# Finite range effects in trapped bosons systems

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**Abstract**: We consider a system of two bosons trapped in a one-dimensional harmonic oscillator potential interacting by a finite-range gaussian potential. We study the dependence of its energy spectrum as a function of the strength and range of the interaction. The dynamic structure function associated with the monopolar excitation is computed and analysed by explicitly employing the eigenstates of the system. We also characterise the dynamic structure function with the energy sum rules. Finally, a comparison with the results provided by a contact interaction is also presented.

## I. INTRODUCTION

Recent advances in ultra-cold atomic gases have provided opportunities to study systems of few atoms, fermions or bosons, trapped in potentials with different geometries[1].

In the case of bosons, we consider the most straightforward example: two non-interacting particles confined in a harmonic oscillator potential. In the ground state, the two particles condense in the same lowest single-particle state [2][3]. Now, if we introduce a contact interaction and explore the limit of infinite strength, we see how the two bosons resemble two spinless non-interacting fermions, producing the so-called Tonks-Girardeau state[4].

In this paper, we want to study the effects of considering a finite-range force instead of a contact one. To this end, we concentrate on a system of two identical bosons interacting through a finite-range gaussian interaction confined in a 1D harmonic oscillator potential. We study the energy spectrum of the system when we vary the interaction strength for a given range of the interaction potential. In addition, we analyse the response of the system to a monopolar excitation by the calculation of its associated dynamic structure function, exploring its dependence on the strength and range of the interaction. We also compare all the results with the ones produced by a contact interaction[5][6].

The paper is organised in the following way: In Sec.II we characterise the Hamiltonian of the system and explain the procedure to obtain the eigenvalues and eigenstates. A brief discussion of the convergence of the results is also presented. In Sec.III, we show the dependence of the ground and excited states on the intensity of the finite-range interaction. In Sec.IV, we compute the dynamic structure function associated with the monopolar excitation for several interactions strengths and evaluate the energy sum rules of the dynamic structure function. Finally, in Sec.V, we summarise our conclusions.

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## II. THEORETICAL METHOD

The system is formed by two bosons confined in 1D harmonic oscillator (h.o) interacting through a Gaussian potential.

$$V(x_i - x_j) = \frac{\bar{g}}{\sqrt{2\pi\bar{\sigma}^2}} e^{-\frac{(x_i - x_j)^2}{2\bar{\sigma}^2}}\,, \tag{1}$$

being $\bar{g}$ and $\bar{\sigma}$ the parameters that characterize the strength and range of the potential respectively. Thus, the Hamiltonian of our system reads:

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx_1^2} - \frac{\hbar^2}{2m}\frac{d^2}{dx_2^2} + \frac{1}{2}m\omega^2 x_1^2 + \frac{1}{2}m\omega^2 x_2^2 + \frac{\bar{g}}{\sqrt{2\pi\bar{\sigma}^2}} e^{-\frac{(x_1 - x_2)^2}{2\bar{\sigma}^2}}\,. \tag{2}$$

This Hamiltonian can be split in two pieces by defining the centre of mass (c.m.) and relative coordinates as, $X = \frac{(x_1+x_2)}{2}$ and $x_r = x_1 - x_2$. In addition, from now on we will use harmonic oscillator units. Finally one gets:

$$H_{c.m.} = -\frac{1}{4}\frac{d^2}{dX^2} + X^2\,,$$
$$H_r = -\frac{d^2}{dx_r^2} + \frac{1}{4}x_r^2 + g\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x_r^2}{2\sigma^2}}\,. \tag{3}$$

### A. Numerical method

As a result of splitting the Hamiltonian, the wave function can be factorized in a c.m. and relative wave functions:

$$\Psi(X, x_r) = \phi(X)\psi(x_r)\,. \tag{4}$$

Paying attention to (Eq.3) we can see that $H_{c.m.}$ has a similar form as an harmonic oscillator Hamiltonian. Hence, the spectrum of this $H_{c.m.}$ is $E_k^{c.m.} = k + 1/2$, $(k = 0, 1, 2, ...)$.

To solve $H_r$ we have to diagonalise the matrix of the relative Hamiltonian (Eq.3). We choose a finite number

of eigenstates of the non-interacting part of the relative Hamiltonian $\{\psi_0(x_r), \psi_2(x_r), ..., \psi_{2M}(x_r)\}$ and compute the matrix elements of $H_r$ (Eq.5). Notice that to fulfil the symmetry requirements of boson wave functions, we only contemplate the modes corresponding to even functions.

The matrix elements are given by:

$$\langle \Psi_{2m} \mid H_r \mid \Psi_{2n} \rangle = \left(\frac{1}{2} + 2n\right) \delta_{m,n} + \int_{-\infty}^{\infty} \Psi^*_{2m} V(x_r) \Psi_{2n} dx_r = \left(\frac{1}{2} + 2n\right) \delta_{m,n} + N_{2m} \frac{g}{\sqrt{2\pi\sigma^2}} N_{2n} \int_{-\infty}^{\infty} H_{2m}\left(\frac{x_r}{\sqrt{2}}\right) H_{2n}\left(\frac{x_r}{\sqrt{2}}\right) e^{\frac{-x_r^2}{2}} e^{\frac{-x_r^2}{2\sigma^2}} dx_r \,. \quad (5)$$

The final result is[7]:

$$< \Psi_{2m} \mid H_r \mid \Psi_{2n} >= \left(\frac{1}{2} + 2n\right) \delta_{m,n} + N_{2m} g \frac{1}{\sqrt{2\pi\sigma^2}} N_{2n} \sqrt{2}\, I_{2m,2n} \,, \quad (6)$$

where $N_{2m}$ and $N_{2n}$ are normalization factors and $I_{2m,2n}$ is the result of the integral indicated above:

$$N_{2m} = \frac{1}{\sqrt[4]{2\pi}} \frac{1}{\sqrt{2^{2m}(2m)!}} \,. \quad (7)$$

$$I_{2m,2n} = \sum_{k_1=0}^{m} \sum_{k_2=0}^{n} \frac{(2m)!(-1)^{k_1}\, 2^{2m-2k_1}}{k_1!(2m-2k_1)!} \frac{(2n)!(-1)^{k_2}\, 2^{2n-2k_2}}{k_2!(2n-2k_2)!} A^{-\frac{1+q}{2}}\, \Gamma\left(\frac{1+q}{2}\right) \,. \quad (8)$$

### B. Convergence

In practice, the factorials in the integral of (Eq.8) grow rapidly, even for low modes. For that reason, we have tried to simplify the expressions involving the factorials. However, the maximum number of modes that we can use is M=85. That limits the convergence of our results to a specific range of $g$ and $\sigma$.

Analysing the convergence of the energy as a function of the number of modes for a given value of $g$ and different $\sigma$ we observe that for small values of $\sigma$, $\sigma \lesssim 0.1$, we need a higher number of modes.

One way to study the convergence of the procedure is by checking the fulfilment of the virial theorem. For this specific finite-range interaction it is expressed as:

$$-2E_{kin} + 2V_{h.o} - \frac{\langle x_r^2 V_{int}(x_r)\rangle}{\sigma^2} = 0 \,. \quad (9)$$

The number of modes M=85 seems to provide a good convergence in the full range of $g$ and $\sigma$ considered, see Fig. 1. In that figure we represent the virial and its different contributions where the negative sum part $-2E_{kin} - \frac{\langle x_r^2 V_{int}(x_r)\rangle}{\sigma^2}$ compensates the harmonic potential factor $2V_{h.o}$ fulfilling the virial.

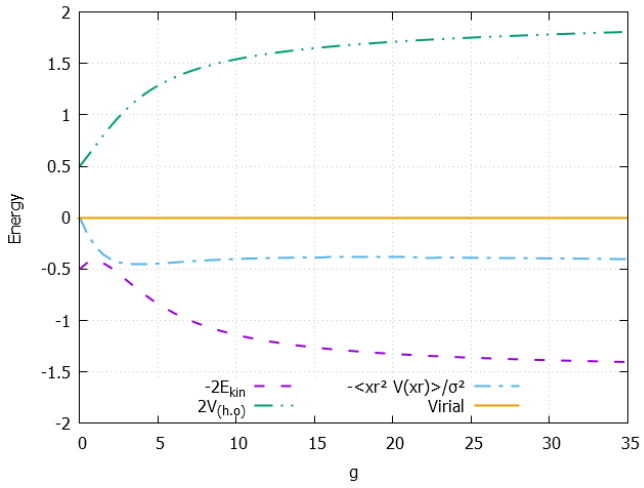


FIG. 1: Virial and its different contributions as a function of the strength interaction $g$ for $\sigma = 0.2$ and M=85.

## III. STATIC PROPERTIES

By diagonalizing $H_r$ (Eq.6) in a finite Hilbert space (a finite number of modes), we get approximate solutions, whose eigenvalues are upper bounds of the exact solutions.

$$H_r \tilde{\Psi}_l = \tilde{E}_l^{(r)} \tilde{\Psi}_l \,. \quad (10)$$

### A. Ground state

In Fig. 2 we show the dependence of the ground state energy and its different contributions, including the c.m. energy, on the interaction strength for a given $\sigma = 0.2$. We see that the total ground state energy grows from E=1 when $g = 0$, where the system has no interaction and the eigenvalues are the solutions of the harmonic oscillator problem, to a value slightly greater than 2 for $g = 15$. The harmonic potential energy increases monotonically with $g$ starting at $V_{h.o} = 0.5$ for $g = 0$. However, the kinetic energy goes through a minimum $g \approx 2$ and after rises monotonically with $g$. The interaction energy grows for small values of $g$ until it reaches a maximum at approximately $g = 2.5$; then, it decreases as $g$ grows further.

In the case of a contact interaction the total, kinetic and potential energy reach a limit saturating values, E=2 and $V_{h.o} = E_{kin} = 1$ for $g = \infty$. In this limit, the two bosons resemble two spinless non-interacting fermions. It

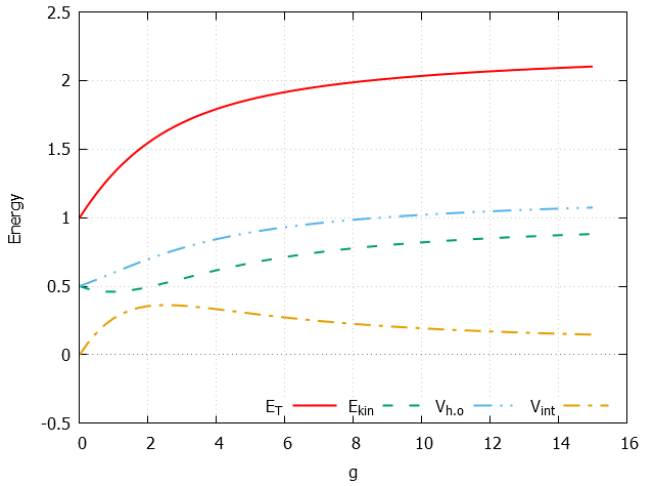


FIG. 2: Total ground state energy (red) and its different contributions: $E_{kin}$(green), $V_{h.o}$(blue), $V_{int}$(orange) as a function of the interaction strength $g$ with $\sigma = 0.2$ and M=85.

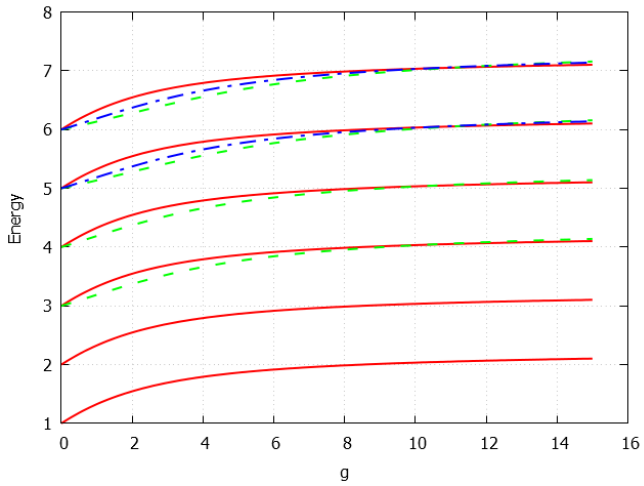


FIG. 3: Lowest energy levels for a system of two bosons with finite range interaction as a function of the interaction strength $g$ for $\sigma$=0.2 and M=85. The red lines correspond to the ground state of the relative motion. The green and blue lines are the first and second relative excitations. The results also consider the centre of mass excitations. For that reason, the red lines are parallel and describe different excitations of the c.m..

is the so-called Tonks-Girardeau limit [4]. For a finite-range interaction, we observe a similar behaviour of the different contributions to the energy. Although, the total, kinetic and potential energies exceed the limit defined by the contact interaction. This phenomenon is also observed in Ref.[6].

### B. Energy spectrum

The full spectrum of the system will be the sum of the centre of mass and relative energies,

$$E_{k,l} = E_k^{(c.m.)} + \tilde{E}_l^{(r)} \,. \tag{11}$$

In Fig. 3, we plot the lowest energy levels of the spectrum as a function of $g$. We observe that all eigenvalues grow monotonically from the non-interacting bosonic system $g = 0$ up to $g = 15$, where the energy exceeds the saturation values found for a contact interaction [5][4],which correspond to the Tonks-Girardeau limit.

This fact can be understood analysing the evolution of the ground state. For $g = 0$, the two bosons are in the ground state of the harmonic oscillator single-particle Hamiltonian (E=1/2). Alternatively, the system occupies the ground state for both the relative and c.m. Hamiltonians. Both descriptions give a total energy E=1. For higher values of $g$ more complicated configurations enter to play. Notice that the total energy is a little larger than the limit that one obtains in the case of contact interaction. This overcoming is a consequence of the finite-range of the interaction.

The first excited state corresponds to the first excitation of the c.m.. Actually, it can be seen that the excitation energies of the c.m. do not depend on $g$ and result in parallel lines (red lines) to the ground state. The second excitation, for $g = 0$, has degeneracy two. One of the states describes two quantum excitations of the c.m. and the ground state of the relative part. While the other corresponds to the ground state of the c.m. and the first excited state of positive parity of the relative motion. Notice that when $g$ increases the degeneracy in $g = 0$ is broken.

## IV. DYNAMIC STRUCTURE FUNCTION

The dynamic structure function (DSF) describes the response of the system to an external perturbation. In our case, we will study the response of the system to a monopolar excitation. This perturbation is described by a one body operator $\hat{F} = \sum_{i=1}^{N} x_i^2$, and the dynamic structure function has the following form:

$$S_F(E) = \frac{1}{N} \sum_{q}^{D} |\langle q|\hat{F}|0\rangle|^2 \delta[E - (E_q - E_0)] \,. \tag{12}$$

Where $|0\rangle$ is the ground state of the system and $|q\rangle$ are the different excited states, $H|q\rangle = E_q|q\rangle$, with $q = \{q_{c.m.}, q_r\}$. The one body operator can be also split in two pieces, corresponding to the c.m. and relative coordinates[5]:

$$\langle q|x_1^2 + x_2^2|0\rangle = \langle q_{c.m.}, q_r|2X^2|0_{c.m.}, 0_r\rangle \delta_{q_r,0_r} + \langle q_{c.m.}, q_r|\frac{x_r^2}{2}|0_{c.m.}, 0_r\rangle \delta_{q_{c.m.},0_{c.m.}} \,. \tag{13}$$

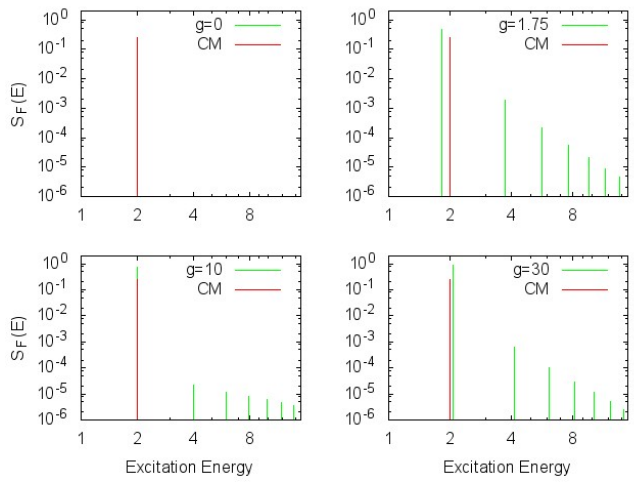


FIG. 4: Dynamic Structure function for a system of two bosons with finite-range interaction as a function of the excitation energy in a logarithmic scale. It is calculated for $g = 0$, 1.75, 10 and 30 for $\sigma = 0.2$ and M=85.

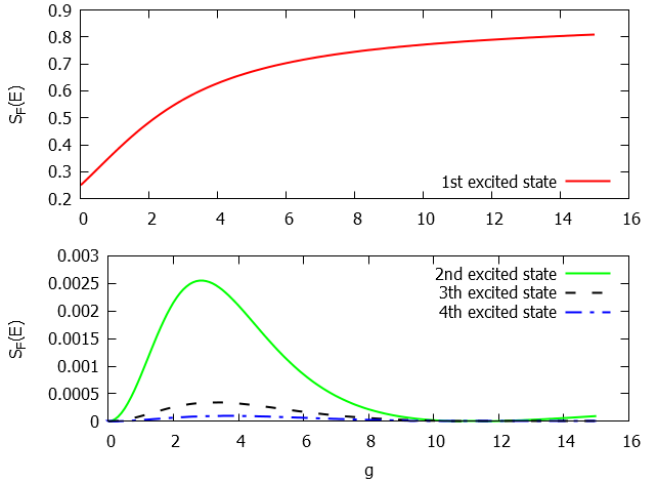


FIG. 5: Strength of the breathing mode (upper) and the next three excited states in function of the interaction strength $g$ with $\sigma = 0.2$.

Therefore, for this one body operator:

$$\langle q_{c.m.} = 2, q_r | X^2 | 0_{c.m.}, 0_r \rangle = \frac{1}{2\sqrt{2}} \delta_{q_r,0_r} \,, \tag{14}$$

the c.m. excitation will always appears at a fixed excitation energy $E_{ex} = 2$ with strength 1/4 independent of the interactions between the particles.

In Fig. 4 we represent the dependence of the DSF on the excitation energy ($E_{ex} = E_q - E_0$). Firstly, when $g = 0$, i.e., non-interacting system, each contribution of the monopolar operator excites two different states, at the same excitation energy $E_{ex} = 2$ being 1/4 the strength of both: the c.m. and the relative one.

For $g$ different than zero, the strength of the DSF is distributed among several excited states, associated with the relative motion. The excitation energy of the main peak (known as breathing mode) decreases for increasing values of $g$ up to a certain value of $g$. If we increase the interaction strength further, the excitation energy of the breathing mode grows again and reaches the value $E_{ex}(g = 0) = 2$ at $g \approx 10$, for $\sigma = 0.2$. This reentrant behaviour has been discussed in Refs.[8][5] for contact interaction. However, in the case of finite-range interaction, if we continue increasing the interaction strength, the excitation energy of the breathing mode grows above $E_{ex}(g = 0) = 2$. This phenomenon can be seen in Fig. 4 for $g = 30$.

The strengths of the different states excited by the monopolar operator are reported in Fig. 5. The strength of the breathing mode (upper panel), starts at the value 1/4 for $g = 0$ and grows monotonically with $g$. This behaviour implies that it is easier to excite the breathing mode for larger $g$. The strengths of the other excited states increase with $g$ until they reach a maximum and then decrease. In comparison with the contact interaction, the strength of this higher states of the DSF is larger for the finite-range interaction with the same strength as the contact one.

In Fig. 6 we represent the reentrance energy ($E_R = E_{ex}(g) - E_{ex}(g = 0)$) for several excited states as a function of $g$. All excited states show the reentrance behaviour, $E_R$ decreases $E_R < 0$ up to a minimum and then grows again reaching the value $E_R = 0$ when $g \approx 10$. For a contact interaction, the value $E_R = 0$ is reached asymptotically when $g \to \infty$. In contrast for a finite-range interaction, and for larger values of $g$, we obtain $E_R > 0$.

### A. Sum Rules

An alternative way to characterize the dynamic structure function is by the energy moments $M_n$[9],

$$M_n = \int_0^\infty E^n S_F(E) dE$$
$$= \frac{1}{N} \sum_q^D (E_q - E_0)^n |\langle q | \hat{F} | 0 \rangle|^2 \,. \tag{15}$$

Furthermore, there are some theorems, called sum rules, that permit to compute the energy moments $M_n$ without knowing the eigenvalues or eigenvectors of the many-body system [9]. A good example is the $M_1$sum rule, which can be written as[5]:

$$M_1 = \frac{1}{2} \langle 0 | [\hat{F}^\dagger, [\hat{F}, \hat{H}]] | 0 \rangle = \frac{4}{N} V_{h.o} \,. \tag{16}$$

In Fig. 7 the energy moment $M_1$ is reported as a function of $g$. The sum rule has been computed in terms of

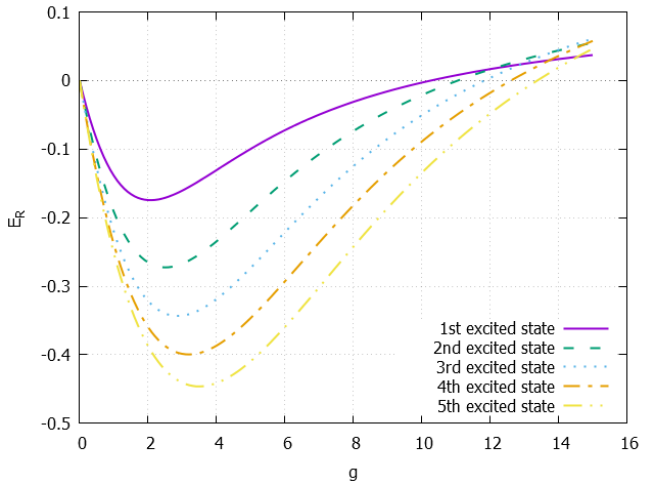


FIG. 6: Reentrance energy ($E_R = E_{ex}(g) - E_{ex}(g=0)$) as function of the interaction strength $g$ for five relative motion excited states. $\sigma = 0.2$ and M=85.

the total harmonic potential energy in the ground state (Eq.16) or by the explicit integration of the DSF. The excellent agreement between both methods, in the full range of $g$ explored, ensures the convergence of our results. The $M_1$ increases monotonically with $g$. This behaviour is due to the increase of $V_{h.o}$ with $g$ or equivalently to the increase of the strength of the breathing mode, Fig. 5. The contributions of the other excited states are lower because of their little strength, which decreases rapidly for greater values of $g$.

## V. SUMMARY AND CONCLUSIONS

In this work, we have investigated a system of two bosons in a 1D harmonic trap interacting by a finite-range potential of gaussian shape.

Firstly, we have studied the energy spectrum of the Hamiltonian by diagonalizing the relative Hamiltonian in a truncated space. This procedure is variational, and the eigenvalues are upper-bounds to the exact solutions. The fulfilment of the virial theorem for the ground state has been used as an additional test of the convergence of our results toward the exact ones. We have also computed the dynamic structure function for a monopolar excitation. The response has a dominating peak (breathing mode), which strength increases with $g$. The location of the main peak has a reentrance behaviour similar to the one observed for contact interactions. However, due to the finite-range interaction, we also observe positive reentrance energies in contrast to a contact interaction. Finally, we have evaluated the $M_1$ energy sum rule to test the accuracy of the calculated DSF.

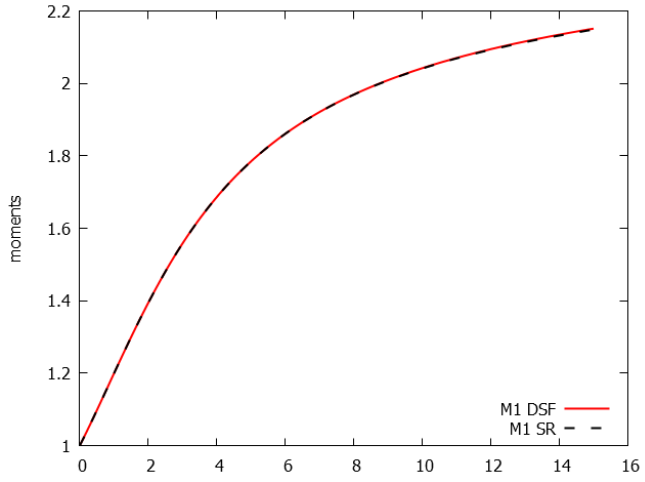


FIG. 7: $M_1$ computed directly from the dynamic structure function (DSF) and with the sum rules(SR).

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