Applicability of Hamilton's equations in the quantum soliton problem

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We test the validity of Hamilton-equation methods for determining the time evolution of trial state vectors in quantum mechanics. Given a trial state vector, we are able to construct a differential operator under which a scalar Hamilton function must be invariant. State vectors composed of single-particle states, coherent-state products, and mixed single-particle states and coherent-state products are considered explicitly. In the latter category, we consider state vectors of the form proposed by Davydov in his treatment of the quantum soliton problem. We find that Davydov's wave vector, as determined by the Hamilton-equation method, is not a solution of the Schrödinger equation for the Fröhlich Hamiltonian except under very restrictive circumstances. The theoretical justification for a number of conclusions about soliton transport in Fröhlich-type systems is thus called into question.

I. INTRODUCTION

In recent years the problem of energy transport in biological macromolecules has been referred to as a "crisis" owing to the fact that estimates of lifetimes for molecular excitations based on linear dynamics are too short to be reconciled with known features of the biological processes to which they contribute.[1,2] A resolution of the problem was proposed by Davydov, who suggested that the dispersion responsible for the short lifetime of an excitation might be offset by a focusing of the excitation through the nonlinear character of the interatomic forces (e.g., as may arise from hydrogen bonding in polypeptides).[2–4] It is possible that nonlinear interactions may stabilize excitations, resulting in solitary waves known as solitons. Soliton mechanisms have been proposed in a number of macromolecular processes, ranging from the dynamics of α-helix proteins[2–4] and solid-state analogs of polypeptides[5,6] to the function of myosine molecules during muscle contraction[4] and that of DNA during protein synthesis.[7] Many such problems may be modeled by the Frölich Hamiltonian,[8] applied by Davydov to resolve the bioenergetic crisis. The result of Davydov's analysis is a nonlinear Schrödinger equation whose soliton solution is well known.

The prevalent interpretation of the microscopic character of the soliton in this context relies heavily on the properties of coherent states. Since their introduction by Glauber,[9] coherent states have proven to be a natural language in which to approach a number of many-boson problems, most notably those posed by the photons of the electromagnetic field. Both pure coherent states and distribution functions over the complex phase plane have become standard tools of quantum optics.[10] The coherent-state formalism may be profitably applied to the study of phonons in condensed matter,[11] though with somewhat less scope.

In the study of quasiparticle transport in deformable media, certain coherent-state products have been found to describe the dynamic organization of vibrational normal modes which results in the development of a persistent deformation of the medium about the region occupied by an immobile perturbing particle.[12] Attempts such as Davydov's have been made to address the more general case of a mobile perturbing particle by seeking solutions of the Schrödinger equation of a particular form and determining the time evolution of the wave function by extremum principles. Coherent states have played a central role in such generalizations,[2–4] which often regard wave function parameters as generalized coordinates and apply the classical Hamiltonian equations to determine their evolution.[2–4,6,13] In such an approach a set of Hamilton equations for the mode amplitudes supplants the single Schrödinger equation for the state vector.

Solutions of the Schrödinger equation are often sought in the form of (a) single-particle states, (b) coherent-state products, or (c) mixtures of single-particle states and coherent-state products. We consider each of these forms in Secs. II, III, and IV, respectively. The premises on which the Hamilton-equation approach is based impose specific constraints that must be satisfied by the Hamiltonian of a system in order for the approach to be consistent with the Schrödinger equation approach. In Secs. II–IV, we construct such consistency conditions explicitly.

In Sec. III we consider, among others, an effective two-body Hamiltonian which has been used to obtain nonlinear Schrödinger equations[13,14] and we show that the nonlinear Schrödinger equations resulting from Hamilton's equations in this case are *not* consistent with the Schrödinger equation.

In Sec. IV, we consider the specific difficulties encountered in the polaron/soliton problem employing the Fröhlich Hamiltonian. We demonstrate that the Hamilton-equation propagation of the state vector proposed by Davydov[2-4] is, in general, inconsistent with the Schrödinger equation.

In the following discussion we are concerned with dynamics and dynamical constraints. Constant contributions to the total energy are neglected below; that is, we ignore the scalar terms remaining after normal-ordering second-quantized Hamiltonian operators.

II. SINGLE-PARTICLE STATES

In this section we consider only single-particle states, which we denote by $|\Psi(t)\rangle$. These are defined to have the form

$$|\Psi(t)\rangle \equiv \sum_m \psi_m(t) a_m^\dagger |0\rangle \tag{2.1}$$

in which $a_m^\dagger$ creates a particle in the state labeled by m, $\psi_m(t)$ is a time-dependent c number, and $|0\rangle$ is the particle vacuum. The Schrödinger equation for this state may be written

$$i\hbar \frac{d}{dt}|\Psi(t)\rangle \equiv i\hbar \sum_m \dot{\psi}_m(t) a_m^\dagger |0\rangle = H|\Psi(t)\rangle \;, \tag{2.2}$$

where H is the system Hamiltonian operator. Since we are considering only single-particle states, only the one-body parts $H^{(1)}$ of number-conserving Hamiltonians are relevant. These have the form

$$H^{(1)} = \sum_{m,n} H_{mn}^{(1)} a_m^\dagger a_n \;, \tag{2.3}$$

where the $H_{mn}^{(1)}$ are the single-particle matrix elements of the Hamiltonian. Left multiplying (2.2) with the bra vector $\langle m| = \langle 0|a_m$ and setting $\langle 0|a_m a_n^\dagger|0\rangle = \delta_{mn}$, we obtain the set of scalar equations for the wave-function expansion coefficients in the chosen basis

$$i\hbar\dot{\psi}_m(t) = \sum_n H_{mn}^{(1)} \psi_n(t) \;, \tag{2.4a}$$

$$i\hbar\dot{\psi}_m^*(t) = -\sum_n H_{mn}^{(1)} \psi_n^*(t) \;. \tag{2.4b}$$

Though dependent on the choice of basis, the complete set of equations (2.4) is collectively equivalent to the Schrödinger equation (2.2).

As an alternative procedure, let us first form the expectation value of the Hamiltonian operator in the state under consideration. Denoting the set of expansion coefficients by $\{\psi(t),\psi^*(t)\}$, we have

$$\begin{aligned} H^{(1)}\{\psi(t),\psi^*(t)\} &= \langle \Psi(t)|H^{(1)}|\Psi(t)\rangle \\ &= \sum_{m,n} H_{mn}^{(1)} \psi_m^*(t)\psi_n(t) \;. \end{aligned} \tag{2.5}$$

If we interpret $\psi_n(t)$ as a generalized coordinate and $i\hbar\psi_n^*(t)$ as the corresponding generalized momentum with respect to the Hamilton function $H^{(1)}\{\psi(t),\psi^*(t)\}$, then the Hamilton equations

$$\dot{\psi}_m(t) = \frac{\partial}{\partial i\hbar\psi_m^*(t)} H^{(1)}\{\psi(t),\psi^*(t)\} \;, \tag{2.6a}$$

$$i\hbar\dot{\psi}_m^*(t) = \frac{-\partial}{\partial\psi_m(t)} H^{(1)}\{\psi(t),\psi^*(t)\} \tag{2.6b}$$

constitute an alternative method for determining the form of $|\Psi(t)\rangle$, provided our interpretation is consistent with the actual formal structure of the dynamics. For the one-body Hamiltonians we consider here, Eqs. (2.6) are entirely equivalent to Eqs. (2.4) and hence to the Schrödinger equation.

Anticipating that more complex Hamiltonians may not admit such direct conclusions, we now illustrate a distinct line of reasoning, which, while weaker in its result, is of wider applicability. We begin with the assumption that the state vector $|\Psi(t)\rangle$ is a solution of the Schrödinger equation; that is, that (2.2) is valid. We left multiply (2.2) with the bra vector $\langle\Psi(t)|$, yielding

$$i\hbar\sum_n \psi_n^*(t)\dot{\psi}_n(t) = H^{(1)}\{\psi(t),\psi^*(t)\} \;. \tag{2.7}$$

Now we *assume* that the Hamilton equations (2.6) are also valid, whereupon the time derivatives in (2.7) may be replaced by the corresponding momentum derivatives of the scalar Hamiltonian function $H^{(1)}\{\psi(t),\psi^*(t)\}$. The result is a differential invariance condition

$$\left[\sum_n \psi_n^*(t)\frac{\partial}{\partial\psi_n^*(t)}\right] H^{(1)}\{\psi(t),\psi^*(t)\} = H^{(1)}\{\psi(t),\psi^*(t)\} \;, \tag{2.8}$$

which $H^{(1)}\{\psi(t),\psi^*(t)\}$ must satisfy if both (2.2) and (2.6) are to be valid. Obviously, the complex conjugate condition with $\psi_n^*(t)\to\psi_n(t)$ must also hold. Both conditions are satisfied for the form of the Hamiltonian and state vector we have considered, so no internal inconsistency is revealed in this simple case, as expected.

The condition (2.8) on the form of the Hamiltonian results from the requirement that two different methods for determining the same set of dynamical quantities be consistent with one another. Generalizations of this differential invariance condition can be developed under quite general circumstances since its development depends only on the assumptions that the state vector $|\Psi(t)\rangle$ is a solution of the Schrödinger equation, and that the parameters bearing the time dependence in $|\Psi(t)\rangle$ may be considered as generalized coordinates with respect to the scalar Hamilton function $H^{(1)}\{\psi(t),\psi^*(t)\}$. Although the *only* conclusion of such a condition is the negative one which follows when the condition is violated, that conclusion is of considerable importance. We find in Secs. III and IV that the relevant conditions are violated in common applications of the Hamilton-equation approach in the study of quantum solitons.

III. COHERENT-STATE PRODUCTS

Throughout this section we will be concerned with a particular kind of state vector or wave function, and with the determination of this state vector's time evolution by methods grounded in the equations of motion for operators. This involves frequent interchanges between the Schrödinger and Heisenberg pictures of the quantum evolution of a dynamical system. For clarity, we consistently indicate the picture in use by the quantities on which time dependence is displayed; thus, $a_n \mid A(t)\rangle$ is understood to indicate the use of the Schrödinger picture, while $a_n(t)\mid A\rangle$ is understood to indicate the use of the Heisenberg picture. We let $\{a,a^\dagger\}$ denote the set $\{a_1,a_1^\dagger,\ldots,a_N,a_N^\dagger\}$ of creation and annihilation operators appearing in the Hamiltonian operator $H\{a,a^\dagger\}$ of a given system. We consider state vectors $\mid A(t)\rangle$ defined by

$$\mid A(t)\rangle \equiv \mid \alpha_1(t)\rangle \otimes \mid \alpha_2(t)\rangle \otimes \ldots \otimes \mid \alpha_N(t)\rangle \ , \tag{3.1}$$

wherein $\mid \alpha_n(t)\rangle$ is a pure coherent state defined by[9-11]

$$\mid \alpha_n(t)\rangle \equiv \exp[-\tfrac{1}{2}\mid \alpha_n(t)\mid^2]\exp[\alpha_n(t)a_n^\dagger]\mid 0\rangle \ . \tag{3.2}$$

The complex scalar $\alpha_n(t)$ is the coherent-state amplitude, which may take on all values in the complex plane. The product state $\mid A(t)\rangle$ may be defined by the property that

$$a_n \mid A(t)\rangle = \alpha_n(t)\mid A(t)\rangle \tag{3.3}$$

for all of the a_n. The expectation value of a Hamiltonian operator $H\{a,a^\dagger\}$ in the state $\mid A(t)\rangle$ is therefore a real scalar function $H\{\alpha(t),\alpha^*(t)\}$ of all the $\alpha_n(t)$ and their complex conjugates. We presume that our starting Hamiltonian operator is in normal ordered form so that there is no ambiguity in the relationship between $H\{a,a^\dagger\}$ and $H\{\alpha(t),\alpha^\dagger(t)\}$.

The following relationships between commutators of the Hamiltonian operator and derivatives of the scalar Hamilton function follow from the properties of the coherent state $\mid A(t)\rangle$:

$$\langle A \mid [a_n(t),H(t)]\mid A\rangle = \langle A(t)\mid [a_n,H]\mid A(t)\rangle = \frac{\partial}{\partial \alpha_n^*(t)}H\{\alpha(t),\alpha^*(t)\} \ , \tag{3.4a}$$

$$\langle A \mid [a_n^\dagger(t),H(t)]\mid A\rangle = \langle A(t)\mid [a_n^\dagger,H]\mid A(t)\rangle = \frac{-\partial}{\partial \alpha_n(t)}H\{\alpha(t),\alpha^*(t)\} \ . \tag{3.4b}$$

Applying these relations to the expectation value of the corresponding Heisenberg equations of motion for the creation and annihilation operators yields

$$i\hbar\dot{\alpha}_n(t) = \frac{\partial}{\partial \alpha_n^*(t)}H\{\alpha(t),\alpha^*(t)\} \ , \tag{3.5a}$$

$$i\hbar\dot{\alpha}_n^*(t) = \frac{-\partial}{\partial \alpha_n(t)}H\{\alpha(t),\alpha^*(t)\} \ , \tag{3.5b}$$

where we have used the fact that $\langle A \mid \dot{a}_n(t)\mid A\rangle = d\langle A\mid a_n(t)\mid A\rangle/dt = \dot{\alpha}_n(t)$. The relations (3.5) are the classical Hamilton equations for generalized coordinates $\alpha_n(t)$ and momenta $i\hbar\alpha_n^*(t)$ with respect to a Hamiltonian function $H\{\alpha(t),\alpha^*(t)\}$, and follow without approximation directly from the definition of coherent-state $\mid A(t)\rangle$, the Heisenberg equations of motion, and Bose commutation relations for the operators $\{a(t),a^\dagger(t)\}$. The set of coherent-state indices $\{\alpha(t),\alpha^*(t)\}$, and therefore $\mid A(t)\rangle$, may be determined for any Hamilton function $H\{\alpha(t),\alpha^*(t)\}$ for which the classical Hamilton equations (3.5) are solvable. The procedure outlined above is attractive as a means of determining particular solutions of the Schrödinger equation corresponding to the less-tractable Heisenberg equations of motion for the operators $\{a(t),a^\dagger(t)\}$. We find, however, that for most Hamiltonians the vectors $\mid A(t)\rangle$ so determined are *not* solutions of the corresponding Schrödinger equation, due to the existence of a constraint on the form of the Hamilton function $H\{\alpha(t),\alpha^*(t)\}$.

Consider the Schrödinger equation for the state vector $\mid A(t)\rangle$

$$i\hbar\frac{d}{dt}\mid A(t)\rangle = H\mid A(t)\rangle \ . \tag{3.6}$$

Inserting into (3.6) the form of $\mid A(t)\rangle$ given by (3.1) and (3.2) and carrying out the differentiation with respect to time, we find

$$i\hbar\sum_m\{-\tfrac{1}{2}[\dot{\alpha}_n^*(t)\alpha_n(t)+\alpha_n^*(t)\dot{\alpha}_n(t)] + \dot{\alpha}_n(t)a_n^\dagger\}\mid A(t)\rangle = H\mid A(t)\rangle \ . \tag{3.7}$$

Left multiplying (3.7) with the bra vector $\langle A(t)\mid$, we obtain the scalar relationship

$$\tfrac{1}{2}i\hbar\sum_n[\dot{\alpha}_n^*(t)\alpha_n(t)-\alpha_n^*(t)\dot{\alpha}_n(t)] = H\{\alpha(t),\alpha^*(t)\} \ . \tag{3.8}$$

Using the Hamilton equations (3.5) to eliminate the time derivatives in (3.8), we obtain an invariance condition on the Hamilton function,

$$\tfrac{1}{2}\sum_n\left[\alpha_n(t)\frac{\partial}{\partial\alpha_n(t)}+\alpha_n^*(t)\frac{\partial}{\partial\alpha_n^*(t)}\right]H\{\alpha(t),\alpha^*(t)\} = H\{\alpha(t),\alpha^*(t)\} \ . \tag{3.9}$$

This condition may be cast in a simpler from by transforming to the "action-angle" variables[11] defined by $\alpha_n \equiv J_n^{1/2}\exp(i\vartheta_n)$, for which the partial derivative operators take the form

$$\frac{\partial}{\partial\alpha_n} = J_n^{1/2}\exp(-i\vartheta_n)\left[\frac{\partial}{\partial J_n}+\frac{1}{2iJ_n}\frac{\partial}{\partial\vartheta_n}\right] , \tag{3.10}$$

whereupon the condition (3.9) becomes

$$\sum_n\left[J_n(t)\frac{\partial}{\partial J_n(t)}\right]H\{J(t),\vartheta(t)\} = H\{J(t),\vartheta(t)\} \ . \tag{3.11}$$

The requirement that the Hamilton function be invariant under the action of a specific differential operator strongly limits the class of Hamiltonians admitting the state vectors $\mid A(t)\rangle$ as solutions of their Schrödinger equations. The invariant Hamilton functions $H\{J,\vartheta\}$ satisfying (3.11) have the form

$$H\{J,\vartheta\} = \sum_m f_m(\vartheta_1,\vartheta_2,\ldots,\vartheta_N)J_1^{x_{m1}}J_2^{x_{m2}}\cdots J_n^{x_{mN}} \ , \tag{3.12}$$

wherein the functions f_m are arbitrary real functions of the phases only and the x_{mi} are real numbers subject to the restriction that $x_{m1}+x_{m2}+\cdots+x_{mN}=1$.

The scalar Hamilton function to which the invariance condition is applied is derived from a Hamiltonian operator represented in a given basis. A Hamiltonian operator admitting coherent-state Schrödinger solutions in a given basis may not admit solutions of the same form constructed in another basis and vice versa, even if the bases are related by a canonical transformation. This observation underscores the fact that what is being tested by the condition (3.11) is the admissibility of a class of trial state vectors having a specified form, the form being represented in a basis-specific way.

Hamiltonians used to describe unperturbed excitons or vibrons often take forms which yield Hamilton functions satisfying condition (3.11). The Hamiltonian for pure Frenkel excitons is often represented as

$$H_{\text{ex}}=\sum_m E_m a_m^\dagger a_m+\sum_{m,n} V_{mn} a_m^\dagger a_n \;, \tag{3.13}$$

in which $a_m^\dagger$ (a_m) creates (annihilates) an exciton in the site state labeled by m. Forming $\langle A \mid H_{\text{ex}} \mid A\rangle$ and making the transformation to action-angle variables yields

$$H_{\text{ex}}\{J,\vartheta\}=\sum_m E_m J_m + \sum_{m,n} V_{mn}(J_m J_n)^{1/2}\exp[-i(\vartheta_m-\vartheta_n)] \;. \tag{3.14}$$

Since the degree of the action polynomial is unity (degree 2 in the square roots of the action variables), (3.11) is satisfied.

The Hamilton for pure vibrons is sometimes written[15]

$$H_{\text{vib}}=\sum_n \hbar\omega_n(b_n^\dagger b_n+\tfrac{1}{2})+\sum_{m,n} L_{mn}{:}(b_m^\dagger+b_m)(b_n^\dagger+b_n){:} \tag{3.15}$$

in which $b_n^\dagger$ (b_n) creates (annihilates) a quantum of vibrational energy in a molecular mode labeled by n. Casting H_{vib} into explicit normal-ordered form as indicated by $:\cdots:$ and neglecting the zero-point energy gives

$$H_{\text{vib}}=\sum_n \hbar\omega_n b_n^\dagger b_n + \sum_{m,n} L_{mn}(b_m^\dagger b_n^\dagger+b_m^\dagger b_n+b_n^\dagger b_m+b_m b_n) \;. \tag{3.16}$$

Forming $\langle A \mid H_{\text{vib}} \mid A\rangle$ and making the transformation to action-angle variables yields

$$H_{\text{vib}}\{J,\vartheta\}=\sum_n \hbar\omega_n J_n + 4\sum_{m,n} L_{mn}(J_m J_n)^{1/2}\cos\vartheta_m\cos\vartheta_n \;. \tag{3.17}$$

Again, the degree of the action polynomial is unity, so that (3.11) is satisfied.

For an example of a Hamiltonian violating the condition (3.11) one need look no farther than the general two-body interaction

$$H^{(2)}=\sum_{i,j,k,l} H_{ijkl}^{(2)} a_j^\dagger a_i^\dagger a_k a_l \;. \tag{3.18}$$

Such two-body operators have appeared in effective Hamiltonians obtained as approximations to the Fröhlich Hamiltonian[13,14] to be discussed in Sec. IV. When transformed into the action-angle representation, $H^{(2)}$ takes the form

$$H^{(2)}\{J,\vartheta\}=\sum_{i,j,k,l} H_{ijkl}^{(2)}(J_j J_i J_k J_l)^{1/2} \times\exp[-i(\vartheta_j+\vartheta_i-\vartheta_k-\vartheta_l)] \;. \tag{3.19}$$

The degree of the action polynomial is 2, not 1 as required for $H^{(2)}\{J,\vartheta\}$ to satisfy the invariance condition. Since the Hamilton equations (3.3) are exact for the coherent states, the necessary conclusion is that *the Schrödinger equation for a Hamiltonian containing the two-body interaction $H^{(2)}$ does not admit pure coherent-state products as solutions.*

If $H^{(2)}$ (or its continuum analog) is added to the Hamiltonian of an otherwise free particle, the Hamilton equations for the coherent-state amplitudes are of the nonlinear Schrödinger type. The violation of the invariance condition implies that these nonlinear equations for the coherent-state amplitudes do *not* describe the quantum evolution of a system with two-body interactions.

IV. MIXED SINGLE-PARTICLE STATES AND COHERENT-STATE PRODUCTS

A state vector of mixed single-particle—coherent-state character has played a central role in the theory of solitons in deformable molecular chains. First introduced by Davydov,[3] state vectors of the form

$$\mid D(t)\rangle \equiv \sum_m \psi_m(t)a_m^\dagger \mid 0\rangle\otimes\mid\beta_{1m}(t)\rangle\otimes\mid\beta_{2m}(t)\rangle \otimes\ldots\otimes\mid\beta_{nm}(t)\rangle \tag{4.1}$$

are sought as solutions of the Schrödinger equation, wherein $\mid\beta_{qm}(t)\rangle$ is a pure coherent state defined by

$$\mid\beta_{qm}(t)\rangle\equiv\exp[-\tfrac{1}{2}\mid\beta_{qm}(t)\mid^2]\exp[\beta_{qm}(t)b_q^\dagger]\mid 0\rangle \;. \tag{4.2}$$

The operator $a_m^\dagger$ creates an exciton in the site state labeled by m, and $b_q^\dagger$ creates a phonon with the wave vector q. The exciton component of the proposed state vector is clearly a single-particle state, while the phonon component is a product of coherent states in each phonon mode.

As in previous sections we may proceed to develop a differential invariance condition on the scalar Hamilton function without specific reference to the form of the Hamiltonian of interest. We assume $\mid D(t)\rangle$ satisfies the Schrödinger equation

$$i\hbar\frac{d}{dt}\mid D(t)\rangle=H\mid D(t)\rangle \;. \tag{4.3}$$

Explicitly differentiating the proposed form of $\mid D(t)\rangle$ with respect to time and left multiplying (4.3) with the bra vector $\langle D(t)\mid$ yields

$$i\hbar\left[\sum_n \psi_n^*(t)\dot{\psi}_n(t) + \tfrac{1}{2}\sum_{q,n}\psi_n^*(t)\psi_n(t)[\beta_{qn}^*(t)\dot{\beta}_{qn}(t)-\dot{\beta}_{qn}^*(t)\beta_{qn}(t)]\right] = \langle D(t)\,|\,H\,|\,D(t)\rangle \ . \quad (4.4)$$

Now assuming that Hamilton's equations may be applied to determine the time dependence of the wave-function parameters, we have

$$i\hbar\dot{\psi}_m(t) = \frac{\partial}{\partial\psi_m^*(t)}\langle D(t)\,|\,H\,|\,D(t)\rangle \ , \quad (4.5a)$$

$$i\hbar\dot{\psi}_m^*(t) = \frac{-\partial}{\partial\psi_m(t)}\langle D(t)\,|\,H\,|\,D(t)\rangle \ , \quad (4.5b)$$

$$i\hbar\dot{\beta}_{qm}(t) = \frac{\partial}{\partial\beta_{qm}^*(t)}\langle D(t)\,|\,H\,|\,D(t)\rangle \ , \quad (4.5c)$$

$$i\hbar\dot{\beta}_{qm}^*(t) = \frac{-\partial}{\partial\beta_{qm}(t)}\langle D(t)\,|\,H\,|\,D(t)\rangle \ . \quad (4.5d)$$

Using Eqs. (4.5) to eliminate the time derivatives in (4.4), we obtain the following differential invariance condition for $\langle D(t)\,|\,H\,|\,D(t)\rangle$:

$$\left[\sum_n \psi_n^*\frac{\partial}{\partial\psi_n^*} + \tfrac{1}{2}\sum_{q,n}\psi_n^*\psi_n\left[\beta_{qn}^*\frac{\partial}{\partial\beta_{qn}^*}+\beta_{qn}\frac{\partial}{\partial\beta_{qn}}\right]\right] \times\langle D\,|\,H\,|\,D\rangle = \langle D\,|\,H\,|\,D\rangle \ . \quad (4.6)$$

We are now in a position to test the internal consistency of the Hamilton-equation approach as applied to the Fröhlich-type Hamiltonian

$$H = \sum_{m,n} V_{mn}a_m^\dagger a_n + \sum_q \hbar\omega_q b_q^\dagger b_q + \sum_{q,m}\chi_m^q\hbar\omega_q(b_q^\dagger + b_{-q})a_m^\dagger a_m \quad (4.7)$$

for which we require the expectation value $\langle D(t)\,|\,H\,|\,D(t)\rangle$:

$$\langle D\,|\,H\,|\,D\rangle = \sum_{m,n} V_{mn}\psi_m^*\psi_n + \sum_{q,n}\hbar\omega_q\psi_n^*\psi_n\beta_{qn}^*\beta_{qn} + \sum_{q,m}\chi_m^q\hbar\omega_q(\beta_{qm}^*+\beta_{-qm})\psi_m^*\psi_m \ . \quad (4.8)$$

Denoting the differential operator in (4.6) by $\mathscr{D}$, we find on applying $\mathscr{D}$ to the Hamilton function (4.8) that

$$\mathscr{D}\langle D\,|\,H\,|\,D\rangle = \langle D\,|\,H\,|\,D\rangle + \sum_{q,n}\hbar\omega_q\beta_{qn}^*\beta_{qn}(\psi_n^*\psi_n)^2 + \tfrac{1}{2}\sum_{q,m}\chi_m^q\hbar\omega_q(\beta_{qm}^*+\beta_{-qm})(\psi_m^*\psi_m)^2 \ . \quad (4.9)$$

Clearly, in general $\mathscr{D}\langle D\,|\,H\,|\,D\rangle \neq \langle D\,|\,H\,|\,D\rangle$. We find, therefore, that the application of the Hamilton equations (4.5) for the evaluation of the parameters $\{\psi(t),\beta(t)\}$ results in a vector $|\,D(t)\rangle$ which is *not* a solution of the Schrödinger equation for the Hamiltonian (4.7), in contradiction of the original premise. Thus, in the general case the parameters $\{\psi(t),\beta(t)\}$ solving the equations (4.5) do not describe the actual quantum evolution. This conclusion follows directly from the form of the Hamiltonian and the form assumed for $|\,D(t)\rangle$ and is thus independent of any technical approximations which may be required to solve the Hamilton equations (4.5) in practice.

The general inequivalence found in (4.9) serves to illustrate how the invariance condition may at once both guide and mislead. There exists at least one class of solutions $\{\beta_{qm}(t),\psi_m(t)\}$ for which the condition *is* satisfied, namely, $\{\beta_{qm}(t),\psi_m(t)\}=\{-\chi_m^q,\psi_m(t)\}$. The state vectors $|\,D(t)\rangle$ to which such solutions correspond are precisely the single-polaron states.[12] These states *do*, in fact, solve the Schrödinger equation with the Hamiltonian (4.7), but *only* in the $V_{mn}=0$ limit. This serves to underscore the assertion made throughout this paper that the invariance condition provides only negative information. [It is worth noting that an alternate form of $|\,D(t)\rangle$ used by Davydov in Refs. 2 and 4 in which the dependence of $\beta_{qm}(t)$ on the site index m is neglected also results in a violation of an invariance condition, though all quantities entering the condition must be redefined.]

V. CONCLUSION

In this paper we have shown how manipulations of a system Hamiltonian can provide (negative) information about the solutions of the corresponding Schrödinger equation. These results are motivated by a method often used for analyzing the evolution of a quantum system in which the classical Hamilton equations are used to describe the time dependence of parameters appearing explicitly in a trial state vector. Given a trial state vector, it proves possible to construct an invariance condition which is a necessary (but not sufficient) condition for the set of Hamilton equations to be equivalent to the Schrödinger equation. The differential operator and scalar Hamilton function are simply constructed without any knowledge, exact or approximate, of the solutions of the Schrödinger equation.

We have illustrated the use of the differential invariance condition for trial state vectors consisting of single-particle states, coherent-state products, and mixed single-particle and coherent-state products. The construction of an invariance condition is not limited to such states, but may be carried out whenever state-vector parameters are assumed to satisfy the classical Hamilton equations.

In the course of our illustration, we showed that the form of the state vector assumed by Davydov in his application of the Hamilton-equation method to the Fröhlich Hamiltonian leads to a violation of the associated invariance condition except under very restrictive circumstances. The implication is that the wave vectors $|\,D(t)\rangle$ produced by the Hamilton-equation method are not solutions of the Schrödinger equation for the Fröhlich Hamiltonian. Care must be taken not to overinterpret this result. Our result does not indicate that the Fröhlich Hamiltonian does not admit soliton excitations. If such excitations exist, however, our result indicates that their state vectors are not of the form $|\,D(t)\rangle$ determined by

Hamilton's equations.

Unfortunately, the differential invariance condition we have derived does not provide a measure of the deviation of Hamilton-equation solutions from corresponding Schrödinger-equation solutions having the same initial form. An extensive examination of this difficulty is presented in the following paper and will be further considered elsewhere.[16]

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