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ACCURACY OF THE GENERALIZED HARTREE-FOCK METHOD IN NUCLEAR PHYSICS

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A simple procedure is suggested for decreasing the errors which arise when the Schrödinger equation is solved by methods which do not take into account with sufficient accuracy any of the conservation laws. The procedure is based on an approximate representation of the operators of function projection on the space of functions with the required value of the quantum number corresponding to the conservation law. The method may be employed for refinement of the u, v transformation in the superfluid model of the nucleus and for more accurate determinations of the moments of inertia. In the present paper the method is employed for estimating the accuracy of the u, v transformation method. It is shown that the errors in the values of the excitation energies of the low states determined by the u, v transformation method do not exceed 15 per cent. It is also shown that an account of the projecting greatly reduces the variation of the correlative function C for various excited states of the system.

In nuclear theory, extensive use is made of methods in which the conservation law for any quantum number is taken approximately into account. An example is the method of u, v transformation in the superfluid model of the nucleus. In this case approximate account is taken of the law of conservation of the number of particles N. The possibility of using similar methods and the advantages of their use in the description of expansive systems were indicated by Bogolyubov[1]. Great interest is attached, however, to estimates of the accuracy of such methods when solving real problems in nuclear physics. In the present article we propose one very simple procedure with which to improve the accuracy of the methods described above. It entails the use of approximate expressions for the operator of projection on the space of functions with the required value of the quantum number corresponding to the conservation law. Using as an example the superfluid model of the nucleus, it is shown that such a procedure leads only to a slight complication in the formulas of the initial method (in this case, the u, v transformation method).

In the concluding part of the paper, a comparison is made of the results of calculations based on formulas obtained in that investigation, and the data obtained in accordance with the papers of Pawlikowski and Rybarska[2] for a model system consisting of six parts, distributed over five doubly degenerate levels. Comparison shows that the proposed method actually gives a more accurate solution of the Schrödinger equation with Hamiltonian

$$\hat{H} = \sum_{s,\sigma} E(s)\, \overset{+}{a}_{s\sigma} a_{s\sigma} - G \sum_{ss'} \overset{+}{a}_{s+} \overset{+}{a}_{s-} a_{s'-} a_{s'+}. \tag{1}$$

The method developed has been employed by us to estimate the accuracy of the u, v transformation method for systems that simulate real nuclei. Analogous estimates were given by Solov'ev[3]. However, the method used in the cited paper was too complicated to obtain information on the accuracy with which the wave functions of the system were determined. Nonetheless, it is shown even there (and confirmed by the estimates of the present article), that the errors of the u, v transformation method can lead in some cases to excessive deviations in the description of real nuclei.

Let Ĥ and N̂ be, respectively, the Hamiltonian and the particle-number operator of the system. We assume that the following condition is satisfied

$$[\hat{H}, \hat{N}] = 0, \tag{2}$$

and that the specific form of the operators has no significance for the derivation of our main formulas. Let there also be defined some class of functions Ψ, which will be assumed to contain in addition to a defined function Ψ_1 also the functions

$$\Psi_1(z) = z^{\hat{N}} \Psi_1, \tag{3}$$

which correspond to all values of the complex variable z. We emphasize that the functions Ψ are not generally speaking the eigenfunctions of the operator $\hat{N}$, so that the function $\Psi(z)$ can differ appreciably from $\Psi = \Psi(0)$.

It is easy to verify that the expression

$$\frac{1}{2\pi i}\oint \frac{dz}{z}\frac{\Psi(z)}{z^{N_0}} \tag{4}$$

is the projection of the function Ψ on the space of the states of the system of N_0 particles, while the expression

$$H_B = \frac{1}{2\pi i}\oint \frac{dz}{z}\frac{\langle\Psi, \hat{H}\Psi(z)\rangle}{z^{N_0}}\left[\frac{1}{2\pi i}\oint\frac{dz}{z}\frac{\langle\Psi, \Psi(z)\rangle}{z^{N_0}}\right]^{-1} \tag{5}$$

defines the mean value of the energy operator in state (4). (In (4) and (5) the integration is along a closed contour in the z plane, enclosing the point z = 0.)

The purpose of the present work is to obtain a sufficiently simple formulation of the variational problem posed by Bayman[4]:

$$\delta H_B = 0, \tag{6}$$

which defines the function Ψ_B and the minimum value of the functional (5) $E_B = \min H_B$, approximating the wave function and the energy of the ground state of the system. When speaking of a simple formulation, we have in mind that the solution of the problem

$$\delta\langle\Psi, \hat{H}\Psi\rangle = 0, \qquad \langle\Psi, \hat{N}\Psi\rangle = N_0 \tag{7}$$

is known, and we attempt to reduce the problem (5) to a problem similar to (7).

We introduce the notation

$$O(z) = \langle\Psi, \hat{O}\Psi(z)\rangle / \langle\Psi, \Psi(z)\rangle = \overline{O}_z \tag{8}$$

for the matrix element of an arbitrary operator $\hat{O}$. This matrix element depends also on all the parameters which define the function Ψ. Let us define also a function

$$\Phi(z) = \ln\frac{\langle\Psi, \Psi(z)\rangle}{z^{N_0}}. \tag{9}$$

The expression for the mean value of the arbitrary operator $\hat{O}$ in the state (4) has in the new notation the form

$$O_B = \oint \frac{dz}{z} O(z) e^{\Phi(z)} \Big/ \oint \frac{dz}{z} e^{\Phi(z)}. \tag{10}$$

We assume that the function $\Phi(z)$ has a sharply pronounced saddle point, so that the integrals involved in (10) can be calculated by the saddle-point method. From (3) it also follows that z_0 is a saddle point of the function $\Phi(z)$ if

$$N(z_0) = N_0, \tag{11}$$

and that the function has in the vicinity of this point the form

$$\Phi(z) = \Phi(z_0) + \frac{(z - z_0)^2}{2z_0^2}\Delta N_{z_0}^2, \tag{12}$$

where

$$\Delta N_{z_0}^2 = \overline{(\hat{N} - N_0)_{z_0}^2}. \tag{13}$$

We assume that only one saddle point contributes to the integrals of (10), and that the following inequality is satisfied

$$\Delta N_{z_0}^2 \gg 1. \tag{14}$$

We assume also that the dependence of the matrix element of some operator $O(z)$ on z is much weaker than the dependence of the function $\Phi(z)$. We then obtain for the mean value of this operator an estimate

$$\begin{aligned} O_B &\approx O(z_0) - \frac{1}{2\Delta N_{z_0}^2}\left[\frac{\partial^2}{\partial\rho^2} O(z_0 e^\rho)\right]_{\rho=0} \\ &= O(z_0) - \frac{1}{2\Delta N_{z_0}^2}[\overline{O(\hat{N} - N_0)_{z_0}^2} - \overline{O}\Delta N_{z_0}^2]. \end{aligned} \tag{15}$$

Equation (11) has in the general case a large number of solutions, but if only one point z_0 is significant, then it can be stated that it is located on the real axis and has a positive value. It follows therefore that $N(z_0)$, $\Delta N_{z_0}^2$, and $O(z_0)$ have the meaning of mean values of the corresponding operators in the state $\Psi(z^{1/2})$ (see [4]).

Using (15), we can easily obtain the following expression for the mean value of the number of particles and of the energy:

$$\begin{aligned} H_B &\approx H(z_0) - \frac{1}{2\Delta N_{z_0}^2}\left(\frac{\partial^2 H}{\partial\rho^2}\right)_{\rho=0} \\ &= H(z_0) - \frac{1}{2\Delta N_{z_0}^2}[\overline{H(\hat{N} - N_0)_{z_0}^2} - \overline{H}\Delta N_{z_0}^2], \end{aligned} \tag{16}$$

$$N_B \approx N(z_0) - \frac{1}{2}\frac{\Delta N_{z_0}^3}{\Delta N_{z_0}^2}. \tag{17}$$

The last term in (17) characterizes the error introduced by the approximate method of calculating the contour integrals. It is easy to see that the more symmetrical the representation of the states with $N > N_0$ and $N < N_0$ in the function $\Psi(z_0^{1/2})$, the smaller this error.

Formulas (11) and (16) are the principal result of [4] and show that the mean value of the energy in state (4), under the formulations made above, differs little from the mean value in the state $\Psi(z_0^{1/2})$, defined by (11). The second term in the right half of (16) enables us to estimate the errors due to replacing the variational problem (6) by the simpler problem (7). If the use of the saddle-point method is justified, the problem (6) reduces to the determination of the minimum of (17) subject to the additional condition (11), which can be replaced, remaining within the limits of the accuracy of the method, by the condition

$$N_{\mathrm{B}} = N_0. \tag{18}$$

The difference in the energy and in the values of the parameters which define those functions Ψ that satisfy the conditions under which the functionals (7) and (6) are stationary, should then be small. Confining ourselves to first-order corrections in the magnitude of the additional terms in (16) and (17), we can obtain for $\Delta E = \min H_{\mathrm{B}} - \min H$ the expression

$$\Delta E \approx -\frac{1}{2\Delta N^2_{z_0}}\left[\frac{\upsilon}{\partial\rho^2}\left(H\left(z_0e^{\rho}\right) - \lambda N\left(z_0e^{\rho}\right)\right)\right]_{\rho=0}$$
$$= \frac{1}{2\Delta N^2_{z_0}}\left[\overline{(H-\lambda N)(\hat{N}-N_0)^2} - \overline{(H-\lambda N)}\ \overline{(\hat{N}-N_0)^2}\right]. \tag{19}$$

In (19) the mean values of the operators $\hat{H}$, $\hat{N}$, $(\hat{N}-\hat{N}_0)^2$ and the chemical potential λ are determined by the solution of the problem (7). We note that owing to the fact that the second derivative of $H-\lambda N$ is positive at the minimum point, the correction to the energy is negative in the approximation under consideration.

So far we have not used at all the specific form of the Hamiltonian, of the trial functions, or even the form of the operator $\hat{N}$. The only property of the operator $\hat{N}$ which is essential to the derivation of (16)—(19) is the presence of a spectrum of eigenvalues that differ from one another by an integer. Therefore, analogous derivations can be carried out, for example, to make more precise the methods in which the angular momentum conservation law is not accurately taken into account.

Let us proceed to determine the errors resulting from the expressions given above when solving the Schrödinger equation with Hamiltonian (1). We have

$$\hat{N} = \sum_{s,\sigma} a^+_{s\sigma}a_{s\sigma}. \tag{20}$$

The functions Ψ are defined in the usual manner

$$\Psi = \prod_s \left(u_s + v_s a^+_{s+}a^+_{s-}\right)|0\rangle. \tag{21}$$

It is easier to obtain in this case simpler calculations

$$\Delta E = -\frac{1}{G\Delta N^2}\left(C^2 - C_1^2\right), \tag{22}$$

where

$$\Delta N^2 = 4\sum_s u_s^2v_s^2, \qquad C = G\sum_s u_sv_s,$$
$$C_1 = G\sum_s u_sv_s\left(u_s^2 - v_s^2\right). \tag{23}$$

For the mean value of the particle-number operator we obtain the expression

$$N_{\mathrm{B}} = \sum_s \overline{N}_s = 2\sum_s v_s^2\left[1 - \frac{1}{\Delta N^2}u_s^2\left(u_s^2 - v_s^2\right)\right]. \tag{24}$$

In order to obtain the correction to the wave functions of the system, it is advantageous to simplify the problem by using the fact that for a sufficiently smooth dependence of $u_s^2(v_s^2)$ on s the following inequalities are satisfied

$$\Delta N^3 \ll \Delta N^2, \quad C_1 \ll C. \tag{25}$$

We have seen that the ratio $\Delta N^3/2\Delta N^2$ determines, strictly speaking, the accuracy of the method. It is therefore natural to neglect the quantities ΔN^3 and C_1 in (22) and (24), after which the functionals H_{B} and N_{B} assume the form

$$H_{\mathrm{B}} \approx 2\sum_s E_sv_s^2 - G_{\mathrm{eff}}\left(\sum_s u_sv_s\right)^2, \quad N_{\mathrm{B}} \approx 2\sum_s v_s^2, \tag{26}$$

where

$$G_{\mathrm{eff}} = \left(1 + 1/\Delta N^2\right)G. \tag{27}$$

In this approximation the projection leads to renormalization of the interaction constant G. By varying Equation (26) we readily obtain the usual equations of superfluidity, in which the constant G is replaced by G_{eff}, and the renormalized values of the energy levels are

$$\widetilde{E}_i = E_i - v_i^2G_{\mathrm{eff}} - \frac{2\left(u_i^2 - v_i^2\right)}{G\left(\Delta N^2\right)^2}\,\frac{\widetilde{C}^2}{\left(1 + 1/\Delta N^2\right)^2},$$
$$\widetilde{C} = G_{\mathrm{eff}}\sum_s u_sv_s.$$

The formulas given above enable us to obtain corrections both for the energy of the ground state of the system and for the parameters u and v, which determine the solution of the variational problem. However, before we proceed to the calculations, we must note the following. In the superfluid model of the nucleus, G is a parameter determined from the condition relating the experimentally known value of the pair energy and the different values of this quantity (see [3]). The correlation function C and the parameters u and v are related in a rather complicated manner to the physical parameters of the system. It is therefore of great interest to investigate the spectrum of the excited states of the system as a function of the pair energy. In the case considered here, when the Hamiltonian has the form (1), the formulas presented above describe a considerable part of the low-lying excited states. Indeed, the function of the state with nonvanishing quantum numbers ν_i, ν_j (see [2]) has in terms of the second quantization the form

$$\Psi_{i,j} = \overset{+}{a}_{i\mu}\overset{+}{a}_{j\eta}\Psi'_{i,j}(\overset{+}{a}_{s\sigma})|0\rangle, \qquad (28)$$

where Ψ' contains the operators $\overset{+}{a}_{s\sigma}$ with $s \neq i, j$. The function is an eigenfunction of the Hamiltonian (1), from which terms corresponding to $s = i, j$ or $s' = i, j$ have been excluded. In the theory of the u, v transformation, states described by these functions are called two-quasiparticle states with quasiparticles at levels i and j.

The formulas presented above are based on the assumption that the saddle point in the integrals of (5) is quite sharply pronounced. As applied to the superfluid model of the nucleus, this means that the variance ΔN^2 of the number of particles is assumed to be large compared with unity. Calculations for systems simulating real nuclei show that this quantity usually assumes values $\Delta N^2 \sim 5-7$ in describing ground states of nuclei, and values $\Delta N^2 \sim 2-5$ in describing two-quasiparticle states. This raises the question whether the described method provides a real improvement in the accuracy of the calculations.

Table I

	G			
	0.5	0.8	1.0	1.25
E_{0ex}	10.00	8,21	6,83	4,95
E_0	10.22	8,42	7,00	5,09
E_{0uv}	10.56	9,22	8,08	6.51

Remark. The energy of the ground state E_0 of the model system, described by Pawlikowski and Rybarska[2], for different values of the constant G (the quantities are given in multiples of the distance between the single-particle levels E_i).

Table II

State	Parameters	Exact value for G = 1.0	Value obtained by the u, v transformation method		Value obtained by the method described in the article	
			$G = 1,0$	$G=1,09$	$G = 0,94$	$G = 1,0$
0	P	3.603	3,083	3,603	3.605	3,954
	E_0	6.828	8,084	7.532	7,442	7,004
	G_{eff}	—	1	1,09	1.182	1,251
	$\widetilde{C}$	—	2,092	2.338	2,585	2.771
	λ	—	3.654	3.688	3,723	3,751
	$N-N_0$	—	0	0	—0,133	—0,138
	δ	0	0.025	0.032	0,024	0,029
3.4	ε	3,850	2,916	3.288	3.722	4,025
	G_{eff}	—	1	1,09	1.639	1.697
	$\widetilde{C}$	—	0,010	0,024	1,619	1.733
	λ	—	3,000	3,214	3,776	3.798
	$N-N_0$	—	0	0	—0.127	—0.137
	δ	0	0,012	0,012	0,008	0,009
1,2	ε	7,394	6,867	7.171	7.101	7,329
	G_{eff}	—	1	1.09	1,347	1,426
	$\widetilde{C}$	—	1.218	1.360	1.755	1,857
	λ	—	4.651	4,684	4.785	4,819
	$N-N_0$	—	0	0	—0.247	—0.256
	δ	0	0.031	0.037	0.036	0,040

Remark. A comparison of the results of the calculation of the model system, obtained by the u, v transformation method and by the method described in the present article, with the exact values $P = 2(E_0)_{N-1} - E_N - E_{N-2}$—pair energy of the system, consisting of N particles; ϵ—excitation energy; $\widetilde{C}$—correlation function, equal to $C = G\Sigma_s u_s v_s$ in the u, v transformation method and $\widetilde{C} = G_{eff}\Sigma_{s'} u_s v_s$ in the method described in the present article; λ—chemical potential of the system, $N - N_0 = -\Delta N^3/2\Delta N^2$; finally, $\delta = \frac{1}{5}\left[\sum_{s=1}^{5}(N_s - N_{s,ex})^2\right]^{1/2}$—mean square error in the determination of the degree of filling of the single-particle levels.

Table III

P	Parameters	0	K—2 K	K—2 K+1	K—1 K	K—1 K+1	K—1 K+2	K K+1	K K+2	K K+3
0.170	G_{eff}	0.0236	0.0250	0,0255	0.0256	0,0263	0.0254	0,0267	0.0257	0,0254
	ε	0	0,400	0.363	0.258	0.222	0,297	0.190	0,278	0.344
	$\varepsilon_{u,v}$	0	0,398	0.353	0,254	0,204	0.294	0,164	0,273	0,340
	$\widetilde{C}$	0,150	0,125	0,124	0.121	0,120	0,121	0,120	0.120	0.122
	$\widetilde{C}_{u,v}$	0.120	0.073	0.041	0,061	0,003	0,070	0	0.060	0,065
	λ	1.342	1,400	1.381	1,391	1,368	1,332	1,354	1,318	1.314
	$\lambda_{u,v}$	1.341	1,409	1,387	1.408	1.402	1.331	1,313	1,313	1,311
	$N—N_0$	—0.014	0.122	0,056	0.170	0,080	—0.018	0.037	—0.061	—0,038
0,205	G_{eff}	0.0246	0.0259	0,0262	0.0264	0.0269	0,0263	0.0272	0.0265	0.0262
	ε	0	0,420	0.388	0,282	0.251	0,320	0,222	0.303	0.367
	$\varepsilon_{u,v}$	0	0,418	0.380	0.278	0,236	0,316	0,196	0.297	0.362
	$\widetilde{C}$	0.170	0,141	0.140	0.136	0.135	0,136	0.134	0.136	0.138
	$\widetilde{C}_{u,v}$	0.139	0.090	0,068	0,077	0,039	0,083	0,002	0.075	0,081
	λ	1,342	1,396	1.380	1,387	1,366	1,332	1,353	1.320	1,315
	$\lambda_{u,v}$	1,342	1.406	1,386	1,404	1,379	1,331	0.329	1,314	1.312
	$N—N_0$	—0.007	0.120	0,060	0,163	0,078	—0,018	0,037	0.060	—0,040

Remark. Comparison of the results of the u, v transformation method and the method described in the article for a system that simulates a nucleus with 102 neutrons at two values of the pair energy. The energies are given in units of $\hbar\omega_0^0 = 7.37$ MeV. The notation is the same as in Table II.

Tables I—III and Figs. 1 and 2 enable us to compare the accuracy of the method presented and the method of u, v transformation in accordance with the data of Pawlikowski and Rybarska[2] concerning the exact solution of the model problem which they considered. In Figs. 1 and 2 and in Table I the quantities with the subscript "ex" represent the exact value of the corresponding quantity, while the subscript u, v denotes that the quantity was obtained by the u, v transformation method; quantities without indices were determined from the formulas of the present article. The data presented show that the described method greatly reduces errors in the determination of the energy spectrum of the system.

A comparison of the exact results for G = 1 with the results of the u, v transformation method and our method for the same values of the constant G, which give the required identical pair energy of the system, shows that the procedure used leads to a reduction in the error of the first-level excitation energy by a factor greater than 4 (the inaccuracy with which the excitation is determined by our method is in this case merely 3.4%). The changes in distribution of the particles over the levels, to which the described method leads, turn out to be small (it can be shown that when $\Delta N^2 \gg 1$ the change in the degree of filling of the s level is $s\delta N_s \sim 1/(\Delta N^2)^2$).

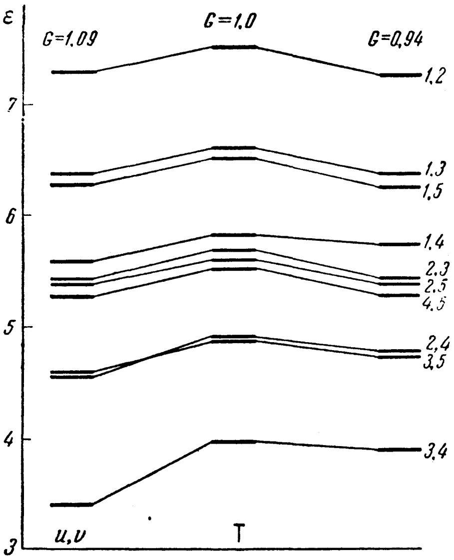

FIG. 2. Excitation energy of two-quasiparticle states of the model system obtained by different methods for a fixed value of the pair energy (P = 3.603).

Analogous calculations were made for two systems close to those describing real nuclei (nuclei with N = 102 neutrons). The results of these calculations are listed in Table III, which also shows the results of the calculations by the u, v transformation method. The comparison of these results shows that a refinement of the u, v trans-

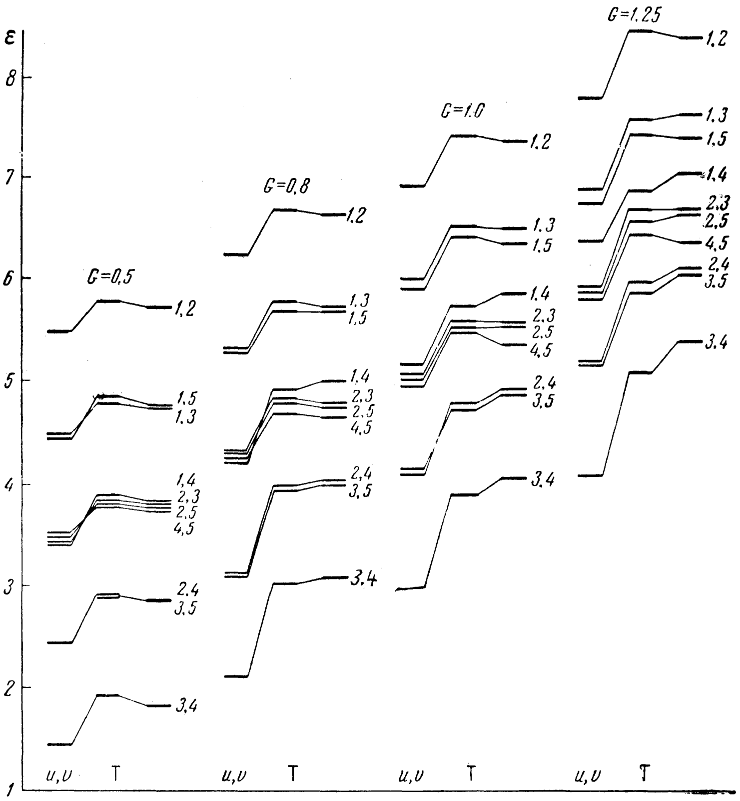

FIG. 1. Excitation energy of two-quasiparticle states of the model system for different values of the constant G.

formation method can lead to 15% changes in the energy of the first excited state of even-even nuclei. The change in the excitation energy of the higher lying levels is insignificant. It is also seen from Table III that the change in the correlation function $\tilde{C}$ brought about by an account of the projection is significant even for the ground state and is quite large for the low excited states. Analogous results also follow from the calculations of the model problem. In accordance with our calculations, all the two-particle states have very nearly equal values of $\tilde{C}$. We note that in our method $\tilde{C}$ is connected by different relations to the different physical quantities than in the u, v transformation method. Because of this, the change in $\tilde{C}$ compared with the calculations by the u, v transformation method is not accompanied by an appreciable change in the distribution of the particles among the levels. The larger $\tilde{C}$, the greater the difference between the wave function of the system and the antisymmetrized product of the single-particle wave functions. The comparable value of the correlation function in the ground and in the two-quasiparticle excited states of the system shows that the wave function of these excited states is still far from a Hartree-Fock type.

In conclusion, I take this opportunity to express my gratitude to V. G. Solov'ev and I. Petkov for interest in the work and for numerous discussions. The calculations described above were carried out in the computer center of the Joint Institute for Nuclear Research by M. V. Mikhaĭlova, to whom I am sincerely grateful.

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