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Short-range correlations in nuclear matter using Green's functions within a discrete pole approximation

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Abstract

We treat short-range correlations in nuclear matter, induced by the repulsive core of the nucleon–nucleon potential, within the framework of self-consistent Green's function theory. The effective in-medium interaction sums the ladder diagrams of both the particle–particle and hole–hole type. The demand of self-consistency results in a set of nonlinear equations which must be solved by iteration. We explore the possibility of approximating the single-particle Green's function by a limited number of poles and residues. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

The correct treatment of short-range correlations when performing nuclear calculations using realistic NN-interaction is of great importance [1]. Realistic NN-interactions are fitted to the two-nucleon scattering data and the deuteron binding energy and contain a large repulsive core for small internuclear distances [2]. When this interaction is used in quantum-mechanical perturbation theory, convergence is no longer guaranteed as the dominant contribution of the repulsive core will lead to large and repulsive two-body matrix elements. A Hartree–Fock calculation starting from a realistic interaction will lead to an unbound system, and the energy of the ground state will be highly dependent on the specific potential used [3].

Within the self-consistent Green's function (SCGF) formalism short-range correlations are treated by replacing the realistic interaction with a medium-modified effective interaction. This effective interaction is obtained by summing all diagrams of the ladder type.

Short-range correlations will lead to a depletion of the hole states and a partial occupation of the particle states in the ground state of the system. This deformation of the Fermi sea will reduce the pairing correlations [4] and can lead to a non-superfluid ground state at the empirical saturation density. Furthermore an additional density dependence is introduced, which influences the saturation properties of nuclear matter.

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A self-consistent treatment employing the full energy dependence of the spectral function is feasible for nuclear matter at finite temperatures [5], but becomes very difficult at zero temperature, due to the complicated structure of the spectral function. Therefore a number of approximations for the spectral function have been developed in the recent past [6–11]. In this work we propose a discrete pole approximation for the Green's function. Using this approximation the deformation of the Fermi sea is incorporated in the evaluation of the effective interaction. Different discretization schemes are possible. Here the BAGEL scheme has been used to generate the exact location and strength of the discrete poles. Results are displayed for a modified Reid interaction.

2. Formalism

Green's functions constitute a useful tool for investigating the properties of correlated many-particle systems.

When considering infinite nuclear matter, the symmetries of the system will seriously reduce the degrees of freedom and the single-particle Green's function will be completely determined by the magnitude of the momentum p and the energy of the particle ω. This propagator can then be represented in Lehmann's representation as,

$$g(p,\omega) = \int_{-\infty}^{\epsilon_F} d\omega' \frac{S_h(p,\omega')}{\omega - \omega' - i\eta} + \int_{\epsilon_F}^{\infty} d\omega' \frac{S_p(p,\omega')}{\omega - \omega' + i\eta}. \tag{1}$$

The particle spectral function $S_p(p,\omega)$ represents the probability of adding a particle with momentum p to the system, while leaving the resulting system with an excitation energy ω. The hole spectral function $S_h(p,\omega)$ is related in a similar way to the removal of a particle with momentum p.

Using the Dyson equation, the correlated spectral functions can be determined,

$$\begin{aligned} S_h(p,\omega) &= \begin{cases} \dfrac{1}{\pi} \dfrac{\operatorname{Im}\Sigma(p,\omega)}{(\omega - p^2/2m - \operatorname{Re}\Sigma(p,\omega))^2 + (\operatorname{Im}\Sigma(p,\omega))^2}, & \text{if } \omega < \epsilon_F, \\ 0, & \text{if } \omega > \epsilon_F, \end{cases} \\ S_p(p,\omega) &= \begin{cases} 0, & \text{if } \omega < \epsilon_F, \\ -\dfrac{1}{\pi} \dfrac{\operatorname{Im}\Sigma(p,\omega)}{(\omega - p^2/2m - \operatorname{Re}\Sigma(p,\omega))^2 + (\operatorname{Im}\Sigma(p,\omega))^2}, & \text{if } \omega > \epsilon_F. \end{cases} \end{aligned} \tag{2}$$

The irreducible self-energy Σ is a complex quantity and represents the interaction with the other particles. Because of the short-range correlations induced by the repulsive core of a realistic NN-interaction, the self-energy must be expanded in terms of an energy-dependent effective interaction Γ,

$$\Sigma(p,\omega) = \int \frac{d\vec{p}'}{(2\pi)^3} \int \frac{d\omega'}{2\pi i} \langle \vec{q}|\Gamma(P,\omega+\omega')|\vec{q}\rangle g(p',\omega'), \tag{3}$$

with $\vec{P} = \vec{p} + \vec{p}'$ and $\vec{q} = (\vec{p} + \vec{p}')/2$. The summation of both the spin and isospin variables is suppressed for notational convenience. A diagrammatic representation of the self-energy is given in Fig. 1.

The effective interaction Γ is calculated from the realistic NN-interaction by summing the infinite subset of ladder diagrams. In contrast to the Brueckner–Hartree–Fock (BHF) approach, SCGF retains both particle–particle (pp) and hole–hole (hh) propagation in the intermediate two-particle propagator [6],

$$\begin{aligned} \langle \vec{p}|\Gamma(P,\Omega)|\vec{p}'\rangle = \langle \vec{p}|V|\vec{p}'\rangle &+ \int \frac{d\vec{q}}{(2\pi)^3} \langle \vec{p}|V|\vec{q}\rangle \\ &\times \left[\int d\omega \int d\omega' \frac{S_p(p_1,\omega) S_p(p_2,\omega')}{\Omega - \omega - \omega' + i\eta} - \int d\omega \int d\omega' \frac{S_h(p_1,\omega) S_h(p_2,\omega')}{\Omega - \omega - \omega' - i\eta} \right] \\ &\times \langle \vec{q}|\Gamma(P,\omega)|\vec{p}'\rangle, \end{aligned} \tag{4}$$

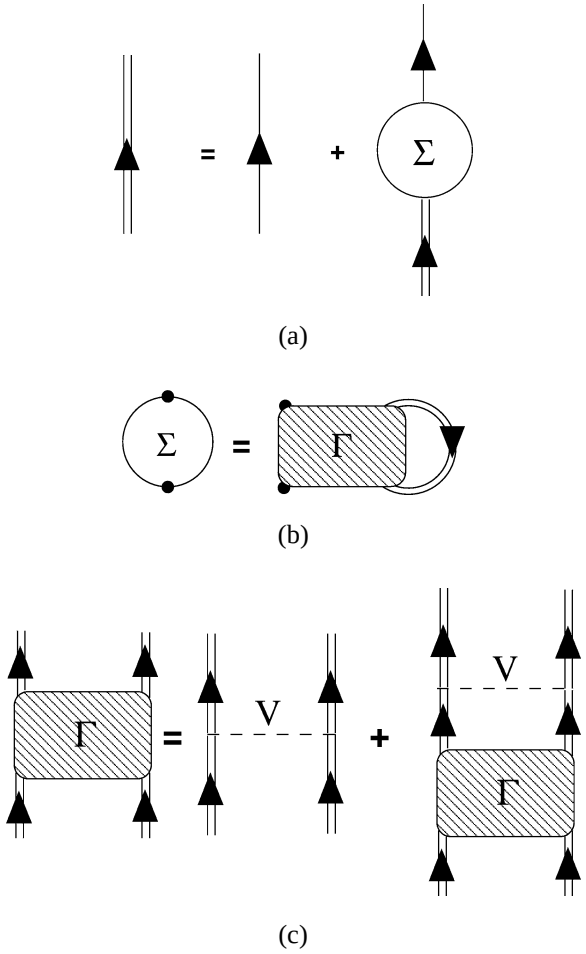

Fig. 1. Diagrammatic representation of (a) the Dyson equation, (b) the self-energy and (c) the effective interaction in the ladder approximation.

with $\vec{p}_{1,2} = \vec{P}/2 \pm \vec{q}$.

Self-consistency becomes a crucial requirement if one wants to fulfill certain elementary conservation laws such as the conservation of the number of particles. Therefore the spectral function obtained from Eq. (2) should be used in the evaluation of the self-energy, Eq. (3) and the effective interaction, Eq. (4). The resulting set of coupled, non-linear equations is solved by iteration. Starting from an initial guess for the Green's function, one calculates the self-energy and the effective interaction. The Dyson equation then leads to a Green's function different from the original one. This Green's function can again be used in the evaluation of the effective interaction and the self-energy. This procedure continues until both self-energy and Green's function have converged.

At $T = 0$ (zero temperature), the evaluation of the effective interaction through the successive iterations is a cumbersome task. The combination of very sharp peaks as well as a broad background distribution in the spectral function makes an accurate numerical evaluation difficult. It is therefore of importance to look for suitable approximations for this spectral function. These approximations should retain the most prominent features of the full spectral function, Eq. (2), but at the same time they must allow a fast evaluation of the self-energy and the effective interaction.

3. Approximated spectral functions

The most basic approximation for the spectral function is obtained by neglecting the imaginary part of the self-energy, so that the full spectral function of Eq. (2) is replaced by a single delta peak at the 'on-shell energy',

$$\epsilon_{qp}(p) = p^2/2m + \mathrm{Re}\,\Sigma(p, \epsilon_{qp}(p)). \tag{5}$$

This approach corresponds to an extension of the Brueckner–Hartree–Fock (BHF) prescription, including hh-propagation in the effective interaction, and is usually referred to as the quasi-particle scheme. Extended calculations within this scheme were carried out for both model interactions [6] and realistic NN-interactions [7]. In the latter calculation [7] the on-shell energy is replaced by the mean removal energy for hole states. As a result a finite gap in the energy spectrum is obtained at the Fermi energy. This gap is necessary to avoid the pairing instability, that occurs when hh-propagation is included within a quasi-particle scheme.

A major drawback of the quasi-particle approach is the neglect of the broad background distributions in both particle and hole spectral function. These background distributions are assumed to carry about 15–25% of the total strength [1] and are responsible for a serious deformation of the Fermi sea. The incorporation of the effects of this deformed Fermi sea in the calculation of the effective interaction leads to an additional density dependence, that contributes to a full description of the saturation mechanism of nuclear matter.

In recent years several attempts have been undertaken to perform self-consistent calculations using a spectral function more closely related to the full spectral function. The group of Dickhoff parametrizes the spectral function in each iteration [9–11]. In this way the integrals can be carried out in an analytic way. De Jong [8] uses a mixed approach, in which for $p < k_F$ the hole spectral function is replaced by a renormalized delta peak, whereas the complete energy dependence of the particle spectral function is retained. The integration of this particle spectral function does not lead to large difficulties, since there is no sharp quasi-particle peak in the particle spectral function for $p < k_F$. For states with $p > k_F$ a similar mixed approach is then used.

In this Letter we propose an extension of the quasi-particle scheme, that aims at incorporating the off-shell propagation of the particles. The Green's function is represented by a small set of discrete poles,

$$g(p,\omega) = \sum_i \frac{f_i(p)}{\omega - F_i(p) + i\eta} + \sum_j \frac{b_j(p)}{\omega - B_j(p) - i\eta}. \tag{6}$$

The poles labeled B_i are located below the Fermi energy, while those labeled F_i are situated above this energy. The poles and their corresponding residues are chosen in such a way that they form a reasonable approximation of the fully dressed Green's function. In addition to a peak corresponding to the quasi-particle peak, additional peaks are used to simulate the background distribution for both positive and negative energies.

Several discretization schemes for the spectral function can be proposed. For each scheme one should obtain poles F, B and residues f, b that are continuous functions of the momentum p. Furthermore one wants to recover the complete spectral function in the limit of an infinite number of poles. The specific discretization scheme used in this Letter is based on the BAGEL approach, which has proven to be very successful in the description of the long-range correlations in finite nuclei [12–15].

The poles and residues obtained within the BAGEL scheme reproduce the correct lowest order energy-weighted moments of the continuous spectral function at each iteration,

$$m_k(p) = \sum_i f_i(p)\big(F_i(p)\big)^k + \sum_j b_j(p)\big(B_j(p)\big)^k = \int_{-\infty}^{+\infty} \omega^k S(p,\omega)\,d\omega, \quad \forall p. \tag{7}$$

The BAGEL algorithm allows for a direct calculation of the poles and the residues of the Green's function from the imaginary part of the self-energy, without having to calculate the integral on the right-hand side of Eq. (7). For an approximation using D poles, one expects the moments up to $2D-1$ to be reproduced. However, due to the large

asymmetry in the self-energy, the BAGEL algorithm must be applied separately to both the forward ($\omega > \epsilon_F$) and backward ($\omega < \epsilon_F$) part of the self-energy. Therefore only moments $k \leqslant D$ will be reproduced.

4. Results

We first display results for the most simple extension of the quasi-particle scheme: a three pole BAGEL approximation. A modified version of the Reid93-interaction [2] was used for these results. In order to avoid pairing instabilities, the $^1S_0$ and the $^3S_1$–$^3D_1$ partial waves of this interaction are multiplied by a factor 0.75 and 0.5, respectively.

This pairing instability leads to the appearance of complex poles [16] in the effective interaction, which makes a calculation along the lines of the scheme sketched out above impossible. However a self-consistent calculation, using the full energy dependence of the spectral function might lead to the disappearance of these pairing instabilities. In this case the projection operators used in the calculation of the effective interaction relate to a Fermi sea that is deformed due to short-range correlations, rather than to the uncorrelated Fermi sea. This causes a reduction of the effective interaction for energies close to $2\epsilon_F$ and will also reduce the pairing correlations [4]. Such a mechanism can lead to a normal ground state at the empirical saturation density ($k_F = 1.36$ fm^{-1}) instead of a superfluid ground state, provided the short-range correlations are strong enough. As a consequence a self-consistent procedure using the full realistic interaction would become feasible, without having to treat the possible pairing of nucleons. The discrete pole approximation is a suitable tool to incorporate the effects of the deformed Fermi sea in the calculation of the effective interaction. If the specific discretization scheme fails to include the complete effects of the correlated Fermi sea, the pairing instability remains unless a reduced interaction is used. When using such a modified interaction, one cannot expect to reproduce the correct empirical values of the binding energy and the occupation probabilities, but the results nevertheless hint at the new mechanisms at work when off-shell propagation is included in the calculation.

Fig. 2 displays the poles and the residues of a three-pole BAGEL scheme as a function of the momentum.

• The central pole (labeled "c") has a behaviour similar to the quasi-particle pole, but carries more than 97% of the strength for all momenta. This is considerably more than the strength carried by the quasi-particle pole, which is typically 65–75% for hole states [1]. Furthermore this central pole is located about 20 MeV above the on-shell energy for all momenta (dotted line). These observations indicate that in the BAGEL scheme the central pole will not only represent the quasi-particle pole, but will also contain a considerable fraction of the forward background distribution.

• The remainder of this background distribution is represented by a pole located at high positive energies (labeled "+"). This behaviour is typical for nuclear matter calculations using a realistic force. The large value for the energy of the "+"-pole is a result of the the short-range correlations induced by the repulsive core of the interaction. The exact location of this pole depends strongly on the specific interaction used.

• Finally the background distribution at negative energies is represented by the pole labeled "−", whose location equals roughly

$$B_-(p) \sim -p^2/2m. \tag{8}$$

This pole corresponds to the high-momentum components in the nuclear wave function [17].

The full energy dependence of the spectral function calculated from Eq. (2) is displayed in Fig. 3 after convergence, in a quasi-particle scheme (dashed line) and in a three-pole BAGEL scheme (full line), for two momenta. The most pronounced difference is the energy range where the spectral function is non-vanishing. In the quasi-particle calculation the hole spectral function will only be different from zero above a threshold energy. This is no longer the case in a BAGEL calculation, where the hole spectral function extends to $-\infty$. One should also note the shell-like structure of the BAGEL spectral function. This behaviour is a result of the discrete pole approximation for the propagators: the different energy intervals leading to a non-vanishing spectral function can

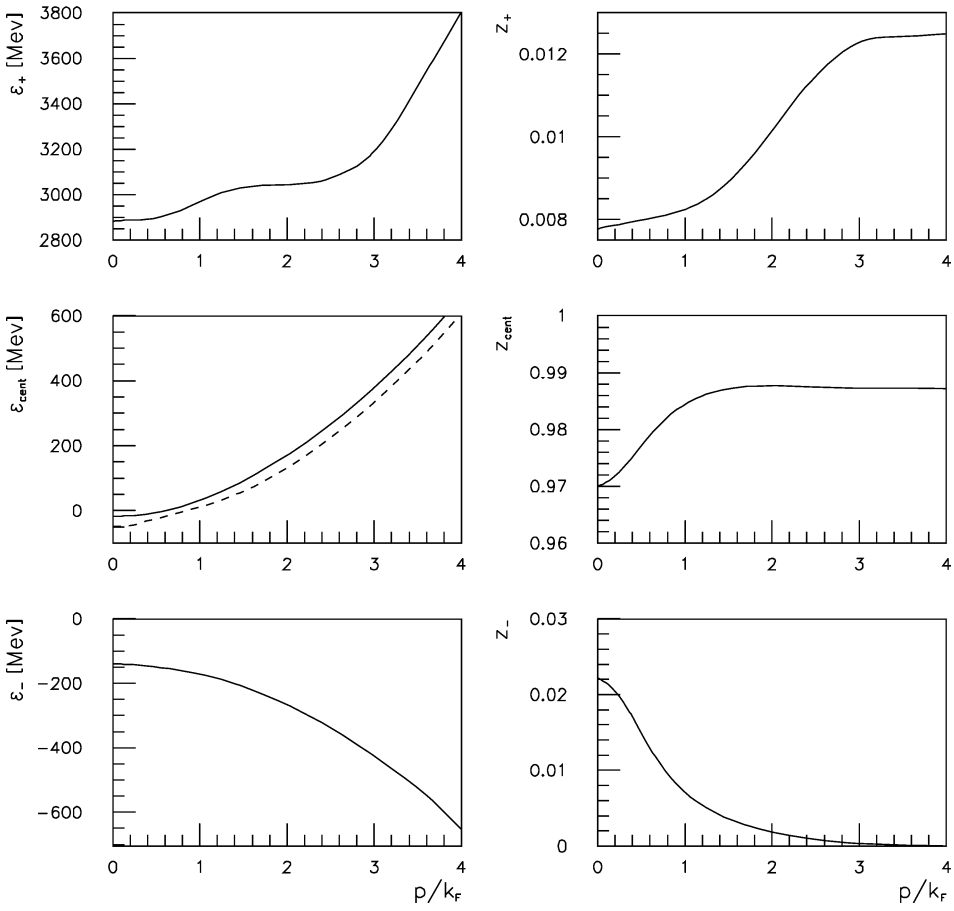

Fig. 2. A three-pole BAGEL spectrum after the convergence of the scheme has been reached ($k_F = 1.36$ fm^{-1}). The left-hand side displays the location of the poles, while the right-hand side shows the corresponding residues. In the central plot on the left the full line corresponds to the central BAGEL pole, while the dashed line corresponds to the on-shell energy corresponding with the self-energy obtained within the same BAGEL approximation.

be attributed to different combinations of the discrete poles contributing to the effective interaction and the self-energy.

The difference in spectral function close to the Fermi energy should be ascribed to the different locations of the central BAGEL pole and the quasi-particle energy. This deviation also causes a number of ambiguities when evaluating the occupation probability and binding energy.

The occupation probability is shown in Table 1. Results are displayed for three different calculations. The column labeled “BAGEL” corresponds to the sum of the backward BAGEL poles. This is the occupation probability used in the evaluation of the effective interaction within the BAGEL scheme. Due to the large amount of strength concentrated in the central pole of the BAGEL spectrum, the induced depletion is not large enough to avoid the appearance of a pairing instability when the full interaction is used. The other columns in Table 1 correspond to the integration of the full hole-spectral function obtained after convergence of the quasi-particle scheme and the three-pole BAGEL scheme. When comparing both dressed approximations we observe that the quasi-particle scheme leads to a larger depletion than the BAGEL scheme. The underlying reason is the feedback of the depleted Fermi sea on the effective interaction. The BAGEL scheme incorporates the effects of this correlated Fermi sea

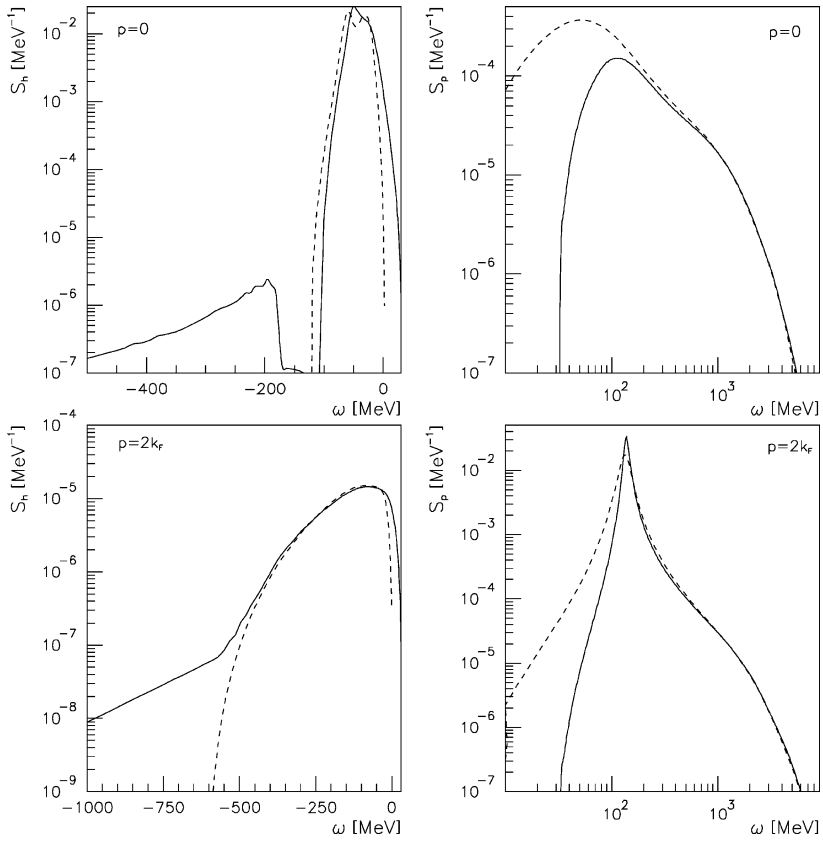

Fig. 3. The hole and particle spectral function calculated using Eq. (2) after the convergence of the BAGEL spectrum, at $k_F = 1.36$ fm^{-1}. The upper plots correspond to a momentum $p = 0$, the lower plots to $p = 2k_F$. Note the use of a logarithmic energy scale for the particle spectral functions, illustrating the large spreading of particle strength due to the short-range correlations. (Also the linear energy scale used for the right-hand side plots differs for both momenta.) The full line corresponds to a BAGEL calculation, the dashed line to the dressed quasi-particle result.

Table 1
The occupation probability calculated in three different approaches, with $k_F = 1.36$ fm^{-1}. The full quasi-particle and full BAGEL results are obtained by integrating the respective spectral functions up to the Fermi energy. The BAGEL result refers to the sum of the BAGEL poles located below the Fermi energy

	Full quasi-particle	BAGEL	Full BAGEL
$p = 0.0$	0.91	0.99	0.94
$p = 0.7k_F$	0.87	0.99	0.92
$p = 1.2k_F$	2.8×10^{-2}	5.1×10^{-3}	3.4×10^{-2}
$p = 2.0k_F$	3.2×10^{-3}	1.8×10^{-3}	3.4×10^{-3}

to some extent, which causes a reduction of the effective interaction around $2\epsilon_F$. These preliminary calculations suggest that the inclusion of off-shell propagation leads to a reduction of the depletion. It should be noted that the BAGEL approximation does not conserve the total number of particles, since one finds a particle excess of 4%

Table 2
The location and strength of the central pole for $p = 0$ and $k_F = 1.36$ fm^{-1}, in the BAGEL-scheme after the first iteration, when larger sets of $d = 3, 5, \ldots, 13$ BAGEL-poles are included in the calculation. The quasi-particle energy for this momentum equals -49.47 MeV

d	ϵ_c [MeV]	z_c
3	-16.88	0.87
5	-17.24	0.83
7	-17.93	0.80
9	-18.89	0.77
11	-19.95	0.73
13	-20.97	0.67

Table 3
Results of a five pole BAGEL calculation for the first three iterations with $p = 0$, $k_F = 1.36$ fm^{-1}

Iterations	ϵ_c [MeV]	z_c
1	-17.24	0.83
2	-12.66	0.92
3	-9.58	0.96

using the occupation probabilities obtained by summing the discrete poles and an excess of 8% using the integrated hole spectral function. This is again caused by the specific features of the BAGEL scheme and such a behaviour is not expected to show up when other discretization schemes are used. One should note that these occupation probabilities were obtained using a reduced interaction. Calculations with a full interaction should yield a larger depletion. Both a quasi-particle calculation using the soft-core Reid interaction [7] and a CBF-calculation using the Urbana V_{14} potential [18] predict an occupation probability of $n(0) = 0.82$.

The problems associated with the position and strength of the central pole, cannot be avoided within a BAGEL scheme. When larger sets of BAGEL poles are included in the description of the Green's function, the central pole after the first iteration will show a closer resemblance with the quasi-particle pole as is shown for $p = 0$ in Table 2. Table 3 displays the second and third iteration of a five-pole calculation. One can see that already in the second iteration, the feedback-mechanism embedded in the self-consistent calculation will reattribute part of the strength of the outward poles to the central pole, which at the same time shifts to higher energies. Hence, the self-consistent inclusion of a larger set of BAGEL poles does not improve the correspondence between the central BAGEL pole and the quasi-particle behaviour.

One can try to alleviate the problems caused by the location of the central BAGEL pole by performing a shift of the central BAGEL pole or of the complete BAGEL spectrum. However, such a scheme does not converge, and due to this shift the correct lowest order moments of the spectral function are no longer reproduced. Furthermore this shift does not alter the strength attributed to the central pole so that the pairing-instability is not avoided when the full realistic interaction is used.

It should be clear at this point that if one wants to benefit from the advantages of the discrete pole scheme, a new discretization scheme should be devised. When constructing this scheme, one should focus on a better description of the quasi-particle behaviour, by fixing the location of the central-pole at the quasi-particle energy. The other poles can be used to describe the features of the extended background distribution, including the sum rules of the spectroscopic strength. Work along these lines is currently in progress.

5. Summary

The discrete pole approximation proposed in this letter is an extension of the quasi-particle scheme, incorporating the off-shell propagation of the nucleons. This off-shell propagation is absent in a one-pole scheme, since the background distributions are neglected within such a scheme. Using a multiple-pole approximation for the Green's function, the deformation of the Fermi sea, originating from the short-range correlations is taken into account in the evaluation of the effective interaction. This opens the possibility of studying the effects of self-consistency on pairing properties of nuclear matter. The deformation of the Fermi sea also introduces an additional density dependence in the binding-energy which is important for the correct description of the saturation mechanism. Preliminary calculations using a BAGEL-discretization scheme and a model potential, suggest a reduction of the depletion caused by a new feedback mechanism originating from the use of a correlated Fermi sea. The BAGEL scheme however is plagued by a weak correspondence between the central pole and the quasi-particle pole. The use of an improved discretization scheme should solve this problem.

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