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Time-dependent variational approach to solitons in the quantum Toda chain

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Abstract. We consider the quantum Toda chain in a semiclassical approximation. If the chain is initially in a coherent state and we constrain it to preserve the coherence, its motion is described by effective classical equations. These turn out to be of the same form as the classical equations of motion, but have a renormalized coupling constant. We call the solitons arising from this effective model 'quantum solitons'.

1. Introduction

Since Bethe's pioneering article on the spin-$\frac{1}{2}$ Heisenberg chain in 1931 [1] much work on exactly solvable many-particle quantum systems has been done. In particular, the quantum inverse spectral method (QISM) developed by Fadeev and co-workers provides a powerful means for both finding and solving exactly solvable models [2].

We emphasize, however, that there is still a need to apply approximate methods if one is interested in local quantities like, for instance, the wavefunction corresponding to a soliton. The variational approach described later gives an explicit approximate expression for a *time-dependent* wavefunction of a many-body system, which has the additional advantage of being quite simple. At the present time, this still lies beyond the scope of the exact methods.

The system in which we are interested is the well known Toda chain, a chain of equal particles connected by equal springs. The potential of one of these springs is $V(r) = (\omega^2/\gamma^2)(\exp(-\gamma(r-r_0)) + \gamma(r-r_0) - 1)$, where the parameters γ, ω have been chosen so as to give the potential of a harmonic spring with frequency ω as $\gamma \to 0_+$. If the system is constrained on a ring of length L and the particle mass is chosen to be unity the Hamiltonian reads

$$H = E_0 + \sum_{n=1}^{N} \left\{ \frac{p_n^2}{2} + \frac{\omega^2}{\gamma^2} e^{-\gamma(a-r_0)} (e^{-\gamma(x_{n+1}-x_n)} - 1) \right\}. \tag{1.1}$$

Here x_n is the position of the nth particle relative to its position at rest, $x_{N+1} = x_1$, E_0 is the classical ground-state energy and $a = L/N$ is the lattice constant. In the following H_h denotes the harmonic limit of H.

The Toda chain is integrable in the classical [3, 4] as well as in the quantum mechanical case [5]. The Bethe ansatz [6] and QISM [7] have been applied to it. Note that Bethe's wavefunctions serve merely as an approximation, yielding, however, the exact ground-state energy and excitation spectrum in the thermodynamic limit [8]. The correct wavefunctions for few particles have been found by Gutzwiller [9] and they are implicit in the QISM treatment due to Sklyanin [7].

Semiclassical quantization procedures have also been applied to the Toda system [8, 10]. Shirafuji [10] used a path integral WKB method to quantize the periodic Toda chain. In this approach the energy levels of the quantum system arise from the classical periodic orbits, i.e. the classical soliton becomes a stationary state when it is quantized. A similar interpretation results from Bethe's ansatz and from QISM. One branch of the elementary excitation spectrum turns out to yield the classical soliton dispersion curve, $E = E(p)$, in the classical limit. This fact clearly supports the view of a 'quantum soliton' as a stationary state.

Our work was strongly motivated by the question whether a soliton on a quantum chain could also be thought of as a dynamical object. The answer is affirmative at least within the frame of the variational method described later. We look for the best dynamics of Gaussian wavepackets, which we constrain to preserve their shape. The centres of the wavepackets move according to effective classical equations of motion. In general these would be different from the original classical ones. But in the case of the Toda chain the effective Lagrangian turns out to be of the same form as the original one. Only the coupling parameter ω is renormalized.

2. Variational principle

If a physical equation of motion is of Lagrangian form, i.e. derivable from Hamilton's principle, this always provides a formally simple approach for getting approximate solutions by restricting the functions to be varied to a smaller and more palpable family [11]. A starting point for obtaining approximate solutions to Schrödinger's time-dependent equation may be the Lagrangian

$$L = \langle\varphi|(\mathrm{i}\hbar\partial_t - H)|\varphi\rangle. \tag{2.1}$$

It results in Schrödinger's equation if varied with respect to φ, an arbitrary normalized quantum state. But if φ is constrained to be a $2N$ parameter family $\varphi_{\dot\alpha_1,\ldots,\dot\alpha_N,\alpha_1,\ldots,\alpha_N}$ of test functions, we will get N second-order ordinary differential equations in the parameters α instead. These may be interpreted as classical equations of motion for a system with N degrees of freedom.

It is an unpleasant feature of variational methods that the error is always difficult to estimate. The crucial point is to guess some appropriate test functions. In the case of the Toda chain it seems quite natural to use coherent phonon states, for they give the exact solution for vanishing anharmonicity γ and should still give useful results if γ is not too large and the energy of the considered excitation is not too high. Using coherent phonon states (CPS) means nothing else but restricting the allowed wavefunctions to Gaussian form.

3. Coherent states

We use the following notation for CPS:

$$|\beta\rangle = \exp\left\{\sum_k(\beta_k b_k^+ - \beta_k^* b_k)\right\}|0\rangle = \exp\left\{\frac{1}{\mathrm{i}\hbar}\sum_n(\xi_n p_n - \pi_n x_n)\right\}|0\rangle \tag{3.1}$$

where b_k^+ creates a phonon of wavenumber k, $|0\rangle$ is the phonon vacuum and p_n, x_n are the momentum and position operators, respectively. The relation between ξ_n, π_n and β_k^*, β_k is exactly the same as that between x_n, p_n and b_k^+, b_k.

$$\xi_n = \frac{1}{\sqrt{N}} \sum_k e^{ikna} \sqrt{\frac{\hbar}{2\omega_k}} (\beta_k + \beta_k^*) \qquad \pi_n = -\frac{i}{\sqrt{N}} \sum_k e^{ikna} \sqrt{\frac{\hbar\omega_k}{2}} (\beta_k - \beta_k^*). \tag{3.2}$$

As usual ω_k denotes the phonon frequency, $\omega_k = 2\omega \sin|ka/2|$. Let us note three basic properties of (3.1):

(i) $b|\beta\rangle = \beta|\beta\rangle \qquad \langle\beta|\beta\rangle = 1$ (3.3)

(ii) $\langle\beta|x_n|\beta\rangle = \xi_n \qquad \langle\beta|p_n|\beta\rangle = \pi_n$ (3.4)

(iii) $(i\hbar\partial_t - H_h)|\beta\rangle = 0$ if ξ_n, π_n follow the classical equation of motion. (3.5)

(iii) led us to use CPS here. With (i) and (ii) $L[\beta]$ is readily computed.

4. Effective Lagrangian

The difference $x_{n+1} - x_n$ may be written as

$$x_{n+1} - x_n = \sum_k \alpha_{nk}(b_k + b_{-k}^+). \tag{4.1}$$

Here all operator independent quantities have been collected in α_{nk}. Let $A = \sum_k \alpha_{nk} b_k$, $B = \sum_k \alpha_{nk} b_{-k}^+$. This yields

$$\begin{aligned}[A, B] &= \sum_k |\alpha_{nk}|^2 = \frac{\hbar}{N\omega} \frac{\sin(\pi/N)}{1 - \cos(\pi/N)} \\ &= \langle 0|(x_{n+1} - x_n)^2|0\rangle =: \langle\Delta x^2\rangle \overset{N\to\infty}{\longrightarrow} 2\hbar/\pi\omega \end{aligned} \tag{4.2}$$

$$[A, [A, B]] = [B, [A, B]] = 0.$$

We may now use the Baker–Kempe–Hausdorff formula and property (i) to determine the potential part of $L[\beta]$.

$$\langle\beta| \exp\{-\gamma(x_{n+1} - x_n)\}|\beta\rangle = \exp\{\gamma^2\langle\Delta x^2\rangle/2\} \exp\{-\gamma(\xi_{n+1} - \xi_n)\}. \tag{4.3}$$

And in a similar way:

$$\langle\beta|p_n^2|\beta\rangle = \pi_n^2 + \omega^2\langle\Delta x^2\rangle \tag{4.4}$$

$$\langle\beta|i\hbar\partial_t|\beta\rangle = \tfrac{1}{2}\sum_n(\dot{\xi}_n \pi_n - \xi_n \dot{\pi}_n) + N\omega^2\langle\Delta x^2\rangle. \tag{4.5}$$

Hence it turns out that

$$\langle\beta|H|\beta\rangle = \sum_{n=1}^{N}\left\{\frac{p_n^2}{2} + \frac{\omega^2}{\gamma^2}\mathrm{e}^{-\gamma(a-r_0)}(\mathrm{e}^{\gamma^2\langle\Delta x^2\rangle/2}\mathrm{e}^{-\gamma(\xi_{n+1}-\xi_n)} - \varepsilon'(\gamma,a))\right\} \tag{4.6}$$

where some constants have been combined in $\varepsilon'(\gamma, a)$. In order to keep $\langle\beta|H|\beta\rangle$ finite in the thermodynamic limit $\varepsilon'(\gamma, a)$ must be replaced by some other constant ε. This may be called infrared renormalization.

We want $\min\langle\beta|H|\beta\rangle$ to be zero and thus get $\varepsilon = \exp(\gamma^2\langle\Delta x^2\rangle/2)$. Inserting $\langle\beta|H|\beta\rangle$ in the expression for the effective Lagrangian we finally arrive at

$$L_{\text{eff}} = \sum_n\left\{\frac{1}{2}\dot{\xi}_n^2 - \frac{\omega^2}{\gamma^2}\mathrm{e}^{-\gamma(a-r_0-\gamma\langle\Delta x^2\rangle/2)}(\mathrm{e}^{-\gamma(\xi_{n+1}-\xi_n)} - 1)\right\} \tag{4.7}$$

where we have already inserted the equation of motion for π_n and suppressed a total time derivative as well as a constant term as both are irrelevant for the equation of motion. Equation (4.7) is valid for the N-particle chain as well as for the infinite chain.

5. Discussion

L_{eff} in (4.7) is the classical Lagrangian for the Toda chain except for the extra factor $\varepsilon = \exp\{\gamma^2\langle\Delta x^2\rangle/2\}$, which therefore contains all quantum effects. It reduces to unity in the classical limit, i.e. for $\hbar \to 0$ or $\omega \to \infty$, respectively, but also in the harmonic limit, $\gamma \to 0$. Hence, as one would have expected the chain behaves classically in the harmonic limit.

The fact that L_{eff} is again of Toda's form makes it possible to give explicit analytical corrections to all classically known quantities by simply replacing ω by $\omega\exp(\gamma\langle\Delta x^2\rangle/4)$. In particular, L_{eff} gives rise to the familiar Toda solitons. We are tempted to call these solitons 'quantum solitons', because they describe the motion of the test wavefunction. They are broadened compared with classical solitons moving with the same velocity.

We stress again that the existence of these solitons is no triviality. If the effective potential in (4.7) had turned out to be of different form, no solitons would have resulted. An arbitrary potential suffers different corrections for each order in its Taylor expansion, which do not necessarily sum up to a simple factor (see the appendix). Thus, in general, the dynamics of the effective problem differs in structure from that of the underlying classical one.

The quantum correction ε is easy to understand. The zero point motion of the particles causes an additional pressure, as if the lattice were compressed by an amount $\gamma\langle\Delta x^2\rangle/2$ per lattice constant. The total force per lattice constant exerted on a spring is in the ground state

$$\langle 0| - V'(x_{n+1} - x_n)|0\rangle = (\omega^2/\gamma r_0)(\varepsilon\mathrm{e}^{-\gamma(a-r_0)} - 1) =: P. \tag{5.1}$$

Instead of fixing the lattice constant one could also fix the pressure

$$\gamma r_0 P/\omega^2 + 1 = \mathrm{e}^{-\gamma(a-r_0-\gamma\langle\Delta x^2\rangle/2)}. \tag{5.2}$$

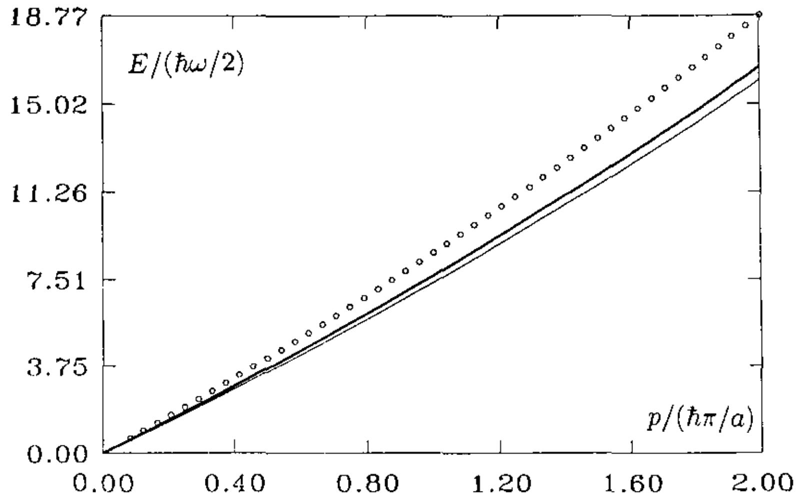

Figure 1. Dispersion curves for fixed a: The thin curve is the classical curve, the thick curve is the curve obtained from the Bethe ansatz, and the hexagons denote the curve obtained from the variational approach, which always overestimates the energy.

For zero P the chain is streched. The new lattice constant is

$$a = r_0 + \gamma\langle\Delta x^2\rangle/2. \tag{5.3}$$

In this case L_{eff} agrees with the classical Lagrangian for zero pressure and the quantum correction does not affect the dynamics.

It is always difficult to estimate the error involved in a variational approximation. Here we are in the lucky situation that we can test our results for the dispersion curve $E(p)$ by comparing them directly with the exact ones [13]. The parameters in figure 1 have been chosen such that $C = (\omega^2/\gamma^2)/(\hbar\omega) = 1$ and the lattice constant a has been fixed at $a = r_0$. In fact, C is the only free parameter if the Toda Hamiltonian (1.1) is written in scaled form, see [13]. The semiclassical regime is characterized by $C \gg 1$. In this regime it is scarcely possible to distinguish the three curves.

If we consider the case $P = 0$, the classical and variational curves are identical, whereas the curve from Bethe's ansatz lies slightly under the classical one.

After having finished this work, we became aware that Dancz and Rice [13] obtained the same effective equations some years ago, starting from the Heisenberg equations of motion. However, our derivation is technically much less involved and uses a variational principle, that guarantees the best possible dynamics within the CPS approximation.

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Appendix. Effective potential for an arbitrary nonlinear spring

First we compute the expectation value taken in a CPS for an arbitrary monomial in the displacement of the spring: Defining

$$U := \exp\left\{\frac{1}{i\hbar}\sum_n(\xi_n p_n - \pi_n x_n)\right\} \tag{A1}$$

we get $U^+ x_n U = x_n + \xi_n$. Thus

$$\begin{aligned}\langle\beta|(x_{n+1}-x_n)^m|\beta\rangle &= \langle 0|(x_{n+1}-x_n+\xi_{n+1}-\xi_n)^m|0\rangle \\ &= \sum_{j=0}^{m}\binom{m}{j}\langle 0|(x_{n+1}-x_n)^j|0\rangle(\xi_{n+1}-\xi_n)^{m-j}.\end{aligned} \tag{A2}$$

It remains to compute

$$\langle 0|(x_{n+1}-x_n)^j|0\rangle = \sum_{k_1,\ldots,k_j}\alpha_{k_1}\ldots\alpha_{k_j}\langle 0|A_{k_1}\ldots A_{k_j}|0\rangle \tag{A3}$$

with $A_{k_i} := b_{k_i} + b^+_{-k_i}$, and $\alpha_{k_i} := \sqrt{\hbar/2N\omega_{k_i}}\exp(ik_i na)(\exp(ik_i a)-1)$ as in (4.1). Obviously $\langle 0|A_{k_1}\ldots A_{k_j}|0\rangle$ is zero if j is odd. With the aid of Wick's theorem we get for $j = 2l$

$$\langle 0|A_{k_1}\ldots A_{k_{2l}}|0\rangle = \frac{1}{2^l l!}\sum_{P\in S^{2l}}\langle 0|A_{k_{P1}}A_{k_{P2}}|0\rangle\ldots\langle 0|A_{k_{P(2l-1)}}A_{k_{P2l}}|0\rangle. \tag{A4}$$

The summation is over all permutations of the $2l$ indices. Now

$$\langle 0|A_{k_{P(2i-1)}}A_{k_{P2i}}|0\rangle = \delta_{k_{P(2i-1)},-k_{P2i}} \tag{A5}$$

and thus

$$\begin{aligned}\langle 0|(x_{n+1}-x_n)^{2l}|0\rangle &= \frac{1}{2^l l!}\sum_{P\in S^{2l}}\sum_{k_1,\ldots,k_{2l}}\alpha_{k_1}\ldots\alpha_{k_{2l}}\delta_{k_{P1},-k_{P2}}\ldots\delta_{k_{P(2l-1)},-k_{P2l}} \\ &= \frac{1}{2^l l!}\sum_{P\in S^{2l}}\left(\sum_k|\alpha_k|^2\right)^l = (2l)!(\langle\Delta x^2\rangle/2)^l/l!.\end{aligned} \tag{A6}$$

Inserting (A6) in (A2) we get the following: Given the potential $V(r) = r^m$ the corresponding effective potential is

$$\begin{aligned}V_{\mathrm{eff}}(r) &= \sum_{l=0}^{[m/2]}\binom{m}{2l}\frac{(2l)!}{2^l l!}\langle\Delta x^2\rangle^l r^{m-2l} \\ &= (-i\langle\Delta x^2\rangle)^m He_m(ir/\langle\Delta x^2\rangle)\end{aligned} \tag{A7}$$

with He_m the Hermite polynomial of order m (see [14]). We now pick up two more formulae from [14],

$$\begin{aligned}He_m(r) &= 2^{-m/2}H_m(r/\sqrt{2}) \\ H_m(r) &= \frac{e^{r^2}2^{m+1}}{\sqrt{\pi}}\int_0^\infty dz\, e^{-z^2}z^m\cos(2rz - m\pi/2)\end{aligned} \tag{A8}$$

and arrive at

$$(-\mathrm{i}\langle\Delta x^2\rangle)^m He_m(\mathrm{i}r/\langle\Delta x^2\rangle) = \frac{1}{\sqrt{2\pi\langle\Delta x^2\rangle}} \int_{-\infty}^{\infty} \mathrm{d}z\, z^m \mathrm{e}^{-(z-r)^2/2\langle\Delta x^2\rangle}. \tag{A9}$$

Thus for every potential which can be represented as a series of polynomials we get

$$V_{\mathrm{eff}}(r) = \frac{1}{\sqrt{2\pi\langle\Delta x^2\rangle}} \int_{-\infty}^{\infty} \mathrm{d}z\, V(z) \mathrm{e}^{-(z-r)^2/2\langle\Delta x^2\rangle}. \tag{A10}$$

This may be checked again for the Toda potential (see also [12]).

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