Quantization of weakly nonlinear lattices: Envelope solitons

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A method of quantizing weakly nonlinear lattices is proposed. It is based on introducing ''pseudofield'' operators. In this formalism quantum envelope solitons together with phonons are regarded as elementary quasiparticles making up a boson gas. In the classical limit the excitations corresponding to frequencies above a linear cutoff frequency are reduced to conventional envelope solitons. The approach allows one to identify a quantum soliton that is localized in space and to understand the existence of a narrow soliton frequency band.

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One of the most important tasks of the modern physics of atomic lattices is the experimental observation of the nonlinear localized excitations that are believed to exist. Although in specially prepared chains of coupled oscillators such excitations have been obtained experimentally [1], in the microscopic world their observation is hardly possible in a direct way. A report on the observation of intrinsic localized modes, although in a magnetic model, appeared only recently [2]. This raises the problem of construction of the statistical mechanics of nonlinear lattices covering both linear and nonlinear excitations and allowing one to describe the contribution of the localized modes to macroscopic (measurable) characteristics of solids. As a first step one has to provide the quantization of the atomic chains.

Anharmonic quantum lattices have been considered in the literature. Of two approaches developed so far, one can be classified following [3] as the number state method [3] and the quantum inverse scattering tecnique [4]. Another method based on exact numerical diaganonalization of a Hamiltonian was developed in [5,6], where breather modes were obtained in a lattice with ϕ^4 on-site potential [5] and in a coupled electron-phonon system [6], both nonintegrable. The breather modes were identified through the spectra and dynamic correlation functions.

The approaches mentioned deal with nonlinear quantum Hamiltonians given *a priori*. An alternative and somewhat complementary way of introducing quantum systems is quantization that starts with a classical Hamiltonian. As is evident, canonical quantization, i.e., substitution of c numbers by their operators satisfying canonical commutation relations, can be provided formally in the case of nonlinear lattices also. However, in a generic situation this method is not tractable either analytically or numerically.

At the same time, methods for the analytical description of nonlinear classical lattices are well elaborated today. They are based on introducing different small parameters and result in various spatially localized excitations. Among them we mention envelope solitons (ES's) (see, e.g., [7]), which appear when the wave amplitude is considered as a small parameter, and intrinsic localized modes or breathers (see, e.g., [8]). In the case where a small parameter can be identified as coupling between neighbor sites quantization can be performed by the method proposed in [9]. The role of the coupling constant magnitude in the context of quantum lattices was discussed in [5].

In the present article we concentrate on quantization of a nonlinear lattice when the small parameter is the nonlinearity, thus allowing the existence of ES's in the classical limit. The appropriate physical limit can be interpreted as opposite to the one considered in [9]. Also, in contrast to previous studies of nonintegrable quantum nonlinear lattices, the ES appears to be a dynamical object, and thus allows one to construct a kinetic theory of interacting solitons and phonons.

There are several points to be reflected by the theory. It has been established that quantum nonlinear lattices have a well pronounced soliton band in the spectrum which is extremely narrow for a given nonlinearity [3]. This means that the associated object can be unambiguously identified either as an ES or as an intrinsic localized mode depending on the value of the frequency. Another point is the identification of the quantum ES, which must go beyond computing the frequency alone. Indeed, an important difference between an ES and a phonon is that the soliton is spatially localized while the phonon is localized only in momentum space. Thus we intend to obtain a quantum soliton as an object, a quasiparticle, localized in space (a possible method of construction of such wave packets is described in [3]). This is in contrast to the quantization used in field theory [10], where a kink, being a topological object, is considered as a vacuum state. Finally, an important property of the classical theory is that ES's are governed in leading order by the nonlinear Schrödinger equation [7], which means that in leading order they do not interact with linear phonons and can be regarded as independent quasiparticles. Thus in leading order the quantum theory must allow one to introduce creation and annihilation operators for the quantum soliton and neglect its interactions with other quasiparticles. In this way the interaction Hamiltonian will naturally appear as a perturbation and thus the gas of interacting quasiparticles—solitons and phonons—can be considered within the conventional perturbation technique of field theory.

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We note that the approach developed below has some points similar to one proposed in [11] for quantum optical solitons. In particular, the quantum ES in [11] is described in terms of the field operators (we call them pseudofield operators) which are the Fourier transforms of the conventional creation and annihilation operators. However, there are several essential differences between our method and the approach of [11] (apart from the different systems to be quantized). First, we start with the original (i.e., not approximated) classical dynamical system. Second, we introduce the soliton as a quasiparticle. Third, we consider a highly rarified gas of quasiparticles in the quasiclassical limit (while in [11] the Hartree approximation for a photon gas was exploited). Finally, the quantum ES emerges as a matrix element of the creation operator applied to the vacuum state [12] (notice that in the classical theory envelope solitons are not necessarily real). If, however, one considers an ES as an excitation of the displacement field (see u_n below), then the quantum ES appears to be an observable.

Speaking about quantization of the ES, one can identify one essential feature of the quantum model. In the classical theory the ES amplitude (and frequency detuning) is not a fixed value (see, e.g., [7]). That is why the energy associated with the classical ES is not a fixed quantity. The quantum problem has a scale defined by the Planck constant: it is natural to expect that the excitation characterized by the frequency ω will have energy $\hbar\omega$. Taking into account that the linear oscillator energy is given by $m\omega^2A^2$ (here m is a mass and A is the amplitude) one concludes that the amplitude of the quantum ES must be of the order of $\lambda=\sqrt{\hbar/\omega m}$. On the other hand the amplitude of the soliton must be small. In order to specify this last requirement, let us assume that the interaction energy of neighboring sites is $U(x)$ and define the characteristic scale of the energy variation: $L\sim\{|[1/U(x)][d^2U(x)/dx^2]|\}^{-1/2}$. Then the relation between the nonlinear and linear terms in the classical model is of order $(A/L)^2$. It is this value that appears to be a small parameter in the classical theory, or more precisely $A/L\ll 1$. Then substituting the estimate for the amplitude obtained above on the basis of the quantum approach one gets the requirement $\hbar/\omega mL^2\ll 1$ as a condition for the validity of the small amplitude expansion. Scaling out all the quantities and assuming that the characteristic spatial size of the excitation is 1, $L\sim 1$, we conclude that the effective small parameter of the problem is $\hbar$, i.e., we are dealing with the quasiclassical limit.

We consider quantization of a one-dimensional monatomic lattice described by the Hamiltonian

$$H=\frac{1}{2}\sum_n\frac{p_n^2}{m}+\frac{1}{2}\sum_{n_1,n_2}K_2(n_1,n_2)x_{n_1}x_{n_2}+\frac{1}{4}\sum_{n_1,\ldots,n_4}K_4(n_1,\ldots,n_4)x_{n_1}\cdots x_{n_4},\qquad(1)$$

where x_n and $p_n=m\dot{x}_n$ are displacements of atoms from their equilibrium positions and their linear momenta, and $K_2(n_1,n_2)$ and $K_4(n_1,\ldots,n_4)$ are linear and nonlinear real force constants. The overdot hereafter stands for the derivative with respect to time. We concentrate on the case of force coefficients symmetric with respect to permutation of the indices, e.g., $K_2(n_1,n_2)=K_2(n_2,n_1)$. Also it is assumed that $\Sigma_{n_1}K_2(n_1,n_2)=0$.

First of all we recall some facts of the theory of linear lattices. Consider vibrations of a one-dimensional (possibly disordered) lattice described by the Hamiltonian

$$H=\frac{1}{2}\sum_n\frac{p_n^2}{m_n}+\frac{1}{2}\sum_{n,l}K(n,l)x_nx_l\qquad(2)$$

where m_n is the mass of the nth atom and $K(n,l)=K(l,n)$ are real force constants. It is convenient to introduce new dependent variables $u_n=\sqrt{m_n}x_n$ and force constants $J(l,n)=K(l,n)/\sqrt{m_lm_n}$. The equation of motion reads

$$\ddot{u}_n+\sum_l J(n,l)u_l=0.\qquad(3)$$

It will be assumed that the lattice consists of $\mathcal{N}$, $\mathcal{N}\gg 1$, atoms and is subject to cyclic boundary conditions. Then Eq. (3) can be associated with the linear spectral problem $[\psi_q(n)=\psi_q(n+\mathcal{N})]$

$$\sum_l J(n,l)\psi_q(l)=\omega_q^2\psi_q(n),\qquad(4)$$

where the real eigenvalues ω_q^2 are squared eigenfrequencies and q denotes the eigenmodes. Eigenfunctions $\psi_q(n)$ and $\overline{\psi}_q(n)$ correspond to the same eigenfrequency (the overbar stands for complex conjugation). Introducing the matrix $\mathbf{J}$ with the element $J(n,l)$ placed at the nth row and lth column, a ket vector $|q\}=\mathrm{col}(\ldots,\psi_q(n-1),\psi_q(n),\psi_q(n+1),\ldots)$, and a bra vector $\{q|=(\ldots,\overline{\psi}_q(n-1),\overline{\psi}_q(n),\overline{\psi}_q(n+1),\ldots)$, we rewrite the eigenvalue problem (4) in the form $\mathbf{J}|q\}=\omega_q^2|q\}$. We assume that $\omega_q=\omega_{-q}$, i.e., $\overline{\psi}_q(n)=\psi_{-q}(n)$. $\psi_q(n)$ constitute an orthonormal complete set $\{q|q'\}=\Sigma_n\overline{\psi}_q(n)\psi_{q'}(n)=\delta_{q,q'}$, and $\Sigma_q\overline{\psi}_q(n)\psi_q(l)=\delta_{n,l}$ (here $\delta_{l,n}$ is the Kronecker delta).

The quantization of lattice (3) can be reduced, first, to the problem of diagonalization of the matrix $\mathbf{J}$ and, second, to the quantization of independent linear oscillators. In normalized variables the kinetic energy is written in the form $\{\pi|\mathbf{I}|\pi\}$ where $|\pi\}=\mathrm{col}(\ldots,\pi_{n-1},\pi_n,\pi_{n+1},\ldots)$, $\pi_n=\dot{u}_n$ is the momentum conjugate to u_n, and $\mathbf{I}$ is the unit matrix. Thus any matrix diagonalizing the potential energy will preserve the diagonal form of the kinetic energy. To provide diagonalization of the potential energy we construct an $\mathcal{N}\times\mathcal{N}$ matrix $\mathbf{\Psi}=(\ldots,|q_{j-1}\},|q_j\},|q_{j+1}\},\ldots)$ (here numbering of the discrete eigenvalues is introduced). As is clear $\mathbf{J\Psi}=\mathbf{\Psi\Omega}^2$, where

$$\mathbf{\Omega}=\mathrm{diag}(\ldots,\omega_{q_{j-1}},\omega_{q_j},\omega_{q_{j+1}},\ldots),$$

i.e., the matrix $\mathbf{\Psi}$ diagonalizes $\mathbf{J}$: $\mathbf{\Psi}^{-1}\mathbf{J\Psi}=\mathbf{\Omega}^2$. If one represents $|u\}=\mathbf{\Psi}|X\}$ and $\{u|=\{X|\mathbf{\Psi}^{-1}$ where

$$|u\} = \mathrm{col}(\ldots, u_{n-1}, u_n, u_{n+1}, \ldots)$$

and

$$|X\} = \mathrm{col}(\ldots, X_{q_{j-1}}, X_{q_j}, X_{q_{j+1}}, \ldots)$$

is a column matrix of the normal coordinates with $X_q = \overline{X_{-q}}$, the potential energy will take the form $\{X|\mathbf{\Omega}^2|X\}$. Finally

$$H = \frac{1}{2}\{P|P\} + \frac{1}{2}\{X|\mathbf{\Omega}^2|X\}, \tag{5}$$

where $|P\} = \mathrm{col}(\ldots, P_{q_{j-1}}, P_{q_j}, P_{q_{j+1}}, \ldots)$ is related to the representation $|\pi\} = \mathbf{\Psi}|P\}$.

In order to quantize the linear disordered lattice one introduces phonon annihilation and creation operators

$$\hat{a}_q = \sqrt{\frac{\omega_q}{2\hbar}}\hat{X}_q + \frac{i}{\sqrt{2\hbar\omega_q}}\hat{P}_{-q},$$
$$\hat{a}_q^\dagger = \sqrt{\frac{\omega_q}{2\hbar}}\hat{X}_q - \frac{i}{\sqrt{2\hbar\omega_q}}\hat{P}_q, \tag{6}$$

where $\hat{X}_q$ and $\hat{P}_q$ are operators of the c numbers X_q and P_q satisfying the canonical commutation relations. Then the Hamiltonian is reduced to the conventional form $\hat{H}_l = \Sigma_q \hbar\omega_q(\hat{a}_q^\dagger\hat{a}_q + \frac{1}{2})$. The operators of displacements and of linear momenta read

$$\hat{u}_n = \sum_q \sqrt{\frac{\hbar}{2\omega_q}}[\psi_q(n)\hat{a}_q + \overline{\psi}_q(n)\hat{a}_q^\dagger],$$
$$\hat{\pi}_n = -i\sum_q \sqrt{\frac{\hbar\omega_q}{2}}[\psi_q(n)\hat{a}_q - \overline{\psi}_q(n)\hat{a}_q^\dagger]. \tag{7}$$

Let us introduce Schrödinger *pseudofield operators* according to the relations

$$\hat{\psi}_n = \sum_q \psi_q(n)\hat{a}_q, \quad \hat{\psi}_n^\dagger = \sum_q \overline{\psi}_q(n)\hat{a}_q^\dagger. \tag{8}$$

They describe creation and annihilation of a quasiparticle at site n. We emphasize the main distinguishing feature of these operators compared with the canonical field operators: $\psi_q(n)$ is an eigenfunction of the classical problem rather than a wave function.

It is not difficult to verify that

$$\hat{a}_q = \sum_n \overline{\psi}_q(n)\hat{\psi}_n, \quad \hat{a}_q^\dagger = \sum_n \psi_q(n)\hat{\psi}_n^\dagger, \tag{9}$$

and there exist commutation relations

$$[\hat{\psi}_{n_1}, \hat{\psi}_{n_2}] = [\hat{\psi}_{n_1}^\dagger, \hat{\psi}_{n_2}^\dagger] = 0, \quad [\hat{\psi}_{n_1}, \hat{\psi}_{n_2}^\dagger] = \delta_{n_1,n_2}.$$

The operator of number of quasiparticles is given by

$$\hat{N} = \sum_q \hat{a}_q^\dagger\hat{a}_q = \sum_n \hat{\psi}_n^\dagger\hat{\psi}_n. \tag{10}$$

Finally, following the conventional procedure we introduce the Heisenberg pseudofield operator

$$\hat{\mathbf{\Psi}}_n(t) = \exp\left(i\frac{\hat{H}t}{\hbar}\right)\hat{\psi}_n\exp\left(-i\frac{\hat{H}t}{\hbar}\right). \tag{11}$$

It solves the equation

$$\frac{\partial^2}{\partial t^2}\hat{\mathbf{\Psi}}_n(t) + \sum_l J(n,l)\hat{\mathbf{\Psi}}_l(t) = 0. \tag{12}$$

Let us now consider a nonlinear lattice with the classical Hamiltonian (1) after the renormalization $J_2(n_1,n_2) = K_2(n_1,n_2)/m$ and $J_4(n_1,\ldots,n_4) = K_4(n_1,\ldots,n_4)/m^2$. To obtain the explicit form of the quantum Hamiltonian we assume that the definition (7) holds in the nonlinear case. We substitute the operators of displacement and linear momentum (7) into the Hamiltonian, and express the result through the pseudofield operators, rearranging the last in normal order and dropping the constant that corresponds to the energy of the lattice vacuum. Then $\hat{H} = \hat{H}_0 + \hat{H}_{int}$. The operator $\hat{H}_0$ has the form

$$\hat{H}_0 = \sum_{n_1,n_2} S_{n_1,n_2}\hat{\mathbf{\Psi}}_{n_1}^\dagger\hat{\mathbf{\Psi}}_{n_2} = \sum_q \hbar\omega_q\hat{a}_q^\dagger\hat{a}_q \tag{13}$$

with the kernel $S_{n_1,n_2} = \Sigma_q\hbar\omega_q\psi_q(n_1)\overline{\psi}_q(n_2)$. Now $\psi_q(n)$ is an eigenfunction and ω_q is a frequency of the ''nonlinear'' eigenvalue problem. The ''nonlinearity contribution'' emerges from the ordering procedure. More precisely, the eigenvalue problem (4) is now considered with the kernel

$$J(n,l) = J_2(n,l) + J_d(n,l), \tag{14}$$

where $J_2(n,l)$ is the force constant of the underlying linear lattice and the ''deformation'' $J_d(n,l)$ is given by

$$J_d(n_1,n_2) = \frac{3\hbar}{2\omega_q}\sum_q\sum_{l_1,l_2} J_4(n_1,n_2,l_1,l_2)\psi_q(l_1)\overline{\psi}_q(l_2).$$

The interaction potential $\hat{H}_{int}$ has the form

$$\hat{H}_{int} = \sum_n S_{n_1n_2n_3n_4}[\hat{\mathbf{\Psi}}_{n_1}\hat{\mathbf{\Psi}}_{n_2}\hat{\mathbf{\Psi}}_{n_3}\hat{\mathbf{\Psi}}_{n_4} + \hat{\mathbf{\Psi}}_{n_1}^\dagger\hat{\mathbf{\Psi}}_{n_2}^\dagger\hat{\mathbf{\Psi}}_{n_3}\hat{\mathbf{\Psi}}_{n_4} + \hat{\mathbf{\Psi}}_{n_1}^\dagger\hat{\mathbf{\Psi}}_{n_2}^\dagger\hat{\mathbf{\Psi}}_{n_3}^\dagger\hat{\mathbf{\Psi}}_{n_4} + \hat{\mathbf{\Psi}}_{n_1}^\dagger\hat{\mathbf{\Psi}}_{n_2}^\dagger\hat{\mathbf{\Psi}}_{n_3}^\dagger\hat{\mathbf{\Psi}}_{n_4}^\dagger]$$

with the kernel

$$S_{n_1n_2n_3n_4}=\frac{\hbar^2}{16}\sum_q\sum_l\frac{J_4(l_1,l_2,l_3,l_4)}{\sqrt{\omega_{q_1}\omega_{q_2}\omega_{q_3}\omega_{q_4}}}\psi_{q_1}(l_1)\psi_{q_2}(l_2)\times\psi_{q_3}(l_3)\psi_{q_4}(l_4)\overline{\psi}_{q_1}(n_1)\overline{\psi}_{q_2}(n_2)\times\overline{\psi}_{q_3}(n_3)\overline{\psi}_{q_4}(n_4).$$

In the small amplitude limit which corresponds to small J_4, $\hat{H}_{int}$ can be considered as a perturbation. That is why we introduce pseudofield operators in the interaction representation $\hat{\Psi}_n^{(0)}(t)$ by formula (11) where $\hat{H}_0$ is used instead of $\hat{H}$. Then one can verify that $\hat{\Psi}_n^{(0)}(t)$ solves Eq. (12) with $J(n,l)$ given by Eq. (14).

In order to show how the ES comes out from the above approach we note that the ES solution corresponds to the situation when only one quasiparticle is excited in the lattice. In what follows quasiparticles corresponding to frequencies inside the spectral band of the linear lattice, $\omega\in[0,\omega_0)$ where ω_0 is the cutoff frequency of the underlying linear lattice, are called phonons, while excitations with $\omega>\omega_0$ will be referred to as solitons. Then $\hat{\Psi}=\hat{\Psi}_{ph}+\hat{\Psi}_s$.

Let us introduce the notation $|n_{q_1},\ldots,n_{q_N}\rangle$ for the wave function of a state when n_{q_j} quasiparticles with wave number q_j are excited. Then the ''one-soliton'' state, when there exists only one eigenvalue ω_s bigger than ω_0, is $|0,\ldots,0;1\rangle$ and $\psi_s(n)=\langle 0,\ldots,0;0|\hat{\Psi}|0,\ldots,0;1\rangle$ [we use the notation $\psi_s(n)\equiv\psi_{q=\pi/a}$, $\omega_s=\omega_{q=\pi/a}$]. In order to obtain ψ_s we rewrite Eq. (4) in the form

$$\omega_s^2\psi_s(n)=\sum_m\psi_s(m)J_2(n,m)+\frac{3\hbar}{2\omega_s}\times\sum_{m_1,m_2,m_3}J_4(n,m_1,m_2,m_3)\psi_s(m_1)\times\overline{\psi}_s(m_2)\psi_s(m_3). \tag{15}$$

As long as the small amplitude limit is under consideration, the frequency ω_s is close to the cutoff frequency of the underlying linear lattice, ω_0, and one can introduce a small parameter ϵ ($\epsilon\ll 1$) through the relation $\omega_s^2-\omega_0^2=\epsilon^2\omega_0^2$ where $\epsilon^2=2(\omega_s/\omega_0-1)$ is the frequency detuning toward the forbidden zone.

We look for the solution of Eq. (15) in the form

$$\psi_s(n)=\epsilon\sqrt{\frac{2\omega_s}{3\hbar}}\varphi_n A(\epsilon n), \tag{16}$$

where φ_n is the eigenvalue of the problem for the perfect linear lattice, i.e., $J(n,l)=J_2(n,l)$ in Eq. (4). Then expanding $A(\epsilon(n-l))$ (here l depends on the number of nearest neighbors interacting with the given atom) in a Taylor series with respect to ϵl, introducing $x=\epsilon a n$ (treated as a continuum spatial variable), and taking into account that $\psi_s(n-l)=\psi_s(n+l)$, one arrives at

$$-\frac{a^2}{2}\sum_{n_1,n_2}(n_1-n_2)^2J_2(n_1,n_2)\overline{\varphi}_{n_1}\varphi_{n_2}\frac{\partial^2A}{\partial x^2}+\sum_n J_4(n_1,\ldots,n_4)\varphi_{n_1}\overline{\varphi}_{n_2}\varphi_{n_3}\overline{\varphi}_{n_4}|A|^2A=\omega_0^2A,$$

which is obtained for a monochromatic solution of the one-dimensional nonlinear monatomic lattice within the framework of conventional multiscale analysis [7].

The results obtained agree with the known ones. In particular, it has been shown that for the given nonlinearity the frequency of the quantum soliton is fixed by the normalization condition [11]. This condition defines ϵ introduced in Eq. (16) and must be computed for each lattice separately. It is clear, however, that in any case the result gives $\epsilon\sim\sqrt{\hbar}$, which shows the consistency of the expansion. On the other hand, this result does not contradict the existence of a narrow soliton band, which was explained in [3,9,11] with the help of different arguments. Indeed, the quantum ES is characterized not only by the ''carrier wave'' frequency but also by frequency smearing which is of the order of $(\hbar/m)^{3/2}\omega_0^{-1/2}L^3$. Our results agree also with recent findings in the classical statistical mechanics of nonlinear systems, namely, it is well known that bosons display the tendency of creating clusters (see, e.g., [13]). This means that creation of a phonon and a quantum ES sufficiently close to each other will end up in clustering of the two quasiparticles. This can be viewed as absorption of the phonon by the soliton. This phenomenon was observed recently in numerical experiments [14]. Finally, to leading order with respect to the nonlinearity, solitons and phonons are noninteracting objects. Interaction is taken into account in higher orders of the expansion.

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