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ЕРЕВАНСКИЙ ФИЗИЧЕСКИЙ ИНСТИТУТ
YEREVAN PHYSICS INSTITUTE

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ELECTRON CORRELATIONS IN THE EFFECTIVE HUBBARD MODEL

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ԷԼԵԿՏՐՈՆԱՅԻՆ ԿՈՌԵԼՅԱՑԻԱՆԵՐ ՀԱԲԱՐԴԻ ԱՐԴՅՈՒՆԱՎԵՏ ՄՈԴԵԼՈՒՄ

Առաջարկված է նոր ունիտար ձևափոխություն, որը թույլ է տալիս ստանալ Հաբարդի արդյունավետ համիլտոնյան՝ U ներատոմային հաստատունի կամայական նշանի ու մեծության և ատոմի վրա n-էլեկտրոնների լըցման կամայական թվի դեպքում։ Ցույց է տրված, որ U<0 դեպքում արդյունավետ համիլտոնյանը ունի թյուրսպինային փոխանակման տեսք, և Հիլբերտի սահմանափակ տարածությունում գոյություն ունի թաքնված տեղային SU(2) և U(1) տրամաչափային սիմետրիա։

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A.N.KOCHARIAN, P.S.OVNANIAN

ELECTRON CORRELATIONS IN THE EFFECTIVE HUBBARD MODEL

A new general unitary transformation is obtained, which allows to get in a controllable manner the effective Hamiltonian of the Hubbard model at an arbitrary sign and value of the intraatomic constant U and for any given n filling number of electrons per atom. It is shown that at U<0 the effective Hamiltonian has a multipseudospin exchange form for an arbitrary filling and there exist hidden local SU(2) and U(1) gauge symmetries in the restricted Hilbert space.

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Yerevan 1990

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А.Н.Кочарян, П.С.Овнанян

ЭЛЕКТРОННЫЕ КОРРЕЛЯЦИИ В ЭФФЕКТИВНОЙ МОДЕЛИ ХАББАРДА

Найдено новое унитарное преобразование, которое позволяет конролируемым образом получить эффективный гамильтониан модели Хаббарда при произвольном значении и величине внутриатомной константы U и для произвольного числа электронов на атоам n. Показано, что в ограниченном гильбертовом пространстве при U<0 и при произвольном заполнении эффективный гамильтониан имеет вид многоспинового обмена и обладает скрытой SU(2) и U(1) симметриями.

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Ереван 1990

1. Introduction

The interest in strongly correlated electron systems, which may be realized in high T_c superconductors (HTSC) has considerably increased in recent years [1]. The remarkable progress in the investigations of the properties of strongly correlated electrons is owing to the perturbation expansion theory [2].

The effective Hubbard Hamiltonian in the limit of the small parameter t/U has been calculated on the basis of this theory for a degenerate system with many particles [3]. However, there are many difficulties for taking into account all the terms of the same order of t/U sequentially into account [4]. Later on, the method of projection operator was developed in the form of a canonical perturbation expansion (CPE) of the Hubbard Hamiltonian at an arbitrary filling [5,6], in which many-body interactions result from even numbers of inter-configurational transitions. However, it should be noted, that the CPE method is valid only for the leading order in t/U [7].

Below we propose a new modified method of unitary transformation [8], which allows us to take into account in a controllable manner all contributions of any given order of t/U in the effective Hamiltonian in the unrestricted Hilbert space $H_{0,1,2}$. This canonical transformation is valid for an arbitrary value and sign of U and for any given filling. For half filling in the restricted Hilbert space $H_{0,1}$ ($H_{0,2}$) with no empty and doubly (single) occupied sites the Hubbard Hamiltonian at $U>0$ ($U<0$) and $|U|>t$ is equivalent to the multi-spin (pseudospin)

Hamiltonian. At $U>0$ it is shown that the local gauge $U(1)$ and $SU(2)$ symmetries exist only at half filling, whereas at $U<0$ and even number of electrons the hidden $U(1)$ and $SU(2)$ local symmetries hold for any filling.

2. The Two-Site Hubbard Model

We consider the Hubbard Hamiltonian at an arbitrary value and sign of the parameter U

$$H = -t \sum_{\sigma\langle ij\rangle} c^{+}_{i\sigma} c_{j\sigma} + U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \tag{1}$$

Introducing new operators in terms of the Hubbard operators $X^{ab} = |a\rangle\langle b|$ [8] we obtain:

$$B_{ij} = B_{ji} = 1/2 \sum_{\sigma} \sigma (X_i^{\sigma 0} X_j^{-\sigma 2} + X_j^{\sigma 0} X_i^{-\sigma 2}) \tag{2}$$

$$\tau_{ij} = \tau^{+}_{ji} = \sum_{\sigma} (X_i^{\sigma 0} X_j^{0\sigma} + X_j^{2-\sigma} X_i^{-\sigma 2}) . \tag{3}$$

The Hamiltonian (1) can be rewritten in the symmetrized form of the sum of two-site Hubbard models

$$H = \sum H_{ij} = -t \sum_{\vec{i}\vec{\Delta}} \left((\tau^{+}_{\vec{i},\vec{i}+\vec{\Delta}} + h.c.) + 2(B^{+}_{\vec{i}\,\vec{i}+\vec{\Delta}} + h.c) - \frac{U}{zt}(X^{22}_{\vec{i}} + X^{22}_{\vec{i}+\vec{\Delta}}) \right) \tag{4}$$

where summation over the lattice vectors $\vec{\Delta}$ is made over the half of all the nearest-neighbor pairs, $z/2$ (z is the coordination number).

For simplicity let us at first consider the unitary canonical transformation for a diatomic molecule (dimer) with $i,j=1,2$ ($z=1$).

$$T = \exp\,[c(B^{+}_{ij} - B_{ij})] \tag{5}$$

Using the properties of B and B^{+} operators

$$B^{+}_{ij} B_{ij} B^{+}_{ij} = B^{+}_{ij} , \quad \tau^{+}_{ij} \tau_{ij} \tau^{+}_{ij} = \tau_{ij} ,$$
$$(B_{ij})^2 = (\tau^{+}_{ij})^2 = (\tau_{ij})^2 = \tau_{ij} B_{ij} = \tau_{ij} B^{+}_{ij} = 0 , \tag{6}$$

the expression (5) is reduced to

$$T = (1 + (u-1)(B^{+}_{ij} B_{ij} + B_{ij} B^{+}_{ij}) - v(B^{+}_{ij} - B_{ij})) , \tag{7}$$

where $u=\cos(c)$, $v=\sin(c)$. Then, the diatomic Hamiltonian can be rewritten in the form

$$\tilde{H}_{ij} = T H_{ij} T = -t(\tau^{+}_{ij} + \tau_{ij}) + (Uuv - 2t(u^2 - v^2))(B^{+}_{ij} + B_{ij}) +$$
$$+ (Uv^2 - 4tuv)[B_{ij}, B^{+}_{ij}] + U(X_i^{22} + X_j^{22}) . \tag{8}$$

The condition of disappearance of linear $(B^{+}+B)$ in (8) gives

$$Uuv - 2t(u^2 - v^2) = 0 \tag{9}$$

which allows to get the parameters u, v and c

$$u^2 = \frac{1}{2}(1 + U\,\mathrm{sign}(U)(U^2+16t^2)^{-1/2})$$
$$v^2 = \frac{1}{2}(1 - U\,\mathrm{sign}(U)(U^2+16t^2)^{-1/2}) \tag{10}$$
$$c = 1/2\ \mathrm{arctg}(4t/U) .$$

Then the effective Hamiltonian of the diatomic molecule has the form

$$\tilde{H}_{ij} = -t(\tau_{ij} + h.c.) + E(U)\,[B_{ij}, B^{+}_{ij}] + U(X_i^{22} + X_j^{22}) \tag{11}$$

where $E(U) = \frac{U}{2} - \mathrm{sign}(U)\,(U^2/4 + 4t^2)$ and

$$[B_{ij} B^{+}_{ij}] = \frac{1}{2} \left(\sum_{\sigma\sigma'} \sigma\sigma' X_i^{\sigma\sigma'} X_j^{-\sigma-\sigma'} - \sum_{\alpha\alpha'=0,2} X_i^{\alpha\alpha'} X_j^{\bar{\alpha}\bar{\alpha}'} \right)$$

The eigenfunctions and eigenvalues of $\tilde{H}_{ij}$ can be obtained

[8], and the spectrum is the same as in [9]. Turning again to the electron representation, we get the exact expression for the effective Hamiltonian for dimers, which coincides with the formula (24) of Ref.[3], but instead of the expansion coefficient t^2/U we have the exact factor $E(U)$.

In states with one electron per atom $n=1$, the term linear over τ vanishes, and the normalized eigenfunction of the singlet state at arbitrary sign and value of the parameter U has the form:

$$\Psi_{GS}=2^{-1/2}\left[v\sum_{\alpha=0,2} X_i^{\alpha 0}X_j^{\bar{\alpha}0}+u\sum_{\sigma}\sigma X_i^{\sigma 0}X_j^{-\sigma 0}\right]|0_i0_j\rangle . \qquad (12)$$

The action of the electron operators on the vacuum state $|0_i0_j\rangle$ is equivalent to transition to the Hubbard operators

$$c_{i\sigma}^{+}|0_i0_j\rangle = X^{\sigma 0}|0_i0_j\rangle \qquad \sigma c_{i\sigma}^{+}c_{i-\sigma}^{+}|0_i0_j\rangle = X^{20}|0_i0_j\rangle \ . \qquad (13)$$

For the main-state energy we correspondingly have

$$E_{GS}=U/2-\mathrm{sign}(U)(U^2/4+4t^2)^{1/2}+U\,\theta(-U). \qquad (14)$$

Further it is convenient to introduce the projection operators

$$B_{ij}B_{ij}^{+} = 1/2\sum\sigma\sigma' X_i^{\sigma\sigma'}X_j^{-\sigma-\sigma'} \qquad B_{ij}^{+}B_{ij} = 1/2\sum X_i^{\alpha\alpha'}X_j^{\bar{\alpha}\bar{\alpha}'} . \qquad (15)$$

which satisfy the relations

$$(B_{ij}B_{ij}^{+})^n=(B_{ij}B_{ij}^{+}) \quad (B_{ij}^{+}B_{ij})^n=(B_{ij}^{+}B_{ij}) \quad (B_{ij}B_{ij}^{+})(B_{ij}^{+}B_{ij})=0 .$$

With the help of the projection operators one can easily find the spectrum of the two-atom molecule at $U>0$ and $U<0$. The energy of triplet excitations is independent of the parameter U and is equal to zero. There are two more singlet excited states with energy

$$E=U \quad \text{and} \quad E=U/2+\mathrm{sign}(-U)(U^2/4+4t^2)^{1/2}+U\theta(U). \qquad (16)$$

To study the spin structure, it is convenient to use the constraint between the spin and electron operators

$$S^{+}=c_{\sigma}^{+}c_{-\sigma}=\bar{c}_{\sigma}^{+}\bar{c}_{-\sigma}=X^{\sigma-\sigma} \qquad S^{z}=\sum\sigma\bar{n}_{\sigma}=\sum\sigma n_{\sigma}=\sum\sigma X^{\sigma\sigma} . \qquad (17)$$

Obviously, $B_{ij}B_{ij}^{+}$ is simply expressed through the spin operators

$$B_{ij}B_{ij}^{+}=1/2\left[\bar{n}_i\bar{n}_j/2 - 2\vec{S}_i\vec{S}_j\right], \qquad (18)$$

where $\bar{n}_i = \sum \bar{n}_{i\sigma}$.

Introducing the charge operators for holons (h) and doublons (d)

$$X^{00}=h^{+}h=(1-n_{\sigma})(1-n_{-\sigma}) \ , \quad X^{22}=d^{+}d=n_{\sigma}n_{-\sigma} , \qquad (19)$$

and the transition operators between them expressed through the pseudospin variables $L^{\pm}$ and L^{z}

$$L^{+}=X^{20}=d^{+}h=\sigma c_{\sigma}^{+}c_{-\sigma}^{+} \ , \quad 2L^{z}=d^{+}d-h^{+}h=Q_i , \qquad (20)$$

as well as using the constraint between the doublons and holons, $d^{+}d + h^{+}h=M$, the operator $B^{+}B$ is expressed by

$$B_{ij}^{+}B_{ij}=1/2\left[\frac{M_iM_j}{2} - 2L_i^zL_j^z + L_i^{+}L_j^{-}+ \text{h.c.}\right].$$

By an invariant transformation over the pseudospins with a 180° winding round z axis, $L^{\pm}\rightarrow -L$ and $L^{z}\rightarrow L^{z}$, one obtains

$$B_{ij}^{+}B_{ij}=1/2\left[\frac{M_iM_j}{2} - 2\vec{L}_i\vec{L}_j\right]. \qquad (21)$$

In a uniform magnetic field the triplet state is split and a transition to a ferromagnetic state at the critical field H_c takes place.

$$g\mu H_c = (U^2+16t^2)^{1/2} - U . \qquad (22)$$

Not dwelling upon the properties of the two-atom Hubbard molecule, let us consider the one- and two-dimensional Hubbard model.

III. The One- and Two-Dimensional Hubbard Model

The canonical transformation for an infinite linear chain with $j=i+1$ ($z=2$) may be taken in the form:

$$T = \prod_i \exp\,[1/2(B^+_{ij}-B_{ij})\ \mathrm{arctg}\ 4t/U] \tag{23}$$

for which the following relation takes place

$$THT^{-1} = \sum_i \tilde{H}_{i,i+1} = \sum_i TH_{i,i+1}T^{-1} \tag{24}$$

Our approach is close to that of [10], but instead of summation in the exponent, we use the product of the exponents. This allows us to get a more convenient expression for the unitary transformations (7) and (23) and get exact results even without small parameter expansion.

The operators B and τ with no coinciding indexes always commutate

$$[B_{ij},B^+_{kl}] = [B_{ij},B_{kl}] = [\tau_{ij},B_{kl}] = [\tau_{ij},\tau^+_{kl}] = 0 \tag{25}$$

At one coinciding index of the τ and B operators, some commutators vanish

$$[\tau_{i,i+1}B^+_{i-1,i}] = [B_{i,i+1}\ B_{i-1,i}] = 0 \tag{26}$$

others, $[\tau\tau]\neq0$, $[BB]\neq0$, $[\tau B]\neq0$, have a complicated form and are not presented here. There are interesting anticommutating relations for the linked complexes of operators, e.g.,

$$\{B_{ij}B^+_{ij},B_{jk}B^+_{jk}\} = (B_{ij}B^+_{ij} + B_{jk}B^+_{jk} - B_{ik}B^+_{ik})/2 \tag{27}$$

Due to this relation the three-site interaction ijk can be reduced to the two-site nearest and next nearest neighbor interaction $(ij)(kl) + (kl)(ij) = ((ij) + (jk) - (ik))/2$.
Using (23), the effective Hamiltonian (4) may be expressed as:

$$\tilde{H} = \sum_i \ldots T_{i+1,i+2}T_{i,i+1}T_{i-1,i}H_{i,i+1}T^{-1}_{i-1,i}T^{-1}_{i,i+1}T^{-1}_{i+1,i+2}\ldots \tag{28}$$

As in the former case, one can be easily convinced that due to the Eq.(25) the Eq.(28) does not contain the linear term $B^+_{ij}+B_{ij}$.

In the general case of a non-restricted chain, $\tilde{H}_{ij}$ contains an infinite number of terms. However, if one makes use of the expression for the parameters $v\sim2t/U$, $u=1-4t^2/U^2$ at strong coupling $|U|\gg t$, then one obtains the effective Hamiltonian with a given precision at an arbitrary filling n in an unrestricted Hilbert space $H_{0,1,2}$.

$$\begin{aligned} H = &-t\sum(\tau^+_{i,i+1} + h.c.) - \frac{4t^2}{U}\left[B_{i,i+1}, B^+_{i,i+1}\right] + UX^{22}_i - \\ &-\frac{4t^2}{U}\left[(B_{i,i+1}+ h.c.)\,,(B^+_{i-1,i}+B^+_{i+1,i+2} - h.c.)\right] - \\ &-\frac{2t^2}{U}\left[(\tau_{i,i+1}+ h.c.)\,,(B^+_{i-1,i}+B^+_{i+1,i+2} - h.c.)\right] - \\ &-\frac{4t^2}{U}(B^+_{i,i+1}B_{i+1,i+2}X^{22}_{i+1} - h.c.)\,. \end{aligned} \tag{29}$$

Projection of (29) on the states without doubly occupied sites ($X^{22}=0$) at $n\leq1$ and $U>0$ in a restricted Hilbert space $H_{0,1}$ without charge fluctuations, yields

$$PHP^{-1} = -t \sum_i (X_i^{\sigma 0} X_{i+1}^{0\sigma} + h.c.) - \frac{4t^2}{U} \sum_i B_{i,i+1} B^+_{i,i+1} - \frac{t^2}{U} \sum_{i\sigma\sigma'} (\sigma\sigma' X_i^{\sigma 0} X_{i+1}^{-\sigma-\sigma'} X_{i+2}^{0\sigma'} + h.c.) \tag{30}$$

where $P=\prod_i (1-X_i^{22})$ is the Gutzwiller projection operator. The second term in (29) can be expressed strictly through the spinon operators (18).

Besides the two-site interaction of the t^2/U order here arises a three-site neighbor interaction of the same order. The three-site terms contribute to (29) only in the presence of a hole. The last term in (29) describes the next nearest neighbor hop with and without an associated spin flip. Comparing our results (29) with the formula (3) of Ref.[4], we notice that they coincide, except for the factor in the last term. At half filling the complete effective Hamiltonian is rewritten in the form of the sum of different complexes of product of the in series linked operators, e.g. $B_{ij}B^+_{ij}B_{jk}B^+_{jk}\dots$ and hence, can be expressed by (21) in the form of a multispin exchange.

With the help of a recursion relation one can collect all similar terms. Their coefficients contain different powers of the parameters $(1-u)$ and v, which does not change their sign when substituting t by $-t$, that is why the complete effective Hamiltonian at $n=1$ on the subspace H_1 is invariant to the electron-hole transformation. Beginning from four-site interactions, along with the Heisenberg interactions S_iS_j and S_iS_k, there appear multispin (double exchange, $(S_iS_j)(S_kS_l)$, and so on) interactions.

At half filling the resonance valence bond (RVB) [1] corresponds to covering a system by the singlet dimers $(B^+_{ij}B_{ij}=1)$.

Let us consider also the cases with $U<0$ and an even number of electrons, at which only empty and doubly occupied sites without spin fluctuations occur in the restricted Hilbert space $H_{0,2}$ $(X^{00}+X^{22}=1)$. Then one may be easily convinced, that the operator $P=\prod_i(1-\sum_\sigma X_i^{\sigma\sigma})$ projects the Hamiltonian on the sites without $(X^{\sigma\sigma})$ spinons, which yields the expression

$$\tilde{H} = -\frac{4t^2}{|U|} \sum B^+_{i,i+1}B_{i,i+1} + U \sum X_i^{22} \tag{31}$$

The Hamiltonian (31) may be rewritten in the form:

$$\tilde{H} = -\frac{4t^2}{|U|} \sum_i (X_i^{22}X_{i+1}^{00} + X_i^{00}X_{i+1}^{22} + X_i^{20}X_{i+1}^{02} + X_i^{02}X_{i+1}^{20}) \tag{32}$$

The operators X^{02}, X^{20}, X^{22} and X^{00} generate an $SU(2)$ algebra and hence, their commutation relations are isomorphous to those of the pseudospin operator L

$$2L^z = X^{00}-X^{22}, \quad L^+=X^{20} \tag{33}$$

Like X^{02} and X^{20} operators, L^+ and L^- are locally fermionic in $H_{0,2}$ and satisfy the relation for the pseudospin 1/2

$$[L^+L^-] = 2L^z, \quad \{L^+L^-\} = 1 \tag{34}$$

Using the important relation

$$B^+_{ij}B_{ij}B^+_{jk}B_{jk}B^+_{ij}B_{ij} = \frac{1}{4}(X_k^{00} + X_k^{22})B^+_{ij}B_{ij} \tag{35}$$

one can easily obtain the slightly frustrated effective Heisenberg Hamiltonian with accuracy t^4/U^3:

$$H = \left(\frac{4t^2}{|U|} - \frac{16t}{|U|^3}\right)\sum_i(\vec{L}_i\vec{L}_{i+1} - \frac{1}{4}) + \frac{4t^4}{|U|^3}\sum(\vec{L}_i\vec{L}_{i+1} - \frac{1}{4}) + U\sum_i X_i^{22} \tag{36}$$

The first term is the Hamiltonian of the isotropic

Heisenberg antiferromagnetic which describes the superexchange with the charged quasiparticles – holons (X^{00}) and doublons (X^{22}). The next term is the pseudospin exchange of the next nearest neighbors. In general, for any filling, the complete $\tilde{H}$ consists of infinite sums of different products of all possible linked bioperators, $B^{+}_{ij}B_{ij} = 1/2\,(1/2 - 2\vec{L}_i\vec{L}_j)$, and has a form similar to the effective Hamiltonian at half filling and U>0.

In case of the two-dimensional Hubbard model the corresponding unitary transformation has a similar form

$$T = \prod_{\vec{i},\vec{\Delta}} \exp\,[c(B^{+}_{\vec{i},\vec{i}+\vec{\Delta}} - h.c.)]\,, \qquad (37)$$

for which it is necessary to choose a definite order of operators in (28). As in the previous case, the condition eliminating the linear term ($B^{+}+B$) in (4) brings us to Eq.(10) for the parameter c, u and v. Hence, the unitary transformation has a form similar to (7)

$$T = \prod_{\vec{i},\vec{\Delta}} \Big(1+(u-1)(B^{+}_{\vec{i},\vec{i}-\vec{\Delta}}B_{\vec{i},\vec{i}+\vec{\Delta}} + B_{\vec{i},\vec{i}+\vec{\Delta}}B^{+}_{\vec{i},\vec{i}+\vec{\Delta}}) - v(B_{\vec{i},\vec{i}+\vec{\Delta}} - h.c.)\Big) \qquad (38)$$

One can show strictly, that the effective Hamiltonian in 2-D case on the alternative lattice is invariant under the electron-hole transformation at any filling (at n=1) and at U>0 (U<0). For arbitrary u, v and n we have obtained a complete expression for $\tilde{H}$ through all possible linked operators, which is too long to be given here.

IV. Conclusion

So, the proposed canonical transformation obtained for arbitrary U, t, n, allows us to take consistently into account all the necessary contributions in the effective Hamiltonian in the unrestricted Hilbert space $H_{0,1,2}$ in any order of the perturbation theory over the parameter t/U. In case of half

filling at U>0 and for any filling at U<0, the effective Hamiltonian can be strictly expressed by the spin or pseudospin operators. Our transformation has a global gauge symmetry and for that reason does not change the internal symmetry of the Hubbard model.

Though B^{+} and B operators are not invariant at local gauge transformation, nevertheless, their product, BB^{+}, which is equal to $b^{+}_{ij}b_{ij}$ [1], becomes local invariant under the transformation $c_{i\sigma}=c_{i\sigma}\exp(i\phi_i)$.

Since at n=1 the complete Hamiltonian on the Hilbert space $H_{0,1}$ contains only BB^{+}-type terms, then it is obvious that the gauge symmetry is a general internal property, which is attributed to the Hubbard model at half filling and is not connected with its approximation in the Heisenberg model.

At attraction (U<0) there is a hidden local gauge SU(2) symmetry

$$c_{i\sigma} \rightarrow uc_{i\sigma} + \sigma v c_{i-\sigma}, \qquad (39)$$

and what is more, there is a global and a local gauge U(1) symmetry at the transformation $c_{i\sigma} \rightarrow c_{i\sigma}\exp(\sigma\phi_i)$ as well as at an arbitrary filling on the $H_{0,2}$ subspace.

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ЭЛЕКТРОННЫЕ КОРРЕЛЯЦИИ В ЭФФЕКТИВНОЙ МОДЕЛИ ХАББАРДА

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