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## On the semiclassical treatment of anharmonic quantum oscillators via coherent states—the Toda chain revisited

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**Abstract.** We use coherent states as a time-dependent variational ansatz for a semiclassical treatment of the dynamics of anharmonic quantum oscillators. In this approach the square variance of the Hamiltonian within coherent states is of particular interest. This quantity turns out to have a natural interpretation with respect to time-dependent solutions of the semiclassical equations of motion. Moreover, our approach allows for an estimate of the decoherence time of a classical object due to quantum fluctuations. We illustrate our findings with the example of the Toda chain.

### 1. Introduction

Coherent states are an important notion in quantum physics, in particular with respect to semiclassical approximations; for general references see [1–3].

The coherent states of the harmonic oscillator were introduced by Schrödinger [4] and were re-examined by Glauber [5] in circumstances of quantum optics. For spin systems, spin-coherent states, i.e. the coherent states of  $SU(2)$ , were introduced by Radcliffe [6]. These two types of coherent states provide an immediate connection to the classical limit of generic quantum systems and are the most important examples of coherent states in physics.

The connection to the classical limit is obtained by using coherent states as a time-dependent variational ansatz to investigate the dynamics of a quantum system. Recently, this approach has been reconsidered by the present authors with respect to interacting spin systems given by a general Heisenberg model [7]. The central result in that work is the evaluation of the square variance of the Hamiltonian within coherent states. This quantity turns out to have a natural interpretation with respect to time-dependent spin structures and also allows for an estimate of the validity of the variational approach. In the present work we extend these results to the case of oscillator systems.

In classical nonlinear lattices, as well as in classical spin systems, certain nonlinear excitations like solitary waves are of particular interest. However, it is an open question whether such dynamic and spatially localized excitations can also exist in the corresponding quantum systems. The results of this work provide an estimate for the lifetime of such objects. We demonstrate this for the example of the Toda chain.

The outline of this paper is as follows: in section 2 we summarize the essential properties of the coherent states of the harmonic oscillator, and in section 3 we introduce the time-dependent variational method in quantum mechanics. This method is used in the next section to treat a generic anharmonic oscillator. In particular, the square variance of the Hamiltonian is evaluated. This quantity shows very analogous properties to those obtained in [7] for the case

of quantum spin systems. These findings can be extended to the case of several anharmonically coupled degrees of freedom; as an example we examine the quantum Toda chain in sections 5 and 6.

## 2. Coherent states of the harmonic oscillator

The Hamiltonian of the quantum harmonic oscillator is given in standard notation by

$$\mathcal{H}_h = \frac{p^2}{2m} + \frac{m\omega^2}{2}q^2 = \hbar\omega \left( a^+a + \frac{1}{2} \right) \quad (1)$$

with

$$a = \frac{1}{\sqrt{2}} \left( \sqrt{\frac{m\omega}{\hbar}}q + \frac{i}{\sqrt{\hbar m\omega}}p \right) \quad a^+ = (a)^+ \quad (2)$$

and the well known commutation relations

$$[p, q] = \frac{\hbar}{i} \Leftrightarrow [a, a^+] = 1. \quad (3)$$

The quantities  $\sqrt{\hbar/m\omega}$  and  $\sqrt{\hbar m\omega}$  arising in the operators (2) are the characteristic length and momentum, respectively. The system has an equidistant spectrum. Eigenstates are naturally labelled by  $n \in \{0, 1, 2, \dots\}$ ,

$$\mathcal{H}_h|n\rangle = \hbar\omega(n + \frac{1}{2})|n\rangle. \quad (4)$$

Coherent states of the harmonic oscillator are eigenstates of the lowering operator  $a$  with complex eigenvalues  $\alpha$ ,

$$a|\alpha\rangle = \alpha|\alpha\rangle. \quad (5)$$

They can be expressed as

$$|\alpha\rangle = \exp(\alpha a^+ - \alpha^* a)|0\rangle = \exp(-\frac{1}{2}|\alpha|^2) \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle. \quad (6)$$

The parameter  $\alpha$  is naturally decomposed into its real and imaginary part as

$$\alpha = \frac{1}{\sqrt{2}} \left( \sqrt{\frac{m\omega}{\hbar}}\xi + \frac{i}{\sqrt{\hbar m\omega}}\pi \right). \quad (7)$$

Denoting an expectation value within a coherent state (6) by  $\langle \cdot \rangle$  it holds

$$\langle q \rangle = \xi \quad \langle p \rangle = \pi. \quad (8)$$

Coherent states maintain their shape in the time evolution of the harmonic oscillator,

$$e^{-\frac{i}{\hbar}\mathcal{H}_h t}|\alpha\rangle = e^{-\frac{i}{2}\omega t}|\alpha e^{-i\omega t}\rangle \quad (9)$$

and the time dependence of the expectation values (8) follows exactly the classical motion of the harmonic oscillator. This fact justifies the term ‘coherent states’. A further important property of these objects is their completeness,

$$\frac{1}{\pi} \int d^2\alpha |\alpha\rangle\langle\alpha| = 1 \quad (10)$$

but it should be mentioned that an arbitrary linear combination of coherent states does not have property (5). Thus, the coherent states do not form a subspace of the Hilbert space but rather a submanifold.

### 3. The time-dependent variational method

The Schrödinger equation of quantum mechanics can be derived by extremizing the action functional

$$S = \int_{t_i}^{t_f} dt \langle \psi | i\hbar \frac{d}{dt} - \mathcal{H} | \psi \rangle \quad (11)$$

with respect to the quantum state  $|\psi(t)\rangle$  (or  $\langle\psi(t)|$ ) which is kept fixed at the times  $t_i$  and  $t_f$  [8]. An approximate approach to the dynamics of a quantum system can be performed by restricting the states in (11) to a certain submanifold of the Hilbert space. In the context of semiclassical approximations coherent states are a natural choice. For example, for a single particle moving in a potential the appropriate objects are coherent oscillator states as described in the foregoing section. Thus, our restricted action functional reads in this case

$$\tilde{S} = \int_{t_i}^{t_f} dt \langle \alpha | i\hbar \frac{d}{dt} - \mathcal{H} | \alpha \rangle = \int_{t_i}^{t_f} dt (\pi \partial_t \xi - \langle \mathcal{H} \rangle) \quad (12)$$

where we have left out a total time derivative in the last integrand. The coherent state  $|\alpha\rangle$  is employed here as a time-dependent variational ansatz, i.e. its time dependence is assumed to be given by time-dependent parameters  $\pi(t)$ ,  $\xi(t)$ . This restricted variational principle can be recognized as the stationary phase condition for the quantum mechanical transition amplitude between fixed states  $|\alpha(t_i)\rangle$  and  $|\alpha(t_f)\rangle$  when expressed as a path integral over coherent states [9],

$$U(t_i, t_f) = \int \mathcal{D}\alpha \exp\left(\frac{i}{\hbar} \int_{t_i}^{t_f} dt \langle \alpha | i\hbar \frac{d}{dt} - \mathcal{H} | \alpha \rangle\right). \quad (13)$$

The variational equations of motion obtained from (12) are

$$\partial_t \xi = \frac{\partial \langle \mathcal{H} \rangle}{\partial \pi} \quad \partial_t \pi = -\frac{\partial \langle \mathcal{H} \rangle}{\partial \xi} \quad (14)$$

which have the same form as the classical Hamilton equations.

The time-dependent variational ansatz of coherent states becomes exact if the potential in the Hamiltonian is harmonic. Therefore, our approximate description of the quantum dynamics should be valid for not too large anharmonicities. This will be examined further in the next section.

### 4. The anharmonic oscillator

Let us consider a generic anharmonic quantum oscillator

$$\mathcal{H} = \frac{p^2}{2m} + \frac{m\omega^2}{2}q^2 + \frac{a}{3}q^3 + \frac{b}{4}q^4. \quad (15)$$

With coherent states as a time-dependent variational ansatz we find for the expectation value of the energy

$$\begin{aligned} \langle \mathcal{H} \rangle = & \frac{1}{2m} \left( \pi^2 + \frac{1}{2} \hbar m \omega \right) + \frac{m\omega^2}{2} \left( \xi^2 + \frac{1}{2} \frac{\hbar}{m\omega} \right) + \frac{a}{3} \left( \xi^3 + \frac{3}{2} \xi \frac{\hbar}{m\omega} \right) \\ & + \frac{b}{4} \left( \xi^4 + 3\xi^2 \frac{\hbar}{m\omega} + \frac{3}{4} \left( \frac{\hbar}{m\omega} \right)^2 \right) \end{aligned} \quad (16)$$

which is, of course, constant in time. The variational equations of motion (14) read

$$\partial_t \xi = \frac{\pi}{m} \quad (17)$$

$$\partial_t \pi = -m\omega^2 \xi - a \left( \xi^2 + \frac{1}{2} \frac{\hbar}{m\omega} \right) - b \left( \xi^3 + \frac{3}{2} \frac{\hbar}{m\omega} \xi \right). \quad (18)$$

It is worthwhile to note that the same equations can be obtained from the Heisenberg equations of motion for the operators  $q$  and  $p$ ,

$$\partial_t q = \frac{i}{\hbar} [\mathcal{H}, q] \quad \partial_t p = \frac{i}{\hbar} [\mathcal{H}, p] \quad (19)$$

when the expectation values of both sides of the equations are taken within the state  $|\alpha\rangle$  and the same assumption about its time evolution is made as above. This approach has been used by Krivoslykov *et al* [10].

Equations (16)–(18) reduce to the classical ones in the limit  $\hbar \rightarrow 0$ . Therefore, the coherent states reproduce the classical limit.

Next let us examine the square variance of the energy, i.e.  $\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2$ . This quantity is non-zero only in the quantum case and, as well as  $\langle \mathcal{H} \rangle$ , strictly an invariant of the system, whatever the exact quantum mechanical time evolution of the coherent state is. The square variance can be written in the form

$$\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2 = \Omega_1 + \Omega_2 \quad (20)$$

with

$$\Omega_1 = \frac{1}{2} \left( (\hbar m\omega) \left( \frac{\pi}{m} \right)^2 + \frac{\hbar}{m\omega} \left( m\omega^2 \xi + a \left( \xi^2 + \frac{1}{2} \frac{\hbar}{m\omega} \right) + b \left( \xi^3 + \frac{3}{2} \frac{\hbar}{m\omega} \xi \right) \right)^2 \right) \quad (21)$$

$$\Omega_2 = \frac{1}{2} \left( \frac{\hbar}{m\omega} \right)^2 \left( a\xi + \frac{3}{2} b\xi^2 \right)^2 + \left( \frac{\hbar}{m\omega} \right)^3 \left( \frac{a^2}{12} + 2b^2\xi^2 + \frac{5}{4} ab\xi \right) + \left( \frac{\hbar}{m\omega} \right)^4 b^2 \frac{3}{8}. \quad (22)$$

The quantity  $\Omega_1$  is of leading order  $\hbar$ , while  $\Omega_2$  contains only higher orders. The squared expressions in  $\Omega_1$  can be recognized as the right-hand sides of (17), (18). Thus, we have

$$\Omega_1 = \frac{1}{2} \left( (\hbar m\omega) (\partial_t \xi)^2 + \frac{\hbar}{m\omega} (\partial_t \pi)^2 \right). \quad (23)$$

Within our variational approach, the first order in  $\hbar$  of the square variance of the Hamiltonian is purely due to the time dependence of the state vector. On the other hand, for a quantum state which has a non-trivial time evolution and is consequently not an eigenstate of the Hamiltonian, the energy must definitely have a finite uncertainty. Following this observation, the first order in (20) is not to be considered as an artifact of our variational ansatz, but as a physically relevant expression for the uncertainty of the energy for a time-dependent solution to the variational equations of motion (17), (18). Therefore, the variational approach with coherent states does not only reproduce the classical limit, but is also meaningful for a semiclassical description of the anharmonic oscillator.

The contributions of higher order summarized in  $\Omega_2$  indicate limitations of our variational ansatz, i.e. they are a measure of decoherence effects due to the quantum mechanical time evolution. To clarify this, let us consider the temporal autocorrelation function

$$\langle \alpha | e^{-\frac{i}{\hbar} \mathcal{H} t} | \alpha \rangle \quad (24)$$

i.e. the projection of the time-evolved state onto the initial coherent state. The modulus of this quantity depends on time for two different reasons: firstly the quantum state has a non-trivial semiclassical time evolution described by equations (17), (18). In real space the coherent

state is represented by a Gaussian. Within our *semiclassical* description of the dynamics the wavefunction remains a Gaussian, but its centre is moving. Therefore the overlap of the initial state and the time-evolved state is reduced. Secondly, defects of our variational approach, which lead to decoherence effects, also diminish the scalar product (24). Such quantum fluctuations affect the shape of the wavefunction which will not remain strictly of the Gaussian form under the *exact* quantum mechanical time evolution in the anharmonic potential. The latter effects become significant on a time scale given by the uncertainty relation, where the relevant contribution to the uncertainty of the energy is given by  $\Omega_2$ ,

$$\sqrt{\Omega_2} \Delta t \geq \frac{\hbar}{2}. \tag{25}$$

Alternatively one may consider the following correlation amplitude

$$C(t) := \langle \alpha(t) | e^{-\frac{i}{\hbar} \mathcal{H} t} | \alpha \rangle \tag{26}$$

with  $\alpha(t)$  given by time-dependent functions  $\xi(t)$  and  $\pi(t)$  which are solutions of (17), (18) with the initial condition  $\alpha(0) = \alpha$ . This quantity is the projection of the coherent state evolved under the exact quantum mechanical time evolution onto the state given by the semiclassical time evolution. If the potential in the Hamiltonian is purely harmonic we have  $|C(t)| = 1$  and  $\Omega_2$  vanishes. In this case our variational ansatz of coherent states is of course exact and no decoherence effects occur. This observation also supports our interpretation of the different contributions to  $\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2$ .

Thus deviations of the modulus of (26) from unity measure decoherence effects due to the exact quantum mechanical time evolution under the anharmonic Hamiltonian. These effects manifest themselves in the additional contribution  $\Omega_2$  to the square variance of the energy. The leading order  $\Omega_1$  can be interpreted purely as an effect of the semiclassical time evolution which does not incorporate decoherence effects since it assumes the state vector to remain within the submanifold of coherent states throughout the time evolution.

If one inserts a generic time-dependent solution  $\xi(t)$ ,  $\pi(t)$  of the semiclassical equations of motion (17), (18) in  $\Omega_1$  and  $\Omega_2$ , these quantities will not be constant in time separately (although their sum  $\Omega_1 + \Omega_2$  is strictly constant in the exact quantum mechanical time evolution). However, as an approximation, one may use in (25) the value of  $\Omega_2$  given by the initial value of  $\xi$ . This is justified if the semiclassical motion of the particle is not too fast, i.e. the semiclassical momentum  $\pi$  is not too large. In particular, if the initial coherent state is chosen to have  $\pi(0) = 0$  and a certain value of  $\xi$ , the particle will move in the semiclassical description to smaller  $\xi(t)$  because of the attractive potential. In this case the  $\Omega_2$  evaluated for the initial value  $\xi(0)$  is an upper bound for  $\Omega_2$  evaluated for later times, since this quantity grows with increasing  $\xi$ . Conversely, quantum fluctuations summarized in the quantity  $\Omega_2$  become larger if the  $\xi$  approaches the turning point of the semiclassical motion governed by the equations (17), (18). This feature is well known from the usual WKB-approximation and is therefore consistent with the interpretation of  $\Omega_2$  given above. Moreover, in the following we will also examine other systems which exhibit stationary semiclassical dynamics with  $\Omega_1$  and  $\Omega_2$  being constant in time separately.

Another example where the validity of our considerations can be checked explicitly is the free particle with  $\mathcal{H} = p^2/2m$ . Let the particle be initially in a coherent state with the wavefunction

$$\langle q | \alpha \rangle = \left( \frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} \exp \left( -\frac{m\omega}{2\hbar} (q - \xi)^2 + \frac{i}{\hbar} \pi \left( q - \frac{\xi}{2} \right) \right). \tag{27}$$

The quantity  $\omega$  is not a frequency here but a parameter which determines the localization of the particle in real and momentum space around the expectation values (8). The square variance

of the Hamiltonian reads the same as in (20) with

$$\Omega_1 = \frac{1}{2}\hbar m\omega \left(\frac{\pi}{m}\right)^2 \quad \Omega_2 = \frac{1}{8}(\hbar\omega)^2. \quad (28)$$

Since the expectation value of the momentum is constant for such a translationally invariant system,  $\Omega_1$  and  $\Omega_2$  are conserved separately. The time-evolved wavefunction can be readily obtained as

$$\langle q | e^{-\frac{i}{\hbar}\mathcal{H}t} | \alpha \rangle = \left( \frac{m\omega/\pi\hbar}{1+(\omega t)^2} \right)^{\frac{1}{4}} \exp\left( -\frac{m\omega}{2\hbar} \frac{(q - \xi - \frac{\pi}{m}t)^2}{1+(\omega t)^2} \right) e^{i\varphi(q,t)} \quad (29)$$

with a real phase  $\varphi(q, t)$ . Thus, the width of the wavefunction increases, i.e. its spatially localized structure is smeared out, on a timescale of  $\Delta t = 1/\omega$ , which is consistent with the estimate given by (25). This result also strongly supports the above interpretation of the quantities  $\Omega_1$  and  $\Omega_2$ .

In the next section we will make further use of the estimate of the decoherence time  $\Delta t$  provided by (25).

The findings described above are completely analogous to the results obtained recently on interacting spin systems with spin-coherent states as a time-dependent variational ansatz [7]. The particular case corresponding to the harmonic limit of an oscillator is given here by a paramagnet, where all spins are independent of each other and coupled only to a static magnetic field. In this case all spins perform a Larmor precession around the field axis, and this motion is described exactly by spin-coherent states. A further common aspect of the harmonic oscillator and a spin in a magnetic field is the equidistance of the spectra of both systems.

## 5. Anharmonic lattices: the Toda chain

It is an obvious idea to generalize the results of the foregoing section to systems with many anharmonically coupled degrees of freedom. Let us consider a Hamiltonian  $\mathcal{H} = \mathcal{T} + \mathcal{V}$  with

$$\mathcal{T} = \sum_{n=0}^{N-1} \frac{p_n^2}{2m} \quad \mathcal{V} = \sum_{n=0}^{N-1} V(q_n - q_{n-1}) \quad (30)$$

where  $N$  is the number of degrees of freedom and periodic boundary conditions are imposed. The two-particle potential  $V(x)$  contains, in general, anharmonic terms. To give a semiclassical description of the dynamics, one may proceed similarly as for the single anharmonic oscillator, but for a general potential  $V(x)$  such an approach leads to quite complicated expressions, in particular for the square variance of the energy. Fortunately, a special case exists where the results can be given in a concise form. This case is the Toda chain, which is well known in the theory of nonlinear lattices [11],

$$V(x) = \frac{\eta}{\gamma^2} (e^{-\gamma x} + \gamma x - 1) = \frac{m\omega^2 e^{-\gamma\lambda}}{\gamma^2} (e^{-\gamma x} + \gamma x - 1). \quad (31)$$

The potential  $V$  contains the two parameters  $\eta$  and  $\gamma$ ; for further convenience we have rewritten  $\eta$  in terms of the new parameters  $\omega$  and  $\lambda$  to be determined below. In the limit  $\gamma \rightarrow 0$  the system is just the harmonic chain having independent phonon modes labelled by the wavenumber  $k$  with the acoustic phonon dispersion  $\omega(k) = 2\omega \sin(|k|/2)$ . The usual phonon operators read

$$b_k = \frac{1}{\sqrt{2N}} \sum_{n=0}^{N-1} \left[ \left( \sqrt{\frac{m\omega(k)}{\hbar}} q_n + \frac{i}{\sqrt{\hbar m\omega(k)}} p_n \right) e^{-ikn} \right] \quad b_k^+ = (b_k)^+. \quad (32)$$

An appropriate variational ansatz is given by coherent phonon states,

$$|\beta\rangle = \bigotimes_{k \in 1.\text{BZ}} |\beta_k\rangle \tag{33}$$

where the coherent state of the mode  $k$  fulfils  $b_k|\beta_k\rangle = \beta_k|\beta_k\rangle$  and the tensor product runs over the first Brillouin zone. Again we denote expectation values within (33) by  $\langle \cdot \rangle$ . The parameters  $\beta_k$  are related to the local expectation values  $\langle q_n \rangle = \xi_n, \langle p_n \rangle = \pi_n$  by

$$\beta_k = \frac{1}{\sqrt{2N}} \sum_{n=0}^{N-1} \left[ \left( \sqrt{\frac{m\omega(k)}{\hbar}} \xi_n + \frac{i}{\sqrt{\hbar m\omega(k)}} \pi_n \right) e^{-ikn} \right]. \tag{34}$$

Such an approach to the dynamics of the quantum Toda chain has been performed by Dancz and Rice [12], and by Göhmann and Mertens [13]. Here we add instructive results on the square variance of the Hamiltonian.

The expectation value of the Hamiltonian reads

$$\langle \mathcal{H} \rangle = \sum_{n=0}^{N-1} \frac{\pi_n^2}{2m} + \sum_{n=0}^{N-1} \frac{m\omega^2}{\gamma^2} e^{-\gamma(\lambda - \frac{\gamma}{2} \Delta_0)} (e^{-\gamma(\xi_n - \xi_{n-1})} - 1) \tag{35}$$

where  $\Delta_0$  is a correlation in the phononic vacuum  $|0\rangle$ . More generally, one has

$$\begin{aligned} \Delta_p &:= \langle 0 | (q_{n+p} - q_{n+p-1})(q_n - q_{n-1}) | 0 \rangle \\ &= \frac{\hbar}{m\omega} \frac{1}{2N} \frac{-\sin(\frac{\pi}{N})}{\sin(\frac{2p+1}{2N}\pi) \sin(\frac{2p-1}{2N}\pi)} \xrightarrow{N \rightarrow \infty} \frac{-1}{(4p^2 - 1)} \frac{2}{\pi} \frac{\hbar}{m\omega} \end{aligned} \tag{36}$$

where the following relations hold:

$$\sum_{p=0}^{N-1} \Delta_p = 0 \quad \sum_{p=0}^{N-1} (\Delta_p)^2 = \frac{1}{2} \left( \frac{\hbar}{m\omega} \right)^2. \tag{37}$$

The expectation value (35) has the same form as the classical Toda Hamiltonian up to a renormalization of the parameter  $\lambda$ . The equations of motion are obtained analogously as in (14) and therefore also have the same functional form as the classical ones. It was shown in [13] that this is a peculiarity of the Toda potential.

From the equations of motion one obtains

$$\begin{aligned} &\sum_k [\hbar^2 (\partial_t \beta_k) (\partial_t \beta_k^*)] \\ &= \sum_{n,n'} \left[ \frac{\pi_n}{m} (m^2 \omega^2 \Delta_{n-n'}) \frac{\pi_{n'}}{m} + \left( \frac{m\omega^2}{\gamma} e^{-\gamma(\lambda - \frac{\gamma}{2} \Delta_0) - \gamma(\xi_n - \xi_{n-1})} \right) (\Delta_{n-n'}) \right. \\ &\quad \left. \times \left( \frac{m\omega^2}{\gamma} e^{-\gamma(\lambda - \frac{\gamma}{2} \Delta_0) - \gamma(\xi_{n'} - \xi_{n'-1})} \right) \right]. \end{aligned} \tag{38}$$

Note that the left-hand side of (38) is of leading order  $\hbar$ , since the parameters  $\beta_k$  contains a factor  $1/\sqrt{\hbar}$  (cf (34)).

The square variance of the Hamiltonian reads

$$\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2 = R_1 + R_2 + R_3 \tag{39}$$

with

$$R_1 = \langle \mathcal{T}^2 \rangle - \langle \mathcal{T} \rangle^2 = \sum_{n,n'} \left[ \frac{\pi_n}{m} (m^2 \omega^2 \Delta_{n-n'}) \frac{\pi_{n'}}{m} \right] + \frac{N}{4} (\hbar\omega)^2 \tag{40}$$



$$R_2 = \langle \mathcal{V}^2 \rangle - \langle \mathcal{V} \rangle^2 = \sum_{n,n'} \left[ \left( \frac{m\omega^2}{\gamma^2} e^{-\gamma(\lambda - \frac{\gamma}{2}\Delta_0) - \gamma(\xi_n - \xi_{n-1})} \right) (e^{\gamma^2 \Delta_{n-n'}} - 1) \right. \\ \left. \times \left( \frac{m\omega^2}{\gamma^2} e^{-\gamma(\lambda - \frac{\gamma}{2}\Delta_0) - \gamma(\xi_{n'} - \xi_{n'-1})} \right) \right] \quad (41)$$

$$R_3 = \langle TV + VT \rangle - 2\langle T \rangle \langle V \rangle = -(\hbar\omega)^2 \frac{1}{2} \sum_n [e^{-\gamma(\lambda - \frac{\gamma}{2}\Delta_0) - \gamma(\xi_n - \xi_{n-1})}]. \quad (42)$$

These expressions can be derived by similar methods as described in [13]. The technical advantage of the Toda potential lies in the fact that the contribution  $R_2$  has a comparatively simple form and can be obtained via the Baker–Campbell–Hausdorff identity.

Expanding the factor  $(\exp(\gamma^2 \Delta_{n-n'}) - 1)$  in (41) and using equations (38), (37) one can rewrite these formulae as

$$\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2 = \sum_{\mu=1}^{\infty} \Omega_{\mu} \quad (43)$$

with

$$\Omega_1 = \sum_k [\hbar^2 (\partial_t \beta_k) (\partial_t \beta_k^*)] \quad (44)$$

$$\Omega_2 = \frac{1}{2} \sum_{n,n'} \left[ \left( \frac{m\omega^2}{\gamma^2} (e^{-\gamma(\lambda - \frac{\gamma}{2}\Delta_0) - \gamma(\xi_n - \xi_{n-1})} - 1) \right) (\gamma^2 \Delta_{n-n'})^2 \right. \\ \left. \times \left( \frac{m\omega^2}{\gamma^2} (e^{-\gamma(\lambda - \frac{\gamma}{2}\Delta_0) - \gamma(\xi_{n'} - \xi_{n'-1})} - 1) \right) \right] \quad (45)$$

and for  $\mu > 2$

$$\Omega_{\mu} = \sum_{n,n'} \left[ \left( \frac{m\omega^2}{\gamma^2} e^{-\gamma(\lambda - \frac{\gamma}{2}\Delta_0) - \gamma(\xi_n - \xi_{n-1})} \right) \frac{1}{\mu!} (\gamma^2 \Delta_{n-n'})^{\mu} \cdot \left( \frac{m\omega^2}{\gamma^2} e^{-\gamma(\lambda - \frac{\gamma}{2}\Delta_0) - \gamma(\xi_{n'} - \xi_{n'-1})} \right) \right]. \quad (46)$$

Each term  $\Omega_{\mu}$  is of leading order  $\hbar^{\mu}$  because  $\Delta_{n-n'} \propto \hbar$ . As seen from (44) the lowest order in  $\hbar$  in the square variance of the Hamiltonian is purely given by the time dependence of the semiclassical variables. Therefore, the same conclusions apply as in the foregoing section. Note also that again in the harmonic limit  $\gamma \rightarrow 0$  all  $\Omega_{\mu}$  for  $\mu > 1$  vanish and the variational ansatz is exact.

We have demonstrated the result given in equations (43), (44) for the Toda chain as an example, mostly to reduce technical difficulties. In fact, from experience with an analogous semiclassical treatment of quite general Heisenberg spin models in arbitrary spatial dimension [7], these findings are expected to hold for more general lattice models.

## 6. Decoherence effects to semiclassical solitary waves in the Toda chain

In the last decades an immense literature has emerged on solitons in solid state physics. In those publications, the solid is usually modelled (at least effectively) as a classical system, while in fact it generally carries quantum degrees of freedom. We will see below how our approach can be used to make contact between the classical and the quantum mechanical description. In particular, the validity of theories based on classical solitary excitations can be estimated.

The one-dimensional Toda lattice is an integrable system in the classical [11, 14] as well as in the quantum mechanical case [15]. Moreover, a formal identification can be made between the dispersion law of the one-soliton solution of the classical system and a certain branch

of the excitation system of the quantum model, which is obtained by the Bethe ansatz [16]. Both dispersions are identical in form, and in this sense the quantum analogue of a classical soliton may be viewed as a certain stationary state of the quantum system; see also [17] for a discussion of that issue in a semiclassical context. Nevertheless, such an eigenstate obtained from the Bethe ansatz is not a dynamical object and naturally translationally symmetric, i.e. not localized like a classical soliton. Moreover, such an explicit identification is in general only possible if the quantum and the classical system are both integrable. Therefore, the question arises whether quantum states exist which have the essential properties of classical solitary waves, which are required in many classical descriptions of phenomena like energy transport etc. As such a quantum state is not translationally symmetric, it cannot be expected to be an eigenstate of the quantum system. Moreover, its time evolution is in general not fully coherent, but decoherence effects due to quantum fluctuations cause a finite lifetime of such a localized state. In the following we give an estimate for this lifetime of semiclassical solitary waves built up from coherent states in the quantum Toda chain. Let us first consider the variational ground state of the Toda chain with  $\xi_n = \pi_n = 0$  for all  $n$ . Here we clearly have  $\Omega_1 = 0$ , and for  $\Omega_2$  we find

$$\Omega_2 = \frac{N}{4} (\hbar\omega)^2 (1 - e^{-\gamma(\lambda - \frac{\gamma}{2}\Delta_0)})^2 \tag{47}$$

which is also zero for  $\lambda = (\gamma/2)\Delta_0$ . With respect to the parameter  $\eta$  entering the potential (31) this means

$$m\omega^2 \exp\left(-\frac{\gamma^2}{2} \frac{\hbar}{m\omega} \frac{1}{N} \frac{\sin(\pi/N)}{1 - \cos(\pi/N)}\right) = \eta. \tag{48}$$

This relation determines the frequency  $\omega$  which enters the variational ansatz (33) via the phonon dispersion  $\omega(k)$ . One obviously always has a non-negative solution  $\omega$  for any non-negative  $\eta$ . Note that with this choice for  $\omega$  the quantum corrections in the exponential factor in the variational expression (35) and also in the equations of motion cancel with the parameter  $\lambda$ , but are of course present compared with the original Hamiltonian. However, the higher order terms  $\Omega_\mu$  with  $\mu > 2$  are in general non-zero for this classical ground state solution. Thus, our variational ground state approximates the exact ground state within the first two orders of  $\hbar$ . To account for higher corrections one has to implement a more complicated state than (33). Therefore, in the spirit of the WKB approximation scheme we can be confident in giving a valid description of the quantum system within the first two orders of  $\hbar$ .

Let us now turn to a solitary solution to the variational equations of motion (which are practically the same as the classical equations). As mentioned above, such solutions do not correspond to (approximate) eigenstates of the system like the variational ground state, but suffer decoherence effects in their time evolution. Nonlinear excitations in the classical Toda chain with periodic boundary conditions are so-called cnoidal waves which can be expressed in terms of Jacobi elliptic functions. As a limiting case, a pulse soliton arises which is given by elementary expressions [11],

$$\pi_n = \pm \frac{vm}{\gamma} (\tanh(\kappa(n - 1) \pm vt) - \tanh(\kappa n \pm vt)) \tag{49}$$

$$e^{-\gamma(\xi_{n+1} - \xi_n)} - 1 = \frac{\sinh^2 \kappa}{\cosh^2(\kappa n \pm vt)} \tag{50}$$

with the soliton parameter  $\kappa$ , which is the inverse soliton width, and  $v = \omega \sinh \kappa$ . Although this solution of the variational equations of motion is, strictly speaking, not compatible with periodic boundary conditions, it is an excellent numerical approximation for the cnoidal waves

for large wavelength and system size. For simplicity, we shall concentrate on the above expressions in the following. With this solution the quantities  $\Omega_\mu$  can be written as

$$\Omega_\mu = (\hbar\omega)^2 \left( \frac{m\omega^2/\gamma^2}{\hbar\omega} \right)^{2-\mu} Q_\mu(\kappa) \quad (51)$$

where the  $Q_\mu$  depend only on  $\kappa$ . In particular, the  $Q_\mu$  (and therefore the  $\Omega_\mu$ ) are time independent since our soliton solution describes a stationary movement, where a translation in time is equivalent to a translation in space. Therefore, the time dependence drops out when the summations over the system in equations (44)–(46) are performed. The dimensionless quantity  $(m\omega^2/\gamma^2)/(\hbar\omega)$  is the ratio of the energy scales of the nonlinear interaction and of the linear phonon excitations. In a semiclassical regime this quotient is large and suppresses all orders  $\Omega_\mu$  with  $\mu > 2$  (which are not further considered here, cf above). For  $\mu = 2$  we have for an infinite system

$$Q_2(\kappa) = \frac{4 \sinh^4 \kappa}{\pi^2} \sum_{l=-\infty}^{\infty} \frac{1}{(4l^2 - 1)^2} \left[ \sum_{n=-\infty}^{\infty} \frac{1}{\cosh^2(\kappa n) \cosh^2(\kappa(n-l))} \right]. \quad (52)$$

The above summations are non-elementary. The largest contribution stems from the summand with  $l = 0$ . Replacing the remaining sum over  $n$  by an integral, one concludes that this quantity should scale approximately like  $1/\kappa$ . Indeed, a numerical evaluation of the full double sum for  $\kappa \in ]0, 0.5]$  shows that a very accurate value for this expression is  $(4/3\kappa)$ ; deviations from this occur only for large  $\kappa$  and are of order  $10^{-5}$ . Therefore, we may write in a very good approximation

$$\Omega_2 = (\hbar\omega)^2 \frac{4 \sinh^4 \kappa}{\pi^2} \frac{4}{3\kappa} \quad (53)$$

and the estimate of the decoherence time according to (25) is

$$\Delta t \geq \frac{1}{\omega} \frac{\pi \sqrt{3}}{8} \frac{\sqrt{\kappa}}{\sinh^2 \kappa}. \quad (54)$$

Multiplying with the soliton velocity  $c = v/\kappa$  one finds for the decoherence length  $\Delta l = c \Delta t$  for small  $\kappa$

$$\Delta l \geq \frac{\pi \sqrt{3}}{8} \kappa^{-3/2}. \quad (55)$$

Remarkably, no system parameter or Planck's constant itself, but only the soliton width enters (55). The decoherence length is large for small  $\kappa$ , i.e. broad solitons. For instance, a soliton with a width of 100 lattice units may travel (at least) about ten times this distance until decoherence effects become significant. With respect to the classical picture of solitons, this appears rather restrictive. On the other hand, the relation (55) provides only a lower bound for the coherence length; e.g. in the classical limit  $\hbar \rightarrow 0$  all decoherence effects vanish and the decoherence length becomes infinite. However, for not too large values of the ratio  $(m\omega^2/\gamma^2)/(\hbar\omega)$  the decoherence length should be assumed to be of the order of the right-hand side of (55), at least as a 'conservative' estimate.

## 7. Conclusions

In this work we have examined coherent states as a time-dependent variational ansatz for a semiclassical description of anharmonic oscillators. In particular, the square variance of the Hamiltonian  $\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2$  within coherent states is considered. For a single anharmonic oscillator, the first order in  $\hbar$  of this quantity turns out to be purely given by the variational

time dependence of the quantum state, cf equations (20)–(23). Therefore, this contribution has a natural interpretation, which can be confirmed rigorously in the cases of the harmonic oscillator and the free particle. Compared with recent results on spin-coherent states [7] this appears to be a general property of coherent states with respect to generic quantum systems. The remaining contributions to  $\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2$  can be used to estimate decoherence effects which arise from quantum fluctuations. In the foregoing section we illustrated this by the example of the Toda chain. We have chosen this system because it provides comparatively simple expressions for the quantities considered here, and explicit solitary solutions of the classical equations are available. In fact, we expect our approach to be useful for much more general anharmonic lattices.

## References

- [1] Perelomov A 1986 *Generalized Coherent States and Their Applications* (Berlin: Springer)
- [2] Klauder J R and Skagerstam B S 1985 *Coherent States* (Singapore: World Scientific)
- [3] Zhang W-M, Feng D H and Gilmore R 1990 *Rev. Mod. Phys.* **62** 867
- [4] Schrödinger E 1926 *Naturwissenschaften* **14** 664
- [5] Glauber R J 1963 *Phys. Rev.* **131** 2766
- [6] Radcliffe J M 1971 *J. Phys. A: Math. Gen.* **4** 313
- [7] Schliemann J and Mertens F G 1998 *J. Phys.: Condens. Matter* **10** 1091
- [8] Kramer P and Saraceno M 1981 *Geometry of the Time-Dependent Variational Principle in Quantum Mechanics (Springer Lecture Notes in Physics 140)* ed J Ehlers *et al* (Berlin: Springer)
- [9] Klauder J R 1978 Continuous representations and path integrals, revisited *Proc. NATO Advanced Summer Institute* ed G J Papadopoulos and J T Devreese (New York: Plenum)  
Klauder J R 1979 *Phys. Rev. D* **19** 2349
- [10] Krivoshlykov S G, Man'ko V I and Sissakian I N 1982 *Phys. Lett. A* **90** 165
- [11] Toda M 1981 *Theory of Nonlinear Lattices (Springer Series in Solid-State Sciences 20)* (Berlin: Springer)
- [12] Dancz J and Rice S A 1977 *J. Chem. Phys.* **67** 1418
- [13] Göhmann F and Mertens F G 1992 *J. Phys. A: Math. Gen.* **25** 649
- [14] Flaschka H 1974 *Phys. Rev. B* **1974** 9 1924  
Manakov S V 1974 *Sov. Phys. JETP* **67** 269
- [15] Olshanetsky M A and Perelomov A M 1977 *Lett. Math. Phys.* **2** 7  
Sklyanin E K 1985 *Non-Linear Equations in Classical and Quantum Field Theory (Springer Lecture Notes in Physics 226)* ed N Sanchez (Berlin: Springer)
- [16] Sutherland B 1978 *Rocky Mt J. Math.* **8** 413  
Mertens F G 1984 *Z. Phys. B* **55** 353  
Siddharthan R and Shastry B S 1997 *Phys. Rev. B* **55** 12 196
- [17] Göhmann F, Pesch W and Mertens F G 1993 *J. Phys. A: Math. Gen.* **26** 7589