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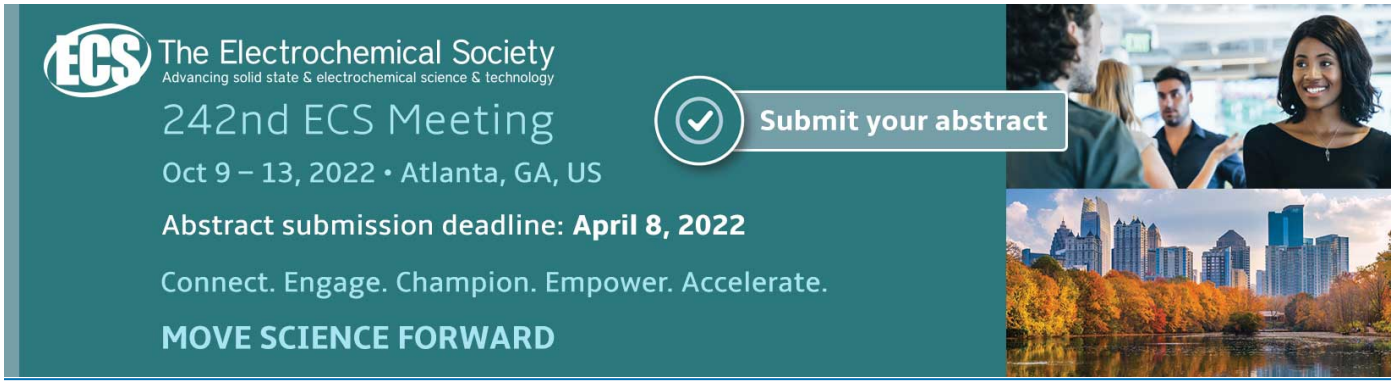

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Use of the Sumudu transform to extract response functions from Quantum Monte Carlo calculations

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Abstract. We review an *ab-initio* method for calculating the dynamical structure function of an interacting many–body quantum system. The method consists in coupling a generalized integral transform approach with imaginary time Quantum Monte Carlo calculations. The strength of the method has been tested on the excitation spectrum of bulk atomic ^{4}He. The peculiar form of the kernel as a representation of the delta-function has allowed to minimize the ill-posedness of the integral transform inversion. In fact it has been possible to obtain, at a considerable degree of reliability, both position and width of the collective excitations in the maxon–roton region, as well as the second collective peak. What we stress here is the ability of such a δ-function-like kernel, for which one can control position and width, to maintain in the transformed space the characteristics of the collective structures. The application to the coherent and incoherent density excitation spectrum of liquid ^{4}He is discussed.

1. Introduction

The computation of microscopic dynamic quantities is routinely performed for classical systems by numerically solving Newton equations and collecting the information of interest from the generated trajectories. In quantum mechanics this process is not possible, since there is no reliable method for solving the time-dependent Schroedinger equation for a general many-body system. Information about the dynamical evolution must be obtained by the computation of spectral function relative to some excitation operator. It is possible, by a simple mathematical manipulation, to show that some *integral transform* of the spectral function can be easily obtained as a ground-state expectation value. While this fact is extremely valuable, since there are many reliable *ab-initio* methods available for ground state calculations, the price to pay is the ill-posedness of the inversion problem that needs to be faced to extract the excitation spectrum.

In this paper we will discuss the problem of extending in a reliable way a class of Quantum Monte Carlo (QMC) algorithms to make it possible to determine the Dynamical Structure Function (DSF) for a generic quantum many-body system and a generic excitation operator. As already mentioned, we will follow the general approach of computing an Integral Transform (IT) of the DSF with generalized kernels. As an example, we will present an application to the study of the coherent and incoherent density excitation spectrum in ^{4}He.

At present, QMC calculations provide benchmark-quality results for the study of a variety of many-body systems as, for example, in quantum chemistry, physics of ultra-cold gases, and


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nuclear physics. One of the most severe limitation of QMC methods is their inability to treat dynamical properties in a similarly reliable way. This failure is essentially due to the fact that the propagators required to implement the time evolution are usually not normalizable, and cannot be sampled. However, by Monte Carlo methods it is possible to implement an imaginary-time evolution, which yields the projection of some generic state belonging to an arbitrary Hilbert space on the component along the eigenstate of the Hamiltonian with lowest eigenvalue. Quantities that do not directly translate into imaginary-time language, are affected by statistical noise when analytically continued to real time. This noise can be hardly reduced and make calculations unfeasible.

The standard approach to the problem is to compute the Laplace transform of the DSF as an imaginary-time autocorrelation function and then to attempt a numerical inversion. However, this inversion is an exponentially ill-posed problem [1]. Sophisticated regularization techniques [2, 3] are needed to correctly extract the physical information. In this context, the reliability of the calculation becomes strongly dependent on the employed inversion scheme. As an example, one of the most powerful inversion schemes, the Maximum Entropy Method [4, 5], cannot resolve the (measured) double peaked structure of $S(\mathbf{q},\omega)$ in superfluid ^{4}He [6], corresponding to a higher energy collective roton mode. In a recent paper this structure was eventually resolved inverting the imaginary time correlation function in a Path Integral Ground State calculation by using a falsification method based on a genetic algorithm [7].

For strongly interacting few-body systems the problem of computing various DSF of density and current excitations is solved by using a generalized integral transform approach, i.e. the Lorentz Integral Transform (LIT) method [8, 9]. The success of this approach, so far applied in nuclear physics, is based on the specific choice of a Lorentzian function as kernel of the IT. On the one hand this choice allows to calculate the transform with bound state techniques, such as expansions on localized many-body basis functions, even when the response is defined in the continuum. On the other hand, and most important, the fact that the kernel is a representation of the δ-function allows for a reliable and stable inversion. So far, the application of this technique has been limited to a small number of particles (up to N=6 [10] and 7 [11]), due to the huge computational costs of the diagonalizations needed to calculate the LIT. In the following we will discuss how it is possible to extend the same ideas to many-body system. In general, QMC methods do not allow for computing generic integral transforms, due to the fact that not all kernels easily translate into functions that can be sampled in coordinates space. However, we will see that it is possible to write a kernel that is suitable for QMC evaluation, and at the same time retains the main features of the Lorentz kernel, i.e. being a peaked function (and a δ-function in some limit), and having a controllable width.

2. Integral transforms

At zero temperature the contribution to the response of a system of interacting particles due to a perturbative probe transferring momentum $\mathbf{q}$ and energy ω to it, can be expressed using a spectral representation

$$\begin{aligned} S_{\hat{O}}(\mathbf{q},\omega) &= \sum_\nu |\langle\Psi_\nu|\hat{O}(\mathbf{q})|\Psi_0\rangle|^2\delta(E_\nu-\omega) \\ &= \langle 0|\hat{O}^\dagger(\mathbf{q})\delta(\hat{H}-\omega)\hat{O}(\mathbf{q})|0\rangle, \end{aligned} \tag{1}$$

where $|\Psi_0\rangle$ is the ground state of the system, $|\Psi_\nu\rangle$ are the final states of the reaction, $\hat{O}$ is an excitation operator, $\delta(\hat{H}-\omega)$ is the spectral-density of the hamiltonian and the summation is extended to all discrete and continuum spectrum states in the set.

The cost of a direct calculation of $S_{\hat{O}}(\mathbf{q},\omega)$ becomes rapidly not affordable when the number of particles or the energy transfer ω increases. The latter problem is due to the fact that to account for continuum states one would need to solve the many-body scattering problem. It is instead possible to consider an integral transform of $S_{\hat{O}}(\mathbf{q},\omega)$ with a generic kernel $K(\sigma,\omega)$

$$\Phi(\mathbf{q},\sigma) = \int K(\sigma,\omega)\, S_{\hat{O}}(\mathbf{q},\omega)\, d\omega. \tag{2}$$

Substituting the expression (1) for $S_{\hat{O}}(\mathbf{q},\omega)$ one obtains:

$$\begin{aligned} \Phi(\mathbf{q},\sigma) &= \sum_{\nu} \langle\Psi_0|\hat{O}^{\dagger}(\mathbf{q})|\Psi_\nu\rangle K(\sigma,\omega)\langle\Psi_\nu|\hat{O}(\mathbf{q})|\Psi_0\rangle \\ &= \langle\Psi_0|\hat{O}^{\dagger}(\mathbf{q})\, K(\sigma,\hat{H})\, \hat{O}(\mathbf{q})|\Psi_0\rangle \end{aligned} \tag{3}$$

Equation (3) can be viewed as a generalization of the energy-weighted sum rules, which now depends on a continuous parameter σ. Provided that the kernel and the excitation operator have suitable analytic properties, the right hand side of equation (3) can be calculated using bound-state type methods. This is the case both for the Stieltjes kernel [12, 13], and for the Lorentz kernel. However, while in the former case the inversion of the transform is as problematic as in the case of the Laplace kernel, in the latter case even a rather simple regularization procedure allows to obtain accurate and stable results. The reason can be easily understood. In the case of the Laplace or the Stieltjes kernels, or, in general, kernels that are significantly non-zero over a wide σ range, the information about $S_{\hat{O}}(\mathbf{q},\omega)$ in the ω domain is spread in a large σ domain. On the contrary the Lorentz kernel, as well as any function that is a δ-function representation, keeps that information in an arbitrarily narrow σ domain, governed by the width of the kernel. In the δ function limit of the kernel no inversion is needed. Once the transform is available we can obtain $\mathcal{R}(\omega)$ via a proper inversion of the transform, using a suitable regularization procedure.

3. Sumudu transform

As we already mentioned, the way to the success for a method based on IT is using kernels that are δ-function representations. While there is a large number of them, very few have a practical implementation. In the past the use of Gaussian kernels has been investigated in different fields from condensed matter [14, 15], to non perturbative QCD [16, 17], but with limited results.

Quite fortunately, it is possible to recast one specific δ-function representation in the imaginary-time propagation language, typical of QMC methods.

Consider the following family of integral kernels built out of the so-called Sumudu transform:

$$K_P(\sigma,\omega;a,b) = \frac{1}{\sigma}\left[\left(\frac{b}{a}\right)^{-a\frac{\omega}{\sigma}} - \left(\frac{b}{a}\right)^{-b\frac{\omega}{\sigma}}\right]^P, \tag{4}$$

where the parameters $b > a$ are integer numbers. This kernel function converges to a scaled delta function $\delta(\omega-\sigma)$ in the $P\to\infty$ limit, independent of the choice of a and b. For a finite P the kernel is still centered around $\omega=\sigma$ but has a finite width that depends on σ and the integers P,a and b. This property makes the choice of the resolution in a given energy range extremely flexible.

The simplest possible choice of the parameters is $a=1$ and $b=2$. In this case, using a binomial expansion, and rewriting powers as exponential functions, leads to a more transparent form of the kernel:

$$K_P(\sigma,\omega) = \sum_{k=0}^{P} \left(\begin{array}{c} P \\ k \end{array}\right) (-1)^k e^{-\ln(2)(P+k)\frac{\omega}{\sigma}}, \tag{5}$$

By operating the substitution $\omega \rightarrow \hat{H}$ according to equation (3), we are lead to a simple linear combination of imaginary-time propagators ($\hbar$=1), taken at imaginary-time points $\tau_{Pk} = \ln(2)(P+k)/\sigma$.

4. Integral transforms in projection Monte Carlo methods

Projection QMC methods are all based on the implementation of such an imaginary-time propagation. The underlying idea is to solve the corresponding integral equation:

$$\Psi(R,\tau) = \int dR' G(R,R',\tau)\Psi(R',0). \tag{6}$$

This can be achieved, for instance, sampling a representation in coordinate space of the Green's function $G(R,R',\tau)$ to propagate a set of configurations representing in turn an expansion of the function $\Psi(R,\tau)$ in eigenstates of the position operator (Diffusion Monte Carlo methods). Alternatively, it is possible to break up the Green's Function in a product of short time propagators in coordinate space:

$$\begin{aligned}\Psi(R,\tau) &= \int dR' \dots dR^n G(R,R^n,\Delta\tau)\times \\ &\quad \times G(R^n,R^{n-1},\Delta\tau)\cdots G(R'',R',\Delta\tau)\psi(R',0),\end{aligned} \tag{7}$$

with $\tau = n\Delta\tau$. This formulation is implemented in the so-called Path-Integral Ground State methods [18], and in the Reptation Monte Carlo (RMC) algorithm [19], where the whole path $\{R,R',R'',\dots,R^n\}$ is sampled from the product of the short-time propagators G, possibly modified with the use of a suitable importance function Ψ_T to be determined in a variational calculation. The fact that estimating $\Phi(\sigma)$ reduces to the computation of an imaginary time correlation function makes this second formulation more convenient and straightforward. In particular, path-based methods yield estimates that never depend on the (necessary) importance function used to improve the convergence of the calculation.

In order to evaluate the transform (2) within a QMC approach, we need to compute the imaginary-time correlation functions, and then construct the corresponding linear combinations. When needed, a smaller width of the kernel could be achieved using a large value of P or reducing the value of the ratio b/a. In both cases the imaginary time correlation function needs to be evaluated for long imaginary time, severely increasing the computational time. In any case, the guiding criterion is that the kernel should have a width at least comparable to the distance between the structures of the DFT.

5. Application to liquid helium

As a first application to a realistic physical problem, we have computed the density excitation response in bulk atomic ^{4}He at $T = 0$. The system is modeled as a periodic box containing $N = 64$ or $N = 125$ ^{4}He atoms. The chosen interaction is the HFDHE2 potential [20, 21], which quantitatively reproduces the binding energy of bulk ^{4}He up to the freezing point. Calculations were performed at the experimental saturation density ($n_0 = 0.02186$ Å^{-3}). The density excitation operator is defined as:

$$\hat{O}(\mathbf{q}) \equiv \hat{\rho} = \sum_{i=1}^{N} e^{i\mathbf{q}\cdot\mathbf{r}_i}\,, \tag{8}$$

and the transformed DSF in equation (2) becomes

$$\Phi(\sigma) = \langle\Psi_0| \sum_{i,j=1}^{N} e^{i\mathbf{q}\cdot\mathbf{r}_i(0)} K_P(\sigma,\hat{H}) e^{-i\mathbf{q}\cdot\mathbf{r}_j(\sigma)} |\Psi_0\rangle.$$

Computations have been performed by means of a RMC algorithm, as described in Ref. [19]. The variational importance function includes two- and three-body correlations expanded in a basis set [22] and optimized using a variational Monte Carlo procedure. Ground state properties are well reproduced: the ground-state energy per particle is $\epsilon_0^{RMC} = -7.23 \pm 0.01$ K, in good agreement with previous calculations using the same potential [19], and with the experimental value $\epsilon_0^{exp} = -7.17$ K. In the computation of the Sumudu transform, we have found by numerical testing that the values of $P = 2$, $a = 1$, and $b = 2$ satisfy this criterion in the range of energy and momenta explored.

As it is customary in neutron spectroscopy one can distinguish the contribution coming from the so-called *coherent* part, given by the terms with $i \neq j$, related to collective excitations, and an *incoherent* part with $i = j$ that essentially picks up contributions from single particle excitations. We have obtained results for both the full and for its incoherent part, in the most studied region of the spectrum: the low momentum phonon-maxon-roton part $q \approx 0.3 \div 3.5\,\text{Å}^{-1}$. The computed static structure factor $S(\mathbf{q})$ is consistent with experimental data and previous calculations [19, 22].

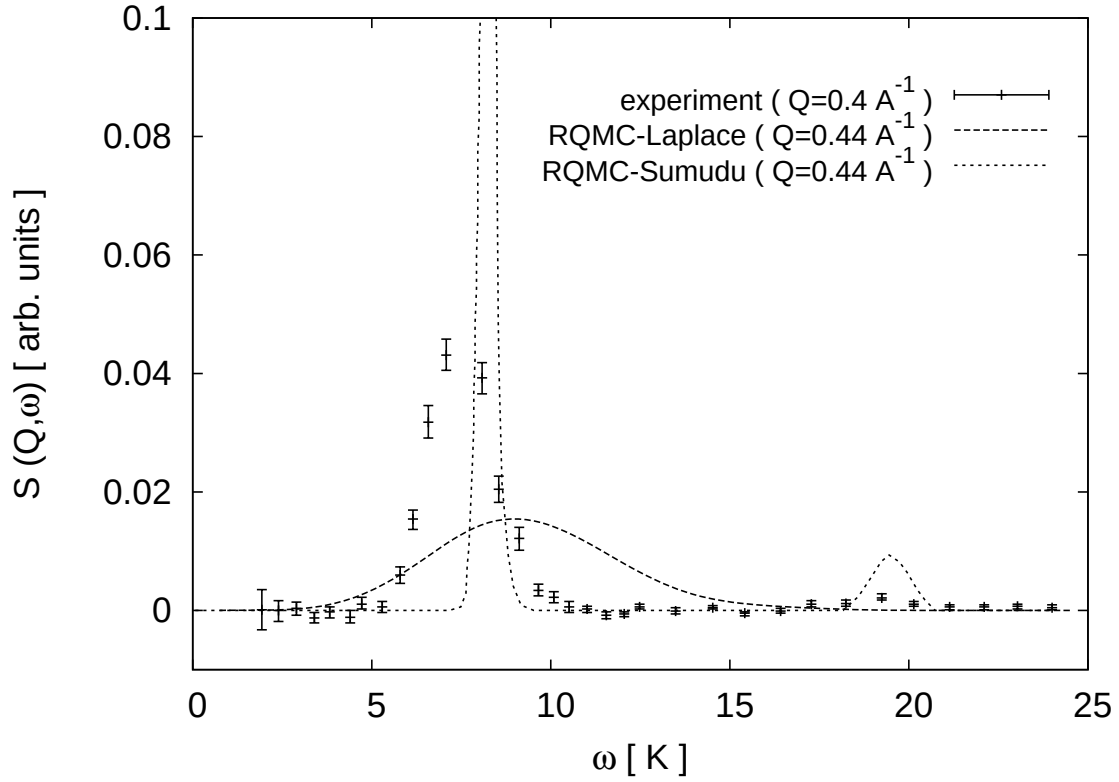

Figure 1. A typical result for the response function (Q, ω) in liquid ^{4}He. Points with errorbars are experimental results at $Q = 0.4\text{Å}^{-1}$. The thick dotted line is the result obtained using a Laplace kernel. The dotted line is the result computed by using the Sumudu kernel. Theoretical calculations refer to $Q = 0.44\text{Å}^{-1}$, value determined by the size of the simulation box.

When looking at the results on $S(\mathbf{q}, \omega)$, the difference between the inversion of the Laplace transform and the transform defined in equation (4) is clearly seen in figure 1, where we compare the results of the inversion obtained from RMC data with both kernels. Momentum discretization due to the finite simulation cell does not allow for a strict comparison to the experimental results. The small shift of the peak might indeed be due to the $0.04\,\text{Å}^{-1}$ difference

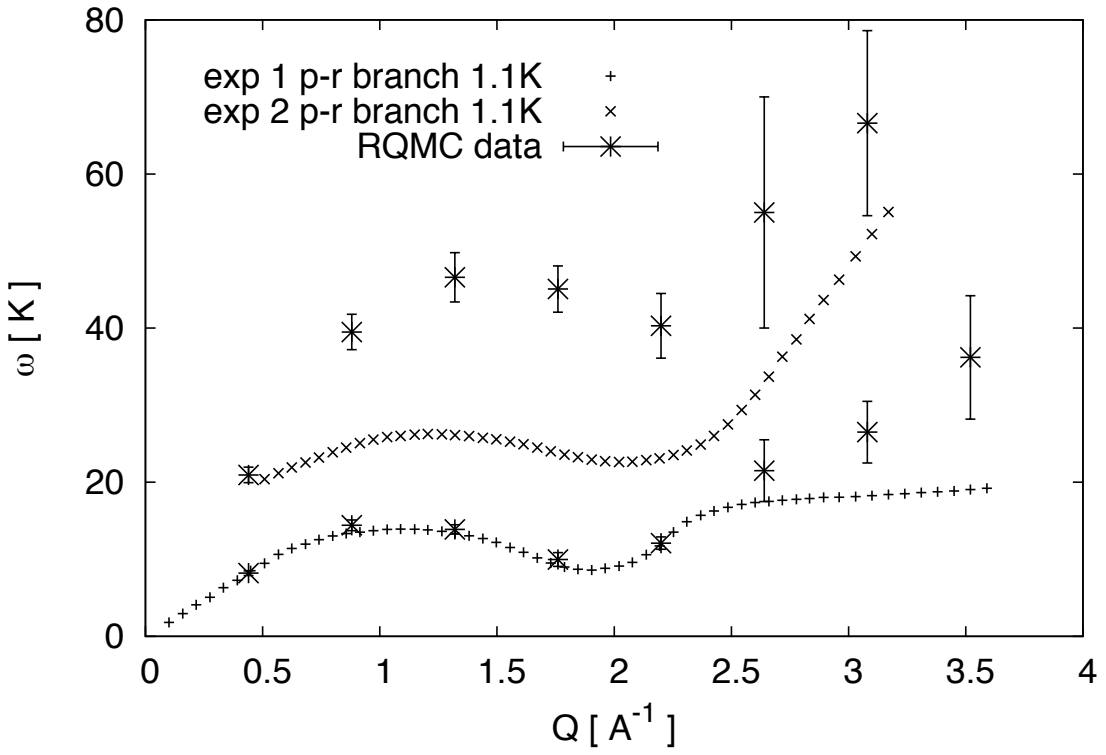

Figure 2. Dispersion of the collective modes in liquid ^{4}He at equilibrium density and $T = 0$. Points with errorbars are the computed values. Errorbars are estimates of the width of the peaks. + and × are the corresponding experimental data from Ref. [24] at $T = 1.1$K.

in the momentum transfer. However, the new kernel permits to retrieve the information on the second peak and gives a much more realistic height and width of the one-phonon peak. It should be pointed out that the width of the peak in the experiments is essentially due to instrumental resolution.

As regards the inversion procedure, we have used both the Entropy Maximization Maximum Likelihood (EMML) [23] and the Simultaneous Algebraic Reconstruction Technique (SMART) [23]. Error bars in the figures are obtained taking the maximum spread between the half-width position obtained from the two methods. We found that for $q \leq 2.4\text{Å}^{-1}$ both methods converge to the same solution, confirming the robustness of the result.

In figure 2 we plot the excitation spectrum obtained using the new transform. The experimental low-lying part [24] is extremely well reproduced up to $q \approx 2.6\text{Å}^{-1}$, where the dispersion does not bend over around 2Δ but continues to raise. In this region (the so-called Pitaevskii plateau), the peak corresponding to the collective excitation is mixing in the single particle excitations spectrum. The resolution that can be reached by the kernel with $P = 2$ is no longer sufficient, and EMML and SMART give different results indicating that the statistical uncertainty in the QMC data is too large to allow a consistent reconstruction. The dispersion corresponds to the centroid of the overall spectrum.

The two-phonon branch is clearly visible and well resolved. As it happens in Ref. [7], it only qualitatively compares to the experiment. The difference might be due either to the fact that measurements are taken at finite temperature, or to a larger sensitivity of the second peak to the details, for instance, of the interatomic interaction (e.g. the presence of effective three-body

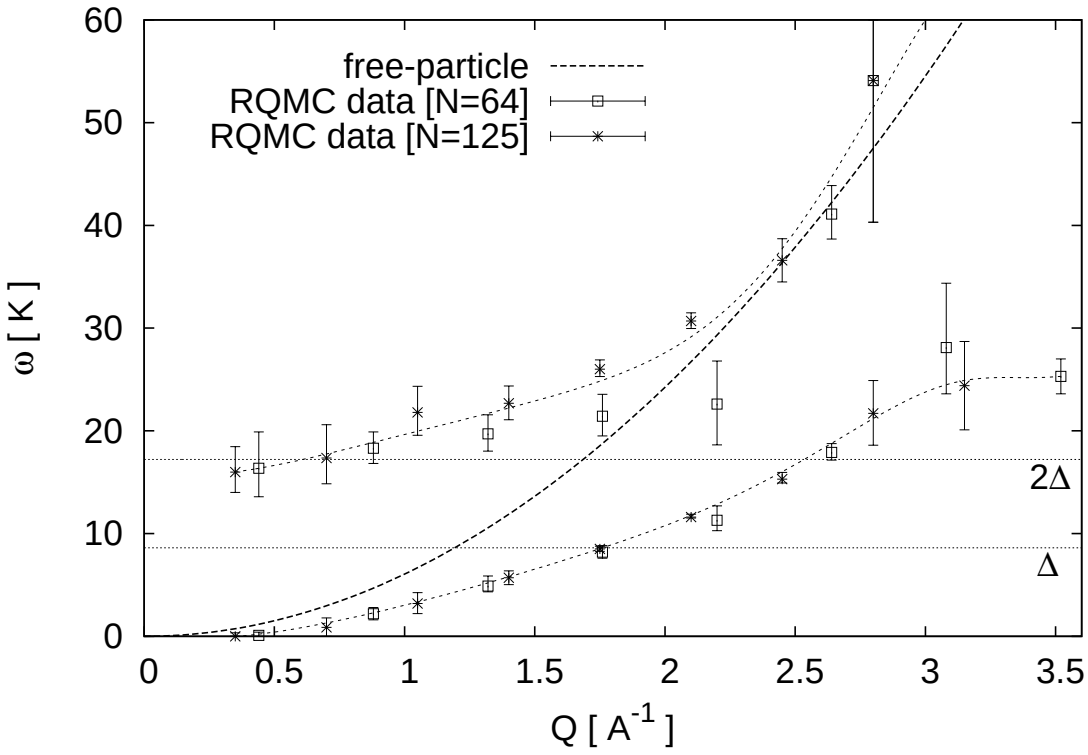

Figure 3. Incoherent Dynamic Structure factor computed by means of the Sumudu integral transform. Empty squares are simulations performed in a simulation box with N=64 atoms, stars refer to a box with N=125 atoms. Dotted lines are plotted as a guid to the eye. The dashed line is the free-particle excitation spectrum. Δ is the roton gap, and the lines at energy Δ and 2Δ are drawn as reference.

forces).

The most useful feature of these calculations is that the resolution is enough to allow for separately compute the incoherent part of the full response function, in order to study single-particle excitations.

In figure 3 we have plotted the calculated excitation spectrum of single-particle excited states. The spectrum shows at least two distinct branches. A lower energy excitation starts from $Q \approx 0.5A^{-1}$ and propagates with a velocity resulting slightly higher than the superfluid critical velocity $Ve/Vc \approx 1.57$. A second branch can be observed starting at an energy slightly below two times the roton energy, tending asymptotically to the free particle spectrum. Interestingly enough, the lower energy branch crosses the collective excitation spectrum exactly at the roton minimum, thereby reinforcing the picture of the roton as a single particle excitation of an atom exiting the superfluid. All these single-particle excitations might be related to the quantum correlations induced by the particle-particle interaction. An extensive experimental analysis of the single particle excitations properties in superfluid ^{4}He is unfortunately not available.

6. Conclusions

We have proposed a method to reliably extract well resolved spectra from numerical calculations implementing imaginary time propagation of an initial state, such as DMC or RMC. The computations might be easily extended to the $T \neq 0$ case by using standard PIMC methods.

The application to the study of the collective and single-particle excitations in ^{4}He shows the robustness and the higher resolution power of this technique. The limit to the accuracy of the spectra is in principle limited only by the available computer power available.

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