WAVE FUNCTIONS OF CONDENSED STATES

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An extremal-type wave function is constructed for an N-fermion system. This function leads to a reduced s-order density matrix having a maximal occupation number. When the rank is unlimited, this number is close to $\binom{n}{p}$, where n = N/a, p = s/a, and a is an even number equal to the number of fermions in the minimal "aggregate" that experiences nondiagonal long-range correlations. At large N and at a = 2, this occupation number tends to the limit indicated by Yang, namely $N^{s/2}/(s-1)!!$. It is shown that the mechanism leading to the appearance of these maximal characteristic numbers of the density matrix is connected with the increasingly more symmetrical inclusion of the individual aggregates into the total wave function of the system.

1. In 1962, Yang advanced the hypothesis that the formation of the condensed state in a multi-particle system is connected with the presence of a "nondiagonal long range order" (NLRO). Speaking more concretely, this means that if all the coordinates x_i in the coordinate representation of the reduced density matrix (RDM) of s-th order $P_s(x_1 \dots x_s | x_1' \dots x_s')$ are microscopically close to x_0, and all the x_i' are close to x_0', then P_s remains finite also when x_0 and x_0' are macroscopically distant from each other. In this case the condensation is characterized by the fact that the macroscopic number of "aggregates" of s particles falls in one s-particle natural state. Thus, individual bosons are responsible for the superfluid state (the NLRO appears in P_1), and Cooper pairs of fermions are responsible for the superconducting state (the NLRO appears in P_2).

It was shown later that the model wave functions describing the superconducting state satisfy the Yang criterion[2,3]. To the contrary, the absence of superconductivity in the one-dimensional model agrees with the fact that this criterion is not satisfied[4].

From the formal point of view, the presence of NLRO is characterized by the fact that the matrix P_s has a "large" ($\sim$N) eigenvalue (natural occupation number NOC). Yang proposed that in the limiting case the NOC for a system of fermions should be of the order of $\beta_s N^{s/2}$ (for even s and $N \to \infty$) and $\beta_s N^{(s-1)/2}$ (for s odd), where β_s does not depend on N[1]. He noted that in the presence of NLRO in a certain RDM this property should be possessed also by all RDM of higher orders.

Later Sasaki[5] and Coleman[6] have shown that actually the upper limits of the NOC P_s as $N \to \infty$ are not higher than $N^{s/2}(s-1)!!/s!!$ when s is even and $N^{(s-1)/2}s!!/(s-1)!!$ when s is odd. But the question of the possible approach to these boundaries, with the exception of the case s = 2, remained open.

In this article we construct wave functions (of the extremal type) for a system of fermions, on which the NOC can approach the limits indicated by Yang. We shall find the constants β_s and indicate that these limits correspond to the presence of NLRO in P_2. On the other hand, if NLRO appears at higher s = a, then the largest NOC of the higher-order RDM approach $\alpha_s N^{s/a}$. In a fermion system, the "condensing aggregate" must contain an even number of particles, i.e., the NLRO can appear first in RDM of second, fourth, sixth, etc. orders. It will be shown that the mechanism of increase of the NOC is connected with the increasingly symmetrical entry of the individual aggregates in the total wave function of the system.

2. We make the following construction. Assume that we are considering an RDM of s-th order for a system of N fermions with wave function of rank r. Let a (the dimension of the aggregate) be a common divisor of s, N, and r: s/a = p, N/a = n, and r/a = l. We break up the basis orbits

$$\overbrace{\varphi_1\varphi_2 \dots \varphi_a}^{1}\overbrace{\varphi_{a+1} \dots \varphi_{2a}}^{2} \dots \overbrace{\varphi_{(l-1)a+1} \dots \varphi_r}^{l}$$

into l aggregates of a pieces each, which are subsequently not intermixed. An aggregate will be characterized by its own number i. The wave function of the system is written in the form

$$\Psi_{(N)}(x_1 x_2 \dots x_N) = \sum_{(i)_n} c_{i_1 i_2 \dots i_n} \det_N[i_1 i_2 \dots i_n], \tag{1}$$

where $\det_N[i_1 i_2 \dots i_n]$ is constructed of the orbits of $i_1, i_2, \dots, i_n$ aggregates. The sum is taken over all $\binom{l}{n}$ aggregates of the possible choices of n numbers from the sequence $1, 2, \dots, l$. We shall henceforth assume that a is even. As will be shown below, the function (1) can have an NLRO only under this limitation. Therefore $\det_N[i_1 i_2 \dots i_n]$ will not change when the symbols $i_1 i_2 \dots i_n$ are interchanged, and it can be assumed that the indices of the coefficient $c_{i_1 i_2 \dots i_n}$ are arranged in increasing order. The normalization condition yields

$$\sum_{(i)_n} |c_{i_1 i_2 \dots i_n}|^2 = 1. \tag{2}$$

We now proceed to calculate the RDM for the function (1). Since the transition RDM of order s vanishes between two determinants that differ by more than s orbitals, it is obvious that when s < a

$$P_s(x|x') = \binom{N}{s} \int_u \Psi_{(N)}(xu)\Psi^*_{(N)}(x'u) = \sum_{(j)_s} \lambda_{j_1 j_2 \dots j_s} \det_s[\varphi_{j_1}\varphi_{j_2} \dots \varphi_{j_s}](x) \det_s{}^*[\varphi_{j_1}\varphi_{j_2} \dots \varphi_{j_s}](x') \tag{3}$$

This expression has the form of a natural expansion. The summation is over all possible $\binom{r}{s}$ choices of the orbits $\varphi_{j_1}\varphi_{j_2}\dots\varphi_{j_s}$ from the initial basis, regardless of the individual aggregates to which they belong. The NOC $\lambda_{j_1 j_2\dots j_s}$ is equal to the sum of the squares of the moduli of the coefficients $c_{i_1 i_2\dots i_n}$ such, that if the indices $j_1 j_2\dots j_s$ include the numbers of orbits from $i_\alpha\dots i_\gamma$ aggregates, then $i_\alpha\dots i_\gamma$ must be present along the $i_1 i_2\dots i_n$. By virtue of the normalization (2), all

$$\lambda_{j_1 j_2\dots j_s}\leqslant 1. \tag{4}$$

Thus, when $s < a$, there can be no NLRO in the system described by the function (1).

Let us calculate now the RDM for $s = a$. In this case the transition RDM differs from zero if the two determinants differ exactly by one aggregate (the index of which can be assumed to be in the first position):

$$P_a[ii_2\dots i_n, ki_2\dots i_n](x|x') = \binom{N}{s}\int\limits_u \det{}_N[ii_2\dots i_n](xu)\times\det{}_N^*[ki_2\dots i_n](x'u) = O_i(x)O_k^*(x'), \tag{5}$$

where $O_i(x)$ is a determinant of order a, made up entirely of the orbits of the i-th aggregate. Therefore in the diagonal part of the RDM for $\Psi_{(N)}$ we also separate the terms containing determinants of the type O_i, which are fully connected with the individual aggregate. The remaining terms contain determinants of order a, made up of the "randomly" chosen orbits. As a result we obtain

$$P_a(x|x') = \sum_{i,j=1}^{l}\Lambda_{ij}O_i(x)O_j^*(x') + \sum\lambda_{j_1 j_2\dots j_a}O_{j_1 j_2\dots j_a}(x)O^*_{j_1 j_2\dots j_a}(x'), \tag{6}$$

where $O_{j_1 j_2\dots j_a}$ is a determinant made up of the orbits $\varphi_{j_1}\varphi_{j_2}\dots\varphi_{j_a}$, which do not all belong to one aggregate. The NOC $\lambda_{j_1 j_2\dots j_a}$ are determined in accordance with the already mentioned rule, and all satisfy the inequality (4). Therefore "large" NOC can appear only among the eigenvalues of the matrix $\hat{\Lambda}$, pertaining to the nondiagonal part $P_a(x|x')$. The elements of $\hat{\Lambda}$ are determined in accordance with

$$\Lambda_{kj} = \sum_{\{i\}n-1} c_{i_1 i_2\dots k\dots i_n}c^*_{i_1 i_2\dots j\dots i_n},\quad k\neq j. \tag{7}$$

The sum is taken over all $\binom{l-2}{n-1}$ aggregates of $n-1$ indices $i_1 i_2\dots i_n$, taken from the numbers $1, 2, \dots, l$ (the two fixed indices k and j should be excluded from this sequence):

$$\Lambda_{kk} = \sum_{\{i\}n-1}|c_{i_1 i_2\dots k\dots i_n}|^2. \tag{8}$$

The sum here contains $\binom{l-1}{n-1}$ terms.

3. We now ascertain how NOC, close in order of magnitude to the number of the system particles, can appear among the eigenvalues of the matrix $\hat{\Lambda}$ can be partially effected under the following assumptions:

We break down arbitrarily the aggregates into assemblies of $l_1, l_2, \dots, l_t$ each:

$$\sum_{\alpha=1}^{t} l_\alpha = l. \tag{9}$$

The first assembly contains the aggregates with numbers $1, 2, \dots, l_1$, the second those with numbers $l_1 + 1, \dots, l_1 + l_2$, etc. We now assume that the coefficients of expansion of $\Psi_{(N)}$ in (1) depend only on how many aggregates from each separated assembly are present in the determinant, i.e.,

$$c_{i_1 i_2\dots i_n} = c(\nu_1\nu_2\dots\nu_t), \tag{10}$$

where ν_α is the number of indices from the α-th assembly among $i_1 i_2\dots i_n$. In such a case the elements of the matrix $\hat{\Lambda}$ (7) and (8) depend only on the assembly to which its indices belong, but not on their number. Thus, Λ breaks down into blocks

$$\hat{\Lambda} = \begin{pmatrix}\hat{\Lambda}_{11} & \hat{\Lambda}_{12} & \dots & \hat{\Lambda}_{1t}\\ \hat{\Lambda}_{21} & \hat{\Lambda}_{22} & \dots & \hat{\Lambda}_{2t}\\ \dots & \dots & \dots & \dots\\ \hat{\Lambda}_{t1} & \hat{\Lambda}_{t2} & \dots & \hat{\Lambda}_{tt}\end{pmatrix}, \tag{11}$$

where the nondiagonal blocks have the structure

$$\hat{\Lambda}_{\alpha\beta} = \varkappa_{\alpha\beta}\underbrace{\begin{pmatrix}1&1&\dots&1\\1&1&\dots&1\\ &\dots&&\\1&1&\dots&1\end{pmatrix}}_{l_\beta}\Bigg\}l_\alpha, \tag{12}$$

and the diagonal ones are equal to

$$\hat{\Lambda}_{\alpha\alpha} = \begin{pmatrix}\varkappa_\alpha & \varkappa_{\alpha\alpha} & \dots & \varkappa_{\alpha\alpha}\\ \varkappa_{\alpha\alpha} & \varkappa_\alpha & \dots & \varkappa_{\alpha\alpha}\\ \dots & \dots & \dots & \dots\\ \varkappa_{\alpha\alpha} & \varkappa_{\alpha\alpha} & \dots & \varkappa_\alpha\end{pmatrix} = \varkappa_{\alpha\alpha}\underbrace{\begin{pmatrix}1&1&\dots&1\\1&1&\dots&1\\ &\dots&&\\1&1&\dots&1\end{pmatrix}}_{l_\alpha}\Bigg\}l_\alpha + \mu_\alpha\hat{l}_\alpha. \tag{12'}$$

The numbers $\kappa_{\alpha\beta}, \kappa_{\alpha\alpha}, \kappa_\alpha$, and μ_α are determined from (7) and (8):

$$\varkappa_{\alpha\beta} = \sum_{\nu_1+\nu_2+\dots+\nu_t=n}\binom{l_1}{\nu_1}\dots\binom{l_\alpha-1}{\nu_\alpha}\dots\binom{l_\beta-1}{\nu_\beta-1}\dots\binom{l_t}{\nu_t}c(\nu_1\dots\nu_\alpha+1\dots\nu_\beta-1\dots\nu_t)c^*(\nu_1\dots\nu_\alpha\dots\nu_\beta\dots\nu_t),$$

$$\varkappa_{\alpha\alpha} = \sum_{\nu_1+\nu_2+\dots+\nu_t=n}\binom{l_1}{\nu_1}\dots\binom{l_\alpha-2}{\nu_\alpha-1}\dots\binom{l_t}{\nu_t}|c(\nu_1\dots\nu_\alpha\dots\nu_t)|^2,$$

$$\varkappa_\alpha = \sum_{\nu_1+\nu_2+\dots+\nu_t=n}\binom{l_1}{\nu_1}\dots\binom{l_\alpha-1}{\nu_\alpha-1}\dots\binom{l_t}{\nu_t}|c(\nu_1\dots\nu_\alpha\dots\nu_t)|^2,$$

$$\mu_\alpha = \varkappa_\alpha - \varkappa_{\alpha\alpha}. \tag{13}$$

The matrix (11) can be partially diagonalized by a transformation with a quasidiagonal unitary matrix[7]

$$\hat{U} = \begin{pmatrix}\hat{u}_1 & & & \\ & \hat{u}_2 & & \\ & & \ddots & \\ & & & \hat{u}_t\end{pmatrix},\quad \hat{u}_\alpha = \underbrace{(u^{(\alpha)}_{jk})}_{l_\alpha}\}l_\alpha,\quad u^{(\alpha)}_k = \frac{1}{\sqrt{l_\alpha}}\exp\frac{2\pi i(j-1)(k-1)}{l_\alpha}. \tag{14}$$

This transformation retains the block structure of (11), but transforms the blocks of (12) into

$$\hat{\Lambda}'_{\alpha\beta} = \varkappa_{\alpha\beta}\begin{pmatrix}\sqrt{l_\alpha l_\beta} & 0 & \dots & 0\\ 0 & 0 & \dots & 0\\ \dots & \dots & \dots & \dots\\ 0 & 0 & \dots & 0\end{pmatrix}. \tag{15}$$

Consequently, the eigenvalues of $\hat{\Lambda}$ will be μ_1 (of multiplicity $l_1 - 1$), μ_2 (of multiplicity $l_2 - 1$)... and μ_t (of multiplicity $l_t - 1$), and to find the remaining NOC it is necessary to diagonalize a matrix of order t (t – number of assemblies) with elements

$$\hat{\varkappa} = \begin{cases} \sqrt{l_\alpha l_\beta}\,\varkappa_{\alpha\beta} & \alpha \neq \beta \\ \varkappa_\alpha + (l_\alpha - 1)\varkappa_{\alpha\alpha}, & \alpha = \beta \end{cases}, \quad \alpha, \beta = 1, 2, \ldots, t. \tag{16}$$

The most important factor is that large NOC may again turn out to be only among the eigenvalues of the matrix $\hat{\kappa}$. In fact

$$\mu_\alpha = \sum_{\nu_1+\nu_2+\ldots+\nu_t=n} \binom{l_1}{\nu_1} \cdots \binom{l_\alpha - 2}{\nu_\alpha - 2} \cdots \binom{l_t}{\nu_t} |c(\nu_1 \ldots \nu_\alpha \ldots \nu_t)|^2, \tag{17}$$

since

$$\binom{l_\alpha - 1}{\nu_\alpha - 1} - \binom{l_\alpha - 2}{\nu_\alpha - 1} = \binom{l_\alpha - 2}{\nu_\alpha - 2}.$$

And inasmuch as

$$\binom{l_\alpha - 2}{\nu_\alpha - 2} < \binom{l_\alpha}{\nu_\alpha},$$

it follows from the normalization condition

$$\sum_{\nu_1+\nu_2+\ldots+\nu_t=n} \binom{l_1}{\nu_1} \cdots \binom{l_\alpha}{\nu_\alpha} \cdots \binom{l_t}{\nu_t} |c(\nu_1 \ldots \nu_\alpha \ldots \nu_t)|^2 = 1$$

that

$$\mu_\alpha < 1. \tag{18}$$

From (8) it follows that

$$\mathrm{Sp}\,\hat{\Lambda} = \sum_{k=1}^{l} \sum_{\{i\}_{n-1}} |c_{i_1 i_2 \ldots k \ldots i_n}|^2 = n \sum_{\{i\}_n} |c_{i_1 i_2 \ldots i_n}|^2 = n. \tag{19}$$

This means that the more small NOC μ_α are separated from $\hat{\Lambda}$, the larger are the eigenvalues of the matrix $\hat{\kappa}$, i.e., the smaller the number of symmetrical assemblies into which the aggregates are broken down, the sooner the condensation.

The limiting case t = 1 leads to a function of extremal type:

$$\Psi_{(N)} = \frac{1}{\sqrt{\binom{l}{n}}} \sum_{\{i\}_n} \det_N [i_1 i_2 \ldots i_n], \tag{20}$$

in which one of the NOC of the matrix $P_a(x|x')$ is

$$\xi_1^{(a)} = \varkappa_\alpha + (l-1)\varkappa_{\alpha\alpha} = n(l-n+1)/l \to N/a \text{ as } l \to \infty. \tag{21}$$

All the remaining NOC are equal to one another:

$$\mu_1 = n(n-1)/l(l-1) < 1. \tag{22}$$

Thus, for a function of the extremal type (20), made up of a-dimensional aggregates, the NLRO appears in $P_a(x|x')$, and all the aggregates are condensated in a state corresponding to $\xi_1^{(a)}$:

$$Q_{(a)}(x) = \frac{1}{\sqrt{l}} \sum_{i=1}' O_i(x) \tag{23}$$

which itself is a function of the extremal type of the a-particles.

4. It is now easy to prove that for a function of the extremal type the NLRO will be observed also in RDM of higher order. Let, for example, s = pa. We can verify that the extremal function of p aggregates

$$Q_{(s)}(x) = \frac{1}{\sqrt{\binom{l}{p}}} \sum_{\{i\}_p} \det_s [i_1 i_2 \ldots i_p] = \frac{1}{\sqrt{\binom{l}{p}}} \sum_{\{i\}_p} O_{\{i\}_p}(x) \tag{24}$$

is a natural s-state for $\Psi_{(N)}$ (20), belonging to

$$\xi_1^{(s)} = \binom{n}{p} \Big/ \binom{l-n+p}{p} \Big/ \binom{l}{p}. \tag{25}$$

To this end we simply calculate

$$\xi_1^{(s)} = \int_{xx'} Q_{(s)}(x) P_s(x|x') Q_{(s)}^*(x').$$

Substituting $\Psi_{(N)}$ (20) in the determinant P_s and taking $Q_{(s)}$ from (24), we get

$$\int_{xx'} Q_{(s)}(x) P_s(x|x') Q_{(s)}^*(x') = \sum_{j=1}^{k} A_{ij}, \quad k = \binom{l}{p},$$

$$A_{ij} = \binom{N}{s} \int_z \Phi_{\{i\}}(z) \Phi_{\{j\}}^*(z), \quad \Phi_{\{i\}}(z) = \int_x O_{\{i\}_p}(x) \Psi_{(N)}(x, z_j). \tag{26}$$

$\Phi\{i\}$ consists of "remnants" of those $\binom{l-p}{n-p}$ determinants $\Psi_{(N)}$, which contained the i-th set from the p aggregates $i_1 i_2 \ldots i_p$ (we use here the term "set" in order not to confuse it with the "assembly" used in Sec. 3). More accurately speaking, this is the token with a coefficient $\binom{l}{n}^{-1}\sqrt{s!/N!}$, of all the determinants made up of the ordered sets of n – p aggregates, and the aggregates entering in $\{i\}_p$ do not take part in their construction. The possibility of ordering the sequence of aggregates in the determinant is connected with the fact that a is even. How many identical determinants are present in the expansion of $\Phi_{(i)}$ and $\Phi_{(j)}$? If the sets of aggregates $\{i\}_p$ and $\{j\}_p$ differ by m aggregates, then the identical determinants are those from the expansion $\Phi\{i\}$ which do not contain the m remaining aggregates of the set $\{j\}_p$. There will be $\binom{l-p-m}{n-p}$ such determinants. Since upon integration in A_{ij} each of them yields a term (N – s)!, it follows that

$$A_{ij} = \binom{l-p-m}{n-p} \Big/ \binom{l}{n}. \tag{27}$$

Altogether there are $\binom{p}{m}\binom{l-p}{m}$ assemblies, differing in m aggregates from $\{i\}_p$. Therefore

$$\sum_{j=1}^{k} A_{ij} = \sum_{m=0}^{p} \binom{l-p-m}{n-p}\binom{p}{m}\binom{l-p}{m} \Big/ \binom{l}{n} = \binom{l-p}{n-p} \Big/ \binom{l}{n}$$

$$\times \sum_{m=0}^{p} \binom{p}{m}\binom{l-n}{m} = \binom{l-p}{n-p}\binom{l-n+p}{p} \Big/ \binom{l}{n} = \binom{n}{p}\binom{l-n+p}{p} \Big/ \binom{l}{p}, \tag{28}$$

as is obtained from (25). The fact that $Q_{(s)}$ will be an eigenstate for P_s can be seen from symmetry considerations.

With increasing rank ($l \to \infty$) the largest NOC for P_s (25) tends to $\binom{n}{p}$. Obviously, the maximum of this expression is reached at minimum a, i.e., at a = 2. Thus, for even N and s, the largest NOC is as close to $\binom{N/2}{s/2}$ as convenient. Using the Stirling formula,

we find that when $N \to \infty$ the largest NOC can tend to $(N/2)^{S/2}(s/2)! = N^{S/2}/s!!$. This differs from the already mentioned rough upper estimate, given by Coleman, in the absence of the factor $(s-1)!!$. In Yang's normalization we have for the constant β_S

$$\beta_s = s!/s!! \tag{29}$$

The obtained upper bound of the NOC corresponds to the strongest nondiagonal long-range correlation, when the elements of the condensate are pairs of fermions. In the case of a weaker NLRO, when the condensing aggregate consists of a fermions, $\binom{n}{p}$ tends to a lower limit as $N \to \infty$, namely $N^{S/a}/a^{S/a}(s/a)!$.

It is possible that a wave function with such a condensation of large aggregates turn out to be more suitable for the description of the nucleus than the ordinary function of superconductivity theory with pair condensation[8], particularly at $a = 4$, which corresponds to an α particle.

In all the foregoing reasoning a very important factor was that a is even. This has made it possible to order the aggregates which enter in the determinants of the expansion of $\Phi\{i\}$. This reveals the principal difference between fermions, the number of which in the aggregate must be even, and bosons. If a were to be odd for fermions, then roughly half the terms in the calculation of A_{ij} (26) would yield a negative contribution, and the entire construction could not lead to large NOC. For bosons, on the other hand, the entire construction remains in force also when a is even (of course, the determinants should be replaced by symmetrized products). Therefore for bosons the maximum of $\binom{n}{p}$ will occur not at $a = 2$ but at $a = 1$, i.e., the largest NOC approach to $\binom{sN}{N}$, in full agreement with the normalization of P_S to $\binom{N}{S}$. For fermions it is impossible to approach this limit, since they must be grouped into pairs.

From all the foregoing we can see how to carry out a similar construction for odd N and s in the case of fermions. It is necessary to "turn around" by one particle: we exclude temporarily one obit φ_0 from the basis and carry out the preceeding construction for even $N-1$ and $s-1$. At $a = 2$, the largest NOC approaches $\binom{(N-1)/2}{(s-1)/2}$. After this, it remains to include φ_0 in each determinant that enters in $\Psi_{(N-1)}$, and in each determinant from $Q_{(s-1)}$. The $Q_{(s)}$ obtained in this manner will be the natural s-state for $\Psi_{(N)}$, and the occupation number, obviously, remains the same as before: $\binom{(N-1)/2}{(s-1)/2}$. In the limit of large N this yields $N^{(s-1)/2}/(s-1)!!$ In accordance with the Yang hypothesis.

5. In conclusion we call attention to the fact that we did not concern ourselves at all with questions of dynamics, and did not investigate the type of system Hamiltonian necessary in order that functions close to extremal be its eigenfunctions. Now, however, we have at our disposal sufficiently abundant material for its use in the variational principle.

In particular, putting in (1) $c_{i_1 i_2 \ldots i_n} = c_{i_1} c_{i_2} \ldots c_{i_n}$ (with $a = 2$), we obtain the usual function of superconductivity theory[3,7,9]. We have, however, an even simpler possibility of forming a functions containing only one variational parameter, which can go over either into a function of the extremal type or into a Hartree-Fock determinant. To this end, as in Sec. 3, the aggregates must be divided into two sets ($t = 2$) and we must put $c(n, 0) = x$, and $c(\nu_1, n-\nu_1) = y$ for any $\nu_1 < n$, where the coefficients x and y are connected by the normalization

$$x^2 + y^2\left[\binom{l}{n} - 1\right] = 1.$$

The remaining parameter can be obtained from the variational principle, and it is possible to establish from (16) whether NLRO exists in the system. We propose to realize this program in the future.

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