Properties of Bose gas in a lattice model  
(strong interaction)  

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The doubts concerning validity of gas approximation for strong interaction (for example, hard spheres) are expressed. A contradictory example - a Bose system in a lattice model - is considered. Namely, the $X−Y$ model for spin 1/2 is taken. A state with spins directed downwards is considered to be vacuum with respect to the particles. An inverse spin (+1/2) corresponds to a particle. There is an usual band spectrum (one band) for a single particle. A trial function is written for a multiple particle system. This function was shown to be a good one within a macroscopic limit, when the particle and lattice site numbers tend to infinity (the ratio of energy standard deviation to average energy tends to zero). A result within the gas limit (particle number is small compared with the lattice site number) is compared with that obtained via generally accepted approach.

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INTRODUCTION

As is known, a Bose gas model with a weak interaction (repulsion), considered by Bogoliubov [1], is generalized for a case of an arbitrary interaction value provided that a so-called gas approximation is correct (for example, see [2]). The main point of this generalization is a transition from true interaction to scattering length (which is small in comparison with inter-particle distance within the gas approximation). However, the gas approximation, being good for a classical case, is not always suitable for a quantum one. The reason is the absence of a conception about trajectories (no quasi-classics) in ultra-quantum limit (which takes place for Bose system). Therefore one can hardly speak about binary collisions. In fact, interaction of every particle with all the particles at once is rather probable: when particle number is small, most particles are in Bose condensate, i.e. these particles are characterized by an infinite wave length. The aim of the present work is to show this phenomenon within the framework of a simple model. Namely, a Bose gas in the lattice model with infinite interaction is considered, so that no more than one particle can be at each cite (description of interaction like for hard spheres). This model is equivalent to X-Y model for spin 1/2 , where particle vacuum is a state with all spins directed downwards and spin directed upwards (+1/2) corresponds to a particle. An average energy value is calculated using a trial function at given particle number written for the X-Y model and a ratio of a mean-square energy deviation to average energy value is shown to tend to zero within a macroscopic limit. The result of calculation of the basic state energy via the traditional approach (according to the accepted rules) is shown to be different.

Bose gas in the hard spheres model was considered, for example, in the work [3], where pseudo-potential method was used. The pseudo-potential value is selected so that the scattering of two particles at each other was the same as in the case of hard spheres. It is the pseudo-potential, for which the corresponding multi-particle Hamiltonian is written, then the interaction is presented in a more simple form and, finally, the basic state energy value (calculated from this simple form) is given ([3], section 1). This model and mathematical treatment is given in [4] also. Nevertheless, no accuracy estimate of the traditional approach was made as nobody used the trial function for initial interaction (hard spheres). This raises the question of whether this approach is correct in the case of Bose condensate, when no conception about particle trajectory and accordingly about binary collisions exists.

THE MODEL

The Hamiltonian of the $X−Y$ model is:

$$H = -t \sum_{<nn'>} S^+(n)S^-(n') \quad (t > 0) .$$  

(1)

Here $<nn'>$ denotes nearest neighbors (the sum takes place over nearest neighbors), and operators $S^\pm(n)$ relate to spin 1/2 at the site with number $n$:

$$S^\pm(n) = S_x(n) \pm iS_y(n)$$

(corresponding radius - vector of the site is $R_n$). These operators commute at different sites and at one site we have:

$$S^-(n)S^+(n) - S^+(n)S^-(n) = -2S_z(n) ,$$

$$S_z(n)S^+(n) - S^+(n)S_z(n) = S^+(n).$$  

(2)

The following Hamiltonian can be written for the Bose particles in the lattice model instead of (1):

$$H → -t \sum_{<nn'>} A_n^+A_{n'} +$$

$$+ U \sum_n A_n^+A_n^+A_nA_n \quad (U \to \infty) .$$  

(3)
Operators $A_n^+$, $A_n$ are the operators of creation and destruction of a Bose particle at a site with number $n$. It is obvious that these statements of the problem are equivalent. Further the spin approach will be used mainly.

The state $\Phi_0$ with all spins directed down (-1/2) is taken as initial one, i.e.:

$$\Phi_0 \equiv |\downarrow\rangle \quad (H\Phi_0 = 0) \ .$$

It is vacuum with respect to the particles. A wave function $S^+(n) |\downarrow\rangle$ corresponding to one inverse spin is equivalent to a particle (a particle at a site with number $n$). As the state $\left(S^+(n)\right)^2 |\downarrow\rangle = 0$, there can be only one particle at a site (two or more particles can not exist at one site), i.e. it can be considered to be the model with interaction of the hard spheres (equivalent of the condition $U \to \infty$ in expression (2)).

The spectrum $\epsilon$ of a single particle is found by a conventional method: the wave function $\Phi_1$ has the form:

$$\Phi_1 = \sum_n C_n S^+(n) |\downarrow\rangle \ , \quad H\Phi_1 = \epsilon \Phi_1 \ .$$

Hence we have the following:

$$-t \sum_{<nm>} C_m S^+(n) |\downarrow\rangle = \epsilon \sum_n C_n S^+(n) |\downarrow\rangle \ ,$$

$$\epsilon C_n = -t \sum_{\nu} C_{n+\nu} \ .$$

The sum with respect to $\nu$ in the last expression is the sum with respect to the nearest neighbors to the site with number $n$. The solution in the form $C_n \sim \exp (i k R_n)$ is sought. Hence we have the following:

$$\epsilon(k) = -t \sum_{\nu} \exp (i k R_n - i k R_{n+\nu}) \to \quad (4)$$

$$-2t \left\{ \cos(k_x a) + \cos(k_y a) + \cos(k_z a) \right\} \ .$$

Here the expression for a simple cubic lattice is presented ($a$ is the lattice period). In the vicinity to the bottom of the band we have:

$$\epsilon(k) \approx -t \nu_0 + \frac{k^2}{2m} \left( 1/m = 2t a^2 \right) \ .$$

The following values correspond to the ground state of one particle:

$$\Phi_1 \sim \sum_{n=1}^{N_0} S^+(n) |\downarrow\rangle \ , \quad \epsilon(0) = -\nu_0 t$$

($\nu_0$ is the number of nearest neighbors, $N_0$ is the number of the lattice sites).

The value $\epsilon(0)$ is the beginning of the particle energy counting (insignificant value). If the particle number $N$ is small ($N << N_0$), one can talk about the Bose gas. The particle number operator is

$$\hat{N} = \frac{1}{2} \sum_{n=1}^{N_0} \left( 1 + 2S_z(n) \right) = \frac{N_0}{2} + S_z \ .$$

It is integral of motion (commutates with the Hamiltonian). This is obvious from the Hamiltonian form and can be directly confirmed.

**TRIAL FUNCTION**

Above mentioned taken into account, the trial function has the following form:

$$\Phi_N = \left(S^+\right)^N |\downarrow\rangle \quad \left(S^+ = \sum_{n=1}^{N_0} S^+(n) \right) \ . \quad (6)$$

This approximation can be expected to be good (at least for small particle number $N << N_0$), as all the particles are in Bose condensate.

First let us consider normalization, i.e. the value $(\Phi_N, \Phi_N)$. The initial state $|\downarrow\rangle$ (vacuum to particles) corresponds to maximum system spin $(N_0/2)$ with maximum negative projection $(-N_0/2)$. This state is normalized. $S^+$ operator raises the projection by a unity without changing of the full spin value. Matrix elements of the operator (calculated by the normalized functions) are known from the general courses of quantum mechanics:

$$\left(S^+\right)_{M, M-1} = \sqrt{(S + M)(S - M + 1)} \ .$$

Here $M$ is $S_z$ spin projection value. For example, the effect of operation on the particle’s vacuum $(M - 1 = -N_0/2, \ S = N_0/2)$ is:

$$\left(S^+\right)_{M, M-1} = \sqrt{N_0} \to S^+ \Phi_0 = \sqrt{N_0} \Phi_1$$

$$\left(M = -N_0/2 + 1 \right) \ .$$

Consequently, having denoted the corresponding to $\Phi_N$ normalized function by $\tilde{\Phi}_N$ ($\tilde{\Phi}_N \equiv D_N \Phi_N$), one can derive:

$$\frac{1}{D_N} = \prod_{M=1-N_0/2}^{N-N_0/2} \sqrt{(S + M)(S - M + 1)} = \prod_{n=1}^{N} \sqrt{n} (N_0 - n + 1) \ .$$
And, finally:

\[ \Phi_N = D_N \Phi_N ; \quad D_N = \sqrt{\frac{(N_0 - N)!}{N!N_0!}}. \tag{7} \]

**Auxiliary relations**

Some relations are necessary in what follows. The most simple is the calculation of, for example, \( (\Phi_N, \Phi_N(n)) \), where \( \Phi_N(n) \equiv S^+(n)\Phi_{N-1} \). This value does not depend on the cite number \( n \), as all the cites are equivalent. Therefore one can write:

\[ \Phi_N(n) \equiv S^+(n)\Phi_{N-1} ; \]

\[ \left( \Phi_N, \Phi_N(n) \right) = \frac{1}{N_0} \sum_n \left( \Phi_N, \Phi_N(n) \right) = \frac{1}{N_0} (\Phi_N, \Phi_N). \tag{8} \]

Analogous relation can be written for the case of both functions containing the cite number, for example:

\[ \left( \Phi_N(n'), \Phi_N(n) \right)_{n \neq n'} = \frac{1}{N_0 - 1} \left\{ \sum_{n'} \left( \Phi_N(n'), \Phi_N(n) \right) - \left( \Phi_N(n), \Phi_N(n) \right) \right\} = \frac{1}{N_0 - 1} \left( \Phi_N, \Phi_N(n) \right) - \left( \Phi_N(n), \Phi_N(n) \right) \]

As for the value with coinciding numbers \( (n' = n) \), one can notice that one of these states is occupied a fortiori, so a norm of the state is got using the relation 7 and substituting \( N_0 \to (N_0 - 1) \), \( N \to (N - 1) \). The result is the following:

\[ \left( \Phi_N(n), \Phi_N(n) \right) = \frac{1}{N_0 - 1} (\Phi_N, \Phi_N) ; \tag{9} \]

\[ \left( \Phi_N(n'), \Phi_N(n) \right)_{n \neq n'} = \frac{N - 1}{N_0 - 1} \frac{N_0}{N_0(N_0 - 1)} (\Phi_N, \Phi_N). \]

The correctness of the relation is tested by substitution of \( N = 1 \).

**ENERGY**

Now an average energy value can be calculated:

\[ E = (\Phi_N, H\Phi_N) = D_N^2 (\Phi_N, H\Phi_N) = -tD_N^2 N \nu_0 \left( \Phi_N+1(n'), \Phi_N+1(n) \right)_{n' \neq n}. \]

Hence taking into account (7), (9) the following relation is derived:

\[ E = -tD_N^2 \frac{N \nu_0}{(N + 1)(N_0 - 1)} \left( \Phi_N+1, \Phi_N+1 \right) = \tag{10} \]

\[ = (-t \nu_0) N \left\{ 1 - \frac{N - 1}{N_0} \right\}. \]

Note natural symmetry at the substitution \( N \to (N_0 - N) \). The contribution linear in relation to the particle number \( N \) is just particle energy at the band bottom, quadratic contribution is a result of particle interaction being taken into account (the test of correctness: true result after substitution of \( N \) by 1).

It is easy to see, that similar energy value is obtained by simplified approach, namely, when using the trial function in the form:

\[ \Phi^{(0)} = \prod_{n=1}^{N_0} (u + vS^+(n)) \downarrow > \]

\[ (u^2 + v^2 = 1 , \quad v^2 = N/N_0) ; \]

\[ E^{(0)} = (\Phi^{(0)}, H\Phi^{(0)}) = (-tN_0 \nu_0)(uv)^2 = \]

\[ = (-t \nu_0) N \left\{ 1 - \frac{N}{N_0} \right\}. \]

The function (11) is a self-consistent field approximation.

It is interesting to note, that foregoing is true in a two-dimensional case (square lattice and three-dimensional spin).

**Distribution function**

A distribution function can be found for the state (11). The trial function (11) can be rewritten using Bose particles and presented in the form:

\[ \Phi^{(0)} = \prod_{n=1}^{N_0} (u + vA_n^+) \downarrow > . \]

The number of particles with given quasi-momentum is:

\[ < A^+(k) A(k) > = \frac{1}{N_0} \sum_{n,n'} < A_n^+ A_{n'} > \times \]

\[ \times \exp \left\{ ik \left[ R(n') - R(n) \right] \right\} ; \]

\[ \sum_{n,n'} = \sum_{n \neq n'} + \sum_{n = n'}. \]
The forbidding of two(many)fold occupation of the cites should be taken into account. The result of the calculation is:

\[ n(0) = \langle A^+(0)A(0) \rangle = N \left(1 - \frac{N}{N_0}\right) + \left(\frac{N}{N_0}\right)^2, \quad (12) \]

\[ n(k) = \langle A^+(k)A(k) \rangle \mid_{k \neq 0} = \left(\frac{N}{N_0}\right)^2. \]

The summation gives the required result:

\[ \langle A^+(0)A(0) \rangle + \sum_{k \neq 0} \langle A^+(k)A(k) \rangle = N \]

(state number \(N_0 - 1\) should be taken into account in the sum over \(k \neq 0\)). Then the energy value is the same:

\[ E^{(0)} = -\nu_0 < A^+(0)A(0) > + \sum_{k \neq 0} \epsilon(k) < A^+(k)A(k) >. \]

It should be emphasized, that though most particles are in the condensate (see (12)), the approximate wave function of the system cannot be written in the form \((A^+(0))^N|0\rangle\) (in contrast to weak interaction \([1]\)). Otherwise, the forbidden case can take place, i.e. the particles can meet at one cite.

**The traditional approach**

It is interesting to compare obtained energy value with the one obtained using the traditional approach (see \([2]\)) within the gas approximation (in our case it takes place at \(N << N_0\)). The system energy can be estimated within the gas approximation using the scattering amplitude. This means to find a vertex function in stair approximation and then to write interaction energy in main approximation, provided that all the particles are in the condensate.

For this purpose Bose particles and their interaction according to Hubbard is used (see \([3]\)). The relation for interaction energy is:

\[ H_{int} = U \sum_n A_n^+ A_n^+ A_n A_n = \quad (13) \]

\[ = \frac{U}{N_0} \sum_{p_1+p_2=p_3+p_4} A^+(p_1)A^+(p_2)A(p_3)A(p_4) \bigg|_{U \to \infty}. \]

According to \([2]\) a full vertex function \(\Gamma\), describing mutual scattering of two particles, should be found in gas approximation. It is \(\Gamma\), that should be used for estimation of the interaction role within the gas limit instead of the initial interaction \(U\). For this purpose diagram technique is used and calculations in stair approximation are made (sum frequency is equal to double particle energy in the band bottom, total momentum is zero):

\[ \Gamma = U + 2i \frac{\nu_0^2}{N_0} < GG > + \ldots = \frac{U}{1 - 2i(U/N_0) < GG >}; \]

\[ \Gamma \bigg|_{U \to \infty} = \frac{iN_0}{2 < GG >}, \]

\[ < GG > = \sum_p \int \frac{d\omega}{2\pi} G(\Omega + \omega, p)G(-\omega, -p), \]

\[ G(\omega, p) = \frac{1}{\omega - \epsilon(p) + i\delta}. \]

Here sum frequency is \(\Omega = 2\nu(0)\). The result of the calculation is:

\[ \Gamma^{-1} = -\frac{2i}{N_0} < GG > = \frac{1}{N_0} \sum_p \frac{1}{\epsilon(p) - \epsilon(0)}; \quad (14) \]

\[ \Gamma^{-1} \to \frac{0.505}{2\nu}. \]

The last value is given for simple cubic lattice. The expression for energy (all the particles are in the condensate \(A^+(0) = A(0) \to \sqrt{N}\)) is:

\[ E \to \epsilon(0) < A^+(0)A(0) > + \frac{\Gamma}{N_0} < A^+(0)A^+(0)A(0)A(0) > \]

\[ = -\nu_0 N + \frac{N_0}{N} N = -\nu_0 N \left(1 - \frac{2}{0.505\nu_0} \frac{N}{N_0}\right). \]

One can see, that contribution of interaction for cubic lattice (\(\nu_0 = 6\)) is one and a half times less than for used trial function. It should be emphasized, that it is the consequence of binary collision approximation.

**Accuracy evaluation**

Corrections to energy can be estimated using the functions resulting from Hamiltonian action on the function \(\Phi_N\). Thus:

\[ S^{-}(n)\Phi_N \equiv S^{-}(n)S^+\Phi_{N-1} = \left[S^+S^{-}(n) - 2S_z(n)\right]\Phi_{N-1}. \]

First, the value \(S_z(n)\Phi_N\) is found. It is easy to see, that:

\[ S_z(n)\Phi_N = \Phi_N(n) + S^+ \left\{ S_z(n)\Phi_{N-1} \right\}. \]

From this recurrent relation follows:

\[ S_z(n)\Phi_N = N\Phi_N(n) - \frac{1}{2}\Phi_N. \quad (15) \]

It is verified directly or by summation by \(n\). Thus:

\[ S^{-}(n)\Phi_N = \Phi_{N-1} - 2(N-1)\Phi_{N-1}(n) + S^+ \left\{ S^{-}(n)\Phi_{N-1}(n) \right\}. \]

From this recurrent relation follows:

\[ S^{-}(n)\Phi_N = N\Phi_{N-1} - N(N-1)\Phi_{N-1}(n). \quad (16) \]
It is verified by a direct substitution as well as at $N = 1$, $N = 2$.

The result is:

$$H \Phi_N = -t \left\{ N \nu_0 \Phi_N - N(N - 1) \sum_{<nn'>} \Phi_N(n,n') \right\}.$$  \hfill (17)

The first term arises from the particles at the band bottom, the second - from interaction of these particles and orthogonal to $\Phi_N$ states ($\Phi_{N\perp}$). The last should be determined for corrections to the energy of an initial state to be found. Noteworthily, that the same energy value $[10]$ is obtained.

We may write:

$$H \tilde{\Phi}_N = E \tilde{\Phi}_N + w \tilde{\Phi}_{N\perp}.$$ \hfill (18)

Here $\tilde{\Phi}_{N\perp}$ is a normalized function, $w$ is a transition matrix element between the states $\Phi_N$ and $\Phi_{N\perp}$. This element should be found for the corresponding two-level problem to be considered.

Thus, according to (17):

$$H \tilde{\Phi}_N = -t N \nu_0 \left\{ 1 - \frac{N - 1}{N_0 - 1} \right\} \tilde{\Phi}_N +$$

$$+ t D_N (N - 1) \left\{ \sum_{<nn'>} \Phi_N(n,n') - \frac{\nu_0}{N_0 - 1} \Phi_N \right\}.$$ \hspace{1cm}

The second term is a sought quantity:

$$w \tilde{\Phi}_{N\perp} = t D_N (N - 1) \Phi_{N\perp}' ;$$ \hfill (19)

$$\Phi_{N\perp}' = \sum_{<nn'>} \Phi_N(n,n') - \frac{\nu_0}{N_0 - 1} \Phi_N.$$ \hspace{1cm}

First let us find a norm of function $\Phi_N'$:

$$\left( \Phi_{N\perp}', \Phi_N' \right) = \sum_{<m'n'> <mn>} \left( \Phi_N(m',n'), \Phi_N(m,n) \right) -$$

$$- \frac{\nu_0^2}{(N_0 - 1)^2} \left( \Phi_N, \Phi_N \right).$$ \hspace{1cm}

Here the orthogonality of functions $\Phi_N$ and $\Phi_N'$ is used.

Various cases should be taken into account in the calculations: all the numbers are different ($W_{N}^{(0)}$), two numbers are equal ($W_{N}^{(1)}$), two pairs of the coinciding numbers ($W_{N}^{(2)}$). The result is the following:

$$W_{N}^{(0)} = 2 N_0 \nu_0 + W_{N}^{(1)} 4 N_0 \nu_0 (\nu_0 - 1) +$$

$$+ W_{N}^{(2)} \left\{ N_0^2 \nu_0^2 - 4 N_0 \nu_0 (\nu_0 - 1) - 2 N_0 \nu_0 \right\}.$$ \hspace{1cm}

Calculation of coefficients can be illustrated by example of $W_{N}^{(0)}$. We have:

$$W_{N}^{(0)} = \left( \Phi_N(m'n'), \Phi_N(nm) \right) \big|_{\Phi_N} =$$

$$= \frac{1}{N_0 - 3} \sum_{l \neq mn} \left( \Phi_N(ln'), \Phi_N(nm) \right) -$$

$$= \frac{1}{N_0 - 3} \left\{ \sum_l \left( \Phi_N(ln'), \Phi_N(nm) \right) - \left( \Phi_N(m'n'), \Phi_N(nm) \right) - \left( \Phi_N(m'n'), \Phi_N(nm) \right) \right\} \rightarrow$$

$$\rightarrow \frac{1}{N_0 - 3} \left\{ (N - 2) \frac{\Phi_N, \Phi_N}{NN_0(N_0 - 1)(N_0 - 2)} - 2 W_{N}^{(1)} \right\}.$$ \hspace{1cm}

Similar operations are made in the other cases:

$$W_{N}^{(0)} = \frac{1}{N_0 - 3} \left\{ \frac{(N - 2) \left( \Phi_N, \Phi_N \right)}{NN_0(N_0 - 1)(N_0 - 2)} - 2 W_{N}^{(1)} \right\};$$ \hfill (20)

$$W_{N}^{(1)} = \frac{1}{N_0 - 2} \left\{ \frac{\left( \Phi_N, \Phi_N \right)}{NN_0(N_0 - 1)} - W_{N}^{(2)} \right\};$$ \hfill (20)

$$W_{N}^{(2)} = \frac{\left( \Phi_N, \Phi_N \right)}{NN_0(N_0 - 1)(N_0 - 2)}.$$ \hspace{1cm}

The following relations for the sought quantity and for $w$, defined in (19), result from combining of all above mentioned relations:

$$\left( \Phi_{N\perp}', \Phi_{N\perp}' \right) \approx 2 \nu_0 \left( \frac{N_0 - N}{N^2 N_0^2} \right) \left( \Phi_N, \Phi_N \right);$$ \hfill (21)

$$w \approx t \sqrt{2 \nu_0 \frac{N_0 - N}{N_0^3/2}} \left( N, N_0 \rightarrow \infty \right).$$ \hspace{1cm}

Now the correction to the system energy can be estimated. The value $w$ tends to infinity within the macroscopic limit, therefore it is a fortiori much higher than the difference of $\tilde{\Phi}_N$ state energy and the initial one. Consequently, the correction to energy is approximately equal to $-w$. And this value is proportional to the square root of volume, i.e. is much lower than the energy of interest (proportional to volume). Therefore, one can draw a conclusion, that initial test function is a good approximation of the problem.
For reliability, the energy root-mean-square value (i.e. \( < H^2 > \)) is found and compared with the value \( < H >^2 = E^2 \). There are all the data for the following relations:

\[
\left( \tilde{\Phi}_N, H^2 \tilde{\Phi}_N \right) = \left( E \tilde{\Phi}_N + w \tilde{\Phi}_{N,\perp}, E \tilde{\Phi}_N + w \tilde{\Phi}_{N,\perp} \right) = E^2 + w^2;
\]

\[
\frac{<(H-E)^2>}{E^2} = 2\nu_0 t^2 \frac{N^2(N_0 - N)^2}{E^2 N_0^3} \bigg|_{N,N_0 \to \infty} \to 0. \tag{22}
\]

Here a finite concentration is meant (the ratio \( N/N_0 \) is constant).

In (22), the system ground state is shown to be well described by the trial function used. It is true for an \( X - Y \) model in general.

**CONCLUSION**

Within the framework of the model used, the conventional Bose gas theory for the particles with strong interaction was shown to be inconsistent. If most particles are in Bose condensate, description of their interaction based on binary collisions (using binary scattering amplitude) does not suit, as there is no quasi-classics for the particles with an infinite wave length. It turns out, as if every particle interacts with all the particles at once. This fact leads to the increase of the interaction energy, as shown in the model used here.

It should be emphasized, that in present work the conclusion about the accuracy of the approach is made after writing of a trial function. In [3] first the problem is simplified by a transition to a pseudo-potential, then solved by the perturbation theory. However, there are no successful attempts to write a multi-particle function for initial interaction (hard spheres).

Note, that the results obtained suit for two-dimensional case (three-dimensional spin).

So far it is not clear, how the spectrum of elementary excitations can be got. Perhaps, a diagram Belyaev-type technique (see, for example, [3]) or its modified form (?) should be used.

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