

Energy weighted sum rules for spectral functions in nuclear matter

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The energy weighted sum rule of single-particle spectral functions in nuclear matter is studied. The spectral functions include the influence of short-range correlations as generated by the Reid potential in the framework of the self-consistent Green's function method. For the range of momenta studied, the sum rule is rather accurately fulfilled numerically (within 5%). It is observed that the high-energy tail of the particle part of the spectral function exhausts most of the sum rule, which confirms the need for the appearance of single-particle strength at very high energies.

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I. INTRODUCTION

The recent experimental information on the single-particle spectral functions [1-4] has motivated a considerable theoretical effort towards the microscopic calculation of these quantities [5-19]. The general goal of these investigations can be summarized by stating that they establish to what extent a mean-field description of nuclei is meaningful.

Due to the additional difficulties, at both the formal and computational level, implied in the treatment of a finite nucleus, most of the microscopic calculations of spectral functions up to now have been performed for nuclear matter. The presently available techniques to calculate spectral functions are based either on orthogonal correlated basis function theory (CBF) [5,6] or on the perturbation expansion of the one-body propagator [7-19]. Although the spectral functions themselves cannot be calculated exactly and one is forced to resort to approximations, present results have reached a high level of sophistication. It is therefore useful to explore new tools which can shed further light on the properties of spectral functions.

Energy weighted sum rules, which have played an important role in analyzing the response of the nucleus [20], may provide such tools. Energy weighted sum rules for the single-particle spectral functions are well established in the literature [21,22] but to our knowledge they have not been considered from a numerical point of view. Therefore, the main purpose of this paper is to analyze the physical implications of the fulfillment of these sum rules for nuclear matter spectral functions which, in the present case, have been calculated in the framework of self-consistent Green's function (SCGF) theory.

In Sec. II two different derivations of the sum rules are presented. In Sec. III the results are discussed and the consequences on the distribution of single-particle strength analyzed. The conclusions are summarized in Sec. IV.

II. SUM RULES FOR THE SINGLE-PARTICLE SPECTRAL FUNCTIONS

The physical meaning of the single-particle spectral functions is rather simple. The hole spectral function $S_h(k, \omega)$ is the probability of removing a particle with momentum k from the target system of A particles leaving the resulting $(A - 1)$ system with an energy $E^{A-1} = E_0^A - \omega$, where E_0^A is the ground-state energy of the target. Analogously, the particle spectral function $S_p(k, \omega)$ is the probability of adding a particle with momentum k and leaving the resulting $(A + 1)$ system with an excitation energy ω measured with respect to the ground state of the A system, i.e., $\omega = E^{A+1} - E_0^A$. The spectral functions can be directly related to the single-particle propagator of the corresponding many-particle system through the Lehmann representation

$$S_h(k, \omega) = \sum_n |\langle \Psi_n^{A-1} | a_k | \Psi_0^A \rangle|^2 \delta(\omega - (E_0^A - E_n^{A-1})) \quad (1a)$$

$$S_p(k, \omega) = \sum_n |\langle \Psi_m^{A+1} | a_k^\dagger | \Psi_0^A \rangle|^2 \delta(\omega - (E_m^{A+1} - E_0^A)), \quad (1b)$$

where $|\Psi_0^A\rangle$ is the ground state of the target, and $|\Psi_m^{A-1}\rangle$ and $|\Psi_m^{A+1}\rangle$ are excited states of the $(A - 1)$ and $(A + 1)$ systems with energies E_n^{A-1} and E_m^{A+1} , respectively.

Equations (1a) and (1b) are a convenient representation for the derivation of the sum rules. The lowest-order sum rule $m_0(k)$ is obtained by using the completeness relation in the energy integration of the spectral functions. In this way one can express $m_0(k)$ as the expectation value of the anticommutator $\{a_{\mathbf{k}}, a_{\mathbf{k}}^\dagger\}$ which, due to the fermion character of the nucleons, is equal to the unit operator:

$$m_0(k) = \int_{-\infty}^{\epsilon_F} d\omega S_h(k, \omega) + \int_{\epsilon_F}^{\infty} d\omega S_p(k, \omega) \\ = \langle \Psi_0^A | \{a_{\mathbf{k}}, a_{\mathbf{k}}^\dagger\} | \Psi_0^A \rangle = 1, \quad (2)$$

where ϵ_F is the Fermi energy of the system.

The same type of procedure, but with a little more algebra, leads to the first-order energy weighted sum rule (EWSR) $m_1(k)$:

$$m_1(k) = \int_{-\infty}^{\epsilon_F} \omega S_h(k, \omega) d\omega + \int_{\epsilon_F}^{\infty} \omega S_p(k, \omega) d\omega \\ = \langle \Psi_0^A | \{[a_{\mathbf{k}}, H], a_{\mathbf{k}}^\dagger\} | \Psi_0^A \rangle. \quad (3)$$

In order to evaluate the right hand side of the EWSR, it is necessary to assume a Hamiltonian, which in the present case is taken to be nonrelativistic and of the two-body type. Under these assumptions,

$$\langle \Psi_0^A | \{[a_{\mathbf{k}}, H], a_{\mathbf{k}}^\dagger\} | \Psi_0^A \rangle \\ = \frac{k^2}{2m} + \frac{1}{(2\pi)^3} \int d^3 k' n(k') \langle \mathbf{k}, \mathbf{k}' | V | \mathbf{k}, \mathbf{k}' \rangle_a, \quad (4)$$

where $n(k)$ is the occupation probability of the single-particle state $|\mathbf{k}\rangle$

$$n(k) = \langle \Psi_0 | a_{\mathbf{k}}^\dagger a_{\mathbf{k}} | \Psi_0 \rangle = \int_{-\infty}^{\epsilon_F} S_h(k, \omega) d\omega \quad (5)$$

and $\langle \mathbf{k}, \mathbf{k}' | V | \mathbf{k}, \mathbf{k}' \rangle_a$ is the antisymmetrized two-body matrix element of the bare nucleon-nucleon interaction. Notice that in order to simplify the notation the spin-isospin variables have been omitted.

The second term on the right hand side of Eq. (4) can be identified with the energy independent part of the self-energy which is obtained as the high frequency limit of $\Sigma(k, \omega)$ [11],

$$\Sigma^\infty(k) = \lim_{\omega \rightarrow \infty} \Sigma(k, \omega) \\ = \frac{1}{(2\pi)^3} \int d^3 k' n(k') \langle \mathbf{k}, \mathbf{k}' | V | \mathbf{k}, \mathbf{k}' \rangle_a. \quad (6)$$

The limit $\Sigma^\infty(k)$ represents the average potential of a given particle with momentum k resulting from its interaction (V) with all the other particles weighted with their corresponding occupation probabilities. In fact, $\Sigma^\infty(k)$ is the generalization of the Hartree-Fock (HF) approximation to the self-energy:

$$\Sigma^{HF}(k) = \frac{1}{(2\pi)^3} \int_{k' < k_F} d^3 k' \langle \mathbf{k}, \mathbf{k}' | V | \mathbf{k}, \mathbf{k}' \rangle_a. \quad (7)$$

The diagrammatic representations of $\Sigma^\infty(k)$ and $\Sigma^{HF}(k)$ are shown in Figs. 1(a) and 1(b), respectively.

It is interesting to realize that the energy weighted sum rules can be related to the asymptotic behavior of the real part of the Green's function for large ω . In fact, from the one-body Green's function for a homogeneous system

$$G(k, \omega) = \frac{1}{\omega - \frac{k^2}{2m} - \Sigma(k, \omega)}, \quad (8)$$

the following expansion of the real part of $G(k, \omega)$ is readily obtained:

$$\text{Re } G(k, \omega) = \frac{1}{\omega} \left\{ 1 + \frac{\frac{k^2}{2m} + \Sigma^\infty(k)}{\omega} + \dots \right\}. \quad (9)$$

On the other hand, the Lehmann representation of $G(k, \omega)$, namely

$$G(k, \omega) = \int_{-\infty}^{\epsilon_F} \frac{S_h(k, \omega')}{\omega - \omega' - i\eta} d\omega' + \int_{\epsilon_F}^{\infty} \frac{S_p(k, \omega')}{\omega - \omega' + i\eta} d\omega', \quad (10)$$

can be expanded in a similar way to get the real part of the propagator

$$\text{Re } G(k, \omega) = \frac{1}{\omega} \left\{ \int_{-\infty}^{\epsilon_F} S_h(k, \omega') d\omega' + \int_{\epsilon_F}^{\infty} S_p(k, \omega') d\omega' + \frac{1}{\omega} \left(\int_{-\infty}^{\epsilon_F} \omega' S_h(k, \omega') d\omega' + \int_{\epsilon_F}^{\infty} \omega' S_p(k, \omega') d\omega' \right) + \dots \right\}. \quad (11)$$

By comparing the two expansions, one recovers the expressions for m_0 and m_1 . Higher-order sum rules are obtained if more terms are retained in the expansion. For example, the next sum rule relates the spectral function to the imaginary part of the self-energy

$$\int_{-\infty}^{\infty} \omega^2 S(k, \omega) d\omega = \left(\frac{k^2}{2m} + \Sigma^\infty(k) \right)^2 + \frac{1}{\pi} \int_{-\infty}^{\infty} |\text{Im } \Sigma(k, \omega)| d\omega, \quad (12)$$

where the dispersion relation for $\text{Re}\Sigma(k, \omega)$ has been used.

The sum rules are rigorous relations between the energy weighted integrals of the spectral functions and certain expectation values in the ground state of the system. It should be noted that the sum rules involve the exact spectral functions. Consider now the case where a certain approximation is used to calculate the self-energy. It is both interesting and important to know whether the sum rules are satisfied by the approximate spectral functions.

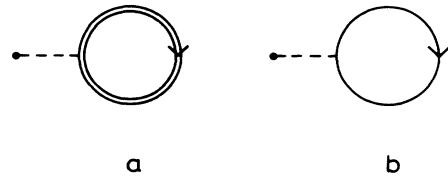


FIG. 1. Diagrammatic representation of the energy independent part of the self-energy (a) and the HF approximation to the self-energy (b).

The asymptotic expansion of the real part of the Green's function can be used to show that a self-consistently determined spectral function satisfies sum rules which have the same form as those of the exact solution. For example, the EWSR is satisfied if the momentum distribution is calculated from the self-consistent spectral function through Eq. (5). The fact that the self-consistent spectral function satisfies sum rules which have the same form as those satisfied by the exact solution, does not constitute a measure of the accuracy of the approximation since any self-consistent solution enjoys this property. It is certainly a guarantee that the numerical solution is correctly carried out. These sum rules would be a strong constraint on the approximation itself if the right hand sides of these rules could be determined experimentally. The availability of the momentum distribution for example determines the first moment of the spectral function if the bare interaction is known (as in many-electron systems) [23].

III. RESULTS AND DISCUSSION

The specific test of the sum rules has been carried out for the Reid interaction [24]. The spectral functions have been calculated in the framework of SCGF theory. The SCGF method and all details necessary for performing the calculations are discussed in Ref. [9]. The basic idea underlying this method is that the properties of a particle are determined by its interaction with the other particles. Due to the short-range repulsion, the minimum meaningful approximation consists in summing up the ladder diagrams which, in the present case, include also hole-hole propagation to all orders. The inclusion of hole-hole propagation is required since at the single-particle level it yields the coupling to the excited states of the $(A-1)$ system and therefore provides the necessary information for the calculation of the hole spectral function. The resulting effective interaction is used to calculate the self-energy from which the spectral functions are obtained. The interaction should then be recalculated since the particles are dressed by their interactions with the medium. A nonlinear formulation of the many-particle system is thus obtained which requires the self-consistent determination of the single-particle propagator. In principle, a complete self-consistent calculation implies the use of fully dressed single-particle propagators in the solution of the ladder equation for the effective interaction. At present, self-consistency has been established only in an averaged way [9] but progress is being made towards obtaining the full solution [25].

Before the numerical analysis is presented, it is useful to comment on the general features of $m_1(k)$. Note that the momentum distribution $n(k)$ on the right hand side of the sum rule is calculated from the hole spectral function S_h [see Eq. (5)] which in turn is used, together with the particle spectral function S_p , in the evaluation of the left hand side of the sum rule [see Eq. (3)]. The first thing to observe is that due to the short-range repulsion present in any realistic interaction, the right hand side of the sum rule, explicitly shown in Eq. (4), is a large positive num-

ber. On the other hand, for nuclear matter at saturation density, one has $\epsilon_F < 0$. This means that the contribution to $m_1(k)$ of the hole part of the spectral function is negative. The same is true for the first portion of the S_p contribution. Therefore, it is the high-energy tail of S_p that should compensate for these negative contributions and bring the sum rule up to the large positive values obtained by evaluating the right hand side. For m_0 , however, the sum rule is already exhausted around 80% by the hole part of the spectral function S_h if $k < k_F$. In the case $k > k_F$, the largest contribution to m_0 comes from the strength around the peak of S_p , the high-energy tail giving only about 6% of the sum rule [8].

The m_0 sum rule is satisfied better than 1% for all k . The hole part of the contribution to m_0 is given by $n(k)$ which has already been discussed for example in Refs. [5,9,11]. Nevertheless, for the following discussion, it is useful to remember that for the Reid potential at normal density the occupation at zero momentum is $n(0) = 0.82$ and the discontinuity at k_F , which measures the strength of the quasiparticle pole at k_F , is $Z(k_F) = 0.72$.

In Fig. 2, the left and the right hand sides of the EWSR are compared as a function of k . The contributions of S_h and S_p are separately shown. Both display a discontinuity with a size equal to $Z(k_F)\epsilon_F = 18$ MeV and of opposite sign making the sum continuous across k_F . The sum rule is well satisfied, especially for low momenta, the maximum discrepancy being about 5% for the momenta shown in the figure. This small discrepancy can be traced to the fact that the effective interaction has been constructed only for the low angular momentum partial waves (3S_1 - 3D_1 , 1S_0) whereas all the other partial waves have been treated in the Born approximation. Therefore, while on the right hand side all partial waves

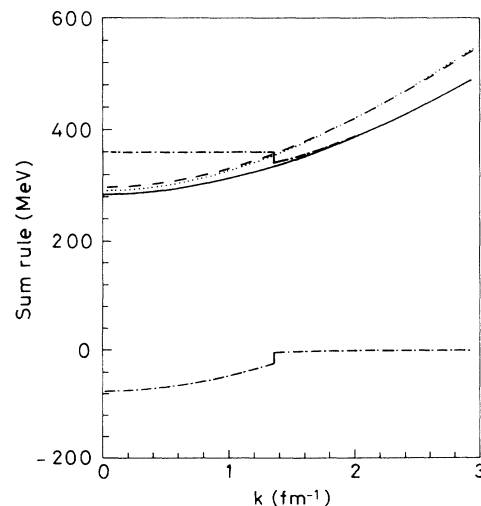


FIG. 2. Illustration of the fulfillment of the EWSR. The dot-dashed lines represent the S_p and S_h contributions to the left hand side of the EWSR [see Eq. (3)] with the latter rapidly approaching zero above k_F . The sum of both terms is represented by the full line which should be compared with the dashed line giving the right hand side. The dotted line gives the HF estimate to the right hand side.

are considered, the spectral functions on the left hand side have been obtained from a self-energy $\Sigma(k, \omega)$ which energy dependence does not contain the contribution of the high angular momenta of the interaction. This may produce slight inaccuracies in the distribution of single-particle strength, especially at high energy and momentum, which are reflected in some deviations in the fulfillment of the sum rule. It has been shown in Ref. [9] that the inclusion of higher partial waves influences the momentum distribution at about the 1% level.

As mentioned before, the fulfillment of the m_1 sum rule is possible due to the existence of a high-energy tail in S_p which compensates for the negative contributions coming from S_h . It is thus clear that m_1 is very sensitive, not only to the amount of single-particle strength, as m_0 is, but also to the way the strength is distributed over energy. Therefore, even if different many-body methods satisfy the lowest-order sum rule m_0 and possibly generate a similar momentum distribution, they can still predict very different results for m_1 if the strength is not distributed similarly. The results of Fig. 2 show that the SCGF method gives a reasonable fulfillment of m_1 .

It is interesting to comment on the result for $m_1(k)$ obtained when one uses the quasiparticle approximation to the spectral function $S_{QP}(k, \omega)$ [8,9]. The resulting $m_1(k)$ is given by $Z(k)\epsilon_{QP}(k)$, where $\epsilon_{QP}(k)$ is the quasiparticle energy at which the Lorentzian approximation to the peak of the spectral function is centered. As S_{QP} misses the high-energy tail of S_p , the quasiparticle estimate of m_1 is very poor. At k_F , for instance, one obtains $m_1^{QP} = 18$ MeV whereas the proper value is 334 MeV.

The evaluation of the right hand side of the EWSR using the HF estimate $\Sigma^{HF}(k)$ is also reported in Fig. 2 (dotted line). It is clearly seen that it gives an excellent approximation since the differences are less than 2% with respect to the calculation with $\Sigma^\infty(k)$, which uses the correlated momentum distribution $n(k)$. Nevertheless, this observation cannot be extended to the higher-order sum rules. A simple inspection of Eq. (12) shows that this is no longer true for the second-order sum rule m_2 , since there are large additional contributions coming from the imaginary part of the self-energy.

It is interesting to notice that the HF approximation to the spectral function, which corresponds to a δ function at the HF energy $\epsilon^{HF}(k) = \frac{k^2}{2m} + \Sigma^{HF}(k)$, satisfies the sum rules exactly in the sense mentioned above. This does not mean that HF provides a good description of the correlated many-body problem but it is a consequence of the self-consistent nature of the HF solution.

The contribution of the interaction to the right hand side of the EWSR [Eq. (6)] is analyzed in Fig. 3 where the contributions to $\Sigma^\infty(k)$ integrating up to k_F , $3k_F$, and ∞ are explicitly shown. The contribution up to k_F gives 79% of the total, reflecting the fact that the momenta smaller than k_F are partially occupied. An additional contribution of 18% comes from momenta between k_F and $3k_F$. The HF approximation to the right hand side of the EWSR has also been included in the figure to emphasize that $\Sigma^{HF}(k)$ is a very good estimate of $\Sigma^\infty(k)$.

The fraction of the sum rule for m_0 and m_1 exhausted by integrating up to a given energy is reported in Fig. 4

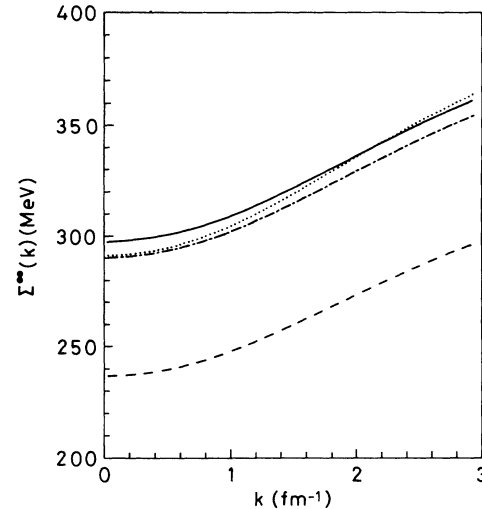


FIG. 3. Contributions to the asymptotic value of the self-energy $\Sigma^\infty(k)$ integrating up to k_F (dashed line), up to $3k_F$ (dash-dotted line) and total (full line). The dotted line is the HF estimate $\Sigma^{HF}(k)$.

for $k = 0.79 \text{ fm}^{-1}$. As expected, the saturation is reached at lower energies for m_0 than for m_1 . For other momenta one obtains approximately the same saturation energy, reflecting the fact that the high-energy tail of S_p is basically the same for all k [8,9]. Notice that for the momentum reported in the figure, which is smaller than k_F , it is necessary to integrate up to approximately 2 GeV to start to overcome the negative contributions to $m_1(k)$.

As a final remark, note that the value of the sum rule depends on the model used for the NN interaction, the short range behavior of which is directly related to the high-energy tail of the spectral function. Clearly, evaluating the sum rule for different potentials would be very useful to make more quantitative statements on the relation between the repulsive core of the interaction and the amount of single-particle strength at high energy.

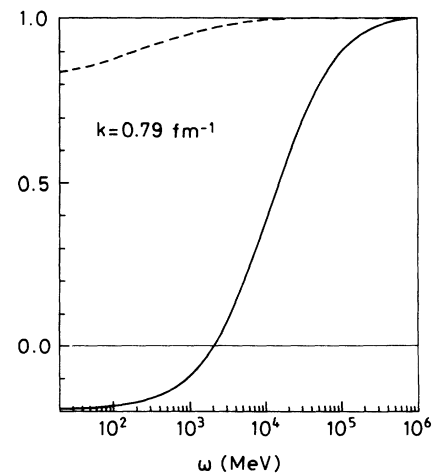


FIG. 4. Illustration of the saturation of the sum rules m_0 (dashed line) and m_1 (full line) for a momentum $k = 0.79 \text{ fm}^{-1}$.

IV. CONCLUSIONS

It has been shown that the spectral functions obtained with the SCGF method fulfill the energy weighted sum rule m_1 to a high degree of accuracy. The discrepancies are less than 5% and can easily be improved if higher angular momentum partial waves are retained in the calculation. Since the sum rules can be used as a test of the numerical accuracy of microscopic calculations of the spectral functions, this result is a measure of the good quality of the spectral functions obtained in SCGF theory. It has also been observed that the HF approximation to the self-energy can be used to get a good estimate of

the right hand side of $m_1(k)$. This observation cannot be generalized to higher-order sum rules. Finally, it has been observed that S_p exhausts most of the EWSR and that a proper fulfillment of the sum rule requires the appearance of strength at very high energy, which corroborates in a quite model independent way the limitations of the mean-field theory.

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