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How the genetic code sees the right amino acid at a nanoscale distance?

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ABSTRACT

How the genetic code is coupled with the protein synthesis at a nanoscale distance is shrouded in mystery. Here we show that the coupling stems from a spin current and its polarization. The codon sends a spin of a certain orientation to the tRNA end. The spin recognizes its counterpart on the amino acid. If the spins are of opposite direction, the synthesis is allowed; if not, the synthesis is forbidden. The rule is flawless and rests on quantum computational experiment. ! 2013 Trade Science Inc. - INDIA

A specific feature of protein synthesis on ribosomes is in its fidelity " one mistake of 10.000 correctly assembled amino acids[1-3]. Such a flawless operation stems from a perfectly-tuned communication between the anticodon-codon (A-C; the codon consists of three nucleotides; the anticodon is its counterpart bound to the codon through the Watson-Crick hydrogen bonds[1]) reading segment (tRNA-mRNA; tRNA is a transport RNA and mRNA is a messenger RNA[1]) and the tRNA charging segment (both segments show a remarkable separation, 6#7 nm[1]) where the amino acid attachment occurs. How these segments see each other is shrouded in mystery[3].

The current publication reveals that high fidelity of operation comes from spin phase recognition existing between the segments. The data are a result of DFT:(L)APW+lo (Wien2k code[4]; the unit cell is a single nucleotide; the localization automatically switches the code to DFT:B3LYP, the A-C and the charging segments), computations (New York Blue Gene/L supercomputer parallel complex, NYCCS) of a simplified tRNA-mRNA structure (this is a necessary requirement because of the system's complexity), Figure 1. The mRNA consists of five nucleotides, G-C-G-U(C,A,G)-G; the U is variable (the core nucleotides, C-G-U(C,A,G), are complementary to the tRNA – the A-C segment). The end of the tRNA is conventional: C-C-A-OH. The end is able to interact with one of amino acids, AA = Arg, Gly, Ser, Gln; $AMP and $OH, Figure 1 (the dot stands for a radical). We treat the tRNA-mRNA core as "frozen" (the atomic positions are from the PDB, Japan). The computation variables are the distances (the computational step does not exceed 0.05) between the tRNA and mRNA (C-G-U(C,A,G) nucleotide sequence), AA, AMP, OH, and the H atom (the A-OH fragment) in the two volumes – 10%4%4 Å[3] (the A-C segment) and 18%2%23 Å[3] (the tRNA end together with the named molecules). Besides finding an optimal structure within the segments, the computations include the hyperfine coupling constants (*hfc*, scalar and vector; they come from interaction between the ^{31}P nuclei, 100% natural abundance[3], and the electrons in the

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places of their localization, the A-C segment and the tRNA end) and the spin polarization tensor. The radicals, •AMP and •OH, arise as a response to the ATP (adenosinetriphosphate) cleavage upon its binding to Mg cation/cations[5], which, first, convert the (Mg)-ATP into a triplet (T) state and, second, decompose it with a radical pair (•AMP and •OH, both spins are parallel that forbids their recombination) production and release the energy, 14.5 kcal/mol[5] (this energy goes on overcoming the two barriers in the two chemical reactions: A + •OH = •A + H_2O and •A + •AA = A-AA, Figure 2). The initial atomic positions in the A-C and tRNA segments are those obtained earlier in[6,7].

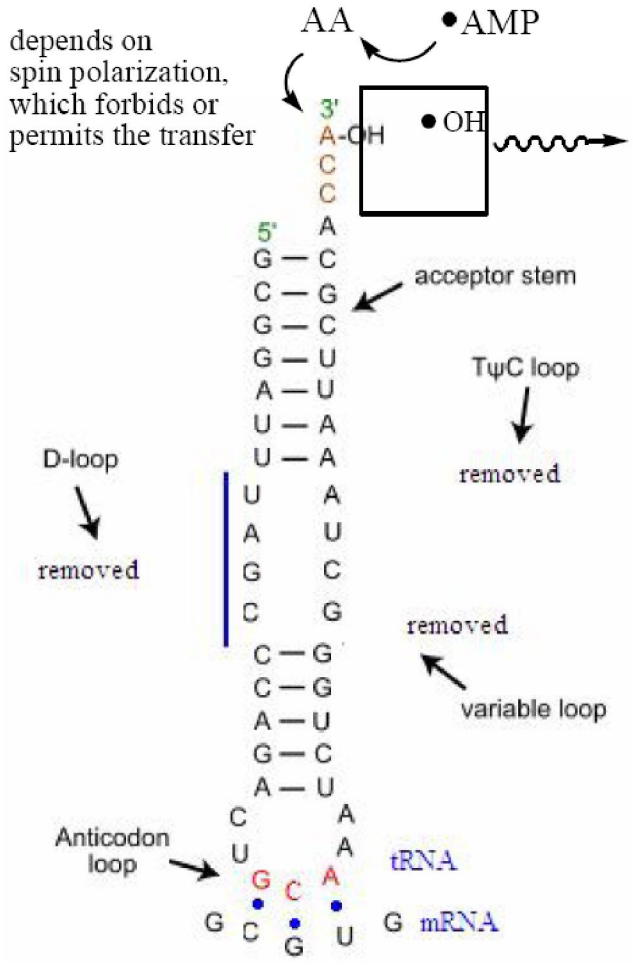

Figure 1 : A simplified structure of the tRNA that is used in quantum computations. The blue dots indicate the A-C segment. The atoms in the box produce the water. The curved arrows indicate spin transfers. The horizontal lines indicate hydrogen bonds. The blue vertical line indicates the nucleotides with no hydrogen bonding like in a real RNA.

The outlined structure reveals some intriguing facts. The complementary pairing, mRNA-tRNA (the A-C segment), shows a triplet-singlet (T-S) crossing[7]. Initially, both electrons are on the mRNA in the T state (the analogue of quantum dots and wires[8]). This state is energetically unfavorable. This assumes that one electron transfers on the tRNA with no spin flip (the T state remains unchangeable)[8]. Further, the electron on the tRNA goes as far as possible from its counterpart and occupies the A terminus nucleotide. The transfer transforms the tRNA end into a radical C-C-A. The named electron changes spin orientation on the •OH radical, opening the way to the •AMP-•OH pair recombination (T→S). However, the recombination does not occur since the HO•-H-O-A interaction appears to be more favorable[6]. The interaction breaks the H-O bond. Consequently, we have the water molecule and the biradical •(O-A•), or simply •A•. The two electrons on the A are unable to exist. Having the same spin orientation, T, they experience repulsion (the Pauli exclusion principle). One electron stays on the A, the other moves back to the A-C segment where it shows a flip (the flip is a response of the electron trap between the two identically oriented spins, Figure 2). When in S, the incoming electron transfers back onto the mRNA. This in turn shifts the reading frame (tRNA-mRNA) to a new position[1-3]. The outlined scenario is displayed in Figure 2. Totally, the spin flips are energetically negligible, ≤ 0.02 cm^{-1}. The energetically consuming are the process with •OH, •A, and •AA (see above). However, even these processes, despite their high energy barriers, release no energy, which supports the idea that biological reactions in living cells do not produce heat in normal state[1-3].

The most important thing for us is that the polarization of the remaining unpaired electron on the •A feels the polarization vector on the •AA, which gains spin density from the •AMP ((c) stage, Figure 2). If •AA and •A spin vectors are of opposite direction, the AA attaches to the oxygen atom of A (S state; initially, the AA and A are separated by 4.38 ¢) through its carbon atom, thus making the tRNA charged[3], if not – there is no interaction (•AA = Gly, Ser, Gln; the AA spin vector is normal to the spin vector on the A; even if we change the spin vector direction through the AA rotation, it makes the carbon(AA)-oxygen(A) interaction impossible since the rotation removes the named atoms from each other!).

The outlined mechanism of the genetic code operation explains the fidelity of the process of tRNA charging. The fidelity is strongly coupled with the spin

polarization between the A and AA, which originates from the spin of the genetic triplet nucleotide sequence. The right tRNA charging in turn determines the correct protein synthesis. The change of U for C,A,G corresponds to the same amino acid – Arg. The degeneracy in the nature of the third nucleotide (sometimes this occurs with the second nucleotide[1]) is strongly coupled with the electromagnetic vector potential A (+"$_l$Adx is a curvature along the path *l*; the A, in turn, determines the magnetic field B = ∇×A), which depends on a three-nucleotide curvature, Berry's phase[9] (if we consider a cloth path on the Poincare sphere), and thus the direction of a spin vector[7]. The latter becomes identical to the named nucleotides, U,C,A,G, since a cosine-dependent nature of the cotangent A space stretched over the phosphorus atoms (their presence enhance the strength of the electron spin through a giant coupling constant, $G_{ij} = 0.07 \div 0.1$ T, our results coincide with the experimental data (the MHz÷GHZ region)[10]; that is why the *hfc* computations are necessary, see above) returns the same total phase angle as a projection onto the Hilbert space, for details see[7].

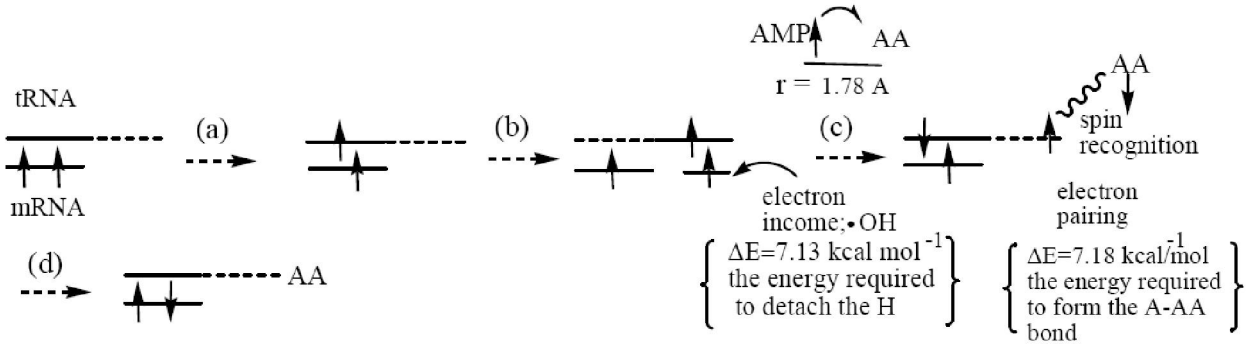

Figure 2 : Spin transfers in the mRNA-tRNA structure. The wavy line indicates interaction between the AA and A. Details are in text.

The *hfc* is an internal feature of living cells (the optimal value of the ^{31}P-electron coupling is reached just at 298-310^0 K, the MD DFT computations[6]). The *hfc* makes A spin-dependent. What we observe in our experiment is no more than a spin current. The driving force of this current is the spin torque[11]. Generally, the spin is a non-conserved value, but its spin momentum is conserved. The traveling of an electron over the tRNA molecule assumes its step-by-step interaction with the phosphorus atoms changing the momentum (the outlined curvature). To conserve the momentum the spin permanently changes its orientation. When coming to the tRNA end, the spin orientation coincides or not coincides (up to the sign) with the oppositely oriented spin on AA (in our experiment the length of tRNA is invariable; the variable segment is only A-C!!!). That is how the genetic code sees the right amino acid and makes the communication between the segments flawless.

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