# Correlation-coupling entropy as a measure of strong electron correlation and fragment-conditional density spin polarization as a measure of electron entanglement

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Quantum entanglement has been one of the hottest topics in current day physics, since it is the driving force behind quantum cryptography, quantum teleportation, and quantum computing. Several measures of quantification of entanglement have been proposed, each of which can often only be applied to a few specific systems. In this paper we derive a kinematic measure of entanglement that is capable of giving a full description of Einstein-Podolsky-Rosen entanglement in molecular systems. The associated "coupled entropy" energy contribution generates the correct amount of strong correlation energy for the $H_2$ and $N_2$ prototype systems, and is shown to be able to perform the same feat if it is explicitly used as the correlation component in the density-matrix functional context. And, finally, we propose a nonkinematic way to measure the entanglement of spins by using the conditional density of the system.

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## I. INTRODUCTION

The first-order density matrix (1RDM) $\gamma(\boldsymbol{x}_1, \boldsymbol{x}_1')$

$$\gamma(\boldsymbol{x}_1, \boldsymbol{x}_1') = N \int \Psi^*(\boldsymbol{x}_1', \ldots, \boldsymbol{x}_N)\Psi(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) d\boldsymbol{x}_2 \ldots d\boldsymbol{x}_N \tag{1}$$

and its diagonal, the electron density $\rho(\boldsymbol{x}_1)$

$$\rho(\boldsymbol{x}_1) = \gamma(\boldsymbol{x}_1, \boldsymbol{x}_1), \tag{2}$$

are the key descriptors of the averaged electron distribution in many-electron systems. In (1) $\Psi(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)$ is the generic wave function, where $\boldsymbol{x} = \{\boldsymbol{r}, s\}$ stands for both spatial $\boldsymbol{r}$ and spin $s$ electron coordinates. The one-electron functions $\rho$ and $\gamma$ serve as the basic arguments of the familiar density functional (DFT) [1–3] and density-matrix functional (DMFT) [4–17] theories, respectively. Useful information is contained in the conditional density

$$\rho^{\text{cond}}(\boldsymbol{x}_2|\boldsymbol{x}_1) = \frac{\rho_2(\boldsymbol{x}_1, \boldsymbol{x}_2)}{\rho(\boldsymbol{x}_1)} \tag{3}$$

extracted from the pair density $\rho_2(\boldsymbol{x}_1, \boldsymbol{x}_2)$, the diagonal of the second-order RDM (2RDM)

$$\rho_2(\boldsymbol{x}_1, \boldsymbol{x}_2) = N(N-1) \int \Psi^*(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N) \times \Psi(\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N) d\boldsymbol{x}_3 \ldots d\boldsymbol{x}_N. \tag{4}$$

The function $\rho^{\text{cond}}(\boldsymbol{x}_2|\boldsymbol{x}_1)$ gives the density of the electrons with the spin $s_2$ at $\boldsymbol{r}_2$ when the reference electron with the spin $s_1$ is at $\boldsymbol{r}_1$ [7].

One of the topics of this paper is the quantification of one of the most intriguing quantum phenomena: quantum entanglement [18–20]. Entanglement became one of the hottest issues in the present-day physics, giving birth to quantum cryptography [21] and quantum teleportation [22], and it is the basic phenomenon in quantum computing [23–26]. Then, the important theoretical point is the adequately defined measure of entanglement [27–33]. In this paper, a local $L^{\text{ent}}(\boldsymbol{r}_2(\in \Omega_B)|\boldsymbol{r}_1(\in \Omega_A)\sigma)$ and a global $G^{\text{ent}}(B|\boldsymbol{r}_1(\in \Omega_A)\sigma)$ measures of entanglement of formation of the mixed states in a bipartite system $AB$ are proposed based on the relaxed $\rho^{\text{cond}}$ (see below).

Apparently, strong electron correlation is a mechanism of electron entanglement in molecular systems, such as the paradigmatic dissociating hydrogen molecule $H_2$. Indeed, in the molecular realization of the Bohm version [19] of the famous Einstein-Podolsky-Rosen (EPR) *Gedanken* experiment [18] strong correlation dictates that the spin of the electron on the hydrogen atom $H_B$ is opposite to that measured on another atom $H_A$ of the entangled dissociating $H_2$ state. Then, the important theoretical point is to provide the kinematic (indirect) measure of strong correlation, which simultaneously can be used to correctly evaluate its energetic effect. In this paper, correlation-coupling entropy $S^{cc}$ is proposed as such a measure (see below).

## II. STRONG ELECTRON CORRELATION VIA CORRELATION-COUPLING ENTROPY

"Metathermodynamic" description of strong correlation with $S^{cc}$ is based on the adopted in DMFT notion of a fictitious ensemble noninteracting system, which has the same $\gamma(\boldsymbol{x}, \boldsymbol{x}')$ as the considered real interacting system [34–36]. This means that both systems have also the same eigenfunctions, the natural orbitals (NOs) $\chi_p$ and eigenvalues, and the natural occupation numbers (NONs) $n_i$ of $\gamma$

$$\gamma(\boldsymbol{x}, \boldsymbol{x}') = \sum_p n_p \chi_p^*(\boldsymbol{x}')\chi_p(\boldsymbol{x}). \tag{5}$$

The introduced noninteracting system is represented with the ensemble $N$-order density matrix ($N$DM) $\Gamma_{es}^N(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)$ constructed from the reference $N$-electron Slater determinant

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$\Phi_0$ (built from the first $N$ strongly occupied spin-NOs $\chi_i$) and its double excitations $\Phi_{ii}^{aa}$ to other NOs $\chi_a$

$$\Gamma_{es}^N = w_0|\Phi_0\rangle\langle\Phi_0| + \sum_{i,a} w_i^a \left|\Phi_{ii}^{aa}\right\rangle\left\langle\Phi_{ii}^{aa}\right|, \Gamma_{es}^N \to \gamma. \tag{6}$$

The ensemble weights $w_0$ and $w_i^a$ are related to the NONs as follows:

$$w_0 + \sum_{i(\neq j),a} w_i^a = n_j \tag{7}$$

for the "strong" occupations $n_j \geqslant \frac{1}{2}$ and

$$\sum_i w_i^a = n_a \tag{8}$$

for the "weak" occupations $n_a < \frac{1}{2}$. Then, the NOs and NONs can be considered as obtained from the minimization of the ensemble energy $E_s^e$

$$E_s^e = \mathrm{Tr}_N\left[H_s^N \Gamma_{es}^N\right], \tag{9}$$

where $H_s^N$ is the Hamiltonian of the noninteracting system, which consists of the one-electron operators

$$H_s^N = \sum_i^N \{h(\boldsymbol{r}_i) + v^{ee}(\boldsymbol{x}_i)\}. \tag{10}$$

Here, $h(\boldsymbol{r})$ is the standard one-electron operator with the local external potential $v(\boldsymbol{r})$

$$h(\boldsymbol{r}) = -\tfrac{1}{2}\nabla_{\boldsymbol{r}}^2 + v(\boldsymbol{r}), \tag{11}$$

while $v^{ee}(\boldsymbol{x})$ is the one-electron nonlocal effective potential of the electron-electron interaction [36,37].

The correlation-induced deviation of $\gamma$ of the introduced ensemble from idempotency can be used to define a measure of the correlation strength. In principle, the Shannon-type symmetrized correlation entropy $S^c$

$$S^c = -\sum_p [n_p \ln n_p + (1-n_p)\ln(1-n_p)] \tag{12}$$

can serve as a kinematic measure of strong correlation [38]. Unfortunately, $S^c$ cannot optimally serve our goal of adequately evaluating the energy of strong correlation $E_{sc}$ as the metathermodynamic entropy contribution of the type

$$E_{sc} = -\Theta S, \tag{13}$$

where $\Theta$ is the effective temperature. $S^c$ cannot differentiate between a system in which multiple isolated bonds are broken and one in which the broken bonds are themselves entangled with each other [17,27]. To this end, we introduce a measure of the departure of $\gamma$ from idempotency

$$S^{cc} = \frac{1}{4\ln 2}\sum_{i,j}\sqrt{-[n_i \ln n_i + (1-n_i)\ln(1-n_i)]} \times \sqrt{-[n_j \ln n_j + (1-n_j)\ln(1-n_j)]}. \tag{14}$$

In (14) the components of $S^c$ of (12) for the NOs are coupled, so we call it correlation-coupling entropy $S^{cc}$. This coupling allows one to use the pairwise correlation interactions of DMFT, the exchange integrals $K_{ij}$

$$K_{ij} = \langle ij|ji\rangle = \int \frac{\chi_i^*(\boldsymbol{x}_1)\chi_j^*(\boldsymbol{x}_2)\chi_j(\boldsymbol{x}_1)\chi_i(\boldsymbol{x}_2)}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} d\boldsymbol{x}_1 d\boldsymbol{x}_2 \tag{15}$$

as the partial effective temperatures (interaction strengths) $\Theta_{ij}$

$$\Theta_{ij} = K_{ij}. \tag{16}$$

With this, $E_{sc}$ is expressed as follows:

$$E_{sc} = -\frac{1}{4\ln 2}\sum_{i,j}\Theta_{ij}\sqrt{-[n_i \ln n_i + (1-n_i)\ln(1-n_i)]} \times \sqrt{-[n_j \ln n_j + (1-n_j)\ln(1-n_j)]}. \tag{17}$$

Then, the total electronic energy $E_{\mathrm{HFE}}$ of a system with strong correlation can be written as the sum

$$E_{\mathrm{HFE}} = E_{\mathrm{HF}}^{\gamma} + E_{sc}, \tag{18}$$

where $E_{\mathrm{HF}}^{\gamma}$ is the Hartree-Fock (HF) energy evaluated using $\gamma(\boldsymbol{x}, \boldsymbol{x}')$ of the ensemble

$$E_{\mathrm{HF}}^{\gamma} = 2\sum_i n_i h_{ii} + \sum_{i,j} n_i n_j (2J_{ij} - K_{ij}), \tag{19}$$

with $J_{ij} = \langle ij|ij\rangle$ being the Coulomb integral and the sums are over all orbitals.

The paradigmatic system with strong nondynamic electron correlation is the (stretched) $H_2$ molecule. In the dissociating limit strong nondynamic correlation is adequately described with the Heitler-London (HL) model with only one antibonding $\chi_u$ orbital in addition to $\chi_g$. The HF energy of $H_2$ (19) in the dissociation limit is given by

$$E_{\mathrm{HF}}^{\gamma} \approx h_{gg} + h_{uu} + \tfrac{1}{4}J_{gg} + \tfrac{1}{4}J_{uu} + J_{gu} - \tfrac{1}{2}K_{gu} \tag{20}$$

and the proposed strong correlation energy expression (17) has the correct asymptotic correction

$$E_{sc} \approx -\tfrac{1}{4}J_{gg} - \tfrac{1}{4}J_{uu} - \tfrac{1}{2}K_{gu}, \tag{21}$$

which renders the correct bond $R$(H-H) dissociation asymptotics also for the total energy (18)

$$E_{\mathrm{HFE}} \approx h_{gg} + h_{uu} + J_{gu} - K_{gu} \approx h_{gg} + h_{uu} + \frac{1}{R}. \tag{22}$$

Table I displays the energies (18) calculated for $H_2$ at the equilibrium $R = 1.4$ bohr and stretched $R = 10.0$ bohr bond distances within the above mentioned two-orbital HL model. The NOs and NONs are taken from the corresponding CASSCF(2,2) calculations with two HL NOs. These NOs are also inserted in the HF part (19) of (18).

TABLE I. All H-H distances are in bohr. 6-31G* basis. CASSCF(2,2) NOs and NONs were used to evaluate the $E_{\mathrm{HF}}^{\gamma}$ and $E_{sc}$ entries.

| $R$ | 1.4 | 10.0 |
|---|---|---|
| $E_{\mathrm{HF}}$ | −1.1267 | −0.7481 |
| $E_{\mathrm{HF}}^{\gamma}$ | −1.0966 | −0.6821 |
| $E_{\mathrm{HF}}^{\gamma} + E_{sc}$ | −1.1369 | −0.9965 |
| $E_{\mathrm{CASSCF(2,2)}}$(NO) | −1.1462 | −0.9965 |
| $E_{\mathrm{FCI}}$ | −1.1517 | −0.9965 |

TABLE II. All N-N distances are in bohr. 6-31G* basis. CASSCF(6,6) NOs and NONs were used to evaluate the $E_{\mathrm{HF}}^{\gamma}$ and $E_{sc}$ entries.

| $R$ | 2.075 | 10.0 |
|---|---|---|
| $E_{\mathrm{HF}}$ | −108.9426 | −107.7976 |
| $E_{\mathrm{HF}}^{\gamma}$ | −108.7928 | −107.5997 |
| $E_{\mathrm{HF}}^{\gamma}+E_{sc}$ | −109.0132 | −108.7646 |
| $E_{\mathrm{CASSCF(6,6)}}$ | −109.0786 | −108.7646 |
| $E_{MRCI}$ | −109.2668 | −108.9368 |

One can see from Table I that the energy (18) reasonably reproduces the reference CASSCF(2,2) energy of the $H_2$, which at $R = 10.0$ bohr coincides with that of the full CI (FCI) in the chosen basis. This means that the proposed metathermodynamical approach fully grasps strong nondynamic electron correlation in this paradigmatic case. Then, the relative lowering of the FCI energy at the equilibrium compared to those of CASSCF(2,2) and (18) is due to the inclusion within the former of a large part of dynamic correlation.

Application to another paradigmatic case of strong nondynamic correlation, the triple-bonded $N_2$ molecule, shows further virtues of the proposed description (14), (17) of strong correlation via the correlation-coupling entropy. The apparent nonadditivity of $S^{cc}$ of (14), in fact, correctly reflects the actual nonadditivity of correlation coupling in the dissociating multiple-bonded molecules. In particular, the correlation coupling in the dissociating $N_2$ does not reduce to the sum of the correlation couplings in the individual bonds. The point is that the $N_2$ dissociates to the symmetrized combination of quartet ground states of two N atoms. This entails extra nonadditive coupling between the electrons of different $\sigma$- and $\pi$-electron pairs [39]. All these couplings are accounted for in the CASSCF(6,6) calculation, which includes all possible excitations in the active space of six frontier $\sigma$- and $\pi$-bonding and antibonding orbitals.

One can see from Table II that the energy (18) is close to the reference CASSCF(6,6) energy of the $N_2$ at the stretched $R = 10.0$ bohr bond distance. At the $R = 2.075$ bohr equilibrium distance the $E_{sc}$ is able to close the majority of the gap between the NO based HF and CASSCF(6,6) energies. It is still missing roughly 0.06 hartree of correlation. The order of magnitude of the missing energy is very close to the amount of energy that has been shown to be related to dispersion type interaction that can only be described by using integrals that use four different orbital indices [17]. This type of correlation is purely dynamical in nature, so the proposed correlation-coupling approach seems to fully grasp both intra- and interpair effects of strong nondynamic correlation.

In addition to being able to describe and extract strong correlation from a one-body density matrix generated by a wave function, $E_{\mathrm{HFE}}$ can also be seen as a full DMFT functional that can be used independently. A relatively faithful approximation of the logarithmic form of $E_{sc}$ in terms of symmetrical particle hole products is given by

$$E_{sc} \approx -\sum_{i,j} \Theta_{ij} \frac{1}{4\left(\frac{1}{16}\right)^p} [n_i(1-n_i)n_j(1-n_j)]^p, \tag{23}$$

with $p = 0.38$. A more commonly known functional, the corrected Hartree Fock or Hartree Fock Bogoliubov (HFB) functional, is recovered in case one sets $p = 0.5$. So one could view this $E_{\mathrm{HFE}}$ functional as a more strongly correlated version of the HFB functional. The HFB functional itself is known to suffer from variational collapse [40], which can be avoided by imposing occupation number contraints [41]. In order to test the self-consistent performance of the HFE functional we have applied the (nonapproximated) logarithmic form to the $H_2$, LiH, $H_2O$, and $N_2$ molecules. We have also performed HFB and CASSCF calculations for comparison purposes. In case of the first three molecules the active space is spanned by two orbitals whose occupation sums up to two electrons. In the case of the $N_2$ molecule the HFB and HFE active space is spanned by three sets of two orbitals whose occupations sum up to two electrons each, while CASSCF uses all six orbitals. The remaining core and deep valence orbitals have their occupations fixed at full occupancy, although the orbitals themselves are still optimized. The potential-energy surfaces are shown in Fig. 1. The $H_2$ and and $H_2O$ curves show that the HFE functional is able to reproduce almost the entire CASSCF curve, only missing a small amount of correlation in the equilibrium region. The "normal" HFB curves, on the other hand, are on top of the HF curves for a relatively long time before separating and going to the CASSCF dissociation limit. So the HFE functional is more capable of giving a balanced description of the change of nondynamical correlation along the entire curve. The same situation can also be seen for the $N_2$ molecule, the only difference being that the presence of dispersive dynamical correlation terms in the CASSCF space causes a larger discrepancy between the HFE and CASSCF equilibrium energies. Both the HFB and HFE functional overestimate the dissociation limit energy for the LiH molecule. This is a known problem of HFB like functionals when they are used in self-consistent calculations of dissociations involving two different atoms or fragments, and can be fixed by adding an appropiate constraint term to the energy [42]. Overall the performance of the HFE functional is good enough to warrant further investigation in the future.

## III. FRAGMENT SPIN POLARIZATION OF THE CONDITIONAL DENSITY AS A MEASURE OF ENTANGLEMENT

Now, we return to the nonkinematic (direct) measure of entanglement in a system $AB$ based on the conditional density. To provide such a measure, it is crucial to use the relaxed $\rho^{\mathrm{cond}}$, which is adjusted to the presence of the reference electron with a certain spin at a certain position. Consider, for example, the $\beta$-spin component $\rho^{\mathrm{cond}}(\boldsymbol{r}_2\beta|\boldsymbol{r}_1\alpha)$ of the conditional density of the dissociating $H_2$ relaxed in the presence of the reference electron with the spin $\alpha$ in the region $\boldsymbol{r}_1 \in \Omega_A$ of a certain H atom $H_A$. Then, strong electron correlation dictates that the relaxed $\rho^{\mathrm{cond}}(\boldsymbol{r}_2\beta|\boldsymbol{r}_1\alpha)$ turns to the electron density of another H atom $H_B$

$$\rho^{\mathrm{cond}}(\boldsymbol{r}_2\beta|\boldsymbol{r}_1(\in \Omega_A)\alpha) \approx \rho_{H_B}(\boldsymbol{r}_2). \tag{24}$$

In a general case of a bipartite closed-shell system $AB$, we propose a local $L^{\mathrm{ent}}(\boldsymbol{r}_2(\in \Omega_B)|\boldsymbol{r}_1(\in \Omega_A)\sigma)$ and a global $G^{\mathrm{ent}}(B|\boldsymbol{r}_1(\in \Omega_A)\sigma)$ measures of entanglement based on the

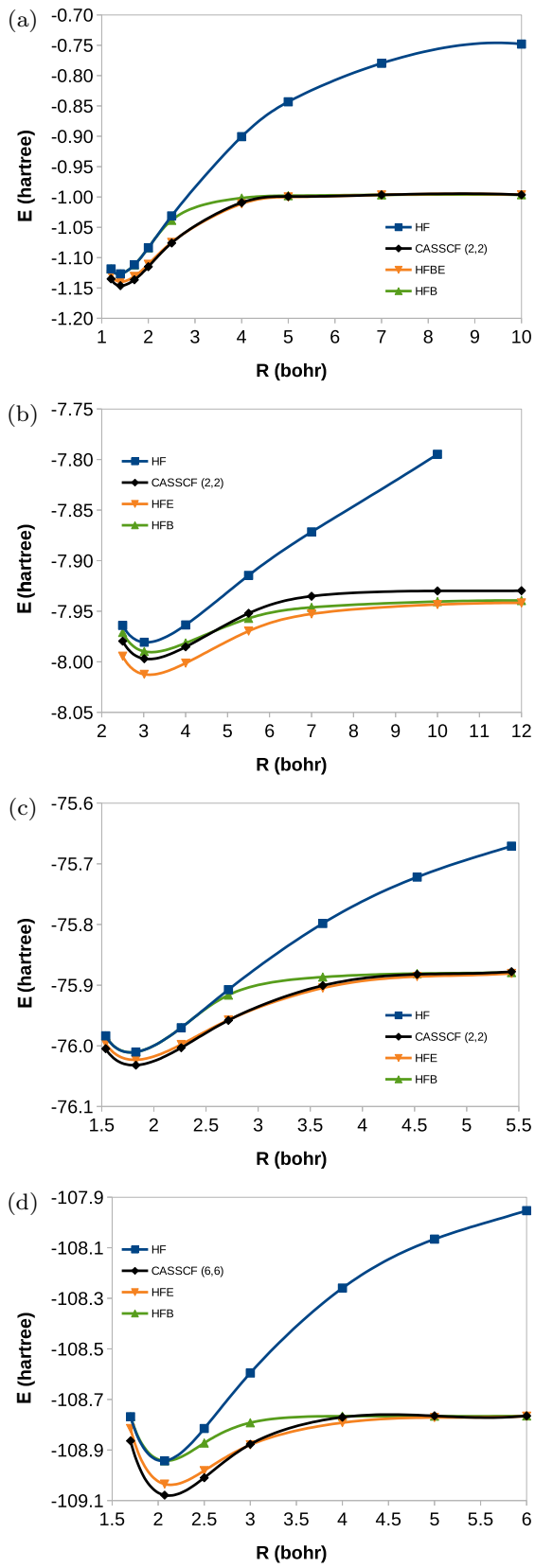


FIG. 1. Potential-energy curves (6-31G*) for $H_2$ (a), LiH (b), $H_2O$ (c), and $N_2$ (d). The $H_2O$ equilibrium geometry is slightly distorted in order to break the symmetry. Only a single O-H bond is broken for the $H_2O$ molecule.

relaxed $\rho^{\text{cond}}$ characterized above. The function $L^{\text{ent}}(\boldsymbol{r})$ is defined as the spin polarization of the conditional density on fragment $B$, which is relaxed in the presence of the reference electron with spin $\sigma$ placed in the (strongly correlated valence) region of fragment $A$

$$\begin{aligned} &L^{\text{ent}}(\boldsymbol{r}_2(\in \Omega_B)|\boldsymbol{r}_1(\in \Omega_A)\sigma) \\ &\quad = \rho^{\text{cond}}(\boldsymbol{r}_2(\in \Omega_B)\sigma'(\neq \sigma)|\boldsymbol{r}_1(\in \Omega_A)\sigma) \\ &\qquad -\rho^{\text{cond}}(\boldsymbol{r}_2(\in \Omega_B)\sigma|\boldsymbol{r}_1(\in \Omega_A)\sigma). \end{aligned} \tag{25}$$

In the considered example of the dissociating $H_2$ the second term in the right-hand side of (25) vanishes due to the strong correlation driven full spin polarization on the individual H atoms. With this, $L^{\text{ent}}$ turns to just $\rho_{H_B}$

$$L^{\text{ent}}(\boldsymbol{r}_2(\in \Omega_B)|\boldsymbol{r}_1(\in \Omega_A)\sigma) \approx \rho_{H_B}(\boldsymbol{r}_2). \tag{26}$$

Next, we introduce the global measure of entanglement $G^{\text{ent}}$ as the number of the unpaired electrons on the fragment $B$ obtained for the relaxed conditional density as the integral of $L^{\text{ent}}(\boldsymbol{r})$ over the fragment $B$:

$$G^{\text{ent}}(B|\boldsymbol{r}_1(\in \Omega_A)\sigma) = \int_{\Omega_B} L^{\text{ent}}(\boldsymbol{r}_2(\in \Omega_B)|\boldsymbol{r}_1(\in \Omega_A)\sigma)d\boldsymbol{r}_2. \tag{27}$$

Apparently, in the considered example of the dissociating $H_2$ the proposed $G^{\text{ent}}$ tends to 1 with $R$ and its parametrical dependence of the position $\boldsymbol{r}_1$ of the reference electron on $A$ is weak

$$\forall \boldsymbol{r}_1 \in \Omega_A, G^{\text{ent}}(B|\boldsymbol{r}_1(\in \Omega_A)\sigma) \to 1, \quad R(\text{H}-\text{H}) \to \infty. \tag{28}$$

Furthermore, in the example considered above of the dissociating $N_2$ the strong intra- and interpair electron correlation makes the spins of three bonding electrons on the nitrogen atom $N_B$ all opposite to the predetermined spin $\sigma$ of the reference electron located in the bonding region $\boldsymbol{r}_1 \in \Omega_A(bond)$ of another nitrogen atom $N_A$ (assuming that atom $A$ has a local maximum $s_z$ value). Then, apparently, the proposed $G^{\text{ent}}$ tends to three with $R$ and its parametrical dependence of the position $\boldsymbol{r}_1$ of the reference electron in the bonding region of $N_A$ is, again, weak:

$$\begin{aligned} &\forall \boldsymbol{r}_1 \in \Omega_A(bond), \quad G^{\text{ent}}(B|\boldsymbol{r}_1(\in \Omega_A)\sigma) \to 3, \\ &qR(\text{N}-\text{N}) \to \infty. \end{aligned} \tag{29}$$

## IV. DISCUSSION AND CONCLUSIONS

The introduced measures of entanglement $L^{\text{ent}}$ and $G^{\text{ent}}$ give a rigorous quantum-mechanical description of the EPR *Gedanken* experiment [18] in its simplified version by Bohm [19]. Indeed, fixing the spin of the reference electron to $\sigma$ on the atom $H_A$ of the entangled state of the dissociating $H_2$ is equivalent to measuring the electron spin of this atom by Alice. Then, because of entanglement, Bob will instantly receive the opposite spin on another atom $H_B$, which is adequately represented with the value 1 of the proposed $G^{\text{ent}}$.

Moreover, the introduced measures adequately describe the multientanglement extension of the EPR experiment with the considered example of the dissociating $N_2$. Fixing the spin of the reference electron to $\sigma$ in the bonding region of the atom

$N_A$ of the entangled state of the dissociating $N_2$ is equivalent to the hypothetical measuring of the spin of the electron of the corresponding breaking bond on the atom $N_A$ by Alice. Then, because of multiple entanglement, Bob will instantly receive three opposite spins on another atom $N_B$, which is adequately represented with the value 3 of the proposed $G^{\text{ent}}$.

We have seen that the metathermodynamical energy correction (17) is perfectly capable of describing the bond breaking processes. However, the entropy component of this energy (14) scales quadratically, which means that it does not have the proper additive property that an entropy measure should have, i.e., adding an identical noninteracting copy of the system to the system does not result in the doubling of the entropy, since additional cross terms appear. The energetic correction does not suffer from any difficulties due to the fact that it uses an exchange integral, which nullifies any entropic terms between noninteracting parts of the system. One could define a spatially modified entropy of the form

$$S^{cco} = \frac{1}{4\ln 2}\left(\sum_i -[n_i \ln n_i + (1-n_i)\ln(1-n_i)] + \sum_{i\neq j} O_{ia}\sqrt{-[n_i \ln n_i + (1-n_i)\ln(1-n_i)]} \times \sqrt{-[n_j \ln n_j + (1-n_j)\ln(1-n_j)]}\right), \tag{30}$$

where

$$O_{ia} = \int |\chi_i(\boldsymbol{r}_1)||\chi_a(\boldsymbol{r}_1)| d\boldsymbol{r}_1. \tag{31}$$

This entropy would not suffer from the additive collapse. We have also proposed a conditional density based scheme that can measure the entanglement directly. Work on both of these schemes is in progress.


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