

Collective proton transport with weak proton-proton coupling

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A mechanism based on the peculiar dynamical properties of the hydrogen bond is suggested to describe fast proton transfers in hydrogen-bonded chains with realistic (weak) intersite proton-proton interactions. For this purpose, a two-sublattice model is suggested and studied analytically that admits an exact soliton solution. The solitons, which are topological objects (kinks and antikinks) on the one hand, but dynamical entities (like Boussinesq solitons) on the other hand, are shown to have a sufficiently large width to allow free propagation along the chain.

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I. INTRODUCTION

There have been numerous attempts to model the proton transport in hydrogen-bonded (HB) chains by *two-component* lattice topological solitons [1–19]. The basic idea in such a soliton modeling was to exploit the following remarkable properties of H bonding: (i) the proton in each H bond of a HB chain can be found in two equilibrium positions separated by a potential barrier, so that two degenerate ground states of the chain $\cdots X-H \cdots X-H \cdots X-H \cdots$ and $\cdots H-X \cdots H-X \cdots H-X \cdots$ are assumed to exist, and (ii) the height of the potential barrier that separates the two states depends strongly on the distance between adjacent X atoms, so that a coupled motion of the protons and the X atoms may provide a barrier-lowering mechanism that allows an easy proton transfer between the two equilibrium positions of the protons. A crucial point for the validity of the soliton mechanism in such a chain was the assumption of the existence of a strong intersite proton-proton coupling. However, according to *ab initio* calculations of this coupling (41 cal/mol Å²) [20], realistic values of the potential barrier in the H bond are too high to allow free soliton propagation because the so-called displacive limit in the chain of coupled double-well oscillators [21,22] is not valid and strong discreteness effects will pin the narrow kink [23]. The coupled motion of the H and X atoms was also shown to be insufficient to lower the barrier enough to provide a free soliton regime. Even when this coupled motion is taken into account, the ionic defects in HB chains with realistic parameter values [24] were shown to be very narrow objects [12].

In fact, this limitation appears because the models do not take into account the full characteristics of the potential energy surface of the chain. We show in this paper that a soliton mechanism that does not require a strong coupling of the protons in adjacent hydrogen bonds may exist if one properly describes the nonlinear features of the hydrogen bonds. The solitons that we obtain are closer to the well-known lattice (Boussinesq or Toda) solitons [25] rather than to the kinks in

the coupled double-well model [21,22]. For instance, they cannot exist as stable *standing* solitary waves. On the other hand, they are still *topological* objects and can be considered as a different type of soliton in one-dimensional lattices.

In Sec. II, we discuss the potential and physical parameters needed to describe the proton dynamics in a single hydrogen bond. The relationship of these parameters to those known for the pairwise proton-ion and ion-ion interactions are explicitly given in this section. In Sec. III, we obtain in the continuum limit an exact two-component soliton solution and study its properties. The last section contains a summary and conclusions.

II. THE MODEL FOR A SINGLE HYDROGEN BOND

The important point in a two-sublattice model for proton transfers is an *explicit* dependence of the shape of the double-well potential on the relative distance between the adjacent ions that form this potential. The natural way to find the analytical expression for such a double-well potential is to construct it from two single pairwise potentials located at varying distance from each other with opposite orientations. In particular, any potential of the standard forms (Morse or Lennard-Jones) can be chosen for this purpose. Although a construction of this type has been implemented in many papers (see, e.g., Refs. [10–13,15–17] and others), nevertheless we need to reconsider it here properly using a revised procedure. This is an important step because we are interested in large-amplitude solutions of the resulting two-component model, when the amplitude of the background sublattice is sufficient to allow the barrier for proton transfers between the wells to vanish. On the other hand, we do not discuss very much in this paper the numerical values for the parameters because they are discussed in many works (see, e.g., Refs. [10,12,16,24,26–29] and references therein) and are not crucial for the validity of our solution.

Consider first a single isolated fragment $X-H \cdots X$ of a

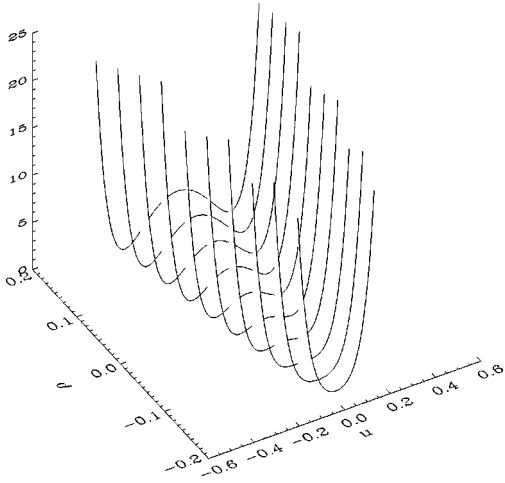


FIG. 1. Potential $V(u, \rho)$ created on the proton by the two lateral X ions. The potential is plotted for various values of ρ , the change of the $X \cdots X$ distance with respect to its equilibrium value.

HB chain. Its total energy can be split into two parts as follows:

$$U(u, \rho) = \varepsilon_0 V(u, \rho) + \frac{1}{2} K \rho^2, \quad (1)$$

where the first term describes the potential for the proton created by the two lateral X atoms (ions) while the second term represents the harmonic approximation of a renormalized (due to the presence of the middle proton) interaction between the X atoms. Here u is the displacement of the proton from the midpoint of the H bond, whereas ρ is the deviation of the distance R between the X atoms from its equilibrium distance (the lattice spacing l), so that $\rho = R - l$. The dimensionless two-dimensional potential energy surface for the proton, $V(u, \rho)$, can be calculated by quantum chemistry by choosing a given distance R between the X atoms and varying the displacement u [26–28]. For the isolated fragment $X-H \cdots X$, it has the shape shown in Fig. 1. When the two X atoms are sufficiently far apart (the relative distance ρ exceeds a certain critical value ρ_c), it has two minima separated by a potential barrier, so that the function $V(u, \rho)$ appears as two valleys separated by a potential hill. The bottoms of these valleys, whose position is given by two symmetric functions $u = \pm u_0(\rho)$ shown in Fig. 2, can be taken as the reference potential level and can be set to $V(\pm u_0(\rho), \rho) = 0$. Moreover, we can normalize the function $V(u, \rho)$ such that $V(0, 0) = 1$ and therefore ε_0 turns out to be the height of the barrier when the lateral X atoms are situated at the equilibrium distance l .

When ρ is reduced below the critical value $\rho_c < 0$, the valleys merge into *one* (symmetric) potential energy minimum. In other words, at this point, the double-well topology of the proton potential $V(u, \rho)$ is transformed into a single well centered at the midpoint ($u = 0$) of the H bond. This behavior can be described by the bifurcation diagram shown in Fig. 2. The adjacent X atoms cannot pass through each other and therefore $|\rho_c| < l$. Obviously, under all these assumptions, the total potential (1) with $K > 0$ will have only two *global* minima ($\pm a, 0$) on the (u, ρ) plane that correspond to the degenerate ground states of the chain.

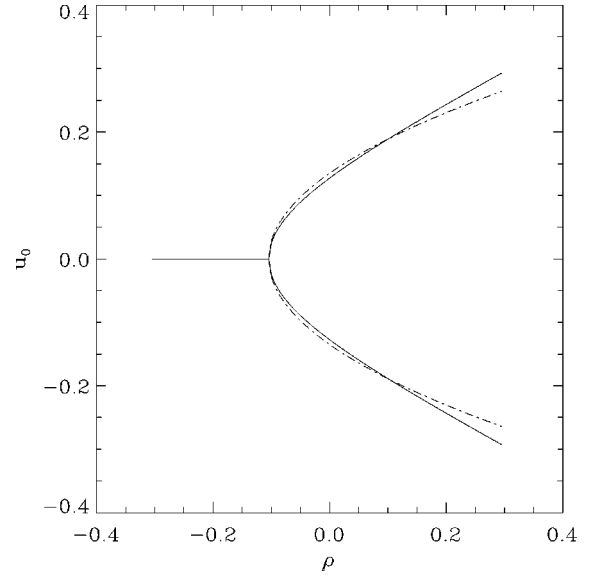


FIG. 2. Bifurcation diagram for the potential $V(u, \rho)$ showing the positions of the minima of the potential versus ρ (full line) and the corresponding bifurcation diagram for the reduced potential defined by Eq. (9) (dot-dashed line).

As shown by the quantum chemistry calculations [27], a good approximation of the potential energy surface (1) can be constructed as the superposition of two symmetrically situated ion-proton Morse potentials as well as an ion-ion coupling, so that one can write [10–12, 15, 16, 28]

$$U(u, R) = D \left\{ 1 - \exp \left[-\beta \left(\frac{R}{2} - r_0 + u \right) \right] \right\}^2 + D \left\{ 1 - \exp \left[-\beta \left(\frac{R}{2} - r_0 - u \right) \right] \right\}^2 + \frac{1}{2} K_0 (R - R_0)^2, \quad (2)$$

where D is the dissociation energy of the ion-proton interaction and r_0 its equilibrium distance. These parameters as well as the parameter β can be evaluated on the basis of the linear dispersion law [12] using available experimental data [24] or fitted from *ab initio* calculations [26, 27, 29]. The stiffness constant K_0 and the distance R_0 are effective (bare) parameters corresponding to a fictitious (“pure”) ion subsystem consisting of only $X \cdots X$ fragments. The spring with stiffness K_0 may be thought of as the result of a Coulomb interaction between nearest-neighbor ions in a one-dimensional lattice with fixed boundary conditions. These parameters are supposed to be sufficiently large as to provide a double-well topology for the function $V(u, 0)$. Sufficient criteria for its existence are given below in the form of inequalities.

Using the condition $\partial U / \partial u = 0$, from Eq. (2) we can explicitly find the dependence $u_0(R)$ that determines the (symmetric) position of the minima as a function of the distance R . Next, representing in Eq. (2) the distance R through the relative displacement ρ by $R = l + \rho$, from the other extremum condition $dU(u = \pm u_0(R), R) / dR = 0$, one finds the equation

$$R_0 - l = (2D\beta/K_0)\exp[\beta(2r_0 - l)], \quad (3)$$

which eliminates the linear (in ρ) term in the sum (2). Equation (3) admits a unique solution if the inequality $2D\beta \exp(2\beta r_0) < K_0 R_0$ holds.

As a result, up to a constant and anharmonic terms in the pure ρ part, the sum (2) can be written in the form (1) where

$$\varepsilon_0 = D \left(1 - \frac{1}{\alpha}\right)^2, \quad \alpha = \frac{1}{2} \exp \left[\beta \left(\frac{l}{2} - r_0 \right) \right], \quad (4)$$

is the height of the double-well potential at $\rho=0$, which itself is given by

$$V(u, \rho) = \left(\frac{\alpha - \cosh(\beta u) \exp(-\beta r/2)}{\alpha - 1} \right)^2. \quad (5)$$

The inequality $\alpha > 1$ ensures a double-well form of the function (5). The parameter condition for this existence can be obtained using Eq. (3). As a result, we obtain the inequality $R_0 > D\beta/2K_0 + 2i[\ln(2)/\beta + r_0]$ as a constraint on the bare parameters.

In order to obtain the form (1) for the ρ part, i.e., to write it as $K\rho^2/2$, one must keep only the harmonic contribution and define the renormalized coupling constant

$$K = K_0 - D\beta^2/2\alpha^2, \quad (6)$$

which must be positive. It is sufficient that $K_0 > D\beta^2/2$. This harmonic approximation is, however, not a severe constraint because the relative distance between the heavy ions shows only small deviations from equilibrium. For this potential, the value of ρ below which the two minima merge is given by $\rho_c = -2\ln(\alpha)/\beta$. The bifurcation diagram in Fig. 2 is given by the equation $\cosh(\beta u_0) = \alpha \exp(\beta\rho/2)$ for $\rho > \rho_c$ and $u_0 = 0$ for $\rho \leq \rho_c$. In particular, when the ions are found in equilibrium ($\rho=0$), the minima $\pm a$, where $a \equiv u_0(\rho=0)$, satisfy the equation

$$\cosh(\beta a) = \alpha. \quad (7)$$

Finally, we need to mention such an important parameter as the frequency of the small-amplitude oscillations of a proton around the minima of both the pairwise proton-ion potential (at $r=r_0$) and the double-well potential (at $u = \pm u_0$). In the former case the frequency ω_0 is given by $\omega_0^2 = 2D\beta^2/m$ where $m = m_p$ is the proton mass, whereas in the latter case the frequency $\Omega_0(\rho)$ defined as $\Omega^2 = (\partial^2 U / \partial u^2)[u = \pm u_0(\rho)]/m$ can be represented through ω_0 as $\Omega^2 = [1 - \alpha^{-2} \exp(-\beta\rho)]\omega_0^2$. This expression demonstrates the softening behavior of the frequency in the double-well potential with decrease of the interionic distance R ($\Omega \rightarrow 0$ as $\rho \rightarrow \rho_c$). When the ions are in equilibrium, the frequencies $\Omega_0 \equiv \Omega(\rho=0)$ and ω_0 are related to each other by

$$\Omega_0 = \sqrt{1 - \alpha^{-2}} \omega_0. \quad (8)$$

Summarizing the results of this section, one may say that we have established one-to-one correspondence between the parameters and variables of the proton-ion interaction together with the bare ion-ion interaction and those of the

“dressed” $X-H \cdots X$ hydrogen bond. In other words, Eqs. (3), (4), and (6)–(8) determine the isomorphism of the two sets, each consisting of five parameters: $\{D, r_0, \omega_0; K_0, R_0\} \leftrightarrow \{\varepsilon_0, a, \Omega_0; K, l\}$. The three inequalities derived above for the bare parameters do not contradict each other. The isomorphism of the variable sets $\{r, R\} \leftrightarrow \{u, \rho\}$, which we already used above, is given by the equations $u = r - R/2$ and $\rho = l - R$.

For small values of the parameter β , an analog of the ϕ^4 approximation can be introduced, and instead of the potential (5) we can use its truncated version as follows:

$$V(u, \rho) = \left(1 - \frac{u^2}{a^2} + \frac{\rho}{b}\right)^2, \quad b = a^2\beta > 0. \quad (9)$$

This simplified form is essential to allow an analytical solution of the coupled dynamics of the H and X ions, but it preserves the two-dimensional topology of the original potential (5), which is a specific property of the hydrogen bond. While it brings some small quantitative changes, the approximation (9) does not change the qualitative properties of the system. And, as we shall show below that the main point that we would like to stress in the paper depends only on the qualitative properties of the solution, the approximation (9) allows us to reach our conclusions from analytical calculations rather than numerical simulations, which is more satisfactory and illustrates the main ideas more clearly.

For the reduced potential (9), the bifurcation diagram is given by $u_0 = 0$ if $\rho < -b$ and $u_0 = a\sqrt{1 + \rho/b}$ for all $\rho \geq -b$. As shown in Fig. 2, it can provide a rather good approximation of the actual bifurcation diagram given by the realistic potential (5) up to values of ρ that approach 0.2 \AA , which corresponds to a very large lattice distortion.

III. DYNAMICS OF THE HB CHAIN: AN EXACT SOLITON SOLUTION

To write the total Hamiltonian of the HB one-dimensional lattice system, we need to add an intersite proton-proton coupling. This interaction is necessary to provide only *two* degenerate ground states in the whole chain, otherwise any disordered state with protons at the left or right of the double-well potential would be a possible state in the system. It is, however, important to stress that, while this interaction is essential to lift the degeneracy of the many possible states of the chain, its magnitude does not need to be large for the validity of the solitonlike solution that we are interested in. As discussed in the Introduction, the realistic proton-proton interaction is expected to be weak, and moreover this is a parameter that is hard to determine accurately. It is therefore fortunate that its value is not crucial for the validity of our results, provided this interaction does not strictly vanish.

Therefore, the Hamiltonian of the chain can be written in the form

$$H = \sum_n \left(\frac{1}{2} m \dot{q}_n^2 + \frac{1}{2} \kappa (q_{n+1} - q_n)^2 + \varepsilon_0 V(u_n, \rho_n) + \frac{1}{2} M \dot{Q}_n^2 + \frac{1}{2} K \rho_n^2 \right), \quad (10)$$

where M is the mass of an X atom, κ and K are the stiffness constants of the proton-proton coupling and the $X \cdots X$ force, respectively, q_n is the displacement of the proton from the midpoint in the n th bond when the X atoms are frozen, and Q_n is the displacement of the n th X atom from its equilibrium position. The displacement in the n th hydrogen bond u_n and its stretching ρ_n are expressed in terms of the displacements q_n and Q_n as follows:

$$u_n = q_n - \frac{1}{2}(Q_n + Q_{n+1}), \quad \rho_n = Q_{n+1} - Q_n. \quad (11)$$

Note that the model Hamiltonian (10) takes into account the fact that the proton potential V is moving together with the adjacent heavy ions. This is an important feature, which was missing in the original soliton model for proton transport [1,4,6].

The corresponding equations of motion are

$$m\ddot{q}_n = \kappa(q_{n+1} - 2q_n + q_{n-1}) - \varepsilon_0 f_n, \quad (12)$$

$$M\ddot{\rho}_n = K(\rho_{n+1} - 2\rho_n + \rho_{n-1}) + \varepsilon_0 \left(\frac{1}{2}(f_{n+1} - f_{n-1}) + g_{n+1} - 2g_n + g_{n-1} \right),$$

where $f_n = \partial V(u_n, \rho_n) / \partial u_n$ and $g_n = \partial V(u_n, \rho_n) / \partial \rho_n$.

In the continuum limit ($nl = x$), the discrete fields $q_n(t)$, $Q_n(t)$, $u_n(t)$, and $\rho_n(t)$ are substituted by the corresponding continuous fields $q(x, t)$, $Q(x, t)$, $u(x, t)$, and $\rho(x, t)$. Then the set of Eqs. (12) becomes

$$m(q_{tt} - c_0^2 q_{xx}) = -\varepsilon_0 f, \quad (13)$$

$$M(\rho_{tt} - v_0^2 \rho_{xx}) = \varepsilon_0 l (f_x + l g_{xx}),$$

where $u = q - Q$ and $\rho = lQ_x$. Here the two characteristic velocities $c_0 = l\sqrt{\kappa/m}$ and $v_0 = l\sqrt{K/M}$ have been introduced. The functions $f = f(u, \rho)$ and $g = g(u, \rho)$ are defined by $f = \partial V / \partial u$ and $g = \partial V / \partial \rho$.

In the moving frame (with velocity v , $\xi = x - vt$), the second equation is trivially integrated once. Next, integrating these equations from $-\infty$ to ξ and setting to zero the integration constant, we find

$$m(c_0^2 - v^2)q'' = \varepsilon_0 \frac{\partial}{\partial q} V(q - Q, \rho), \quad (14)$$

$$m(v^2 - c_0^2)lq' + M(v^2 - v_0^2)\rho = \varepsilon_0 l^2 \frac{\partial}{\partial \rho} V(q - Q, \rho),$$

where the prime denotes a derivative with respect to ξ .

For the particular case of the potential (9), we can look for a solution of this set of coupled equations in which the two fields are proportional to each other. This assumption leads to the two-component kink solution

$$q(\xi) = q_0 \tanh(\mu \xi), \quad Q(\xi) = Q_0 \tanh(\mu \xi), \quad (15)$$

with the amplitudes

$$q_0 = - \frac{b/l\mu \mp a}{1 \pm ab\mu m(v^2 - c_0^2)/2\varepsilon_0 l}, \quad (16)$$

$$Q_0 = - \frac{b}{l\mu} \frac{1 + a^2 \mu^2 m(v^2 - c_0^2)/2\varepsilon_0}{1 \pm ab\mu m(v^2 - c_0^2)/2\varepsilon_0 l},$$

and the inverse half-width

$$\mu^2 = \frac{1}{a^2} \frac{1 + M(v_0^2 - v^2)/m(c_0^2 - v^2)}{(l/b)^2 + M(v_0^2 - v^2)/2\varepsilon_0}. \quad (17)$$

This kink solution can be written in terms of the proton displacements in the hydrogen bond and of the relative displacements of the X atoms:

$$u(\xi) = \pm a \tanh(\mu \xi), \quad \rho = \rho_0 \cosh^{-2}(\mu \xi), \quad (18)$$

where $\rho_0 = l\mu Q_0$. The upper (lower) sign in Eqs. (16)–(18) corresponds to the kink (antikink) solutions.

For realistic parameter values, i.e., weak proton-proton coupling as discussed above, the characteristic velocity c_0 is small. Therefore, it is reasonable to assume that $c_0 < v_0$. Then, the positivity of the right-hand side of Eq. (17) implies the existence of *two bands* of admissible soliton velocities:

$$0 \leq v < c_0, \quad (19)$$

$$v_1 \equiv \sqrt{\frac{Mv_0^2 + mc_0^2}{M+m}} < v < \sqrt{v_0^2 + \frac{2\varepsilon_0 l^2}{b^2 M}} \equiv v_2. \quad (20)$$

The former (slow) mode is actually the standard kink mechanism proposed earlier for proton mobility in hydrogen-bonded chains. However, as shown previously [20,12], these solitons are narrow. This is confirmed by Eq. (17) because, for this low velocity band, the inverse width μ becomes very large for small c_0 . As a result, the continuum approximation breaks down and the kinks are pinned by discreteness effects. In contrast, for the latter (fast) mode, the proton-proton coupling is not important.

IV. CONCLUSIONS

The existence of the solitons studied above, which can be referred to as HB solitons, is due to the specific two-dimensional topology of the proton potential $V(u, \rho)$. It is important to notice that, as shown by Eq. (17), at the left edge of the HB soliton band ($v \rightarrow v_1 + 0$), the solitons become infinitely wide ($\mu \rightarrow 0$), while at the right edge they collapse ($\mu \rightarrow \infty$). Note that a similar behavior occurs for the well-known (supersonic) lattice solitons [25] which become infinitely wide when their velocity is approaching the speed of sound from above. The existence of a velocity range in which the soliton is very broad shows that the solitons belonging to the high velocity band can propagate even at very small proton-proton coupling. It is important to stress that the existence of these broad solitons is not sensitive to the parameter values, provided the two-dimensional potential energy surface has the qualitative shape shown in Figs. 1 and 2.

Another important conclusion is that the heavy-atom deformation component, at least for velocities sufficiently close

to the left edge of the HB band, can be *compressional*, i.e., $\rho_0 < 0$, for both kinks and antikinks. Moreover, this compression for antikinks (positive defects) exceeds that for kinks (negative defects). Finally, one can conclude that there exists in the band (20) an interval such that the reasonable inequalities $a\mu < 1$ and $-l < \rho_0 < 0$ hold.

It should be noticed that for an antikink (positive ionic defect) the potential barrier disappears. The same is also true for the kink solutions, but only for supersonic velocities ($v > v_0$) when $a\mu > b/l$. For subsonic velocities the barrier still exists although it is reduced. It follows from these remarks that the mobility of the positive defects exceeds that of the negative defects, in agreement with experimental data.

Thus, a type of two-component topological soliton that can be called HB solitons has been exhibited in diatomic lattices with H-bonding properties. The results that we have presented here do not rely on specific parameter values of the Hamiltonian. They are based only on general features of the hydrogen bond, the vanishing of the barrier when the heavy ions come close to each other, and the translation of the proton together with the motion of the adjacent heavy ions, which can reasonably be expected to be valid for a hydrogen-bonded chain. In fact, for proton transport in water, quantum

chemistry calculations show that extended proton migration must occur in a concerted fashion requiring an *inward* fluctuation of the O ··· O distance [30], in agreement with the assumptions that underlie our calculations. The validity of the HB soliton for a three-dimensional system is, however, still an open question, as well as its stability in the presence of thermal fluctuations that could destroy the coherence necessary for its propagation.

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