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Balancing the Schrödinger equation with Davydov *Ansätze*

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Two theorems are given governing the general quantum mechanical validity of Davydov *Ansatz* states.

A number of recent developments in the field of polaron-soliton dynamics have shed new light on the proper role to be played by Davydov's *Ansatz* states in the quantum mechanics of polaronic systems;[1-3] i.e., systems described by the Fröhlich Hamiltonian[4]

$$H=\sum_{mn} J_{mn} a_m^\dagger a_n+\sum_q \hbar\omega_q b_q^\dagger b_q +\sum_{qn}\hbar\omega_q(\chi_n^q b_q^\dagger+\chi_n^{q*} b_q)a_n^\dagger a_n . \quad (1)$$

The Davydov *Ansatz* states in question[5] have been referred to as $|D_1\rangle$ and $|D_2\rangle$, where

$$|D_1\rangle\equiv\sum_n \alpha_n a_n^\dagger|\beta_n\rangle \equiv\sum_n \alpha_n a_n^\dagger \exp\left[\sum_q(\beta_{qn}b_q^\dagger-\beta_{qn}^* b_q)\right]|0\rangle , \quad (2)$$

and

$$|D_2\rangle\equiv\sum_n \alpha_n a_n^\dagger \exp\left[\sum_q(\beta_q b_q^\dagger-\beta_q^* b_q)\right]|0\rangle . \quad (3)$$

The $|D_2\rangle$ state is in wider use than $|D_1\rangle$. One reason for this bias is the greater simplicity of $|D_2\rangle$ relative to $|D_1\rangle$. Another reason is that until recently the equations of motion put forward for D_1 states have been plagued with serious flaws.[6,7] On the other hand, one would expect that the greater flexibility of the D_1 states would allow the development of evolution equations which improve on the imperfect dynamics now well known for D_2 states.

A recent variational analysis by Zhang, Romero-Rochin, and Silbey[3] has produced equations of motion for D_1 states which improve on the Hamilton equations used heretofore.[6,7] The defects which had been identified in the former D_1 dynamics are eliminated by the new evolution equations; specifically, the new evolution equations are able to reproduce the exact $J_{mn}=0$ evolution, and hence all known exact results.

The method of Zhang *et al.*[3] consists of applying the variational principle

$$\delta\int_{t_1}^{t_2} dt\left[\langle D_1|i\hbar\frac{d}{dt}-H|D_1\rangle-\lambda\langle D_1|D_1\rangle\right]=0. \quad (4)$$

The success or failure of the variational method depends on the compatibility of the chosen class of trial functions with the evolution generated by H. Ideally, the class of trial functions is exactly closed under the action of the propagator e^{-iHt}, which is to say that every trial function is an exact solution of the Schrödinger equation. In the more realistic case that one is not fortunate enough to have chosen a class of trial functions which solve the Schrödinger equation, the action of e^{-iHt} on a typical initial state within the class of trial functions will cause the initial state to evolve out of the class along a Hilbert space trajectory which cannot be reproduced by the equations of motion obtained from the variational principle. In this case one must question the compatibility of the variational method with quantum mechanics; in proceeding with the variational equations of motion, one is depending on the variational method to produce Hilbert-space trajectories which are in some sense "close" to the unknown exact trajectories.

Zhang *et al.*[3] are able to show that in the $J_{mn}=0$ limit their variational equations of motion are equivalent to the Schrödinger equation. In the language of the preceding paragraph, the set of D_1 states is closed under the action of e^{-iHt} in the $J_{mn}=0$ limit. One does not really expect that this property will continue to hold when $J_{mn}\neq 0$; however, since the variational method is silent on the question, independent methods are required to obtain more definitive information.

In order to obtain definitive answers to the question of the compatibility of D_1 states with quantum mechanics, we substitute $|D_1\rangle$ into the left- and right-hand sides of the Schrödinger equation of the Hamiltonian H and obtain the necessary conditions for their equality. We do this by expanding the right and left sides of the equation

$$i\hbar\frac{d}{dt}|D_1\rangle=H|D_1\rangle$$

in a complete set of orthogonal basis states and equating the coefficients of similar basis states. For this purpose we expand the nonorthogonal coherent states in the orthogonal basis of number states, whereupon we observe that[8]

$$|\beta_r\rangle=\prod_q \exp(-\tfrac{1}{2}|\beta_{qr}|^2)\sum_{v_q=0}^{\infty}[(\beta_{qr})^{v_q}/\sqrt{v_q!}]\,|v_q\rangle , \quad (5)$$

$$b_{q'}|\beta_r\rangle=\beta_{q'r}|\beta_r\rangle , \quad (6)$$

$$b_{q'}^\dagger|\beta_r\rangle=\left[\frac{\beta_{q'r}^*}{2}+\frac{\partial}{\partial\beta_{q'r}}\right]|\beta_r\rangle , \quad (7)$$

$$b_{q'}^\dagger b_{q'}|\beta_r\rangle=\beta_{q'r}\left[\frac{\beta_{q'r}^*}{2}+\frac{\partial}{\partial\beta_{q'r}}\right]|\beta_r\rangle . \quad (8)$$

Now choosing a specific but arbitrary site r and a specific but arbitrary set of phonon occupation numbers $\{v_q\}$, we equate the coefficients of each basis state

$$|r,\{v_q\}\rangle=a_r^\dagger\prod_{\{v_q\}}(b_{q_1}^{\dagger v_{q_1}}/\sqrt{v_{q_1}!})(b_{q_2}^{\dagger v_{q_2}}/\sqrt{v_{q_2}!})\cdots|0\rangle ,$$

with the result

$$i\hbar\frac{d}{dt}a_r\prod_q\exp(-\tfrac{1}{2}|\beta_{qr}|^2)[(\beta_{qr})^{\nu_q}/\sqrt{\nu_q!}]=\sum_n J_{rn}a_n\prod_q\exp(-\tfrac{1}{2}|\beta_{qn}|^2)[(\beta_{qn})^{\nu_q}/\sqrt{\nu_q!}]$$
$$+a_r\sum_{q'}\hbar\omega_{q'}\beta_{q'r}\left[\frac{\beta^*_{q'r}}{2}+\frac{\partial}{\partial\beta_{q'r}}\right]\prod_q\exp(-\tfrac{1}{2}|\beta_{qr}|^2)[(\beta_{qr})^{\nu_q}/\sqrt{\nu_q!}]$$
$$+a_r\sum_{q'}\hbar\omega_{q'}\left[\chi_r^{q'}\left(\frac{\beta^*_{q'r}}{2}+\frac{\partial}{\partial\beta_{q'r}}\right)+\chi_r^{q'*}\beta_{q'r}\right]$$
$$\times\prod_q\exp(-\tfrac{1}{2}|\beta_{qr}|^2)[(\beta_{qr})^{\nu_q}/\sqrt{\nu_q!}]\,. \tag{9}$$

Carrying out the indicated differentiations and collecting related terms, we find

$$i\hbar\dot{a}_r-i\hbar a_r\tfrac{1}{2}\sum_q(\dot\beta^*_{qr}\beta_{qr}+\beta^*_{qr}\dot\beta_{qr})-a_r\sum_q\chi_r^{-q}\hbar\omega_q\beta_{qr}=\sum_n J_{rn}a_n\prod_q\exp[\tfrac{1}{2}(|\beta_{qr}|^2-|\beta_{qn}|^2)](\beta_{qn}/\beta_{qr})^{\nu_q}$$
$$-i\hbar a_r\sum_q\nu_q\frac{\dot\beta_{qr}+i\omega_q\beta_{qr}+i\omega_q\chi_r^q}{\beta_{qr}}\,. \tag{10}$$

(For clarity of presentation we have assumed that the coherent state amplitudes β_{qr} are all nonzero.) Since the a_r and β_{qr} must be independent of the phonon occupation numbers ν_q, we obtain as a condition of balance that the coefficients of each ν_q must independently sum to zero. Considering first the $J_{mn}=0$ case, (10) yields as the balance equation

$$\dot\beta_{qr}=-i\omega_q\beta_{qr}-i\omega_q\chi_r^q\,, \tag{11}$$

which is solved immediately to yield

$$\beta_{qr}(t)=e^{-i\omega_q t}\beta_{qr}(0)+(e^{-i\omega_q t}-1)\chi_r^q\,, \tag{12}$$

in complete agreement with Zhang *et al.*[3] It is straightforward to verify that every solution of (12) determines a family of D_1 states which solve the Schrödinger equation. On the other hand, when $J_{mn}\neq 0$, the balancing conditions for the D_1 equations cannot be fulfilled for arbitrary $\{\nu_q\}$ since the dependence of (10) on ν_q is nonlinear. Since the balance condition must be fulfilled for *every* distribution set $\{\nu_q\}$, this is the indication we have sought which tells us that the D_1 states cannot solve the Schrödinger equation when $J_{mn}\neq 0$. The above reasoning applied to the D_2 states yields

$$i\hbar\dot{a}_r-i\hbar a_r\tfrac{1}{2}\sum_q(\dot\beta^*_q\beta_q+\beta^*_q\dot\beta_q)-a_r\sum_q\chi_r^{-q}\hbar\omega_q\beta_q=\sum_n J_{rn}a_n-i\hbar a_r\sum_q\nu_q\frac{\dot\beta_q+i\omega_q\beta_q+i\omega_q\chi_r^q}{\beta_q}\,. \tag{13}$$

For arbitrary J_{mn} we find the balance equation

$$\dot\beta_q=-i\omega_q\beta_q-i\omega_q\chi_r^q\,. \tag{14}$$

Since β_q cannot depend on the site index r, this condition can be satisfied only if $\chi_r^q=0$. Every $\chi_r^q=0$ solution of (14) determines a family of D_2 solutions which solve the Schrödinger equation. We are thus able to summarize our results in two theorems.

D_1 theorem: Davydov's D_1 states satisfy the Schrödinger equation of the Fröhlich Hamiltonian if and only if $J_{mn}=0$.

D_2 theorem: Davydov's D_2 states satisfy the Schrödinger equation of the Fröhlich Hamiltonian if and only if $\chi_r^q=0$.

These results are valid for any transfer matrix J_{mn}, whether short or long range; any number and type of phonon branches ω_q; and any coupling function χ_n^q, regardless of range, strength, or symmetry.

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[1]David W. Brown, Katja Lindenberg, and Bruce J. West, Phys. Rev. A **33**, 4104 (1986); **33**, 4110 (1986).

[2]W. C. Kerr and P. S. Lomdahl, Phys. Rev. B **35**, 3629 (1987).

[3]Qing Zhang, Victor Romero-Rochin, and Robert Silbey (unpublished).

[4]H. Fröhlich, Proc. R. Soc. London, Ser. A **215**, 291 (1952); Adv. Phys. **3**, 325 (1954).

[5]The results of this paper continue to be valid for a modified form of (2) in which the vacuum state $|0\rangle$ is replaced by a general, but time-independent phonon state

$$|\phi\{\eta_q\}\rangle=\sum_{\{\eta_q\}}C\{\eta_q\}(b_{q_1}^{\dagger\eta_{q_1}}/\sqrt{\eta_{q_1}!})(b_{q_2}^{\dagger\eta_{q_2}}/\sqrt{\eta_{q_1}!})\dots|0\rangle\,.$$

[6]A. S. Davydov, Zh. Eksp. Teor. Fiz. **78**, (1980) [Sov. Phys. JETP **51**, 397 (1980)].

[7]L. Cruzerio, J. Halding, P. L. Christiansen, O. Skovagaard, and A. C. Scott, Phys. Rev. A **37**, 880 (1988).

[8]R. J. Glauber, Phys. Rev. B **131**, 2766 (1963).