\mathrm{d}V/\mathrm{d}u$ term in the equation for $u(\xi)$ and hence does not give any new information, apart from the soliton excitation, which is obtained from all the solvable models. We feel that experimentally one should look for these two types of soliton which will decide in favour of a particular theory and thus also prevent others from presenting new solvable models that are derived from the same old trick!

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References

Laedke E W, Spatschek K H, Wilkens M Jr and Zolotariuk A V 1985 *Phys. Rev.* A **32** 1161
Pnevmatikos St 1987 *Phys. Lett.* **122A** 249
—— 1988 *Phys. Rev. Lett.* **60** 1534
Yomosa S 1983 *J. Phys. Soc. Japan* **52** 1866
Zolotariuk A V, Spatschek K H and Laedke E W 1984 *Phys. Lett.* **101A** 517