Comment on "Self-trapping on a dimer: Time-dependent solutions of a discrete nonlinear Schrödinger equation"

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(Received 31 August 1987)

The equivalence between the discrete self-trapping equation for two degrees of freedom, the pendulum equation, and the space-independent ϕ^4 equation is demonstrated.

The discrete self-trapping (DST) equation was introduced in Refs. 1 and 2 and has been used to account for the dynamics of small molecules, molecular crystals, self-trapping in amorphous semiconductors, and global proteins. In Ref. 3 it was pointed out that the DST equation is integrable for two degrees of freedom and can be reduced to the pendulum equation. However, no details concerning the reduction to the latter equation were given.

Recently, it has been shown in Ref. 4 that the DST with two degrees of freedom can be reduced to the space-independent ϕ^4 equation $\ddot{p}=Ap-Bp^3$. In this Comment we derive the pendulum equation and demonstrate the equivalence with the space-independent ϕ^4 equation.

For two degrees of freedom the DST equation

$$i\dot{\bar{A}}+\underline{H}\bar{A}=0 \tag{1}$$

can be written as

$$i\dot{A}_1(t)+\gamma|A_1(t)|^2A_1(t)+\varepsilon A_2(t)=0\ , \tag{2a}$$

$$i\dot{A}_2(t)+\gamma|A_2(t)|^2A_2(t)+\varepsilon A_1(t)=0\ . \tag{2b}$$

Here, A_1 and A_2 are the probability amplitudes for finding an excitation in the two sites of the system in this case. γ and ε represent the strength of the nonlinear interaction in the system and the coupling between the two sites, respectively.

The density matrix $\underline{\rho}$ with elements

$$\rho_{jk}(t)=A_j(t)A_k^*(t) \tag{3}$$

can be rewritten as

$$\underline{\rho}(t)=\tfrac{1}{2}\left[\underline{I}+\sum_{j=1}^{3}\underline{\sigma}_j r_j(t)\right]\ , \tag{4}$$

where $\underline{I}$ is the identity matrix and $\underline{\sigma}_j$ denote the Pauli matrices. From Eqs. (1) and (3) we get

$$r_1(t)=\rho_{12}(t)+\rho_{21}(t)\ , \tag{5a}$$

$$r_2(t)=i[\rho_{12}(t)-\rho_{21}(t)]\ , \tag{5b}$$

$$r_3(t)=\rho_{11}(t)-\rho_{22}(t)\ . \tag{5c}$$

Rewriting the matrix $\underline{H}$ as

$$\underline{H}(t)=\sum_{j=1}^{3}h_j(t)\underline{\sigma}_j+\frac{\gamma}{2}[|A_1(t)|^2+|A_2(t)|^2]\underline{I}\ , \tag{6}$$

we get

$$h_1(t)=\varepsilon\ , \tag{7a}$$

$$h_2(t)=0\ , \tag{7b}$$

$$h_3(t)=\frac{\gamma}{2}(|A_1|^2-|A_2|^2)=\frac{\gamma}{2}r_3(t)\ . \tag{7c}$$

In Ref. 3 the DST equation (1) was rewritten as

$$\dot{\underline{\rho}}(t)=i[\underline{\rho},\underline{H}]\ . \tag{8}$$

Substituting (4), (6), and (7) into (8) the following equations are obtained:

$$\dot{r}_1(t)=-\gamma r_2(t)r_3(t)\ , \tag{9a}$$

$$\dot{r}_2(t)=\gamma r_1(t)r_3(t)-2\varepsilon r_3(t)\ , \tag{9b}$$

$$\dot{r}_3(t)=2\varepsilon r_2(t)\ , \tag{9c}$$

implying that $|\bar{r}|\equiv(r_1^2+r_2^2+r_3^2)^{1/2}$ remains constant throughout the interaction (as a consequence of unitarity). Note also that Eqs. (9a) and (9b) imply

$$r_1(t)=-\frac{\gamma}{4\varepsilon}r_3^2(t)+\text{const}\ .$$

Equations (9) are best solved by writing them first in the form

$$\dot{r}_1(t)+i\dot{r}_2(t)=i\gamma[r_1(t)+ir_2(t)]r_3(t)-i2\varepsilon r_3(t)\ . \tag{10}$$

Integration of (10) gives

$$r_1(t)+ir_2(t)=\frac{2\varepsilon}{\gamma}+\alpha\exp\left[i\gamma\int_{t_0}^{t}r_3(t')dt'\right]\ , \tag{11}$$

where α and t_0 are real integration constants.

Since, by (5a) and (5b) $r_1(t)$ and $r_2(t)$ are real, we get

$$r_1(t)=\frac{2\varepsilon}{\gamma}+\alpha\cos\gamma\int_{t_0}^{t}r_3(t')dt'\ , \tag{12a}$$

and

$$r_2(t)=\alpha\sin\gamma\int_{t_0}^{t}r_3(t')dt'\ . \tag{12b}$$

Using (12a) and (5a) at $t=t_0$ we obtain

$$\alpha=\rho_{12}(t_0)+\rho_{21}(t_0)-\frac{2\varepsilon}{\gamma}\ . \tag{13}$$

Substituting (12b) into (9c) and defining the real variable q by

$$q=\gamma\int_{t_0}^{t} r_3(t')dt' \ , \tag{14}$$

we get

$$\ddot{q}=2\varepsilon\gamma\alpha\sin q \ , \tag{15}$$

i.e., the pendulum equation.

In Ref. 4 the space-independent ϕ^4 equation

$$\ddot{p}=Ap-Bp^3 \tag{16}$$

is derived from the two degrees of freedom DST equation. Here, p is defined as $p\equiv\rho_{11}(t)-\rho_{22}(t)$. Thus

$$p=r=\frac{\dot{q}}{\gamma} \ . \tag{17}$$

Furthermore, the constants A and B are given by

$$A=\frac{\gamma^2}{2}[\rho_{11}(t_0)-\rho_{22}(t_0)]^2-4\varepsilon^2 +2\varepsilon\gamma[\rho_{12}(t_0)+\rho_{21}(t_0)] \ , \tag{18a}$$

and

$$B=\frac{\gamma^2}{2} \ , \tag{18b}$$

in our notation. (Note that Ref. 4 uses $-V$ instead of ε, which is a positive parameter in the DST model.)

We shall now demonstrate that Eq. (16) is equivalent to Eqs. (15) and (13). Integrating (15) and using (17) and (18b) we obtain

$$Bp^2=-2\varepsilon\gamma\alpha\cos q+c \ , \tag{19}$$

where C is an integration constant. From the definition of p and (14) it follows that $C=A$ is given by (18a).

Substituting $Q=\sin q/2$ into (19) we get

$$Bp^2=2\varepsilon\alpha\gamma(2Q^2-1)+A \ .$$

Differentiation of this equation and use of

$$\dot{Q}=(\dot{q}/2)\cos(q/2)=(\gamma p/2)\sqrt{1-Q^2}$$

yields

$$\dot{p}^2=Ap^2-\frac{B}{2}p^4+\text{const} \ .$$

Repeated differentiation now gives

$$\ddot{p}=Ap-Bp^3 \ ,$$

which is the space-independent ϕ^4 equation.

A. C. Scott and J. C. Eilbeck are gratefully acknowledged for informative discussions. The financial support of the C. Gulbenkian Foundation and The Danish Research Council for Scientific and Industrial Research is acknowledged.

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