Self-consistent theory of spatial structures and dynamic excitations in one-dimensional quantum systems

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We develop a method of self-consistently describing equilibrium spatial structures and the small-oscillation frequency spectrum corresponding to those structures for a one-dimensional quantum system of atoms in an external spatially periodic field. We find numerically the commensurable, incommensurable, and chaotic equilibrium structures and determine the form of the frequency spectrum of the dynamic excitations of such structures. We give a comparison with the classical case.

1. INTRODUCTION

When studying possible structures arising in systems of interacting atoms and spins the method of discrete maps normally used in the theory of dynamic systems[1–7] has turned out to be rather successful. The use of that method has enabled us to construct solutions which describe commensurable, incommensurable, and chaotic structures and to elucidate the main conditions necessary for their realization.

It was shown in Refs. 8,9 that the method of discrete maps, when applied to the analysis of various kinds of structure, can also be developed in the framework of the quantum-mechanical approach. The basis of the method of Refs. 8,9 is to obtain discrete maps for the stationary component of the average positions of atoms and spins in coherent states. It thus turns out to be possible to have a limiting transition to classical equilibrium structures which are determined by the stationary points of the corresponding classical equations of motion and to take quantum corrections, including non-stationary ones, into account. In such an approach the structure is determined as the solution of the quantum maps obtained. The result of the quantum-mechanical treatment is a renormalization of the particle interaction potential. One can classify the solutions obtained in the different regions of the parameters of the initial Hamiltonian by using the additional condition for the minimization of the average energy in the class of employed coherent states. The structures thus obtained are, even under the condition of minimization of the average energy, in general metastable states and the method itself is, with respect of the ground state, one of the modifications of the mean field method. The study of such structures is, however, interesting since it becomes possible to use quantum-mechanical maps which decribe commensurable, incommensurable, and chaotic structures in discrete quantum systems of interacting atoms and spins and thus to determine the role of quantum effects and to study the conditions necessary for transitions between different phases.

Since, however, the spatial structures considered are defined on a class of coherent states, the problem arises of their dynamic stability. In general the analysis of the dynamic stability of such structures encounters great difficulties and can be performed only for the case of small oscillations. The small-oscillation spectrum then obtained depends significantly on the properties of the realized equilibrium structure, and was considered for classical discrete systems in Refs. 10, 11. We note that the analysis of the small oscillation spectrum is possible only with the aid of numerical methods, as the class of realizable equilibrium structures is rather complex even for the simplest one-dimensional systems.[1,10]

We construct in what follows a self-consistent theory which allows us to obtain solutions for possible spatial structures in one-dimensional discrete quantum systems, taking the spectral properties of these structures with regards to small oscillations into account. The method is based upon obtaining a self-consistent set of equations which connects the equilibrium average positions of the atoms in the system with the small-oscillation frequency spectrum. We consider the possible structures in the appropriate coherent states, whose parameters themselves depend on the realizable structures. To a certain degree the method considered is close to the method of the self-consistent theory of anharmonic crystals[12] (see also the references given in Ref. 12), a theory in which the small-oscillation spectrum of a quantum lattice in contact with a thermostat is determined self-consistently.

In section 2 of the present paper we formulate a method for self-consistently considering possible equilibrium structures of a quantum-mechanical system of interacting atoms and the small-oscillation spectrum corresponding to these structures. Our consideration uses as an example Frenkel' and Kontorova's discrete quantum model.[13] We describe in section 3 a scheme for constructing a self-consistent solution. We give in section 4 the results of a numerical experiment on the analysis of various equilibrium structures and the small-oscillation spectrum corresponding to them.

2. FORMULATION OF THE METHOD

We obtain in this section a set of equations for a discrete quantum model which allows us to determine self-consistently equilibrium structures of arranging the atoms in coherent states, taking into account the stability of such structures against small oscillations. It is convenient to expound the essence of the method proposed below by using a specific

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model, with a subsequent indication of ways of generalizing it to more general cases.

We consider Frenkel' and Kontorova's quantum model[13] with the Hamiltonian

$$\hat{H}=\sum_n\left\{\frac{\hat{p}_n^2}{2m}+\frac{\gamma}{2}(\hat{u}_{n+1}-\hat{u}_n-\delta a_0)^2+V_0[1-\cos(q_0\hat{u}_n)]\right\}. \tag{2.1}$$

Instead of the coordinate operator $\hat{x}_n$ we have introduced in (2.1) the operator of the displacement $\hat{u}_n$ of the nth atom relative to the external potential: $\hat{x}_n=\hat{u}_n+na$; $q_0=2\pi/a_0$ (a_0 is the spatial period of the external field); $\delta=(a-a_0)/a_0$ ($-1<\delta<\infty$); a is the equilibrium distance between the atoms of a free chain ($V_0=0$); $[\hat{u}_n,\hat{p}_{n'}]=i\hbar\delta_{n,n'}$; m and γ are, respectively the mass of an atom and the elasticity constant. The index n in (2.1) takes on discrete values in the range S_∞: $-\infty<n<\infty$. For the following analysis we choose formally a finite system of N atoms with n varying in the region of S_N: $1\leqslant n\leqslant N$.

For a system of N atoms we change from the $2N$ operators $\hat{u}_n$, $\hat{p}_n$ to the $2N$ operators $\hat{a}_j$, $\hat{a}_j^+$ using the formulae

$$\begin{aligned}\hat{u}_n(t)&=\sum_{j=1}^{N}\left(\frac{\hbar}{2m|\omega_j|}\right)^{1/2}e(n|j)(\hat{a}_j^+(t)+\hat{a}_j(t)),\\ \hat{p}_n(t)&=i\sum_{j=1}^{N}\left(\frac{\hbar m|\omega_j|}{2}\right)^{1/2}e(n|j)(\hat{a}_j^+(t)-a_j(t)).\end{aligned} \tag{2.2}$$

In (2.2) $e(n|j)$ is the n-th component ($n=1,\ldots,N$) of the jth eigenvector $\mathbf{e}_j$ with the eigenvalue ω_j^2 of some eigenvalue problem which will be defined below. The components of the vector $\mathbf{e}_j$ satisfy the following relations:

$$\sum_{n=1}^{N}e(n|j)e(n|j')=\delta_{j,j'}, \tag{2.3}$$

$$\sum_{j=1}^{N}e(n|j)e(n'|j)=\delta_{n,n'}. \tag{2.4}$$

The expressions (2.3), (2.4) are the orthonormality conditions of the eigenvectors $\mathbf{e}_j$. From the properties (2.3), (2.4) we have $[\hat{a}_j,\hat{a}_{j'}^+]=\delta_{j,j'}$. The operators $\hat{a}_j^+$ and $\hat{a}_j$ have the meaning of creation and annihilation operators. We introduce at time $t=0$ the coherent states $|\alpha_j\rangle$:

$$\hat{a}_j|\alpha_j\rangle=\alpha_j|\alpha_j\rangle,\quad \hat{a}_j\equiv\hat{a}_j(t=0). \tag{2.5}$$

We also define the state

$$|\alpha\rangle=\prod_{j=1}^{N}|\alpha_j\rangle. \tag{2.6}$$

Averaging the Heisenberg equations of motion for the operators $\hat{u}_n(t)$ and $\hat{p}_n(t)$ over the state (2.6) we get

$$\begin{aligned}m\ddot{u}_n(t)&=\gamma[u_{n+1}(t)-2u_n(t)+u_{n-1}(t)]\\&\quad-V_0q_0\langle\alpha|\sin q_0\hat{u}_n(t)|\alpha\rangle,\end{aligned} \tag{2.7}$$

where

$$\begin{aligned}&u_n(t)\equiv\langle\alpha|\hat{u}_n^{(N)}(\{\hat{a}^+,\hat{a}\},t)|\alpha\rangle\equiv u_n^{(N)}(\{\alpha^*,\alpha\},t),\\&p_n(t)\equiv\langle\alpha|\hat{p}_n^{(N)}(\{\hat{a}^+,\hat{a}\},t)|\alpha\rangle\equiv p_n^{(N)}(\{\alpha^*,\alpha\},t),\\&\{\hat{a}^+,a\}\equiv(\hat{a}_1^+,\hat{a}_1;\ldots;\hat{a}_N^+,\hat{a}_N),\\&\{\alpha^*,\alpha\}\equiv(\alpha_1^*,\alpha_1;\ldots;\alpha_N^*,\alpha_N).\end{aligned} \tag{2.8}$$

In (2.8) $\hat{a}_j^+$, $\hat{a}_j$, a_j^*, α_j are, according to (2.5), defined at $t=0$. The upper index (N) indicates that the corresponding operator is written in the normal ordering form with regards to the operators $\hat{a}_j^+$ and $\hat{a}_j$. The average of the operator function $\sin[q_0\hat{u}_n(t)]$ can be written as a series:

$$\begin{aligned}\langle\alpha|\sin[q_0\hat{u}_n(t)]|\alpha\rangle&=\sum_{l=0}^{\infty}\frac{(-1)^l}{(2l+1)!}[q_0u_n(t)]\hat{Q}\\&\times[q_0u_n(t)]\hat{Q}\ldots\hat{Q}[q_0u_n(t)]\equiv\sin[q_0u_n(t)\hat{Q}],\end{aligned} \tag{2.9}$$

where the operator $\hat{Q}$ has the form

$$\hat{Q}=\exp\left(\sum_{j=1}^{N}\frac{\overleftarrow{\partial}}{\partial\alpha_j}\frac{\overrightarrow{\partial}}{\partial\alpha_j^*}\right). \tag{2.10}$$

The power of $q_0u_n(t)$ in the l th term on the right-hand side of (2.9) is equal to $2l+1$. The arrow in (2.10) indicates the direction in which the differential operator acts. In (2.9) each operator $\hat{Q}$ acts on the closest function $u_n(t)$ which stands to the right and on all functions $u_n(t)$ which stand to the left. One can obtain Eq. (2.9) using the rule for normal ordering of functions of non-commuting boson operators, and its derivation is given in Appendix 1.

Using (2.9) we can thus write Eq. (2.7) in the c-number form:

$$m\ddot{u}_n(t)=\gamma[u_{n+1}(t)-2u_n(t)+u_{n-1}(t)]-V_0q_0\sin[q_0u_n(t)\hat{Q}]. \tag{2.11}$$

The spatial structures of the system (2.1) which correspond to the stationary component of the solution $u_n(t)$ ($\dot{u}_n(0)=0$, $\dot{p}_n(0)=0$) were studied in Refs. 8,9. It is shown in Refs. 8,9 that such a method of consideration leads to the standard map for the time-independent average positions of the atoms while quantum effects in that approximation reduce to a renormalization of the potential V_0. By such an approach one can find the solution of discrete quantum maps corresponding to the commensurable and incommensurable phases and to structural chaos.

In the general case the solution of the Cauchy boundary problem for Eq. (2.11) can formally be written in the form

$$u_n(\{\alpha^*,\alpha\},t)=u_n^0(\{\alpha^*,\alpha\})+\mu_n(\{\alpha^*,\alpha\},t), \tag{2.12}$$

$$u_n^0=\sum_m|c_m|^2\langle m|\hat{u}_n|m\rangle, \tag{2.13}$$

$$\mu_n(t)=\sum_{m_1,m_2}c_{m_1}^*c_{m_2}\exp(i\omega_{m_1m_2}t)\langle m_1|\hat{u}_n|m_2\rangle. \tag{2.14}$$

In (2.13), (2.14) $\hat{u}_n\equiv\hat{u}_n(t=0)$; $|m\rangle$ is an eigenfunction of the Hamiltonian (2.1): $\hat{H}|m\rangle=E_m|m\rangle$ ($\omega_{m_1m_2}=(E_{m_1}-E_{m_2})/\hbar$) and the amplitude c_m is the coefficient in the expansion of the coherent state $|\alpha\rangle$ of (2.6) in the functions $|m\rangle$: $|\alpha\rangle=\Sigma_m c_m|m\rangle$.

The explicit form of the functions u_n^0 and $\mu_n(t)$ in

(2.12) can only be approximately determined. We shall in what follows consider a self-consistent theory to determine possible equilibrium structures in (2.11), taking into account their small dynamic excitations. We look accordingly for a solution of Eqs. (2.11) in the form (2.12) where the function u_n^0 is time-independent and determines the equilibrium structure while the function $\mu_n(t)$ describes small dynamic excitations in the system. We shall assume in what follows that the condition

$$|\mu_n(t)/u_n^0| \ll 1, \tag{2.15}$$

is satisfied which means that the amplitude of the oscillations (2.14) is small relative to the u_n^0 of (2.13). Using (2.12), (2.15) we get, to first order in $\mu_n(t)$,

$$\sin(q_0 u_n(t)\hat{Q}) = \sin[q_0(u_n^0+\mu_n(t))\hat{Q}]$$
$$\approx \sin(q_0 u_n^0 \hat{Q}) + q_0\mu_n(t)\cos(q_0 u_n^0\hat{Q}) + O(\mu_n^2(t);\ \partial\mu_n/\partial\alpha;\ \partial\mu_n/\partial\alpha^*). \tag{2.16}$$

In (2.16) we neglected the dependence of $\mu_n(t)$ on $\{\alpha^*,\alpha\}$:

$$\hat{Q}\mu_n(t) \approx \mu_n(t)\hat{Q} \approx \mu_n(t), \tag{2.17}$$

which corresponds to dropping terms containing the derivatives $\partial\mu_n/\partial\alpha$, $\partial\mu_n/\partial\alpha^*$. This approximation corresponds to the mean-field theory method. According to (2.12) we have at time $t=0$

$$u_n(0) = u_n^0 + \mu_n(0), \tag{2.18}$$

where $u_n = u_n(0)$ is the initial value of the function $u_n(t)$ in (2.11). Using (2.2), (2.18) we can write down the initial conditions for α_j, α_j^*:

$$\alpha_j \equiv \alpha_j(t=0) = \alpha_j^0 + \tilde{\alpha}_j(0),\ \alpha_j^* \equiv \alpha_j^*(t=0) = \alpha_j^{0*} + \tilde{\alpha}_j^*(0), \tag{2.19}$$

where α_j^0 and α_j^{0*} correspond to the functions u_n^0 and $\tilde{\alpha}_j(0)$, $\tilde{\alpha}_j^*(0)$ to the functions $\mu_n(0)$. It is convenient for what follows to change in the operator $\hat{Q}$ from differentiating into respect to α_j, α_j^* to differentiating with respect to α_j^0, α_j^{0*}. According to (2.19) we have for the operator $\hat{Q}$ of (2.10) in the approximation (2.17)

$$\hat{Q} \approx \exp\left(\sum_{j=1}^{N} \frac{\overleftarrow{\partial}}{\partial\alpha_j^0}\frac{\overrightarrow{\partial}}{\partial\alpha_j^{0*}}\right). \tag{2.20}$$

Substituting (2.16) into (2.11) and using (2.15) we get a set of equations which determines the equilibrium structure u_n^0 and the excitations $\mu_n(t)$:

$$u_{n+1}^0 - 2u_n^0 + u_{n-1}^0 - (V_0 q_0/\gamma)\exp(-\lambda_n^2)\sin(q_0 u_n^0) = 0, \tag{2.21}$$

$$m\ddot{\mu}_n = \gamma(\mu_{n+1} - 2\mu_n + \mu_{n-1}) - V_0 q_0^2 \exp(-\lambda_n^2)\mu_n \cos(q_0 u_n^0). \tag{2.22}$$

The quantities λ_n^2 are determined in Appendix 2 and have the form

$$\lambda_n^2 = \frac{\hbar q_0^2}{4m}\sum_{j=1}^{N}\frac{1}{|\omega_j|}e^2(n|j). \tag{2.23}$$

3. CONSTRUCTION OF THE SELF-CONSISTENT SOLUTION

We describe the scheme for constructing a self-consistent solution of the set of Eqs. (2.21), (2.22) which will be used in what follows for a numerical analysis.

In the linear substitution of the operators in (2.2) the quantities ω_j^2 and $e(n|j)$ were shown in §2 to be the jth eigenvalue and the nth component of the corresponding j-th eigenvector of the eigenvalue problem:

$$\hat{L}\mathbf{e}_j = \omega_j^2\mathbf{e}_j, \quad j=1,\ldots,N, \tag{3.1}$$

where the operator $\hat{L}$ can be specified by an $N\times N$ matrix. Of course, in the framework of the approach considered here, there is a rather large arbitrariness in the choice of the problem (3.1) and, hence, in the solutions $\{\omega_j^2,\mathbf{e}_j\}$ obtained. In that sense the substitution (2.2) is not unique in the general case and this leads to ambiguities in the choice of the quantities λ_n in (2.23)-to each set $\{\omega_j^2,\mathbf{e}_j\}$ there corresponds a definite value λ_n and, accordingly, a definite class of solutions of the Eqs. (2.21), (2.22). Such an ambiguity is connected with the fact that the equilibrium structure u_n^0 and its excitations $\mu_n(t)$ are considered in well defined coherent states $|\alpha\rangle$ (2.6), the construction of which itself is based upon the solutions of the Eqs. (2.21) and has considerable leeway. All solutions of this kind with possible values of λ_n are metastable and amongst them one can select those which lead to stable solutions of the dynamic Eqs. (2.22). In that sense such solutions are locally stable metastable solutions and may be of independent interest.

However, in what follows we restrict our considerations to only those solutions of the set (2.21), (2.22) in which the quantities λ_n are self-consistently determined by the eigenfrequencies of the dynamic equations (2.22). The eigenvalue problem (3.1) is thus uniquely determined. In the physical sense the choice of such solutions can be justified in the framework of the temperature approach (with the subsequent transition $T\to 0$), in which a structure and its excitations are constructed not in coherent states of the kind considered here but by using a statistical averaging over a temperature-dependent density matrix.[12] This problem goes beyond the framework of the present paper and will be considered later on.

We write down a scheme for constructing a self-consistent solution of the set (2.21), (2.22) of the kind indicated above. First of all we write the set (2.21), (2.22) in dimensionless variables:

$$I_{n+1} = I_n + M_n\sin\varphi_n, \tag{3.2}$$

$$\varphi_{n+1} = \varphi_n + I_{n+1}, \tag{3.3}$$

$$d^2\xi_n/d\tau^2 = \xi_{n+1} - 2\xi_n + \xi_{n-1} - M_n\xi_n\cos\varphi_n, \tag{3.4}$$

where

$$\varphi_n = q_0 u_n^0, \quad I_n = \varphi_n - \varphi_{n-1},$$
$$\xi_n = q_0\mu_n, \quad M_n = K\exp(-\lambda_n^2),$$
$$K = V_0 q_0^2/\gamma, \quad \tau = (\gamma/m)^{1/2}t, \tag{3.5}$$
$$\lambda_n^2 = 2^{1/2}\sigma^2\sum_{j=1}^{N}\frac{1}{|\nu_j|}e^2(n|j),$$
$$\nu_j = \omega_j/(\gamma/m)^{1/2}, \quad \sigma^2 = \hbar q_0^2/4(2\gamma m)^{1/2}.$$

Equations (3.2), (3.3) are equivalent to Eq. (2.21) and determine the equilibrium structure; Eq. (3.4) describes the

small dynamic excitations. In (3.2) to (3.5) we have introduced dimensionless parameters K, ν_j, σ^2. The only dimensionless quantum parameter is σ^2. In this form the parameter σ^2 arose when we construct spatial structures of a system with the Hamiltonian (2.1) in coherent single-particle states, with the additional condition that the average energy of the system be minimized[8,9] (see also Ref. 2 where a similar parameter arose from dimensional considerations).

We construct a self-consistent solution of the set (3.2) to (3.4) as follows. We shall assume that the dimensionless frequencies ν_j occurring in λ_n are determined by the solution of the eigenvalue problem (3.4). In that case the substitution leads to the diagonalization of a quadratic form corresponding to Eqs. (3.4) which determine the small oscillation spectrum of a system of atoms near their equilibrium positions φ_n. The first step in the iteration procedure consists in a choice of quantities $\lambda_n^{(0)}$ (e.g., $\lambda_n^{(0)}=0$, $n=1,\ldots,N$ which corresponds to the classical limit $\hbar=0$). We substitute $\lambda_n^{(0)}$ into (3.2), and specifying I_0 and φ_0, we determine the corresponding equilibrium structure $\{\varphi_n^{(0)}\}$. We further substitute $\lambda_n^{(0)}$, $\varphi_n^{(0)}$ into (3.4) and find the eigenvalues $(\nu_j^{(0)})^2$ and the eigenvectors $\mathbf{e}_j^{(0)}$ corresponding to them ($j=1,\ldots,N$). If the eigenvalues $(\nu_j^{(0)})^2$ are positive, we proceed to the second step of the iterations. To do this, we substitute $\nu_j^{(0)}$ and $e^{(0)}(n|j)$ into the expression for λ_n from (3.5) and we get $\lambda_n^{(1)}$:

$$(\lambda_n^{(1)})^2=2^{1/2}\sigma^2\sum_{j=1}^{N}\frac{1}{|\nu_j^{(0)}|}[e^{(0)}(n|j)]^2. \tag{3.6}$$

We then substitute $\lambda_n^{(1)}$ into (3.2) and find the modified equilibrium structure $\{\varphi_n^{(1)}\}$. We substitute $\lambda_n^{(1)}$, $\varphi_n^{(1)}$ into (3.4) and find the modified spectrum $(\nu_j^{(1)})^2$ and $\mathbf{e}_j^{(1)}$. If the quantities $(\nu_j^{(1)})^2$ are positive we go to the next step, and so on. The convergence of such an iteration process leads to the construction of a self-consistent solution for an equilibrium structure and the spectrum of small oscillations near the equilibrium positions. One must note that each step in the iteration with the set $\{\nu_j^{(m)}, \mathbf{e}_j^{(m)}\}$ can be considered as an independent substitution of Eqs. (2.2). From that point of view each step in the iteration creates independent solutions of the set (3.2) to (3.4). Moreover, as the quantities $\varphi_n^{(m)}$ in (3.4) are assumed to be explicit functions of the number n of the atoms and of the initial conditions I_0 and φ_0 the functions $\mu_n(t)$ depend, as we showed above, explicitly only on the atom number n and the time t. We now turn to a numerical analysis of the set of Eqs. (3.2) to (3.4).

4. RESULTS OF A NUMERICAL EXPERIMENT

It is clear from (3.2), (3.3) that the character of the equilibrium solution $\{I_n,\varphi_n\}$ is determined by the parameters

$$M_n=K\exp(-\lambda_n^2) \tag{4.1}$$

of a standard type map[16] with one difference, however, in that the quantities M_n are functionally connected with the variables $\{I_n,\varphi_n\}$. This property of the set (3.2), (3.3) leads to non-canonical variables $\{I_n,\varphi_n\}$ and one of the consequences of this is the non-conservation of the phase volume in the (I,φ)-plane under the action of such a transformation. In this connection before we proceed to describe the results of a numerical experiment with the set (3.2) to (3.4) we note that we have also performed a numerical calculation of a simpler set of equations in which the quantities λ_n^2 which enter in (3.2) to (3.4) via M_n [Eq. (4.1)] were replaced by the average value λ^2:

$$\lambda^2=\frac{1}{N}\sum_{n=1}^{N}\lambda_n^2=\lambda_0^2\sum_{j=1}^{N}\frac{1}{|\nu_j|}, \tag{4.2}$$

where $\lambda_0^2=2^{1/2}\sigma^2$. This simplification leads, firstly, to the variables $\{I_n,\varphi_n\}$ becoming canonical and, secondly shortens appreciably the time of the calculation as it obviates in each step of the iteration the need for calculating the eigenvectors $\mathbf{e}_j^{(m)}$. In that case the set of Eqs. (3.2) to (3.4) changes to the following:

$$\begin{aligned} &I_{n+1}=I_n+M\sin\varphi_n, \quad \varphi_{n+1}=\varphi_n+I_{n+1},\\ &d^2\xi_n/d\tau^2=\xi_{n+1}-2\xi_n+\xi_{n-1}-M\xi_n\cos\varphi_n. \end{aligned} \tag{4.3}$$

It is clear from (4.3) that the simplification (4.2) causes the equilibrium solution $\{I_n,\varphi_n\}$ to be characterized in this approximation by the dimensionless parameter M:

$$M=Ke^{-\lambda^2}, \tag{4.4}$$

while the frequencies ν_j in λ^2 of (4.2) are the eigenfunctions of the small oscillations determined from the last equation in (4.3). Numerical calculations show that such a simplification does in fact not change the shape of the solutions for I_n, φ_n, ν_j. We shall discuss this "crudeness" of the set of Eqs. (3.2) to (3.4) further in the Conclusion.

When $M_n\gg 1$ the structures generated by the map (3.2), (3.3) turn, as a rule, out to be unstable[7,16] and correspond to chaotic states. The instability of most of the trajectories of the map (3.2), (3.3) at $M_n\gg 1$ leads to the fact that any small perturbation of the initial conditions (I_0,φ_0), however small, causes an exponential growth of the computer rounding-off errors in a numerical study of chaotic structures generated by such trajectories. It is therefore impossible to use an iteration of the maps (3.2), (3.3) to obtain sufficiently long dynamically stable chain sections which correspond to chaotic structures.[10,11] As a rule the computer rounding errors at $M_n\gtrsim 1$ for unstable trajectories become important already after a few tens of iteration steps of the map (3.2), (3.3). Because of this we used for the analysis of chaotic structures a gradient method first employed for this purpose in Ref. 10 and applied also to a study of structural states of spiral systems in external fields.[11] The idea of that method is that to find dynamically stable configurations one solves a set of ordinary differential equations

$$\begin{aligned} &d\varphi_n/d\tau=-\partial\mathcal{H}/\partial\varphi_n=\varphi_{n+1}-2\varphi_n+\varphi_{n-1}-M_n\sin\varphi_n,\\ &n=1,\ldots,N, \end{aligned} \tag{4.5}$$

where $\mathcal{H}$ is the Hamiltonian generating the right-hand side of (4.5). The set (4.5) was solved with free boundary conditions: $\varphi_0=\varphi_1$; $\varphi_{N+1}=\varphi_N$. The solutions $\{\varphi_N(\tau)\}$ determined by the set of Eqs. (4.5) tend, when the time τ in-

creases, to stationary solutions determining the stable equilibrium positions. In the numerical experiment we solved the set of Eqs. (3.4), (4.5) by an iteration method. In the first step we put $M_n = M_n^{(0)} = K$ ($\lambda_n^{(0)} = 0$) and solved the set of Eqs. (4.5). Using next the equilibrium positions found $\{\varphi_n^{(0)}\}$, we evaluated the frequencies $\{\nu_j^{(0)}\}$ from the set (3.4) with $M_n = M_n^{(0)} = K$. Then we calculated the quantities

$$(\lambda_n^{(1)})^2 = \lambda_0^2 \sum_{j=1}^{N} \frac{1}{|\nu_j^{(0)}|} e^2(n|j),$$
$$M_n^{(1)} = K \exp\{-(\lambda_n^{(1)})^2\}, \quad n=1,\ldots,N \tag{4.6}$$

and again solved the set of differential Eqs. (4.5), and so on. To solve the set (4.5) we applied Hamming's fourth-order method. All calculations were performed with double accuracy (seventeen significant figures). The criterion for the ending of the iteration process for the solution of the set (4.5) was given by the smallness of the quantity Δ:

$$\Delta = \frac{1}{N} \sum_{n=1}^{N} \left| \frac{\partial \mathcal{H}}{\partial \varphi_n} \right| . \tag{4.7}$$

In our calculations we terminated the iteration process when the quantity Δ of (4.7) reached values $\Delta \sim 10^{-12}$ to 10^{-10}. Using the iteration process described above we obtain the sets: $\{\varphi_n\}$ determining the equilibrium positions of the atoms, and $\{\nu_j\}$ which is the spectrum of the small oscillations of the chain. We succeeded by the method indicated to show the existence of solutions of the set (3.2)–(3.4), (4.5) corresponding to chaotic structures, to a regular soliton lattice, and to a commensurable phase when all particles are distributed in points commensurable with the period of the external field a_0 (e.g., $\varphi_n = 0$, $x_n = a_0 n$).

We show in Fig. 1 the way the dimensionless difference $y_n = q_0(x_n - x_{n-1}) = 2\pi + I_n$ in the positions of the atoms depends on the site number n for a chaotic structure obtained by solving the set (3.4), (4.5). The random nature of the change in the quantity y_n is very clear. We give in Fig. 2 the small-oscillation spectrum for the structure shown in Fig. 1 (lower "curve"). As the wave vector is not well defined in the case of an irregular lattice, we arranged the frequencies ν_j in Fig. 2 in ascending order so that when we went over to a commensurable structure this curve would change into the dispersion curve of the commensurable phase. For comparison we give in Fig. 2 (upper "curve") the spectrum

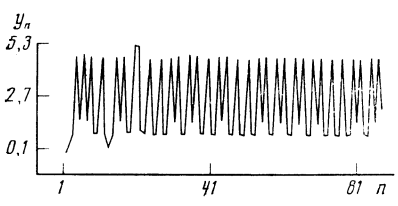

FIG. 1. The n-dependence of $y_n = 2\pi + I_n$, corresponding to a random soliton structure obtained when solving the set of Eqs. (3.2)–(3.4): $K = 6.1$; $\lambda_0^2 = 0.99$; $N = 89$.

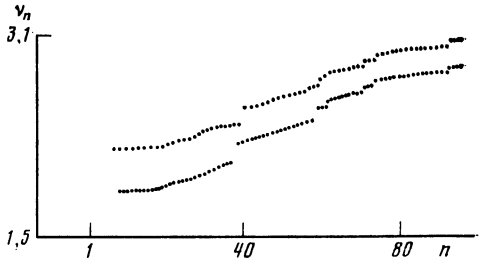

FIG. 2. Small-oscillation spectrum of a random soliton structure for $K = 6.1$ and $N = 89$: $\lambda_0^2 = 0.99$: lower "curve"; $\lambda_0^2 = 0$: upper "curve."

of the corresponding classical chain ($\lambda_n^2 = 0$). From a comparison of these two curves in Fig. 2 it is clear that quantum fluctuations lead to a lowering of the small-oscillation frequencies of the system. In Figs. 3 and 4 (lower "curve") we show the way y_n depends on the site number n for the regular soliton lattice, and the small-oscillation spectrum corresponding to that structure. For comparison we give in Fig. 4 (upper "curve") the small-oscillation spectrum of the corresponding classical lattice ($\lambda_n^2 = 0$). It is clear that just as in the case of the chaotic phase, taking quantum fluctuations into account lowers the small-oscillation frequencies of the system. One can easily see from (3.2) to (3.4) that there always exists a solution corresponding to a commensurable phase $x_n = a_0 n$ ($\varphi_n = 0$). Therefore there is in that case no need to solve Eqs. (3.2) and (3.3), since the equilibrium positions of the atoms are given. The small-oscillation spectrum of this structure can be determined from (3.4):

$$\nu_n^2 = 2[1 - \cos(2\pi n/N)] + M_n, \quad n=1,\ldots,N, \tag{4.8}$$

where the λ_n are given in (3.5). Since the λ_n depend on the ν_j, the set (4.8) can be solved by an iteration method. In the first step of the iteration process we chose $\lambda_n = 0$ and evaluated the spectrum of the commensurable phase ($\nu_j^{(0)}$), neglecting quantum corrections. After that we calculated the $\lambda_n^{(1)}$ and again evaluated the spectrum, and so on. Depending on the magnitudes of K and $\lambda_0^2 = 2^{1/2}\sigma^2$, the iteration process converges to the set $\{\nu_j\}$ in which the zero frequency is either contained or not. If the spectrum contains $\nu = 0$, the quantities λ_n^2 become infinite and this causes the quantities M_n in (4.8) to vanish. In that case, therefore, quantum fluctuations suppress the external field and the commensurable phase turns out in that approximation to be unstable for the given parameters. Indeed, the occurrence of low frequencies ν lead to large mean square fluctuations of the quantities φ_n

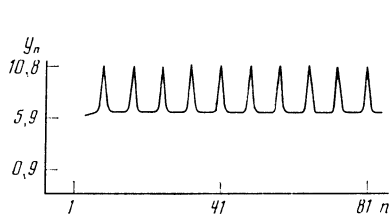

FIG. 3. The n-dependence of y_n corresponding to a regular soliton structure for $K = 6.1$; $\lambda_0^2 = 0.99$; $N = 89$.

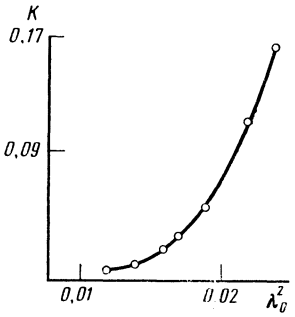

FIG. 4. Small-oscillation spectrum of a regular soliton structure for $K = 6.1$ and $N = 89$: $\lambda_0^2 = 0.99$: lower "curve" and $\lambda_0^2 = 0$: upper "curve."

and to violation of the condition (2.15). The diagram depicted in Fig. 5 thus determines only the region of the linear instability of the commensurable structure considered. If, on the other hand, there is no zero frequency in the spectrum $\{\nu_j\}$ the quantities λ_n^2 turn out to be finite and there occurs merely a renormalization of the amplitudes of the external field. In that case the atoms are arranged in the minima of the external field with period a_0. The curve of Fig. 5 determines in the plane of K and λ_0^2 the boundary for the existence of the commensurate phase considered. In the region above that curve quantum fluctuations lead only to a renormalization of the amplitudes of the external field. Below the curve, quantum fluctuations lead to a suppression of the external field ($\lambda_n \to \infty$, $M_n \to 0$) and to instability of the commensurable phase.

5. CONCLUSION

The method considered above allows us to obtain a whole class of self-consistent solutions describing commensurable, incommensurable, and chaotic structures and the spectrum of the dynamic excitations corresponding to them. All solutions considered are metastable in the general case, since coherent states are the basis of their construction. Since the structures are studied at zero temperature, there arises the problem of how much the solutions obtained in the coherent states are close to those structures ($\bar{u}_n \equiv \langle 0|\hat{u}_n|0\rangle$) which are, say, realized in the ground state $|0\rangle$ of the Hamiltonian $\hat{H}$ of (2.1). In that connection we must note that one of the main effects of the quantum-mechanical consideration of the system (2.1) at zero temperature is the existence of a

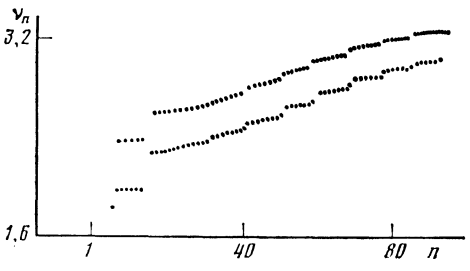

FIG. 5. Curve determining the boundary for the existence for a commensurate phase obtained by numerically solving the set of Eqs. (4.8).

critical value of the magnitude of the quantum fluctuations σ_c above which there occurs the instability of the commensurable phase.[2,17,18] Such an instability is caused by the enhanced role of the long-wavelength component of the quantum fluctuations which lead in final reckoning to a renormalization of the effective potential for the interaction of the atoms with the field. This effect can also be described for the system (2.1) in well chosen coherent states. It was shown in Ref. 9 that the use of collectivized coherent states of some effective system with a quadratic Hamiltonian and a variable magnitude of the gap in the frequency spectrum gives a value of σ_c that agrees with Refs. 2,17. In this case the structures were defined in Ref. 17 as the solutions of standard-type quantum maps for the functions (2.18) with the additional conditions $\dot{\mu}_n(0) = \ddot{\mu}_n(0) = 0$, while quantum fluctuations which are explicitly time-dependent and contained in $\mu_n(t)$ in (2.14) were neglected. From the consideration given above it follows that taking quantum fluctuations approximately into account when constructing a self-consistent solution in coherent states also leads to the existence of a region of instability of the commensurable phase which is caused by the appearance of low frequencies in the spectrum of the self-consistent oscillations of the structure. The actual cause of this instability is that when one varies the parameters some of the energy levels E_m of the initial Hamiltonian (2.1) become degenerate and the corresponding frequencies $\omega_{m_1 m_2}$ in Eq. (2.14) vanish. This, in turn, leads to the need to include this time-independent term from $\mu_n(t)$ in the structural part of the solution u_n^0 of (2.12) and this leads to a renormalization of the structure: $u_n^0 \to \bar{u}_n^0$. In that sense the instability of the commensurable phase in the approximate approach given here means only that the initial commensurable structure itself is unstable.

The method given above allows us to study numerically the different kinds of structure of one-dimensional discrete quantum systems, taking their stability against small oscillations into account. In this connection one should note that the iteration scheme given here for constructing a solution is rather stable even in the case when one considers chaotic structures—it turns out that 3 to 5 iterations are sufficient to arrive at a stationary regime when an equilibrium structure and the small-oscillation spectrum corresponding to it are determined. Moreover, we have noted above that the solutions obtained in the numerical calculation process turn out to be not very sensitive to the procedure of approximating the set (3.2) to (3.4) and to the transition to the set of Eqs. (4.3). This means apparently that the zeroth approximation obtained in that way is to a certain extent stable and that one can use a mean-field type of approximation method. As the main effect of the quantummechanical consideration one must apparently consider the effective lowering of the interaction potential as compared to the classical case: it follows from (3.2), (3.5) that $M_n < M_{cl} \equiv M(\hbar = 0) = K$. Such an effect was noted before in Refs. 8,9 in a somewaht different approach (see also Refs. 2,17). It is possible that such a lowering of the potential when quantum fluctuations are taken into account is a general property of quantum-mechanical considerations and is not connected with the use of coherent states. However, this problem requires further

study. Such a quantal lowering of the interaction potential for a chaotic phase means that the realization of chaotic structures in an essentially quantum case requires more rigid conditions as compared to the classical limit.

In conclusion we note that a generalization of the method considered to the case of more complex one-dimensional quantum systems is possible both in the case where one needs to take into account the non-linearity of the chain and for a more complex form of the interaction potential.

APPENDIX 1

In deriving Eq. (2.9) we use the well known rule for the normal ordering of operator functions of boson operators. We first consider the single-particle case. Let there be given operator functions $\hat{A}$ and $\hat{B}$ depending on the creation and annihilation operators $\hat{a}^+$, $\hat{a}$, with commutator $[\hat{a},\hat{a}^+]=1$. We shall assume that $\hat{A}$ and $\hat{B}$ are normally ordered in the operators $\hat{a}^+$ and $\hat{a}$—all operators $\hat{a}^+$ stand to the left and all operators $\hat{a}$ to the right:

$$\hat{A}(\hat{a}^+,\hat{a})=\sum_{l,m}\gamma_{l,m}(\hat{a}^+)^l(\hat{a})^m\equiv\hat{A}^{(N)},$$
$$\hat{B}(\hat{a}^+,\hat{a})=\sum_{p,q}\mu_{p,q}(\hat{a}^+)^p(\hat{a})^q\equiv\hat{B}^{(N)}. \tag{A1.1}$$

For the normal ordering $\hat{A}^{(N)}\hat{B}^{(N)}$ of normally ordered functions $\hat{A}^{(N)}$ and $\hat{B}^{(N)}$ we use the equation[15]

$$(\hat{a})^m(\hat{a}^+)^p=\hat{N}\left\{\left(a+\frac{\partial}{\partial\hat{a}^+}\right)^m(\hat{a}^+)^p\right\}$$
$$=\hat{N}\left\{(\hat{a})^m\exp\left(\frac{\overleftarrow{\partial}}{\partial\hat{a}}\frac{\overrightarrow{\partial}}{\partial\hat{a}^+}\right)(\hat{a}^+)^p\right\}, \tag{A1.2}$$

where the operator $\hat{N}$ indicates that all operators inside the braces must be arranged in the normally ordered form according to the rule $\hat{N}\{(\hat{a})^m(\hat{a}^+)^p\}=(\hat{a}^+)^p(\hat{a})^m$. Using (A1.1), (A1.2) we have

$$\hat{A}^{(N)}\hat{B}^{(N)}=\hat{N}\left\{\hat{A}^{(N)}\exp\left(\frac{\overleftarrow{\partial}}{\partial\hat{a}}\frac{\overrightarrow{\partial}}{\partial\hat{a}^+}\right)\hat{B}^{(N)}\right\}. \tag{A1.3}$$

Expression (A1.3) is convenient for finding averages in a coherent state:

$$\langle\alpha|\hat{A}\hat{B}|\alpha\rangle=\langle\alpha|\hat{A}^{(N)}\hat{B}^{(N)}|\alpha\rangle=A^{(N)}(\alpha^*,\alpha)\hat{Q}_0B^{(N)}(\alpha^*,\alpha), \tag{A1.4}$$

$$\hat{Q}_0=\exp\left\{\frac{\overleftarrow{\partial}}{\partial\alpha}\frac{\overrightarrow{\partial}}{\partial\alpha^*}\right\}. \tag{A1.5}$$

Choosing, e.g., for $\hat{A}$ and $\hat{B}$ the functions $\hat{u}_n\equiv\hat{u}_n^{(N)}$ and successively applying the ordering process for products of operators $\hat{u}_n^{(N)}$, one easily gets Eq. (2.9) with allowance of generalization of the formulae to a set of N operators $\hat{a}_j^+$, $\hat{a}_j$ satisfying the commutation relation $[\hat{a}_j,\hat{a}_{j'}^+]=\delta_{jj'}$.

APPENDIX 2

We write $\sin(q_0u_n^0\hat{Q})$ in the form of the series (2.9). We consider a term such as

$$[q_0u_n{}^0\hat{Q}]^{2l+1}=[q_0u_n{}^0]\hat{Q}[q_0u_n{}^0]\hat{Q}\dots\hat{Q}[q_0u_n{}^0], \tag{A2.1}$$

where $\hat{Q}$ is given in (2.20) while u_n^0 is connected with α_j^0, α_j^{0*} through the formulae which follow from (2.2):

$$u_n{}^0=\sum_{j=1}^N\left(\frac{\hbar}{2m|\omega_j|}\right)^{1/2}e(n|j)(\alpha_j{}^{0*}+\alpha_j{}^0). \tag{A2.2}$$

Since the operator $\hat{Q}$ acts to the right only on the nearest function, we have from (A2.1)

$$[q_0u_n{}^0\hat{Q}]^{2l+1}=[q_0u_n{}^0(\alpha_j{}^0,\alpha_j{}^{0*})]\left[q_0u_n{}^0\left(\alpha_j{}^0,\alpha_j{}^{0*}+\frac{\overleftarrow{\partial}}{\partial\alpha_j{}^0}\right)\right]\dots$$
$$[q_0u_n{}^0\hat{Q}]^{2l+1}=[q_0u_n{}^0(\alpha_j{}^0,\alpha_j{}^{0*})]\left[q_0u_n{}^0\left(\alpha_j{}^0,\alpha_j{}^{0*}+\frac{\overleftarrow{\partial}}{\partial\alpha_j{}^0}\right)\right]\dots \tag{A2.3}$$

Using (A2.2) and (A2.3) we have

$$[q_0u_n{}^0\hat{Q}]^{2l+1}=\left[q_0\sum_{j=1}^N\left(\frac{\hbar}{2m|\omega_j|}\right)^{1/2}e(n|j)(\alpha_j{}^0+\alpha_j{}^{0*})\right]$$
$$\times\left[q_0\sum_{j=1}^N\left(\frac{\hbar}{2m|\omega_j|}\right)^{1/2}e(n|j)\left(\alpha_j{}^0+\alpha_j{}^{0*}+\frac{\overleftarrow{\partial}}{\partial\alpha_j{}^0}\right)\right]$$
$$\dots\left[q_0\sum_{j=1}^N\left(\frac{\hbar}{2m|\omega_j|}\right)^{1/2}e(n|j)\left(\alpha_j{}^0+\alpha_j{}^{0*}+\frac{\overleftarrow{\partial}}{\partial\alpha_j{}^0}\right)\right]$$
$$=\left[q_0\sum_{j=1}^N\left(\frac{\hbar}{2m|\omega_j|}\right)^{1/2}e(n|j)\left(\alpha_j{}^0+\alpha_j{}^{0*}+\frac{\overleftarrow{\partial}}{\partial\alpha_j{}^0}\right)\right]^{2l+1}. \tag{A2.4}$$

In that case

$$\sin(q_0u_n{}^0\hat{Q})=\frac{1}{2i}\left[\exp\left\{iq_0\sum_{j=1}^N\left(\frac{\hbar}{2m|\omega_j|}\right)^{1/2}\times e(n|j)\left(\alpha_j{}^0+\alpha_j{}^{0*}+\frac{\overleftarrow{\partial}}{\partial\alpha_j{}^0}\right)\right\}\right.$$
$$\left.-\exp\left\{-iq_0\sum_{j=1}^N\left(\frac{\hbar}{2m|\omega_j|}\right)^{1/2}e(n|j)\left(\alpha_j{}^0+\alpha_j{}^{0*}+\frac{\overleftarrow{\partial}}{\partial\alpha_j{}^0}\right)\right\}\right]$$
$$=\frac{1}{2i}\left[\exp\left\{iq_0\sum_{j=1}^N\frac{\overleftarrow{\partial}}{\partial\alpha^0}\left(\frac{\hbar}{2m|\omega_j|}\right)^{1/2}e(n|j)\right\}\right.$$
$$\times\exp\left\{iq_0\sum_{j=1}^N\left(\frac{\hbar}{2m|\omega_j|}\right)^{1/2}e(n|j)(\alpha_j{}^0+\alpha_j{}^{0*})\right\}$$
$$-\exp\left\{-iq_0\sum_{j=1}^N\frac{\overleftarrow{\partial}}{\partial\alpha_j{}^0}\left(\frac{\hbar}{2m|\omega_j|}\right)^{1/2}e(n|j)\right\}$$
$$\left.\times\exp\left\{-iq_0\sum_{j=1}^N\left(\frac{\hbar}{2m|\omega_j|}\right)^{1/2}e(n|j)(\alpha_j{}^0+\alpha_j{}^{0*})\right\}\right]$$
$$\times\left\{-\sum_{j,j'=1}^N\frac{\hbar(iq_0)^2}{4m(|\omega_j||\omega_{j'}|)^{1/2}}e(n|j)e(n|j')\left[\frac{\overleftarrow{\partial}}{\partial\alpha_j{}^0},\alpha_{j'}{}^0\right]\right\}$$
$$=\exp(-\lambda_n{}^2)\sin(q_0u_n{}^0). \tag{A2.5}$$

Similarly

$$\cos(q_0u_n{}^0\hat{Q})=\exp(-\lambda_n{}^2)\cos(q_0u_n{}^0). \tag{A2.6}$$

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