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LETTER TO THE EDITOR

Construction of quantum systems with soluble ground-state properties

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Abstract. We propose transformation of the Langevin equation into an eigenvalue problem as a method to construct systems with soluble ground-state properties. As examples, we discuss quantum systems resulting from the Toda and sine-Gordon chains evolving according to the Langevin equation. Some ground-state properties are then evaluated with methods originally devised to calculate the partition function of one-dimensional classical systems. We also present numeridal results for the two-phonon bound-state frequency and its coupling constant dependence by simulating a generalised quantum sine-Gordon system.

In this work, we present and illustrate a method to construct quantum systems with exactly soluble ground-state properties. This is achieved by considering the Fokker-Planck equation associated with the Langevin equation. In fact, the Fokker-Planck equation can be reduced to the Schrödinger equation by choosing the variance of the random force appropriately. As a result, a system evolving according to the Langevin equation and specified by its potential energy W is related to a quantum system with potential energy V, where $V(W)$ as well as the ground-state wavefunction and its eigenvalue are known. Knowledge of the ground-state wavefunction then allows calculation of the properties of interest. This approach is particularly appealing in one-dimensional many-particle systems, where the resulting multiple integrals can be treated with the transfer integral technique, originally developed to calculate the partition function and related properties of classical systems (Scalapino *et al* 1972).

Other interesting aspects of this relationship between the Langevin equation and an associated quantum problem are (Schneider *et al* 1985): (a) the energy spectrum of the quantum system can be investigated by simulating time-dependent correlation functions in the stationary Langevin process; (b) the critical dynamics of a d-dimensional system evolving according to the Langevin equation can be mapped onto the static critical properties of an associated quantum system and its $(d+1)$-dimensional classical counterpart.

The letter is organised as follows: we sketch the relationship of the model evolving according to the Langevin equation and the associated quantum system, with known ground-state wavefunction and eigenvalue. Invoking the transfer integral technique, we then calculate ground-state properties of interest for a generalised Toda and sine-Gordon chain. Finally, we present some numerical results for the two-phonon bound state and its coupling-constant dependence by simulating a generalised quantum sine-Gordon model in terms of the Langevin process.

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To sketch the method, we consider a one-dimensional N-particle system. The time evolution is given by the coupled Langevin equations

$$\dot{x}_l = \mathrm{d}x_l/\mathrm{d}t = -\partial W/\partial x_l + \eta_l(t). \tag{1}$$

The N-independent Gaussian-noise sources satisfy

$$\langle \eta_l(t) \rangle = 0, \qquad \langle \eta_l(t)\ \eta_{l'}'(l') \rangle = \sigma \delta_{ll'} \delta(t-l'), \tag{2}$$

where σ is the variance of the random force. The associated Fokker–Planck equation for the probability density $P(x_1, \ldots, x_N; t)$

$$\frac{\partial P}{\partial t} = \sum_l \frac{\partial}{\partial x_l}\left(\frac{\partial W}{\partial x_l} P\right) + \frac{\sigma}{2} \sum_l \frac{\partial^2 P}{\partial x_l^2} \tag{3}$$

in the stationary equilibrium state admits the solution

$$P_{\mathrm{eq}} \sim \exp(-2W/\sigma). \tag{4}$$

Invoking the transformation

$$P(x_1, \ldots, x_N; t) = P_{\mathrm{eq}}^{1/2} \Psi(x_1, \ldots, x_N; t), \tag{5}$$

it reduces to the imaginary-time Schrödinger equation

$$-\frac{\partial \Psi}{\partial t} = \left(-\frac{\sigma}{2} \sum_l \frac{\partial^2}{\partial s_l^2} + V \right) \Psi. \tag{6}$$

The potentials W and V are related by the Riccati-type equation

$$V = \frac{1}{2\sigma} \sum_l \left(\frac{\partial W}{\partial x_l}\right)^2 - \frac{1}{2} \sum_l \frac{\partial^2 W}{\partial x_l^2}. \tag{7}$$

The associated eigenvalue problem

$$\left(-\frac{\sigma}{2} \sum_l \frac{\partial^2}{\partial x_l^2} + V \right) \varphi_m = \lambda_m \varphi_m \tag{8}$$

yields a non-negative energy spectrum, with

$$\lambda_0 = 0, \qquad \varphi_0 = P_{\mathrm{eq}}^{1/2} = \mathrm{e}^{-W/\sigma}. \tag{9}$$

This set of equations forms the framework for the correspondence between the Langevin process and a quantum problem. In fact, considering the Schrödinger equation

$$\mathrm{i} \frac{\partial \psi}{\partial t} = \frac{1}{\hbar} \mathscr{H} \psi, \qquad \mathscr{H} = -\frac{\hbar^2}{2m} \sum_l \frac{\partial^2}{\partial x_l^2} + \tilde{V}(x_1, \ldots, x_N), \tag{10}$$

and setting

$$\psi \sim \varphi_m \exp(-\mathrm{i}\lambda_m t), \tag{11}$$

we obtain an eigenvalue problem identical to the corresponding Fokker–Planck expressions (6) and (8), provided that

$$\mathrm{i}t \to t, \qquad \frac{\hbar}{m} = \sigma, \qquad \frac{1}{\hbar} \tilde{V}(x_1, \ldots, x_N) = V. \tag{12}$$

For the purpose of constructing quantum systems with soluble ground-state properties, this correspondence might be used as follows: from (6)–(9) it follows that the quantum

system with Hamiltonian

$$\mathscr{H} = \sum_l \frac{\dot{x}_l^2}{\sigma} + V = -\frac{\sigma}{2}\sum_l \frac{\partial^2}{\partial x_l^2} + V, \tag{13}$$

and V specified by the Riccati equation (7), has the ground state given by (9). On the basis of this ground-state wavefunction, it is now possible to calculate quantities of interest.

To illustrate the method, we first construct a generalised quantum Toda lattice. The potential energy of the one-dimensional Toda lattice might be written as (Toda 1967)

$$W = g^{-2}\sum_l \{\exp[-g(x_{l+1}-x_l)] + g(x_{l+1}-x_l) - 1\}. \tag{14}$$

In the weak-coupling limit ($g \ll 1$), W reduces to the potential-energy expression for a harmonic chain. Using (7), (9) and (14), a generalised quantum Toda lattice with known ground-state wavefunction and eigenvalue is now easily constructed. Its Hamiltonian is

$$\mathscr{H} = \sum_l \frac{\dot{x}_l^2}{\sigma} + \frac{1}{2}\sum_l \left(\frac{1}{\sigma g^2}\{\exp[-g(x_{l+1}-x_l)] - \exp[-g(x_l - x_{l-1}]\}^2 \right.$$
$$\left. - \{\exp[-g(x_{l+1}-x_l)] + \exp[-g(x_l - x_{l-1})]\} \right). \tag{15}$$

The potential energy involves not only nearest-neighbour but also next-nearest-neighbour interactions. Considering a lattice with one open end, the norm as obtained from (9) and (14) is

$$N(p) = \int \mathrm{d}x_0\, \mathrm{d}x_N \exp\left(-\frac{2}{\sigma}p(x_N - x_0)\right) \int \mathrm{d}x_1 \ldots \mathrm{d}x_{N-1} \exp\left(-\frac{2}{\sigma}\sum_{l=1}^{N-1} K_{l+1,l}\right), \tag{16}$$

where

$$K_{l+1,l} = g^{-2}\{\exp[-g(x_{l+1}-x_l)] + g(x_{l+1}-x_l) - 1\} \tag{17}$$

and p denotes the pressure. Evaluation of the multiple integral is completely equivalent to calculation of the partition function of the classical Toda lattice with potential energy W (14) (Takahasaki 1942). Introducing the variables

$$r_l = x_{l+1} - x_l, \tag{18}$$

and observing that

$$\partial(x_0, \ldots, x_N)/\partial(r_1, \ldots, r_N) = 1, \tag{19}$$

the multiple integral reduces to

$$N(p) = (n(\bar{p}))^N, \tag{20}$$

where

$$n(\bar{p}) = g^{-1}\,\mathrm{e}^{\beta}\beta^{-\beta(1+\bar{p})}\Gamma[(1+\bar{p})\beta]$$
$$= g^{-1}\,\mathrm{e}^{\beta}\int_0^\infty \mathrm{d}y \exp\{-\beta[(\mathrm{e}^{-y} + y(\bar{p}+1)]\}. \tag{21}$$

Here we have introduced the scaled variables

$$y = gr, \qquad \bar{p} = pg, \qquad \beta = 2/\sigma g^2. \tag{22}$$

Ground-state properties are now readily obtained. Examples are the zero-pressure linear expansion

$$g\langle r\rangle = \langle y\rangle = \beta^{-1}\,\partial \ln n(\bar{p})/\partial \bar{p} \tag{23}$$

and the zero-pressure mean-square expansion

$$g^2(\langle r^2\rangle - \langle r\rangle^2) = \beta^{-2}\,\partial^2 \ln n(\bar{p})/\partial \bar{p}^2. \tag{24}$$

In the weak-coupling limit ($g \ll 1$), these expressions reduce to (Schneider and Stoll 1981)

$$\langle r\rangle|_{p=0} = \tfrac{1}{4}\sigma g + \tfrac{1}{8}\sigma^2 g^3 - \tfrac{1}{1920}\sigma^4 g^7 + \ldots \tag{25}$$

and

$$\langle r^2\rangle - \langle r\rangle^2|_{p=0} = \tfrac{1}{2}\sigma + \tfrac{1}{8}\sigma^2 g^2 + \tfrac{1}{48}\sigma^3 g^4 + \ldots. \tag{26}$$

As a second example, we construct a generalised sine-Gordon chain with a potential energy of

$$W = \frac{A}{g^2}\sum_l (1 - \cos gx_l) + \frac{C}{2}\sum_l (x_{l+1} - x_l)^2, \tag{27}$$

where g is the coupling constant. For $g \ll 1$, this expression reduces to the potential energy of the harmonic chain. Invoking then (7) and (14), for the Hamiltonian of the generalised quantum sine-Gordon chain we find

$$\mathcal{H} = \sum_l \frac{\dot{x}_l^2}{2\sigma} + \frac{1}{2\sigma}\sum_l \left(\frac{A}{g}\sin gx_l + C(2x_l - x_{l+1} - x_{l-1})\right)^2 - \tfrac{1}{2}\sum_l (A\cos gx_l + 2C) \tag{28}$$

with known ground-state wavefunction and eigenvalue (9) and (27). The calculation of the norm

$$N(A, C, \sigma, g) = \int \prod_l \mathrm{d}x_l\, \mathrm{e}^{-2W/\sigma} \tag{29}$$

is again equivalent to the evaluation of the classical partition function of the sine-Gordon chain, with $1/k_B T$ replaced by $2/\sigma$. As a consequence, the transfer-integral technique can be used to calculate properties of interest (Schneider and Stoll 1980). For

$$C/A \gg 1, \qquad 1/\beta C \gg 1, \qquad \beta = 2/\sigma g^2, \tag{30}$$

the resulting Fredholm integral equation can be transformed into an eigenvalue problem of Mathieu form. For

$$128AC/\sigma^2 g^4 \gg 1 \tag{31}$$

corresponding to the weak-coupling limit ($g \ll 1$), asymptotic expansions are well documented (Schneider and Stoll 1980, 1981), yielding for example

$$\langle \cos gx_l\rangle = 1 - \frac{2}{\beta E_K} - \frac{1}{2(\beta E_K)^3} + \ldots + \mathrm{O}[\exp(-\beta E_K)], \tag{32}$$

$$S_{CC}(q=0) = \frac{1}{\beta A}\left(\frac{1}{\beta E_K} + \frac{3}{2^2(\beta E_K)^3} + \ldots\right) + \mathrm{O}[\exp(-\beta E_K)], \tag{33}$$

$$\lim_{q\to 0} q^2 S_{xx}(q) = \frac{32A\beta}{g^2}\frac{1}{8}(\beta E_K)^{-1/2}\exp(-\beta E_K), \tag{34}$$

where

$$E_K = 8(AC)^{1/2}, \tag{35}$$

$$S_{CC}(q) = \left\langle \left| N^{-1/2}\sum_l e^{iql}(\cos gx_l - \langle \cos gx_l\rangle)\right|^2 \right\rangle, \tag{36}$$

$$S_{xx}(q) = \left\langle \left| N^{-1/2}\sum_l e^{iql}x_l\right|^2 \right\rangle. \tag{37}$$

E_K is the kink-soliton energy of the classical chain. Other ground-state properties might be obtained from the numerical and analytical transfer-integral results of the classical sine-Gordon chain (Schneider and Stoll 1980).

Comparison of the weak-coupling results for the generalised quantum Toda ((25) and (26)) and quantum sine-Gordon ((32) and (34)) chains reveals important differences. In the Toda case, perturbation theory will work, because in the weak-coupling limit the ground-state properties are given by a power-law expansion in the coupling constant, which can be collected in terms of derivatives of the Γ function ((23) and (24)). In the sine-Gordon case, one has to distinguish between properties dominated by power laws and those where the exponential contribution, originating in the classical case from the kink solitons, enters to leading order. In fact, for properties dominated by the exponential term, the weak-coupling limit ($g\to 0$) corresponds to an essential singularity, so that perturbation theory is not applicable. For power-law dominated properties, however, usual perturbation theory is again valid.

Finally, we note that the excitation spectrum of the quantum models can be studied in terms of the long-time behaviour of appropriate correlation functions of the Langevin process defined by (1). A detailed account of this simulation technique was given by Schneider *et al* (1985), Here, we merely note that the correlation function

$$\begin{aligned} S_{CC}(q,t) &= \left\langle \left(N^{-1/2}\sum_l (\cos gx_l(t) - \langle \cos gx_l\rangle)e^{iql}\right)\right. \\ &\quad \left.\times\left(N^{-1/2}\sum_l (\cos gx_l(0) - \langle \cos gx_l\rangle)\, e^{iql}\right)\right\rangle \\ &= \sum_n \left|\left\langle 0\left| N^{-1/2}\sum_l e^{iql}(\cos gx_l - \langle \cos gx_l\rangle)\right| n\right\rangle\right|^2 \exp(-\lambda_n t) \end{aligned} \tag{38}$$

obtained from the Langevin process (1), with W given by (27), corresponds to the imaginary-time correlation function of the generalised quantum sine-Gordon system with Hamiltonian (28). Thus, the numerical determination of the long-time behaviour provides an estimate for the lowest excitation probed by the particular correlation function. In the generalised quantum sine-Gordon equation (28), a weak-coupling treatment suggests that $S_{CC}(q,\omega)$ is dominated by a two-phonon bound state with frequency (Maki 1984)

$$\omega(q=0) = 2\Omega(0)\left[1 - \left(\frac{g^2\sigma}{4(2CA)^{1/2}}\frac{(1+\sigma g^2/8A)^2}{1+\sigma g^2/2A}\right)^2\right]^{1/2}, \tag{39}$$

where

$$\Omega^2(q) = [A + 2C(1-\cos q)]^2 + \tfrac{1}{2}\sigma g^2 A, \tag{40}$$

followed by a two-phonon continuum. To test the limitations of this weak-coupling prediction, we performed a numerical simulation of $S_{CC}(q=0, t)$ (38), with two values for σ, namely, 1 and 8.924. We considered a chain of 200 particles and averaged over 20 independent runs. From the long-time behaviour of the correlation function (38), we estimated the lowest excitation frequency at $q=0$ for various values of g ranging from 0 to 1. A comparison between the weak-coupling prediction (39) and the numerical estimates is given in figure 1. As expected, the weak-coupling prediction is asymptotically correct, but the range of coupling constants providing excellent agreement becomes smaller as σ increases, or in other words, the stronger the quantum fluctuations are. In the limit $g \to 0$, where the harmonic approximation becomes exact, there is no longer a bound state and $\omega(q=0)$ is given by the lower boundary of the two-phonon continuum. In the strong-coupling limit, $g \to \infty$, the system is again equivalent to coupled harmonic oscillators but without a gap. Thus, $\omega(q=0, g \to \infty)$ vanishes.

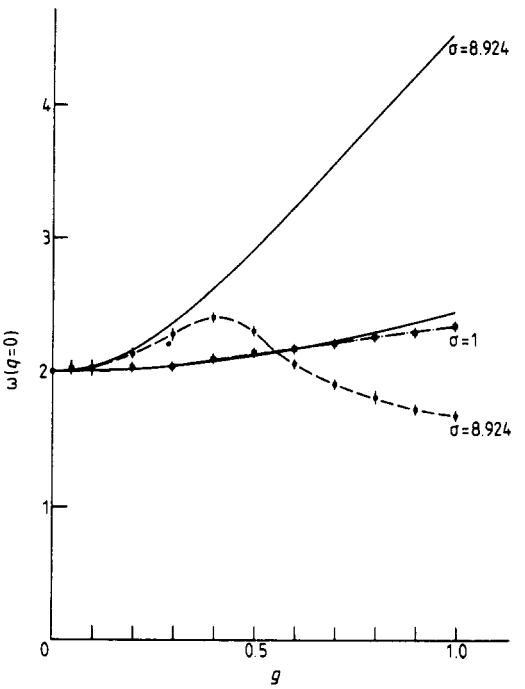

Figure 1. Comparison between the weak-coupling estimates for the two-phonon bound-state frequency (equation (39)) in $S_{CC}(q, \omega)$ and the numerical estimate from the stochastic simulation of $S_{CC}(q, t)$ (equation (38)) for $A=1$, $C=29.22$, $\sigma=1$ and 8.924. The full curve represents the weak-coupling approximation, the broken curve the numerical estimate.

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