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Hamiltonian formulation of energy conservative variational equations by wavelet expansion ☆

Shigeru Maeda[a] and Masami Okada[b,*]

[a] Department of Mathematics & Natural Systems, Faculty of Integrated Arts & Science, The University of Tokushima, Tokushima 770-8502, Japan
[b] Department of Mathematics, Tokyo Metropolitan University, Hachioji 192-0397, Japan

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Abstract

Hamiltonian formulation of various energy conservative evolution equations is given by means of wavelet expansion of solutions on the whole real axis R. The KdV equation, wave equations and Schrödinger equations are treated in a unified similar manner. A matrix representation of operators with respect to a nice wavelet base plays an important role in the formulation. Since the procedure is very concrete, our results can be used to efficiently compute numerical solutions of partial differential equations described in the text. In fact, we may also use symplectic schemes to solve derived Hamiltonian systems.

1. Introduction and preliminaries

According to Lax [9], Gardner gave a Hamiltonian formulation of the KdV equation in the periodic case in [7] and Faddeev and Zakharov briefly pointed out a Hamiltonian formulation on the whole real axis [20]. Here in this note we propose to use a suitable wavelet base on the real axis in order to give a more concrete Hamiltonian formulation of a wide class of general evolution equations, such as the KdV equation, which are derived from energy functionals by the Lagrange–Euler

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* Corresponding author.

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variational argument. We believe that our approach is not without interest from practical as well as theoretical point of view.

In this note, we shall use the complete orthogonal system of Daubechies' wavelets or Coiflets. The system consists of $\psi_{j,k}$, where $\psi_{j,k}(x) = 2^{j/2}\psi(2^j x - k), j, k \in Z$ with the wavelet function ψ, which has the following nice properties [4].

Property. (i) The system $\{\psi_{j,k},\ j, k \in Z\}$ is a complete orthogonal base of $L^2(R)$.

(ii) ψ is a real-valued function with compact support.

(iii) For a given positive number N, there exists ψ such that it is a C^N function and moreover the kth moment of ψ vanishes for $k = 0, 1, 2, \ldots, N-1$.

There are many works where wavelet theory is employed in numerical studies of partial differential equations (PDEs). Let us cite e.g., [1–3,10,14,18] as references which are relevant to this note from our point of view.

Let $\{e_n\}$ be a general complete orthogonal base of $L^2(R)$ for the moment. Later, we shall assume that $\{e_n\}$ is the orthogonal system of wavelet $\{\psi_{j,k}\}$. Then the usual Parseval–Bessel formula is stated as follows.

Lemma 1. *For any $f, g \in L^2(R)$, we have*

$$\sum_n (f, e_n)(e_n, g) = (f, g), \tag{1}$$

where $(,)$ is the inner product.

Let D be the derivation operator $Df = df/dx$ and let D^{-1} be an inverse operator defined by $D^{-1}f(x) = \int_{-\infty}^{x} f(y)\,dy$. Note that in general, D^{-1} is defined only with modulo constants and $D^{-1}f \notin L^2(R)$. Although we have fortunately the following fact which is stated as a lemma for the sake of completeness.

Lemma 2. *Let us assume that f is compactly supported and $\int_{-\infty}^{\infty} x^k f(x)\,dx = 0$, for $k = 0, 1, 2, \ldots, N-1$. Then $D^{-m}f \in L^2(R)$ is uniquely represented by*

$$D^{-m}f(x) = \frac{1}{(m-1)!}\int_{-\infty}^{x} (x-t)^{m-1} f(t)\,dt, \tag{2}$$

for $m = 1, 2, \ldots, N$.

Proof. In order to show that the right-hand side of (2) belongs to $L^2(R)$, it suffices to expand $(x-t)^{m-1}$ into $\sum_{k=0}^{m-1} (-1)^k_{m-1}C_k x^{m-1-k} t^k$ and we see easily that

$$\int_{-\infty}^{x} t^k f(t)\,dt = 0, \quad k = 0, 1, \ldots, m-1, \tag{3}$$

for large $|x|$. The rest of the proof is easy. □

Corollary 1. *Let $\{e_n\}$ be a complete orthogonal system and let f satisfy the conditions of Lemma 2 and let $g \in H^N(R)$, the Sobolev space. Then,*

$$\sum_{n \in Z} (D^{-m} f, e_n)(e_n, D^m g) = (-1)^m (f, g). \tag{4}$$

Proof. Since $D^{-m} f, D^m g \in L^2(R)$, we can use Lemma 1 and the left-hand side is equal to $(D^{-m} f, D^m g)$, from which follows the conclusion by the successive integration by parts. □

Now let us compute the adjoint operators of D^m and D^{-m}.

Proposition 1. *Let ψ_1, ψ_2 be two wavelet functions with preceding nice properties. Then for each positive integer m $(m \leqslant N)$, we have*

$$\text{(i)} \quad (\psi_1, D^m \psi_2) = (-1)^m (D^m \psi_1, \psi_2), \tag{5}$$

$$\text{(ii)} \quad (\psi_1, D^{-m} \psi_2) = (-1)^m (D^{-m} \psi_1, \psi_2). \tag{6}$$

Proof. (i) is immediate by the integration by parts. To prove (ii), note that

$$D^{-m} \psi_2(x) = \frac{1}{(m-1)!} \sum_{k=0}^{m-1} (-1)^k_{m-1} C_k x^{m-1-k} \int_{-\infty}^{x} t^k \psi_2(t) \, dt.$$

Therefore,

$$(\psi_1, D^{-m} \psi_2) = \frac{1}{(m-1)!} \sum_{k=0}^{m-1} (-1)^k_{m-1} C_k \left(x^{m-1-k} \psi_1(x), \int_{-\infty}^{x} t^k \psi_2(t) \, dt \right).$$

Then by Fubini's theorem,

$$\begin{aligned} \left(x^{m-1-k} \psi_1(x), \int_{-\infty}^{x} t^k \psi_2(t) \, dt \right) &= \left(\int_{t}^{\infty} x^{m-1-k} \psi_1(x) \, dx, t^k \psi_2(t) \right)_{L^2(R,dt)} \\ &= - \left(t^k \psi_2(t), \int_{-\infty}^{t} x^{m-1-k} \psi_1(x) \, dx \right)_{L^2(R,dt)}, \end{aligned}$$

which implies

$$(\psi_1, D^{-m} \psi_2) = \frac{1}{(m-1)!} \sum_{k=0}^{m-1} (-1)^{k+1}_{m-1} C_k \left(x^k \psi_2(x), \int_{-\infty}^{x} t^{m-1-k} \psi_1(t) \, dt \right).$$

Now putting $l = m - 1 - k$, the last sum is equal to

$$(-1)^m \frac{1}{(m-1)!} \sum_{l=0}^{m-1} (-1)^l {}_{m-1}C_l \left(x^{m-1-l}\psi_2(x), \int_{-\infty}^{x} t^l \psi_1(t)\, dt \right),$$

which is nothing but $(-1)^m(\psi_2, D^{-m}\psi_1) = (-1)^m(D^{-m}\psi_1, \psi_2)$. $\square$

Fix a given orthogonal system of wavelets $\{e_n\} = \{\psi_{j,k}\}$ with nice properties as before. Then let us associate a matrix to the operators, $P = D^m$ and D^{-m}, $m = 0, 1, 2, \ldots, N$.

Definition 1. For a given real operator P, we define its representing matrix M_P by

$$(M_P)_{ij} = (e_i, Pe_j). \tag{7}$$

Note that M_P is real valued since $\{e_n\}$ is a real-valued base.

Lemma 3. *Let $P = RQ$ where $R = D^{m_1}$, $Q = D^{m_2}$ with integers m_1, m_2 satisfying $|m_1| \leqslant N$, $|m_2| \leqslant N$, $|m_1 + m_2| \leqslant N$. Then we have*

$$M_P = M_R M_Q. \tag{8}$$

Proof. Let us compute any given (i,j) component $(M_R M_Q)_{ij}$. Then

$$\begin{aligned}(M_R M_Q)_{ij} &= \sum_k (e_i, Re_k)(e_k, Qe_j) = \sum_k (R^* e_i, e_k)(e_k, Qe_j) \\ &= (R^* e_i, Qe_j) = (e_i, RQe_j) = (M_P)_{ij},\end{aligned} \tag{9}$$

where the adjoint R^* is equal to $(-1)^{m_1} R$ in view of Proposition 1. $\square$

Let us call P invertible with respect to the base $\{e_n\}$ if and only if $P^{-1}e_k \in L^2(R)$ for each $k \in Z$. Then we have

Corollary 2. *If P is invertible, $M_{P^{-1}} = (M_P)^{-1}$.*

Remark 1. Lemma 3 holds for any invertible operators Q, R in general, and it plays a key role in the sequel.

Remark 2. Note that there exist other notions of invertibility of operators. In fact, if we take $P = I - D^2$, for example, then by easy computation, we have

$$(I - D^2)^{-1} f(x) = \frac{1}{2} \left\{ e^{-x} \int_{-\infty}^{x} f(y) e^{y}\, dy - e^{x} \int_{x}^{\infty} f(y) e^{-y}\, dy \right\},$$

which belongs to $L^2(R)$, for any integrable function f with compact support. This operator $(I - D^2)$ may be called strongly invertible. Furthermore, there exists a weaker notion of invertibility of possible interest. Namely, we may call an operator P weakly invertible if and only if there exists a complete orthogonal base such that P is invertible with respect to this base. However, this issue may need further investigation.

2. Energy functionals and variational method

Let us follow the notation and the functional calculus employed in Gardner [7]. From now on we shall assume $u = u(x,t)$ be a real function of $x \in R$ and $t > 0$, and $G = G(u, u_x, u_{xx}, \ldots)$ be a real function of $u, u_x, u_{xx}, \ldots$. Let

$$F(u) = \int_{-\infty}^{\infty} G(u, u_x, u_{xx}, \ldots)\, dx$$

be the corresponding functional. Then as is well known, its Euler–Lagrange derivative $\frac{\delta F}{\delta u}$ is given by

$$\frac{\delta F}{\delta u} = \frac{\partial G}{\partial u} - \partial_x\left(\frac{\partial G}{\partial u_x}\right) + \partial_{xx}\left(\frac{\partial G}{\partial u_{xx}}\right) - \cdots \ . \tag{10}$$

Now we semi-discretize u, i.e., we expand $u(x,t)$ for each fixed $t > 0$ by means of our orthogonal system $\{e_n\}$, in such a way that

$$u(x,t) = \sum_n c_n(t) e_n(x). \tag{11}$$

Then by the chain rule,

$$\frac{\partial F}{\partial c_n} = \int_{-\infty}^{\infty} \frac{\delta F}{\delta u}\frac{\partial u}{\partial c_n}\, dx = \int_{-\infty}^{\infty} \frac{\delta F}{\delta u} e_n\, dx = \left(\frac{\delta F}{\delta u},\, e_n\right). \tag{12}$$

Therefore, we obtain

$$\frac{\delta F}{\delta u} = \sum_n \frac{\partial F}{\partial c_n} e_n. \tag{13}$$

Note that $F(u)$ can also be considered as a function of an infinite vector $\mathbf{c} = \mathbf{c}(t) = (\ldots, c_{-1}, c_0, c_1, \ldots)^t$ for any fixed t. We shall denote $F(\mathbf{c}) = F(u)$ without ambiguity. Let A be an infinite matrix $A = (a_{ij}), a_{ij} \in R$. Then we put $\mathbf{b} = A\mathbf{c}$ to define a change of variables from $\mathbf{c}$ to $\mathbf{b}$. Let $\nabla_{\mathbf{c}} F$ be the gradient, i.e., the infinite vector defined by $\nabla_{\mathbf{c}} F = (\frac{\partial F}{\partial c_n})_{n \in Z}$ and let $\nabla_{\mathbf{b}} F$ be defined in the same way. Then we have the change of variable formula as follows. Here, keep in mind that $\nabla_{\mathbf{c}}F$ depends only on t.

Proposition 2. *Under the change of variables,* $\mathbf{b} = A\mathbf{c}$, *we have*

$$\nabla_{\mathbf{c}}F = A^t \nabla_{\mathbf{b}}F, \quad \text{where } A^t \text{ is the transpose of } A. \tag{14}$$

3. PDE of type $\partial_t u = P(\frac{\delta F}{\delta u}),\ P^t = -P$

In this section, we assume that the real operator P is invertible and antisymmetric, i.e., $P^* = P^t = -P$. Then we have

Theorem 1. *Let P be a linear and invertible real antisymmetric operator. Then a PDE of type*

$$\partial_t u = P\left(\frac{\delta F}{\delta u}\right) \tag{15}$$

is reduced to a Hamiltonian system with Hamiltonian $H = F$.

Proof. Let u be a solution of the PDE. On the one hand, applying P to (13) we have

$$P\left(\frac{\delta F}{\delta u}\right) = \sum_n \frac{\partial F}{\partial c_n} Pe_n = \sum_n \frac{\partial F}{\partial c_n}\left\{\sum_k (Pe_n, e_k)e_k\right\} = (\dots, e_k, \dots)M_P \nabla_{\mathbf{c}}F. \tag{16}$$

On the other hand, since $\partial_t u = \sum_k \dot{c}_k(t)e_k(x)$, (15) is equivalent to $\dot{\mathbf{c}} = M_P \nabla_{\mathbf{c}}F$. Now we define $\mathbf{d}$ by $\mathbf{d} = M_P^{-1}\mathbf{c}$. Then by Corollary 2,

$$\dot{\mathbf{d}} = M_P^{-1}\dot{\mathbf{c}} = M_P^{-1}M_P\nabla_{\mathbf{c}}F = \nabla_{\mathbf{c}}F.$$

Next, by Proposition 2, $\nabla_{\mathbf{c}}F = (M_P^{-1})^t \nabla_{\mathbf{d}}F$, which implies

$$\dot{\mathbf{c}} = M_P\nabla_{\mathbf{c}}F = M_P(M_P^{-1})^t\nabla_{\mathbf{d}}F.$$

Here recall that P is assumed to be real antisymmetric, i.e., $P^* = P^t = -P$; therefore,

$$M_P^t = -M_P \quad \text{and thus } (M_P^{-1})^t = -M_P^{-1}. \tag{17}$$

Consequently, we have $\dot{\mathbf{d}} = \nabla_{\mathbf{c}}F$ and $\dot{\mathbf{c}} = -\nabla_{\mathbf{d}}F$.

Finally, if we put $\mathbf{p} = \mathbf{c}$ and $\mathbf{q} = \mathbf{d}$, the pair $(\mathbf{q}, \mathbf{p})$ obeys the Hamiltonian dynamics with Hamiltonian $H = F$, i.e.,

$$\begin{cases} \dot{\mathbf{q}} = \nabla_{\mathbf{p}}H, \\ \dot{\mathbf{p}} = -\nabla_{\mathbf{q}}H. \qquad \square \end{cases} \tag{18}$$

Example 1. (i) $P = D^m$ where m is an odd integer, $|m| \leqslant N$.
(ii) $P = D - D^3$.
(iii) $P = D$ and $F(u) = \int (\frac{u^3}{6} - \frac{1}{2}u_x^2)\, dx$.

Note that in the last case, we get the KdV equation on R, $u_t = uu_x + u_{xxx}$.

4. PDE of type $\partial_t^2 u = (-1)^{\chi(P)+1} P^2(\frac{\delta F}{\delta u})$, $P^t = \pm P$

Let us assume that P be an invertible real operator. We assume further that it is either symmetric or antisymmetric. We denote by $\chi(P)$ its signature,

$$\chi(P) = \begin{cases} 0 & \text{if } P \text{ is symmetric,} \\ 1 & \text{if } P \text{ is antisymmetric.} \end{cases}$$

Then we have the following.

Theorem 2. *Let P be a linear and invertible real operator which is either symmetric or antisymmetric. Then a solution u of*

$$\partial_t^2 u = (-1)^{\chi(P)+1} P^2 \left(\frac{\delta F}{\delta u} \right) \tag{19}$$

corresponds to a solution of a Hamiltonian dynamics with the Hamiltonian H derived from F.

Proof. Applying P^2 to (13), we have as before

$$P^2 \left(\frac{\delta F}{\delta u} \right) = \sum_n \frac{\partial F}{\partial c_n} P^2 e_n = \cdots = (\ldots, e_k, \ldots) M_{P^2} \nabla_{\mathbf{c}} F. \tag{20}$$

Therefore, (19) is equivalent to

$$\ddot{\mathbf{c}} = (-1)^{\chi(P)+1} M_{P^2} \nabla_{\mathbf{c}} F. \tag{21}$$

Now we define $\mathbf{q}$ by $\mathbf{q} = M_P^{-1}\mathbf{c}$. Then

$$\ddot{\mathbf{q}} = M_P^{-1}\ddot{\mathbf{c}} = M_P^{-1}(-1)^{\chi(P)+1} M_{P^2} \nabla_{\mathbf{c}} F$$

and since $(M_P)^t = (-1)^{\chi(P)} M_P$,

$$\nabla_{\mathbf{c}} F = (M_P^{-1})^t \nabla_{\mathbf{q}} F = (-1)^{\chi(P)} M_P^{-1} \nabla_{\mathbf{q}} F,$$

which implies

$$\ddot{\mathbf{q}} = (-1)^{\chi(P)+1} M_P^{-1} M_P^2 (-1)^{\chi(P)} M_P^{-1} \nabla_{\mathbf{q}} F = -\nabla_{\mathbf{q}} F. \tag{22}$$

Finally, if we define H by

$$H = \frac{1}{2} \sum_k \dot{q}_k^2 + F(\mathbf{q}), \tag{23}$$

then it is easy to see that the pair $(\mathbf{q}, \mathbf{p} = \dot{\mathbf{q}})$ obeys the Hamiltonian dynamics with the above H. □

Example 2. (i) $P = D^m$ with $|m| \leqslant N/2$, $\chi(P) = \frac{1}{2}\{1 - (-1)^m\}$.
(ii) $P = (I - D^2)^\alpha$, with $\alpha \in R$, $|\alpha| \leqslant N/4$, $\chi(P) = 0$.
(iii) $P = D$ and $F(u) = \int_{-\infty}^{\infty} (e^u - u - 1)\, dx$.

The PDE $u_{tt} = (e^u)_{xx}$ is obtained from the last example, whose numerical solution is computed in [8] by an alternative energy-conserving computational scheme called discrete variational method. See [6,12] and references therein on the discrete variational method.

5. PDE of the form $-i\partial_t u = P(\frac{\delta F}{\delta \bar{u}})$, $P^t = P$

In this section, u is allowed to be complex valued.

Theorem 3. *Let P be a linear and invertible real symmetric operator. Then the equation*

$$-i\partial_t u = P\left(\frac{\delta F}{\delta \bar{u}}\right) \tag{24}$$

is reduced to a Hamiltonian dynamical system in a canonical way.

Proof. We separate u into real and imaginary parts, $u = u_{\mathrm{R}} + iu_{\mathrm{I}}$. Note that

$$\frac{\delta}{\delta \bar{u}} = \frac{1}{2}\left(\frac{\delta}{\delta u_{\mathrm{R}}} + i\frac{\delta}{\delta u_{\mathrm{I}}}\right).$$

Then (24) is equivalent to

$$-i(\partial_t u_{\mathrm{R}} + i\partial_t u_{\mathrm{I}}) = \frac{1}{2}\left(P\frac{\delta F}{\delta u_{\mathrm{R}}} + iP\frac{\delta F}{\delta u_{\mathrm{I}}}\right), \tag{25}$$

namely to

$$\partial_t u_{\mathrm{R}} = -\frac{1}{2}P\left(\frac{\delta F}{\delta u_{\mathrm{I}}}\right) \quad \text{and} \quad \partial_t u_{\mathrm{I}} = \frac{1}{2}P\left(\frac{\delta F}{\delta u_{\mathrm{R}}}\right). \tag{26}$$

Putting

$$u_{\mathrm{R}} = \sum_k c_k e_k \quad \text{and} \quad u_{\mathrm{I}} = \sum_k d_k e_k,$$

where c_k and d_k are real functions of t, we have by the same argument as before,

$$\frac{\delta F}{\delta u_{\mathrm{R}}} = \sum_k \frac{\delta F}{\delta c_k} e_k \quad \text{and} \quad \frac{\delta F}{\delta u_{\mathrm{I}}} = \sum_k \frac{\partial F}{\partial d_k} e_k. \tag{27}$$

Therefore, as in the preceding sections, we see that (26) is equivalent to

$$\dot{\mathbf{c}} = -\tfrac{1}{2} M_P \nabla_{\mathbf{d}} F \quad \text{and} \quad \dot{\mathbf{d}} = \tfrac{1}{2} M_P \nabla_{\mathbf{c}} F. \tag{28}$$

Now we define new coordinates $\mathbf{r}$ and $\mathbf{s}$ by $\mathbf{r} = \sqrt{2} M_P^{-1} \mathbf{c}$ and $\mathbf{s} = \sqrt{2}\mathbf{d}$, from which follows

$$\dot{\mathbf{r}} = -\frac{1}{\sqrt{2}} \nabla_{\mathbf{d}} F \quad \text{and} \quad \dot{\mathbf{s}} = \frac{1}{\sqrt{2}} M_P \nabla_{\mathbf{c}} F.$$

Therefore, by Proposition 2,

$$\nabla_{\mathbf{c}} F = \sqrt{2}(M_P^{-1})^t \nabla_{\mathbf{r}} F = \sqrt{2} M_P^{-1} \nabla_{\mathbf{r}} F, \tag{29}$$

because of the symmetry assumption on P and also we see easily $\nabla_{\mathbf{d}} F = \sqrt{2} \nabla_{\mathbf{s}} F$. Consequently, combining the above equalities, we obtain $\dot{\mathbf{r}} = -\nabla_{\mathbf{s}} F$ and $\dot{\mathbf{s}} = \nabla_{\mathbf{r}} F$.

Finally, putting $\mathbf{p} = \mathbf{r}, \mathbf{q} = \mathbf{s}$, $H = F$, we arrive at the Hamiltonian equation: $\dot{\mathbf{p}} = -\nabla_{\mathbf{q}} H$ and $\dot{\mathbf{q}} = \nabla_{\mathbf{p}} H$. $\square$

Example 3. (i) $P = D^{2m}$ with $|m| \leqslant N/2$.

(ii) $P = (I - D^2)D^2$, $4 \leqslant N$.

(iii) $P = I$ and $F(u) = \int (|u_x|^2 + \gamma |u|^4)\, dx$, with $\gamma \in R$.

Note that the last case corresponds to the Schrödinger equation with cubic nonlinearity.

6. Application to numerical computation—symplectic schemes

Let us briefly indicate a promising application of the preceding Hamiltonian formulation for solutions of energy conservative PDEs. In fact, we have reduced solving PDEs to solving the corresponding infinite-dimensional Hamiltonian dynamical systems:

$$\begin{cases} \dot{\mathbf{q}} = \nabla_{\mathbf{p}} H, \\ \dot{\mathbf{p}} = -\nabla_{\mathbf{q}} H. \end{cases}$$

To solve this Hamiltonian system numerically, we can use symplectic schemes. A symplectic scheme is a difference scheme which preserves the symplectic structure of numerical solutions and furthermore its numerical solutions stay in a small neighborhood of the orbits of the true solutions of the original equations forever. To cite only a few, see e.g., [5,11,13,15] for bibliographies. Let us mention in particular that Yoshida [19] and Suzuki [17] independently found concrete mathematical procedures to derive a symplectic scheme of a desired high order of approximation. Application of the symplectic method to the nonlinear Schrödinger equation is already investigated in [16].

Case studies with numerical simulation may be reported elsewhere.

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