Nonlinear dynamics technique and spatial structures of quantum one-dimensional chains

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A method is proposed for investigating the spatial structures of one-dimensional quantum systems of interacting atoms and spins. The method is based on deriving exact quantum representations for the stationary mean values in a coherent-state basis. Specific examples are considered, and conditions are found for the existence of commensurate and incommensurate phases and for quantum chaos. The physical interpretation of the solutions and their relation to the ground state are discussed.

INTRODUCTION

Theoretical studies of the structure of matter based on nonlinear dynamics[1–9] are attracting increased interest. This method of structural classification is used to describe systems classically and is based on analyzing the solutions of the nonlinear transformations that determine the equilibrium position of the structural elements (atoms, ions, spins, etc.). One of the most important results is that there exist several types of spatial structure (commensurate, incommensurate, chaotic), and their dynamic excitation spectra have been studied. The nonlinear dynamics technique is also of interest for quantum systems, both for studying the possible spatial structures and for analyzing the spectrum of the excitations. Reference 10 introduced one possible scheme for introducing nonlinear transformations for the mean values that describe the spatial structure in the quantum case.

In this paper we offer a quite general approach for studying the structure of quantum chains which employs nonlinear dynamics and consists in the following. We use the Heisenberg picture and take the initial states to be suitably constructed coherent states [either Glauber states $|\alpha\rangle$ (Ref. 11) or spin states $|\mu\rangle$ (Refs. 12, 13)], depending on the system under study. We then average the Heisenberg equations over these states as suggested by Sinitsyn and Tsukernik[14] for boson systems and by Zaslavskiĭ[15] for spin systems. The resulting c-number equations form a closed system of linear partial differential equations for the observables. We can use the stationary points of these dynamic equations of motion to determine the structure of the chains by minimizing the energy of the system with respect to the coherent-state basis. The physical significance of the solutions and the relationship with the ground state problem are discussed below and in the Conclusions.

FORMULATION OF THE METHOD

We consider an arbitrary many-body boson system with the Hamiltonian $\hat{H}=\hat{H}(\{\hat{a}^+,\hat{a}\})$, where

$$\{\hat{a}^+,\hat{a}\}=(\ldots;\hat{a}_1^+,\hat{a}_1;\hat{a}_2^+,\hat{a}_2;\ldots),\quad [\hat{a}_n,\hat{a}_{n'}^+]=\delta_{nn'}$$

and $\hat{a}_n^+$, $\hat{a}_n$ are the boson creation and annihilation operators. To each operator $\hat{a}_n\equiv\hat{a}_n$ $(t=0)$ at initial time $t=0$ we associate the coherent state $|\alpha_n\rangle$ such that $\hat{a}_n|\alpha_n\rangle=\alpha_n|\alpha_n\rangle$. We let $\hat{f}=\hat{f}(\{\hat{a}^+,\hat{a}\})$ be an operator-valued function and project the Heisenberg equation of motion for $\hat{f}$ on the coherent-state basis $\{|\alpha\rangle\}$, where $|\alpha\rangle$ is a product state of the form $|\alpha\rangle=\Pi_n|\alpha_n\rangle$. According to Ref. 14, the closed c-number equation for the function $f(t)\equiv f(t,\{\alpha^*,\alpha\})=\langle\alpha|\hat{f}|\alpha\rangle$ in the basis $\{|\alpha\rangle\}$ reads

$$\dot{f}(t)=\frac{i}{\hbar}\bar{K}_b f(t), \tag{1a}$$

where the operator $\hat{K}_b$ is given by

$$\bar{K}_b=\exp\Big(-\sum_n|\alpha_n|^2\Big)\Big[H\Big(\Big\{\alpha^*,\frac{\partial}{\partial\alpha^*}\Big\}\Big)-H\Big(\Big\{\frac{\partial}{\partial\alpha},\alpha\Big\}\Big)\Big]\exp\Big(\sum_n|\alpha_n|^2\Big). \tag{2a}$$

As noted above, the quantities $\{\alpha,\alpha^*,\partial/\partial\alpha,\partial/\partial\alpha^*\}$ are taken at time $t=0$.

We now consider a spin system with the Hamiltonian $\hat{H}=\hat{H}(\{\hat{S}^+,\hat{S}^-,\hat{S}^z\})$, where

$$\{\hat{S}^+,\hat{S}^-,\hat{S}^z\}\equiv(\ldots;\hat{S}_1^+,\hat{S}_1^-,\hat{S}_1^z;\hat{S}_2^+,\hat{S}_2^-,\hat{S}_2^z;\ldots),$$

and $\hat{S}_n^{\pm}=\hat{S}_n^x\pm i\hat{S}_n^y$ and $\hat{S}_n^z$ are the corresponding spin projection operators for the spin $\hat{S}_n$:

$$[\hat{S}_n^+,\hat{S}_{n'}^-]=2\hbar\hat{S}_n^z\delta_{nn'};\qquad [\hat{S}_n^{\pm},\hat{S}_{n'}^z]=\mp\hbar\hat{S}_n^{\pm}\delta_{nn'}.$$

According to Ref. 15, the Heisenberg equation of motion for an arbitrary operator-valued function $\hat{g}\equiv\hat{g}(\{\hat{S}^+,\hat{S}^-,\hat{S}^z\})$ is given by

$$\dot{g}(t)=\frac{i}{\hbar}\bar{K}_S g(t), \tag{1b}$$

$$\bar{K}_S=\prod_n(1+|\mu_n|^2)^{-2S}\Big[H\Big(\Big\{\hbar\frac{\partial}{\partial\mu^*};2S\hbar\mu^*-\hbar\mu^{*2}\frac{\partial}{\partial\mu^*};\hbar S-\hbar\mu^*\frac{\partial}{\partial\mu^*}\Big\}\Big)-\text{c.c.}\Big]\prod_n(1+|\mu_n|^2)^{2S}, \tag{2b}$$

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after averaging over the initial spin (or generalized) coherent states $|\mu\rangle$ (Refs. 12, 13); here $g(t)\equiv g(t;\{\mu^*,\mu\})=\langle\mu|\hat{g}|\mu\rangle$. In the Heisenberg picture the wave function $|\mu\rangle$ is independent of time and is given by[12]

$$|\mu\rangle=\prod_n|\mu_n\rangle=|1\ldots,\mu_1,\mu_2,\ldots\rangle,$$
$$|\mu_n\rangle=(1+|\mu_n|^2)^{-S}\exp\left(\frac{1}{\hbar}\mu_n\hat{S}_n^-\right)|0\rangle,\quad \hat{S}_n^z|0\rangle=\hbar S|0\rangle, \tag{3}$$

where the spin S is understood to be the same for all n. The linear equations (1a), (2a), (1b), and (2b) describe the evolution of arbitrary c-number functions $f(t)$ and $g(t)$.

In our subsequent analysis of boson and spin chains, we will take the operators $\hat{f}$ to be $\hat{x}_n$ and $\hat{p}_n$, the coordinate and momentum operators for the nth atom; $\hat{g}$ will be one of the spin operators $\hat{S}_n^{(j)}$ ($j=x,y$, or z, and n is the number of the atom in the chain). We thus have $f=\{x,p\}$ and $g=\{S^{(j)}\}$. We want to find the equilibrium positions for the mean values $f(t)$ and $g(t)$, i.e., the solutions of the equations $\dot{f}=0$, $\dot{g}=0$. These solutions determine the stationary points of Eqs. (1a), (1b). The equations for the stationary points can thus be expressed in the form

$$\hat{K}_b f=\begin{cases}\hat{K}_b x_n=0\\ \hat{K}_b p_n=0\end{cases}, \tag{4a}$$

$$\hat{K}_s g=\hat{K}_s S_n^{(j)}=0\quad (j=x,y,z). \tag{4b}$$

The following important fact should be stressed. Since Eqs. (4a), (4b) describe stationary solutions, we have

$$x_n=x_n(t=0),\quad p_n=p_n(t=0),\quad S_n^{(j)}=S_n^{(j)}\ (t=0)$$

and it is easy to find an explicit expression for the action of the operators $\hat{K}_b$ and $\hat{K}_s$ on the functions $x_n, p_n, S_n^{(j)}$. Equations (4a), (4b) are systems of algebraic equations for the stationary mean values of the atomic positions x_n in state $|\alpha\rangle$ and for the stationary means of the spin projections $S_n^{(j)}$ in state $|\mu\rangle$. Of the many solutions of Eqs. (4a) [(4b)], we choose the one that minimizes the functional F defined by

$$F=\begin{cases}F_b=\lim\limits_{N\to\infty}\dfrac{1}{N}\langle\alpha|\hat{H}|\alpha\rangle\\ F_s=\lim\limits_{N\to\infty}\dfrac{1}{N}\langle\mu|\hat{H}|\mu\rangle\end{cases}. \tag{5}$$

The conditions for a minimum are

$$\partial F_b/\partial f_{0,r}=0,\quad \partial^2F_b/\partial f_{0,r}\partial f_{0,r'}>0, \tag{6a}$$
$$\partial F_s/\partial g_{0,r}=0,\quad \partial^2F_s/\partial g_{0,r}\partial g_{0,r'}>0, \tag{6b}$$

where $f_{0,r}$ and $g_{0,r}$ are the parameters with respect to which the minimization is carried out (there are r and r', respectively, such parameters altogether).

We will regard the solutions of Eqs. (4a), (4b) as determining a possible equilibrium structure of the system. The method will be described more fully below; for now we illustrate it in some specific examples.

ONE-DIMENSIONAL QUANTUM CHAIN OF ATOMS IN A PERIODIC EXTERNAL POTENTIAL

Consider a one-dimensional system of atoms interacting with an external spatially periodic field. We write the Hamiltonian in the form[4,16]

$$\hat{H}=\sum_n\frac{\hat{p}_n^2}{2m}+\frac{\gamma}{2}\sum_n(\hat{x}_{n+1}-\hat{x}_n-a)^2+V_0\sum_n(1-\cos q_0\hat{x}_n), \tag{7}$$

where $\hat{x}_n$ and $\hat{p}_n$ are the coordinate and momentum of the nth atom, a is the equilibrium distance between the atoms in the chain for $V_0=0$, m and γ are the atomic mass and the elasticity coefficient, and $q_0=2\pi/a_0$, where a_0 is the spatial period of the external field. We will deal with the displacement operator $\hat{u}_n$ of the nth atom relative to the external potential rather than with $\hat{x}_n$: $\hat{x}_n=\hat{u}_n+na_0$. The Hamiltonian in (7) then becomes

$$\hat{H}=\sum_n\frac{\hat{p}_n^2}{2m}+\frac{\gamma}{2}\sum_n(\hat{u}_{n+1}-\hat{u}_n-\delta a_0)^2+V_0\sum_n(1-\cos q_0\hat{u}_n), \tag{8}$$

where

$$[\hat{u}_n,\hat{p}_{n'}]=i\hbar\delta_{nn'},\quad \delta=(a-a_0)/a_0\ (-1<\delta<\infty).$$

If we write $\hat{u}_n$ and $\hat{p}_n$ in terms of operators $\hat{a}_n^+$ and $\hat{a}_n$ as

$$\hat{u}_n=(\hbar/2\eta)^{1/2}(\hat{a}_n^++\hat{a}_n),\quad \hat{p}_n=i(\hbar\eta/2)^{1/2}(\hat{a}_n^+-\hat{a}_n), \tag{9}$$

we see easily that $[\hat{a}_n\hat{a}_{n'}^+]=\delta_{nn'}$ for arbitrary η. In what follows we will choose η so that (6a) holds, i.e., the mean energy of the system in the class of states $|\alpha\rangle$ is a minimum. In this procedure, the equilibrium structure is sought for a class of wave functions that describe single-node coherent states. We use (5) and (6a) to select the state by varying the parameters, including η (see below). With (2a), Eq. (4a) for the stationary points for system (8) becomes

$$p_n=0,\quad u_{n+1}+u_{n-1}-2u_n-(M/q_0)\sin q_0u_n=0, \tag{10}$$

where

$$M=M(\eta)=(V_0q_0^2/\gamma)\exp(-\hbar q_0^2/4\eta). \tag{11}$$

The exponential is present in (10), (11) because operators of the type

$$e^{-|\alpha_n|^2}\left\{\cos\left[q_0\left(\frac{\hbar}{2\eta}\right)^{1/2}\left(\alpha_n^*+\frac{\partial}{\partial\alpha_n^*}\right)\right]-\cos\left[q_0\left(\frac{\hbar}{2\eta}\right)^{1/2}\left(\alpha_n+\frac{\partial}{\partial\alpha_n}\right)\right]\right\}e^{|\alpha_n|^2}$$

act on the function $p_n=i(\hbar\eta/2)^{1/2}(\alpha_n^*-\alpha_n)$. In analyzing the solutions of (10) it is helpful to transform to canonical "action-angle" variables:

$$I_n=q_0(u_n-u_{n-1});\quad \varphi_n=q_0u_n.$$

Equation (10) then yields the standard recursion formulas[17]

$$I_{n+1}=I_n+M\sin\varphi_n,\quad \varphi_{n+1}=\varphi_n+I_{n+1}, \tag{12}$$

which determines the equilibrium quantum-mechanical

mean positions of the atoms in the states $|\alpha\rangle$. The formal difference between (12) and the classical limit ($\hbar = 0$) is that M depends explicitly on η and $\hbar$ (11). Equation (11) implies that we always have $M(\eta) < M(\hbar = 0) \equiv M_{cl}$, where M_{cl} is the value of M in the classical limit. We will show below that this inequality has several important consequences in the quantum mechanical treatment.

Transformations of the type (12) are presently under active study,[4,7,17-19] and results are available for the isolated resonance approximation,[17] among others. The classical limit for system (7) was analyzed in the isolated resonance approximation in Ref. 6 by employing an effective Hamiltonian. Following that treatment, we write the effective Hamiltonian

$$\mathcal{H}_{\text{eff}} = I^2/2 + M\cos\varphi \sum_{n=-\infty}^{\infty} \delta(z-n) = I^2/2 + M\sum_{l=-\infty}^{\infty} \cos(\varphi - 2\pi l z)$$

for the transformations (12), where z is a continuous atomic variable. The corresponding equations of motion are

$$dI/dz = M\sum_{l=-\infty}^{\infty} \sin(\varphi - 2\pi l z), \quad d\varphi/dz = I. \tag{13}$$

We see easily that the transformations (12) determine the solution of these equations at the points $I_n = I(z = n - 0)$, $\varphi_n = \varphi(z = n - 0)$. Resonances occur at $I_l = 2\pi l$ ($l = 0, \pm 1, \ldots$). The solution simplifies greatly in the isolated resonance approximation,[17] because in this case the motion along I is localized in a neighborhood of I_l if the initial conditions are close to I_l. In this approximation Eqs. (13) become

$$dJ_l/dz = M\sin\psi_l, \quad d\psi_l/dz = J_l,$$

where $J_l = I - I_l$, $\Psi_l = \varphi - 2\pi l z$. These equations correspond to the resonant Hamiltonian $H_l = J_l^2/2 + M\cos\Psi_l$.

The condition

$$\Delta J_l/\delta J_l = 2M^{1/2}/\pi \ll 1 \tag{14}$$

must hold for the isolated resonance approximation to be valid; here $\Delta J_l = 4M^{1/2}$ is the width of the resonance in terms of the action variable (the width of the region inside the separatrix), and $\delta J_l = J_{l+1} - J_l = 2\pi$ is the distance between resonances. The solutions $\Psi_l(z, \varkappa_l)$ and $J_l(z, \varkappa_l)$ inside and outside the separatrix are known to be expressible in terms of elliptic functions; the corresponding phase trajectories are shown in Fig. 1. The solutions will be classified in terms of the parameter

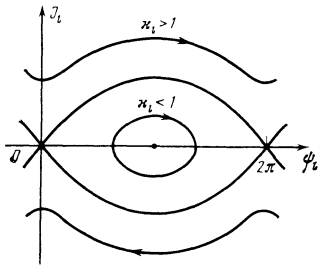

FIG. 1.

$$\varkappa_l = (H_l + M)/2M$$

(we will henceforth drop the subscript l). The solutions inside and outside the separatrix correspond to $0 \leqslant \varkappa \leqslant 1$ and $1 \leqslant \varkappa \ll M^{-1/2}$, respectively, where the condition $\varkappa \ll M^{-1/2}$ is necessary for the isolated resonance approximation (14) to be valid.

Although many solutions Ψ, J exist, we are interested in the one that minimizes F_b [condition (6a)]. The minimization is carried out with respect to the parameters $\varkappa$ and η for a specified value of δ, after which the number of the resonance l is chosen. Moreover, in the isolated resonance approximation we replace the summation by an integration when calculating F_b. The difference from the classical case[6] is due to the fact that F_b is also minimized with respect to the additional parameter η. It is found that the value η_0 of η satisfying (6a) is given by

$$\eta_0 = (2m\gamma)^{1/2}[1 + O(M)^{1/2}]$$

for all $\varkappa$ in the admissible range $0 \leqslant \varkappa \ll M^{-1/2}$. For M in (10)–(14) we thus have

$$M = M(\eta_0) = (V_0 q_0^2/\gamma)\exp(-\sigma^2), \quad \sigma^2 = \hbar q_0^2/4(2m\gamma)^{1/2}. \tag{15}$$

The minimization of F_b with respect to $\varkappa$ gives the critical values of δ:

$$\pm(\delta - l) = 2M^{1/2}(\eta_0)/\pi^2 \equiv \delta_c, \quad \varkappa = \varkappa_0 = 1$$

for which the mean position of the atoms is described by a soliton solution[4] (the resonance number l is chosen to minimize $|\delta - l|$). These critical points are indicated in Fig. 2 by $\delta_c^{cl}, \delta_c^{Q}$. For $|\delta - l|_{\min} > \delta_c$, the relative position of the atoms is periodically modulated with a spatial period

$$\lambda(\delta) = \frac{2\pi}{q(\delta)} = \pi\varkappa_0(\delta)M^{1/2}(\eta_0)/\mathrm{K}\left(\frac{1}{\varkappa_0(\delta)}\right)$$

which is incommensurate with the external field period a_0. Such an atomic configuration is called an incommensurate phase.[4,20] For $|\delta - l|_{\min} < \delta_c$ the atoms are arranged periodically at locations $x_n^{(0)} = na_0(l+1)$ that are multiples of a_0 (these regions are hatched in Fig. 2). The range of δ values for which the commensurate phase exists is given by

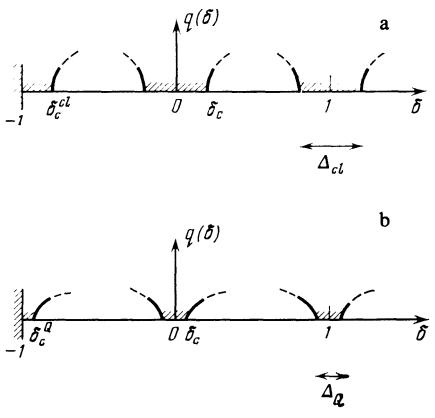

FIG. 2.

$$\Delta_Q = 4M^{1/2}(\eta_0)/\pi^2 = [4q_0(V_0/\gamma)^{1/2}/\pi^2]\exp(-\sigma^2/2).$$

Figure 2a and 2b correspond to the classical ($\hbar = 0$) and quantum cases, respectively. The chief differences between the classical and quantum cases in this approach are due to two factors: 1) the inequality $\Delta_Q < \Delta_{cl} \equiv \Delta_Q(\hbar = 0)$ holds, so that the region of commensurate phase is narrower in the quantum case; 2) the function $q = q(\delta)$ behaves differently for δ close to the critical value δ_c for existence of the incommensurate phase. For instance, if we expand the function $q(\delta)$ at the point $\delta_c = \Delta_Q/2$ and consider values $\delta \geqslant \delta_c$, we get

$$q(\delta) \sim \delta_c/|\ln(\delta - \delta_c)|, \quad (\delta - \delta_c)/\delta_c \ll 1.$$

Since $\delta_c^Q \equiv \delta_c(\hbar \neq 0)$ is less than $\delta_c^{cl}(\hbar = 0)$, $q(\delta)$ changes more slowly in the quantum case (particularly for $\sigma^2 \gg 1$).

The above results imply that in the context of our method, the influence of quantum effects is determined by the parameter

$$\sigma^2 = \hbar q_0^2/4(2m\gamma)^{1/2},$$

which apart from a constant factor coincides with the quantum parameter β^2 introduced in Ref. 4 on the basis of dimensional analysis:

$$\beta^2 = 4 \cdot 2^{1/4}\sigma^2.$$

We note that the quantum parameter σ^2 can be expressed as

$$\sigma^2 = \pi^2\hbar a/2^{1/2}mca_0^2,$$

where $c = (\gamma a/m)^{1/2}$ is the characteristic speed of sound in the chain. Quantum effects may thus be important near the commensurate-incommensurate phase transition because the speed of sound decreases.[4,20]

We will now pause briefly to discuss the properties of the solutions of (12) that describe a chaotic quantum structure.

The transformations (12) for the quantum means admit stochastic solutions even in the isolated resonance approximation (14). Indeed, such solutions form an everywhere-dense subset of the I, φ plane.[17,18] When (14) holds, the width of the stochastic layers is exponentially small. These layers are broadest near the separatrices of the fundamental resonances ($\varkappa \sim 1$, see Fig. 1). Their widths are of order[17,18]

$$\Delta I \sim \exp(-M^{-1/2}).$$

The stochastic layers (deformed tori) alternate with stable trajectories, which dominate when (14) holds. We may regard this as justification for minimizing the functional F_b over the solutions $\psi(z, \varkappa)$, $J(z, \varkappa)$. However, it should be noted that even with the isolated resonance approximation (14), a chaotic phase may be present near the commensurate→incommensurate phase transition.[5,18]

In the opposite case of overlapping resonances:

$$2M^{1/2}/\pi \gg 1, \tag{16}$$

most of the I, φ phase plane for (12) is chaotic and the minimization of F_b becomes a difficult problem.[5,19] However, since the quantum transformations (12) are formally the same as for the classical case, the "quantum trajectories" for the mean atomic positions in the state $|\alpha\rangle$ should have the same formal properties as their classical analogs, and in this sense the classical results in Refs. 5, 7, and 18 should also describe the case (16).

The most important properties of quantum systems when (16) holds are as follows. First, even though the measure of the stochastic trajectories is large while the measure of the stable trajectories is small of order $M^{-1/2} \ll 1$, the stochastic trajectories form numerous metastable states with a close-range order and spatial correlations that decay exponentially with distance. The decay of the phase correlations for the transformations (12) is typically of the form[18,25]

$$R_Q(n) = \frac{1}{2\pi}\int_0^{2\pi} \exp\{i(\varphi_n - \varphi_0)\}d\varphi_0 \sim \exp\left\{-\frac{n}{2}\ln M(\eta)\right\},$$

$$M(\eta) \gg 1, \tag{17}$$

where n in the exponential may be approximated by unity. The formula

$$n_Q \sim 2/\ln M(\eta) \tag{18}$$

thus gives the characteristic correlation length for the average atomic positions. Since $M = M(\eta)$, the correlation length may vary with η. One can choose η only by imposing some additional constraint (e.g., by requiring that F_b be a minimum). Nevertheless, according to (11) n_Q in the quantum case always exceeds the corresponding classical value,

$$\frac{n_Q}{n_{cl}} = \left(1 - \frac{\hbar q_0^2 n_{cl}}{8\eta}\right)^{-1}, \tag{19}$$

where

$$n_{cl} = 2/\ln(V_0 q_0^2/\gamma),$$

$$\hbar q_0^2 n_{cl}/8\eta < 1, \quad M(\eta) > 1.$$

Equation (11) implies that quantum effects always raise the threshold amplitude V_0 of the potential for the onset of chaos. The quantum and classical stochastic parameters $M(\eta)$ and M_{cl} in (12) are related by

$$M(\eta)/M_{cl} = \exp(-\hbar q_0^2/4\eta) < 1, \tag{20}$$

where $M_{cl} = V_0 q_0^2/\gamma$. Expression (20) implies that the stochastic component is strongly suppressed in the ultra-quantum region $\hbar q_0^2/4\eta \gg 1$. We also note that for large m, the influence of the harmonics $\cos(q_0 m\hat{x}_n)$ in the potential (7) is negligible compared to the fundamental harmonic, because the inclusion of quantum effects gives rise to an additional factor $\exp(-m\sigma^2)$ in M in Eqs. (10), (12). This suppression in the quantum case was noted in Ref. 4.

ONE-DIMENSIONAL SPIN CHAIN

We will examine the properties of the solutions of (4b) for spin systems by treating the example of a Heisenberg ferromagnet with spin $S \geqslant 1$ in a field with single-ion anisotropy. The Hamiltonian is of the form

$$\hat{H} = -J\sum_n \hat{\mathbf{S}}_{n+1}\hat{\mathbf{S}}_n + D(\hat{S}_n^z)^2, \tag{21}$$

where $J>0$ is the exchange interaction constant for nearest neighbors and D is the field anisotropy constant. For this system the stationary equations (4b) for the observables become

$$\sin\theta_{n+1}\cos\theta_n e^{i\varphi_{n+1}}-\cos\theta_{n+1}\sin\theta_n e^{i\varphi_n}-\sin\theta_n\cos\theta_{n-1}e^{i\varphi_n}$$
$$+\cos\theta_n\sin\theta_{n-1}e^{i\varphi_{n-1}}+\frac{D}{J}\frac{2S-1}{2S}e^{i\varphi_n}\sin 2\theta_n=0, \qquad (22)$$
$$\sin\theta_{n+1}\sin\theta_n\sin(\varphi_{n+1}-\varphi_n)=\xi=\text{const},$$

where we have made the change of variables

$$\mu_n=\operatorname{tg}(\theta_n/2)e^{i\varphi_n}, \quad 0\leqslant\theta_n\leqslant\pi, \quad 0\leqslant\varphi_n<2\pi.$$

The constant ξ in (22) is determined by the condition that the functional F_s in (6b) be a minimum:

$$\partial F_s/\partial\xi=0, \quad \partial^2F_s/\partial\xi^2>0,$$

which implies that $\xi=0$ and $\varphi_n=\varphi_{n+1}$. Making the change of variables $I_{n+1}=\sin(\theta_{n+1}-\theta_n)$, we can then rewrite the first equation in (22) as a two-dimensional mapping:

$$I_{n+1}=I_n+K\sin 2\theta_n, \qquad (23)$$
$$\theta_{n+1}=\theta_n+\arcsin I_{n+1} \quad (\mathrm{mod}\,\pi),$$
$$K\equiv K(S)=-\frac{D}{J}\frac{2S-1}{2S}. \qquad (24)$$

Transformations similar to (23) have also been derived in Ref. 8 for the DNA model and in Ref. 7 for the classical xy-model for spin chains. The transformations (23) are generated by an equivalent dynamical system with the Hamiltonian[7]

$$\mathcal{H}_{\text{eff}}=I\arcsin I+(1-I^2)^{1/2}+K\cos^2\theta\sum_{n=-\infty}^{\infty}\delta(t-n),$$

which corresponds to the equations of motion

$$\frac{dI}{dt}=-\frac{\partial\mathcal{H}_{\text{eff}}}{\partial\theta}=K\sin 2\theta\sum_{n=-\infty}^{\infty}\delta(t-n)$$
$$=K\sum_{l=-\infty}^{\infty}\sin(2\theta-2\pi lt), \qquad (25)$$
$$d\theta/dt=\partial\mathcal{H}_{\text{eff}}/\partial I=\omega(I)=\arcsin I.$$

System (25) describes a nonlinear pendulum moving at frequency $\omega(I)$ in response to external forces applied at integral times $t=n$. For $D>0$, F_s is minimized by the solutions $\theta_n=\pi/2, I_n=0$, which correspond to a hyperbolic point in the I, θ phase plane for (23). In this case all the spins are ferromagnetically ordered and lie in the xy plane. For $D<0$, the hyperbolic points $\theta_n=0$, $I_n=0$ also minimize F_s; in this case the spins lie along the z axis and F_s is independent of the angles φ_n. Since the minimizing solutions correspond to hyperbolic points with Lyapunov constants

$$\lambda_{\pm}=1+|K|\pm(|K|^2+2|K|)^{1/2}, \quad K<0, \ D>0; \quad K>0, \ D<0,$$

this means that for a nonzero anisotropy D the system may be unstable, i.e., an unordered structure may form. The transformations (23) were studied numerically in Ref. 7, where it was shown that for $K\geqslant 0.3$ an amorphous state forms which consists of an unordered sequence of structures resembling Bloch domain walls.

APPROXIMATION OF THE GROUND STATE

We now consider how well our method approximates the solution for the ground state by considering examples of spin systems for which solutions are known (either exactly or in the mean-field approximation). As a first example we consider an Ising ferromagnet with spin $S=1/2$ in a transverse magnetic field. This model admits an exact solution,[21] and a solution is also available in the mean-field approximation.[22]

We write the Hamiltonian in the form

$$\hat{H}=-J\sum_n\hat{S}^x_{n+1}\hat{S}_n{}^x-G\sum_n\hat{S}_n{}^z, \qquad (26)$$

where $J>0$ is the rate constant for the nearest-neighbor exchange interaction and G is the magnitude of the external magnetic field. In this case expression (4b) takes the form

$$\mu_n=\mu_n{}^*,$$
$$G\frac{\mu_n}{1+\mu_n{}^2}=\frac{J}{2}\left(\frac{\mu_{n+1}}{1+\mu^2_{n+1}}+\frac{\mu_{n-1}}{1+\mu^2_{n-1}}\right)\frac{1-\mu_n{}^2}{1+\mu_n{}^2}. \qquad (27)$$

Making the change of variables

$$\mu_n=e^{i\varphi_n}\operatorname{tg}(\theta_n/2), \quad I_n=\cos\theta_n\sin\theta_{n-1},$$

we find from the first equation in (27) that $\varphi_n=0$ or π. Expressions (27) then reduce to the two-dimensional mapping

$$I_{n+1}=\cos\operatorname{Arcsin}\left[-I_n\cos^{-1}\theta_n+\frac{2G}{J}\operatorname{tg}\theta_n\right]\sin\theta_n,$$
$$\theta_{n+1}=\operatorname{Arcsin}\left[-I_n\cos^{-1}\theta_n+\frac{2G}{J}\operatorname{tg}\theta_n\right]. \qquad (28)$$

The solutions of (28) minimizing the functional F_s (6b) are given by

$$\theta_n=\arcsin(1-G^2/J^2)^{1/2}, \quad I_n=(G/J)(1-G^2/J^2)^{1/2}, \quad G/J<1;$$
$$\theta_n=0, \quad I_n=0, \quad G/J\geqslant 1. \qquad (29)$$

Solution (27) is doubly degenerate in the angle φ: $\varphi_n=\varphi_{n+1}=0$ (π). We see from the solutions (29) that for $G/J<1$

$$S_n{}^x=\pm\frac{1}{2}\left(1-\frac{G^2}{J^2}\right)^{1/2}, \quad S_n{}^z=\frac{1}{2}\frac{G}{J}$$

while for $G/J\geqslant 1$

$$S_n{}^x=0, \quad S_n{}^z=1/2.$$

These results coincide with the ones found by the mean-field method,[22] which also agree with the classical solutions. The mappings (28) in this case coincide with the classical limit for the system with Hamiltonian (26).

For systems with single-ion anisotropy ($S \geqslant 1$), the structure-determining mappings (4b) agree with the classical expressions apart from the renormalization of certain constants. For instance, for system (21) the mappings (23) are the same as the classical ones[7] except for a renormalization of the constant K which makes K depend explicitly on the spin S (24): $K_Q = K(S)$, where K_Q is the quantum value of K. In the classical limit $\hbar \to 0$, $S \to \infty$, $\hbar S \to$ const, K_Q coincides with the classical value K_{cl}. The renormalization is necessary because the spins at a single node are correlated. There are no correlations among spins at different nodes when a coherent-state basis consisting of single-node wave functions is chosen. We note that the usual procedure in the mean-field approximation is to include the single-node correlations and neglect correlations between different nodes. As in the mean-field method (see, e.g., Ref. 23), the minimum principle for the functional F_s (6b) plays an important role. The wave function $|\mu\rangle$ in which the structure is determined is constructed from single-node coherent states $|\mu_n\rangle$, whereas in the mean-field approximation one constructs the wave functions from the eigenfunctions of the one-particle Hamiltonian. We can see how these approaches differ by considering a spin system with the Hamiltonian

$$\hat{H} = -J \sum_n \hat{S}_n{}^z \hat{S}_{n+1}{}^z + 2D(\hat{S}_n{}^x)^2, \tag{30}$$

where $J > 0$ is the exchange interaction constant, $D > 0$ is the anisotropy constant, and the spin $X \geqslant 1$. The mean-field approach for system (30) and $S = 1$ leads to the following solutions.[24] The ground-state energy $E_{\min}$ is equal to $D - J$, and in this case

$$\langle S^z \rangle = \begin{cases} (1 - D^2/J^2)^{1/2}, & D < J \\ 0, & D > J \end{cases}.$$

On the other hand, the method proposed above gives the solutions

$$S_n{}^z = 1, \quad S_n{}^x = 0, \quad S_n{}^y = 0, \quad E_{min} = D - J$$

for (30). In terms of the results for the ground state, our method is thus a modification of the mean-field method and yields a rather crude approximation to the structure of the chain (30).

However, the method can be improved so as to approximate the ground state solution more closely. One approach is to replace the single-node coherent states $|\alpha_n\rangle$ and $|\mu\rangle$ by suitable collective coherent states and then use them to find the structure. We will consider such a modification below for the model (8).

STRUCTURE OF AN ATOMIC CHAIN USING COLLECTIVE COHERENT WAVE FUNCTIONS

We consider a system with the Hamiltonian (8) and introduce the auxiliary Hamiltonian $\hat{H}_0$ for an effective linear chain:

$$\hat{H}_0 = \sum_n \frac{\hat{p}_n{}^2}{2m} + \frac{\gamma}{2} \sum_n (\hat{u}_{n+1} - \hat{u}_n - \delta a_0)^2 + \frac{B}{2} \sum_n \hat{u}_n{}^2. \tag{31}$$

Taking $\hat{n}_n = \hat{u}_{n+N}, \hat{p}_n = \hat{p}_{n+N}$, and using the collective excitation operators $a_k{}^+, a_k$ for system (31), we find

$$\hat{u}_n = \sum_{k=-N/2}^{N/2} \left(\frac{\hbar}{2Nm\omega_k} \right)^{1/2} (\hat{a}_{-k}{}^+ + \hat{a}_k) \exp\left\{ \frac{2\pi i k n}{N} \right\},$$
$$\hat{p}_n = i \sum_{k=-N/2}^{N/2} \left(\frac{\hbar m \omega_k}{2N} \right)^{1/2} (\hat{a}_{-k}{}^+ - \hat{a}_k) \exp\left\{ \frac{2\pi i k n}{N} \right\}, \tag{32}$$
$$\omega_k{}^2 = \frac{1}{m} \left(B + 4\gamma \sin^2 \frac{k\pi}{N} \right).$$

We define the collective states

$$\hat{a}_k |\alpha_k\rangle = \alpha_k |\alpha_k\rangle, \qquad |\alpha\rangle = \prod_k |\alpha_k\rangle, \tag{33}$$

at $t = 0$ and will choose the constant B to minimize the functional F_b (5), where we now use the collective states (33) as the $|\alpha\rangle$ states. Projecting the Heisenberg equation of motion for $\hat{u}_n, \hat{p}_n$ for the chain (8) onto the coherent states $|\alpha\rangle$ (33), we find that Eqs. (4a) for the equilibrium positions of the means u_n lead to transformations (10) with M given by

$$M = \frac{V_0 q_0{}^2}{\gamma} \exp\left[-\frac{\hbar q_0{}^2 k \mathrm{K}(k)}{4\pi (m\gamma)^{1/2}} \right] \tag{34}$$

rather than by (11); here $K(k)$ is the complete elliptic integral of the second kind with modulus

$$k = (1 + B/4\gamma)^{-1/2}. \tag{35}$$

Thus, M is also given by (34) in the transformations (12). We minimize F_b with respect to the parameters $\varkappa$ and k in the isolated resonance approximation (14) and write $\varkappa_0, k_0$ for the minimizing values. The main results are that $F_b(k_0, \varkappa_0) < F_b(\eta_0, \varkappa_0)$, where $F_b(k_0, \varkappa_0)$ and $F_b(\eta_0, \varkappa_0)$ are the minimum values of the functionals F_b (5) for the collective states (33) and single-node coherent states, respectively. In the isolated resonance approximation, the state $|\alpha\rangle_{\min}$ (33) minimizing F_b (5) is energetically more favorable. The chief difference from the case considered above is that no commensurate phase exists in the states $|\alpha\rangle_{\min}$ (33) if the quantum parameter $\sigma \geqslant \sigma_c \equiv 2^{1/4}\sqrt{\pi}$, which agrees exactly with the result found in Ref. 4. We will now show how the parameter σ_c arises. For a commensurate phase, $|\delta - l|_{\min} < \delta_c$, $\varkappa_0 = 1$ and the equation for k_0 is

$$\frac{\mathrm{E}(k_0)}{k_0{}^2} - 1 = \frac{V_0 q_0{}^2}{4\gamma} \exp\left[-\frac{2^{1/2}}{\pi} \sigma^2 k_0 \mathrm{K}(k_0) \right] \equiv \frac{1}{4} M(k_0). \tag{36}$$

Since we are using the isolated resonance approximation, $M(k_0)/4$ is $\ll 1$ in the right-hand side of (36) and k_0 is close to unity [however, the solution $k_0 = 1$ does not give the minimum $F_b(k_0, \varkappa_0)$]. Writing k_0 as

$$k_0 = 1 - \varepsilon, \quad \varepsilon \ll 1, \tag{37}$$

we find from (36) that ε satisfies the equation

$$[\varepsilon a(\varepsilon)]^{-\pi\sqrt{2}/\sigma^2 + 1} = 16 a(\varepsilon) \left(\frac{V_0 q_0{}^2}{4\gamma} \right)^{-\pi/\sqrt{2}/\sigma^2},$$
$$a(\varepsilon) \approx 1.75 + \ln 2 - {}^1\!/_4 \ln \varepsilon, \tag{38}$$

where $a(\varepsilon)$ is slowly varying. Equation (38) has a solution for $\varepsilon \neq 0$ only if $\sigma^2 < \pi\sqrt{2}$. For $\sigma^2 \geqslant \sigma_c^2 = \pi\sqrt{2}$ we have $k_0 = 1$, and in this case the renormalized potential vanishes.

We can interpret this physically as follows. According to (35), $k_0 = 1$ is equivalent to the vanishing of the constant B in (31). For $B = 0$, mean-square quantum fluctuations build up with unbounded magnitude and cause the average potential of the external field in the corresponding states to vanish.

CONCLUSIONS

The above technique for determining the structure of quantum systems differs to some extent from existing methods, in which one analyzes the ground state. In our case, a "structure" is a system in which the means are stationary in certain coherent states. The coherent states $|\alpha\rangle$, $|\mu\rangle$ considered above are in general excited states of the system and include the minimizing states $|\alpha\rangle_{\min}$, $|\mu\rangle_{\min}$. Thus, as far as the ground state is concerned our method is a modification of the mean-field approximation. We note that other modifications may also give a better approximation to the ground state (for instance, collective coherent states can be used, as shown above).

We point out that the coherent states can also be regarded as states that are excited in the system in response to a previous collective excitation (e.g., due to phonons or spin waves). Equilibrium structures of the type considered may thus occur in coherently excited systems. In particular, a nonzero temperature T may cause such an excitation, and the problem then arises of whether one can construct a "temperature coherent state" $|\alpha(T)\rangle$ which provides an equivalent description of thermal effects.

The above results may also be of interest in terms of the possible approach to chaos in quantum systems. To our knowledge no exact quantum mapping leading to chaos have been analyzed in the literature. Although the chaos is "spatial" in our case, it has all of the characteristic features of stochastic trajectories in classical dynamical systems.[4,5,7,18] In a separate paper we will analyze the small-oscillation spectrum for the structures considered above.

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