Inverse problems: Can we obtain more? Quantum dynamics and the $^4$He case

E. Vitali, M. Rossi, L. Reatto, and D.E. Galli

Dipartimento di Fisica, Università degli Studi di Milano, via Celoria 16, 20133 Milano, Italy

(Dated: March 17, 2010)

We introduce a new strategy, called Genetic Inversion via Falsification of Theories (GIFT), to face inverse problems and we apply it to the extraction of information about real time dynamics of a many–body quantum system from noisy imaginary time correlation functions $f(\tau)$ computed via Quantum Monte Carlo (QMC). Production and falsification of model spectral functions $s(\omega)$ are obtained via a survival–to-compatibility with $f(\tau)$ evolutionary process, based on Genetic Algorithms. Statistical uncertainty in $f(\tau)$ is promoted to be an asset via a sampling of equivalent $f(\tau)$ within the noise, which give rise to independent evolutionary processes. We have studied bulk $^4$He at $T = 0$ K; for the first time we recover from exact QMC simulations sharp quasi–particle excitations with spectral functions displaying also the multiphonon branch. As further applications of the method we have studied the impuriton branch of one $^3$He atom in liquid $^4$He and the vacancy–wave excitations in hcp solid $^4$He finding a novel roton like feature.

PACS numbers: 02.30.Zz; 67.40.Db; 67.55.Jd; 67.55.Lf; 67.80.-s

I. INTRODUCTION

Since the earliest days of research in Physics, inverse problems have always provided challenges in a huge variety of physical or even more generally scientific studies. At the most general level, an inverse problem consists in obtaining a (maybe very big) class of features, providing physical properties, that is, since any set of experimental data appears together with statistical uncertainties evaluated starting from suitable measurements, any set of data compatible with the original one has to take part to the falsification test, in order to suppress the possibility of unphysical effects arising from statistical fluctuations.

Once we remain with a set of equivalent “solutions” “survived” to the falsification test, depending on the mathematical details of the space $S$, a natural idea appears to be that of devising a procedure allowing to capture what do the “survived” theories have in common. In this way, even if we won’t succeed in finding out a unique theory $s \in S$, we will be able nevertheless to find out a class of features, providing physical properties, that $s$ has to possess so that it will not be falsified by the limited set of observations.

A. Inverse problems and quantum dynamics

In the last decades new ways of performing “observations”, computer simulations, have emerged in many areas of scientific research and have provided new sources of inverse problems. In this work we focus on one in particular, and namely on the estimation of spectral functions of many–body quantum systems starting from imaginary time correlation functions computed in Quantum Monte Carlo (QMC) simulations. Indeed, the study of dynamical properties requires the evaluation of spectral functions $s(\omega)$:

$$s(\omega) = \int_{-\infty}^{+\infty} \frac{dt}{2\pi} e^{i\omega t} \langle \hat{A} e^{-i\hat{H} t} \hat{B} \rangle , \quad (1)$$

$\hat{A}$ and $\hat{B}$ being given operators acting on the Hilbert space of the system whose Hamiltonian operator is $\hat{H}$. The brackets indicate expectation value on the ground state or thermal average. Unfortunately, general methods to obtain exact real time evolution are not known, thus forcing us to deduce a theoretical $s(\omega)$ from “observations” of imaginary time evolution function $f(\tau) = \langle \hat{O}(t) \rangle$.
In our mathematical framework $\mathcal{S}$ contains a wide class of step functions, providing a compromise between the possibility of suitably approximating any model of spectral function and the feasibility of numerical operations inside it. In the typical case ($A = B^\dagger$) when $s(\omega)$ is known to be real-valued, non-negative and the zero-moment sum-rule holds, we rely on models $\mathfrak{s}$ of the form:

$$\mathfrak{s}(\omega) = \sum_{j=0}^{N_{\omega}+1} \frac{s_j}{M \Delta \omega} \chi_{A_j}(\omega), \quad \sum_{j=0}^{N_{\omega}+1} s_j = M .$$

(5)

$\mathfrak{s}(\omega)$ differs from the physical spectral functions by a factor $c_0$, the zero–moment sum rule, which belongs to the set of observations and its role will become evident below. We introduce a discretization of the codomain:

$$s_j \in \mathbb{N} \cup \{0\},$$

(6)

to make the space finite, and we use the characteristic function $\chi_{A_j}(\omega)$ of the intervals $A_j = [\omega_j, \omega_{j+1})$, $[\omega_0, ..., \omega_N]$ being a partition of width $\Delta \omega$ of an interval of the real line larger than the hypothesized support of $s(\omega)$. $M$ provides the maximum number of quanta of spectral weight available for the ensemble of the intervals $A_j$.

### B. The falsification principle

Once we have defined the space of model spectral functions, we have to devise a practical strategy to implement the falsification principle. We have to rely on the QMC estimations of the imaginary time correlation functions (and, in general, also of the moments):

$$\mathcal{F} \equiv \{ f_0, f_1, \ldots, f_l \} .$$

(7)

Such numbers are averages evaluated during a simulation and appear together with their estimated statistical uncertainties $\{ \sigma_{f_0}, \sigma_{f_1}, \ldots, \sigma_{f_l} \}$. In typical approaches, such information are dealt with inside the framework.
of Bayes’ theorem; they provide the key ingredients to build up the a posteriori probability \( \bar{\omega} \) to be maximized, together with some a priori probability, to extract the most probable spectral function.

On the other hand, we find natural to suggest a new way of exploiting the information contained in \( \{ \sigma_{f_0}, \sigma_{f_1}, \ldots, \sigma_{f_l} \} \): any set \( F^* \) equivalent to \( F \), i.e. such that \( \{ f^*_j - f_j \} \) is of the same order as \( \sigma_{f_j} \), could be a result of another hypothetical simulation. Falsifying the elements of \( S \) should require not only compatibility with \( F \) but also compatibility with a vast population of \( F^* \) equivalent to the set \( \{ F \} \) of data. At a practical level our aim is twofold: on one hand we need a recipe to generate equivalent sets \( F^* \), on the other hand we have to use the generated \( F^* \) to falsify the elements of \( S \). At the simplest level we have addressed the generation of the sets \( F^* \) by sampling independent Gaussian distributions centered on the original observations, with variances which correspond to the estimated statistical uncertainties so that a generic element \( F^* \) is:

\[
F^* \equiv \{ f_0 + \epsilon^*_0, f_1 + \epsilon^*_1, \ldots, f_l + \epsilon^*_l \} = \{ f^*_0, f^*_1, \ldots, f^*_l \} \tag{8}
\]

being \( \epsilon^*_j \) random numbers sampled from Gaussian distributions with zero mean and variances equal to \( \sigma^2_{f_j} \). We stress that the very idea of exploiting the statistical uncertainties in the observations for generating equivalent sets \( F^* \) is the main difference with respect to preexisting statistical approaches to inverse problems. Note that in presence of more complete information in the observations, like an estimation of the full covariance matrix, \( \Sigma \), the generation of the equivalent sets \( F^* \) can be readily generalized by sampling an \((l + 1)\)-variate normal distribution with the following probability density function:

\[
p(F^*) = \frac{\exp \left[ -\frac{1}{2} (F^* - F)^\dagger \Sigma^{-1} (F^* - F) \right]}{(2\pi)^{\frac{l}{2}} \det(\Sigma)^{\frac{1}{2}}} \tag{9}
\]

standard methods to perform efficiently this task are known (see for example Ref.11). To be precise, being the set \( F \) a QMC estimation of the (unknowable) exact correlation function values, the probability density function \( p(F^*) \) in the previous equation does not represent the (unknown) exact distribution of the observations; this situation is typical of the inverse problems we are considering and of the statistical methods developed in this context: we have to rely on what we have observed. Therefore, it is important to estimate the statistical uncertainties connected with the application of a particular statistical method. This can always be obtained comparing models coming from the analysis of independent observations.

The key point is then to falsify the elements of \( S \) relying on each one of these sets: compatibility means small deviations from the observations. Thus, given the set \( F^* \), a very simple measure of the compatibility of a model with this set of observations can be obtained by computing

\[
\Delta(s) = \frac{1}{l + 1} \sum_{j=0}^l \left[ f^*_j - \int d\omega \ e^{-\omega j_\delta} c_0 \bar{s}(\omega) \right]^2 \tag{10}
\]

The normalization of our models requires the multiplication of \( \bar{s}(\omega) \) by \( c_0 \), the zero moment, which however belongs to the set of observations; a natural choice is to sample also its value analogously to how we treat \( F \). This is the reason why a factor \( c_0 \) appears in (10). Each member \( F^* \) of equivalent data leads to a different model; let us call \( \bar{s}_k \) the model found with the \( k \)-th member \( F^* \). Each one of these models cannot be trusted to be the solution of the inverse problem, being at least partially biased by the particular \( F^* \); in other terms we can say that each one of these models will posses spurious information, presumably different in each model, together with some physical information. An averaging procedure is therefore the simplest way to filter out the spurious information and to reveal physical information, which consist in the common features among the models which have not been falsified. Therefore we take as the reconstructed spectral function the average

\[
S_{GIFT}(\omega) = \frac{1}{N_r} \sum_{k=1}^{N_r} c^{(k)} s_k(\omega) \tag{11}
\]

where \( N_r \) is the number of equivalent random set of \( F^* \) used in the computation and \( c^{(k)} \) is the \( c_0^* \) used in the \( k \)-th reconstruction.

The average procedure in the definition of \( S_{GIFT}(\omega) \) points toward some similarities between our strategy and that of ASM. However, in the light of the falsification principle, the two methods are fairly different: in order to obtain its “solution”, ASM averages over spectral functions obtained by exploring model-space regions via a local Metropolis random walk based on a probability distribution \( \mathbf{S} \); thus ASM regards all the sampled spectral functions, also those with a low probability (of course, they are rarely sampled) as models which have not been falsified. Moreover, with ASM the statistical uncertainties in the observations play a different role, appearing only in the definition of the probability. Another issue is the algorithm used to explore the space of models; as explained below, GIFT uses a non-local dynamics induced by a stochastic evolutionary process instead of a local Metropolis random walk which, in principle, could suffer from ergodicity problems, being the high probability model-space regions not guaranteed to be simply connected. Which of the two approaches, GIFT and ASM is superior might well depend on the specific inverse problem or, in practice, it is possible that the reconstruction abilities of GIFT and ASM are essentially equivalent. ASM has never been applied to the \(^4\)He case, it will be interesting in the future to compare the two methods on the same inverse problem.

The natural scale of \( \Delta(s) \) is provided by the value

\[
\delta = \frac{1}{\prod_j \sum_{j=0}^l \sigma^2_{f_j}} \quad \text{models } \bar{s} \text{ such that } \Delta(s) < \delta
\]
may provide unphysical overfitting. In our statistical approach to inverse problems there are two procedures which preserve from overfitting. The first one is that, given a set $F^*$, the exploration of the space of models $S$ should be stopped when a model $\Omega(\omega)$ is found such that $\Delta(\omega) \approx \delta$; a further reduction of $\Delta$ will only represent the intention to give to $F^*$ a strong belief, which is incompatible with the statistical treatment of the observations in our strategy. The second procedure is even more relevant and in some sense it is intrinsic to our strategy: given an $F^*$ the reconstructed model $\Omega(\omega)$ contains some spurious information, but these information will be averaged out in $S_{GIF T}(\omega)$.

At this point the following question urges an answer: How can we practically explore $S$? We want to stress that the answer to this question is not the key point of our strategy; as we explain in the following, we have implemented genetic algorithms as efficient algorithms to explore our huge space of models, $S$. There could be inverse problems and different space of models which could be more efficiently explored with other algorithms; obviously, our strategy, which consists mainly in the new statistical treatment of observations, can be applied also in these cases.

C. The fitness and the genetic dynamics

Genetic algorithms (GA) provide an extremely efficient tool to explore a sample space by a non-local stochastic dynamics, via a survival–to–fitness evolutionary process mimicking the natural selection we observe in natural world; such evolution aims toward “good” building blocks, which, in our case, should recover information on physical spectral functions. The fitness of one particular $\Omega(\omega)$ should be based on the observations, i.e., on the noisy measured set $D = \{F, C\}$. But as explained before, taking into account the estimated statistical noise of $D$, any set $D^*$ compatible with $D$ provides equivalent information to build a fitness function. Thus in our GA any random set $D^* = \{F^*, C^*\}$ gives rise to a fitness, which simply compares “predictions” of theories and “observations”:

$$\Phi_{D^*}(\omega) = -\Delta(\omega) - \sum_n \gamma_n \left[ c_n^* - \int d\omega \omega^n c_n^{\omega}(\omega) \right]^2$$ \hspace{1cm} (12)

In (12) the free parameters $\gamma_n > 0$ are adjusted in order to make the contributions to $\Phi_{D^*}$ coming from $F^*$ and from $C^*$ of the same order of magnitude; the idea is that we are not allowed to prefer some particular observation among the others, thus they should have the same weight in the fitness. If it happens that one $c_n$ is exactly known, no error is added making $c_n^* = c_n$. We stress that (12) provides the simplest and the most natural definition; moreover, as explained below, our GA uses $\Phi_{D^*}$ only to order models in ascending fitness, thus any alternative definition of $\Phi_{D^*}$ which provides the same ordering will give rise to an identical GIFT algorithm.

GA are well known procedures characterized by well defined (genetic–like) operations on populations of candidate solution to optimization problems in applied mathematics. For basic nomenclature and standard implementations one can refer to textbooks (e.g. see [12]). Here we simply sketch our particular realization related to the space of models we have defined. In our GA, we start randomly constructing a collection of $\Omega(\omega)$; each $\Omega(\omega)$ is coded by $N_\omega$ integers, $s_j$ in equation (10). The genetic dynamics then consists in a succession of generations during which an initial population, consisting of $N_\omega$ individuals, is replaced with new ones in order to reach regions of $S$ where high values of the fitness exist, for a given $D^*$.

In practice, in the passage between two generations a succession of “biological–like” processes takes place, and namely selection, crossover and mutation. The selection procedure is meant to make individuals with large fitness preferentially be chosen to give rise to the next generation: we achieved this by ordering the population in ascending fitness and selecting the $k$-th individual with

$$k = \left[ N_\omega r^{1/3} \right] + 1$$ \hspace{1cm} (13)

where $r$ is an uniform random number, $r \in [0, 1)$, and $[\ldots]$ is the integer part; the non linear dependence of $k$ on $r$ ensures that individuals with large fitness are preferentially selected. The crossover then operates on two selected $\Omega(\omega)$, the father and the mother, exchanging subparts of their total number of quanta of spectral weight, $M$, to generate two sons. We have used a special single point crossover by sampling a random integer, $w$, between 0 and $M$ and by exchanging $w$ randomly chosen quanta of spectral weight between the father and the mother. In this way, the second equation in (5) is automatically satisfied, implying that the zero–moment sum rule is also satisfied. Each exchanged quantum remains in the original frequency bin as in its parents, thus ensuring that strong features present in both parents tend to persist in the sons. Successively, with a given probability, mutation takes place on the two new individuals, i.e., a shift of a fraction of spectral weight between two intervals $A_j$. This is repeated till a new generation of $\Omega(\omega)$ replaces the old one, with the exception of the $\Omega(\omega)$ with the highest fitness in the old generation which is cloned (elitism). The number of individuals in the new population is constantly reduced by about 5% at every generation till $N_\omega$ is equal to a given minimal value; from this point over, the number of individuals $N_\omega$ in the new generations is kept constant to this minimum value. The discarded individuals are those with the smallest fitness in the population. This is done to start the genetic evolution from a wide variety of possible models, but to not dissipate computational time on falsified spectral functions.

In our context the GA dynamics performs the falsification procedure: only the $\Omega(\omega)$ with the highest fitness in the last generation provides a model, $\Omega(\omega)$, which has not been falsified by $D^*$. The evolutionary process
III. RESULTS FOR HELIUM SYSTEMS

We are ready now to present applications of our approach on physical systems. Long Monte Carlo runs have been performed in order to get imaginary time correlation functions with a typical statistical uncertainty of 0.1-1%. For bulk superfluid 4He most of the simulations have been for \( N = 64 \) and \( N = 256 \) atoms moving in a cubic box, but also \( N = 128 \) and \( N = 512 \) have been studied; for solid 4He the hcp lattice with \( N = 180 \) and \( N = 448 \) lattice position have been used. Imaginary time correlation functions have been computed for instants \( \tau_i = l \delta \tau \), \( l = 0 \ldots l_{\text{max}} = 60 \) in the superfluid phase and \( l_{\text{max}} = 30 \) in the solid phase, spaced by \( \delta \tau = 1/160 \) K\(^{-1}\). In the present applications on 4He systems the whole covariance matrix has not been computed, thus equivalent sets \( \mathcal{F}^* \) have been sampled simply by using the procedure in equation (8). We have tested on 4He systems the approach on physical systems. Long Monte Carlo runs have been performed also with that in Ref.18.

All the results shown in this article have been obtained in previous studies of superfluid 4He for \( q = 0.7 \) Å\(^{-1}\) at SVP and \( T = 1.3 \) K. Notice the logarithmic scale. Notice also the difference between the wave vector of \( S_{GIFT}(q, \omega) \) and the one of the experimental available dynamic structure factor; the experimental single particle peak position is known to increase by about 0.8 K in moving from \( q = 0.7 \) Å\(^{-1}\) to \( q = 0.783 \) Å\(^{-1}\).

A. The dynamical structure factor of superfluid 4He

Our first case study is the determination of the dynamical structure factor \( S(q, \omega) \) of liquid bulk 4He. We have used the exact SPIGS method\(^{20,21}\) to compute the intermediate scattering function \( F(q, \tau) \) at \( T = 0 \) K near the equilibrium density, \( \rho = 0.0218 \) Å\(^{-3}\), and slightly above the freezing density, \( \rho = 0.0262 \) Å\(^{-3}\); \( F(q, \tau) \) is simply \( f(\tau) \) when \( \hat{A} = \hat{B}^* \) is chosen to be the Fourier transform of the local density operator \( \hat{A} = \hat{\rho} \equiv \sum_{i=1}^{N} e^{-i\vec{q}\vec{r}_i} \). We observe that our reconstructed \( S_{GIFT}(q, \omega) \) exhibits an overall structure in good agreement with experimental data: a sharp quasi–particle peak and a shallow multiphonon maximum are present (see Fig.1). Both features appear for the first time within an analytic continuation procedure applied to a QMC study of a many–body system in the continuum. Notice that it is not appropriate to compare the widths of the two sharp quasi–particle peaks in Fig.1 in fact the experimental peak includes the broadening arising from instrumental resolution and the effect of the finite temperature; on the contrary, as explained in the following, the width of the reconstructed GIFT peak from a \( T = 0 \) imaginary time correlation function is only a measure of the uncertainty in reconstructing its position. In Fig.2 we show one \( S_{GIFT}(q, \omega) \) in the roton region together with the excitation energies \( \epsilon(q) \) i.e., the position of the main peak as function of \( q \). The uncertainties of \( \epsilon(q) \) correspond to the widths of the peaks \( \sigma_\epsilon \); we have checked the consistency of such identification by performing independent QMC estima-
Figure 2: (a) and (b): $S_{GIFT}(q, \omega)$ at $q = 1.755 \text{ Å}^{-1}$ and $\rho = 0.0218 \text{ Å}^{-3}$; (a) single quasi–particle (qp) peak; (b) multiphonon (mp) contribution (notice change of scale). Lines corresponding to a $S_{GIFT}(q, \omega)$ obtained with a nonzero entropic prior ($\eta \neq 0$) are also shown. (c) $\varepsilon(q)$ extracted at $\rho = 0.0218 \text{ Å}^{-3}$ from the position of the qp (circles) peaks and the positions of the maxima of the mp contribution (triangles) are shown. The error–bars represent the 1/2–height widths. (d) $\varepsilon(q)$ and mp contribution extracted at $\rho = 0.0262 \text{ Å}^{-3}$. Lines in (c) and (d): experimental data. (c) (d): experimental data.

Figure 3: Evolution of the deviation $\eta$ during the stochastic evolution of the genetic algorithm for the reconstruction plotted in Fig.2(a,b) for $\eta = 0$ averaged with respect to the sampled sets $D^*$. The dashed horizontal line represents the value $\eta = \frac{\sum_{j=0}^{\infty} \sigma_j^2}{m+1}$.

In principle also a MEM-like algorithm could fit into the GIFT approach: it is enough to modify the fitness function by adding to $\Phi_{D^*}$ in equation (12) an entropic term $-\eta S$, with

$$S = \int d\omega \left\{ \frac{\varphi(\omega)}{m(\omega)} \ln \left[ \frac{\varphi(\omega)}{m(\omega)} \right] - \varphi(\omega) + m(\omega) \right\}, \quad (14)$$

$S$ being the entropy as in Ref.6 and $\eta \geq 0$ a free parameter; $m(\omega)$ is the default model which in previous implementations has been chosen to be simply a constant in absence of any prior knowledge. This is not a faithful implementation of MEM because the entropic term is used in the context of the GIFT method and not within the framework of Bayes’ theorem. Anyway, as we shall show, it provides results for the dynamical structure factor critically dependent on the choice of the parameter $\eta$. This implementation of MEM provides results comparable with those reported in references 6 and 7. The overall double-peak structure is typically lost in presence of the entropic term: no sharp peak is present but only a smooth $S(q, \omega)$ survives, as function of $\omega$, making the extracted excitation energy critically dependent on the value of $\eta$, thus introducing ambiguities in the interpretation of the results. In our original approach, i.e. without $\eta S(\varphi)$, we have checked that none of the parameters (like $M, \Delta, \alpha, \gamma, \ldots$) affects the class of features that we may trust to carry reliable physical information.

As an example of the stochastic evolution, in Fig.3 we show the deviation $\eta$ as a function of the number of generations in the evolutionary process for the reconstruction plotted in Fig.2(a,b) for $\eta = 0$ averaged on the sampled sets $D^*$. One can see that the maximum number of generations, $N_G$, we have used in this reconstruction is optimal in reaching the “compatibility” condition, $\Delta(\varphi) \simeq \frac{1}{m+1} \sum_{j=0}^{\infty} \sigma_j^2$, without overfitting.

By integrating $S_{GIFT}(q, \omega)$ we have access to quantities like the strength of the single quasi–particle peak, $Z(q)$, and thus also to the contribution to the static structure factor, $S(q)$, coming from multiphonon excitations. Remarkably, $Z(q)$ turns out to be in close agreement with experimental data (see upper Fig.4), thus strongly suggesting that the shallow maximum in $S_{GIFT}(q, \omega)$ at large energy carries indeed reliable physical information on the multiphonon branch of the spectrum. The position of such multiphonon maximum (see Fig.2) is in qualitative agreement with experiments as we show in the next section, within the present implementation of
the GIFT method there is no possibility to recover the detailed shape of the spectral function like the multiphonon substructures given by high resolution measurements of $S(q,\omega)$. In the lower panel of Fig.4 we show the static density response function $\chi(q)$ obtained evaluating the $\epsilon_{-1}$ from $S_{GIFT}(q,\omega)$; the agreement with experiments is impressive, also near freezing. The calculation of the excitation spectrum $\epsilon(q)$ in superfluid $^4$He via QMC was addressed for instance in Ref.28 and in Ref.27, but here we are clearly much more ambitious because we aim to reconstruct the full spectral function. Our method is so powerful that it is able to reveal the effects of even fine details of the interatomic interaction. For example, the computed spectrum $\chi(q)$ in the phonon region is about 0.7 K above the experimental value. We understand this as an effect of truncation of the inter–atomic interaction $v(r)$ at a certain distance $r_c$. In most of our computations the interatomic potential is cut-off and displaced to zero at $r_c = 6$ Å, and the equation of state gives rise to an overestimation of the sound velocity by about 16%. We have performed some computations with $r_c = 14$ Å, in a simulation of $N = 512$ $^4$He atoms and in this case the sound velocity turns out to be correct and now the theoretical $\epsilon(q)$ at small $q$ agrees with experiment within the resolution $\Delta \omega$. By computing $\epsilon(q)$ for many wave vectors in the roton region and averaging among the excitation energies nearby the roton minimum, at $\rho = 0.0218$ Å$^{-3}$ we extract a roton energy of $E_R = 8.96 \pm 0.47$ K with the $v(r)$ in Ref.17 and of $E_R = 8.67 \pm 0.29$ K with the $v(r)$ in Ref.18, a potential considered more accurate (Experimental roton energy$^{28}$ at SVP $E_R = 8.608 \pm 0.01$ K). At $\rho = 0.0262$ Å$^{-3}$ we extract a roton energy of $E_R = 7.43 \pm 0.34$ K with the $v(r)$ in Ref.17 and of $E_R = 7.22 \pm 0.27$ K with the $v(r)$ in Ref.18 (Experimental roton energy$^{28}$ at 24 bar $E_R = 7.3 \pm 0.02$ K).

**B. Impurity and vacancy dynamics**

Another interesting test case is provided by liquid $^4$He in presence of one $^3$He impurity, in order to extract the impurity branch which has been experimentally measured. Variational results for such branch are known$^{31,32}$ but no results from exact QMC are available. This calculation requires the choice of $A = e^{-i\vec{r}_{imp}}$, where $\vec{r}_{imp}$ is the position of the impurity. In Fig.5 we show the reconstructed spectral functions together with the estimated dispersion relation obtained from a simulation of $N = 255$ $^4$He atoms and one $^3$He atom at $\rho = 0.0218$ Å$^{-3}$. The agreement with experimental data$^{29}$ is very good, thus providing a robust check of validity of our approach.

As a further application of GIFT we have studied the excitation spectrum of a single vacancy in hcp solid $^4$He at $\rho = 0.0293$ Å$^{-3}$, a density slightly above melting. The behavior of vacancies in solid $^4$He is of high interest because vacancies and other defects are believed to have a key role in the possible supersolid phase of $^4$He at low temperature$^{31,32}$. In order to apply GIFT to vacancy dynamics the first step is the definition of a vector position $\vec{x}_v$ that allows to follow the “motion” of the vacancy in imaginary time during a SPIGS simulation. This problem is much more difficult than the evaluation of the impurity branch, because the very definition of $\vec{x}_v$ is far from trivial due to the large zero–point motion of the atoms in the low density solid. $\vec{x}_v$ turns out to be a many–body variable, depending on all the vector positions of $^4$He atoms, and even not free of ambiguities. We
have employed two different procedures to obtain $\vec{x}_v$: the coarse-grain and the Hungarian. In Fig. 6 we show the vacancy excitation spectrum $\varepsilon_v(\vec{q})$ extracted from the vacancy spectral functions ($\hat{A} = e^{-i\vec{q}\cdot\vec{x}_v}$) obtained with the two methods. The results obtained with the two definitions of $\vec{x}_v$ are very similar, and at first sight make evident a picture of Bloch waves in the crystal; the agreement with a tight binding hopping model is good. Notice that $\varepsilon_v(\vec{q})$ represents the excitation energy with respect to the state with a vacancy with $|\vec{q}| = 0$, i.e., $\varepsilon_v(\vec{q})$ does not include the vacancy activation energy. By fitting $\varepsilon_v(\vec{q})$ with the tight binding expression we extract the vacancy effective mass in the different lattice directions: $m_{v,K}^T = m_{v,M}^T = 0.46 \pm 0.03 m_4$ and $m_{v,A}^T = 0.55 \pm 0.1 m_4$, where $m_4$ is the $^4$He mass; these values for $m^*$ are in agreement with the results obtained with a different method in Ref. 37.

The agreement of $\varepsilon_v(\vec{q})$ with the tight binding model fails dramatically in the $\Gamma M$ direction. In fact, at any reciprocal lattice vector the excitation energy should vanish. On the contrary at the first reciprocal lattice vector along $\Gamma M$ the vacancy excitation spectrum does not vanish but it reveals a novel vacancy–roton mode with an energy of 2.6 $\pm$ 0.4 K and an effective mass of about $m_{v,R}^T = 0.46 m_4$. We have checked that this energy does not depend on the size of the system. Such behavior of $\varepsilon_v(\vec{q})$ in the $\Gamma M$ direction implies that the (non–zero) minimum is not a consequence of the lattice periodicity but it is related to correlated motion of particles like in superfluid $^4$He. It is interesting that neutron scattering from hcp $^4$He gives an unexpected excitation mode beyond the phonon modes exactly in the $\Gamma M$ direction with a roton–like mode at the reciprocal wave vector $\vec{q}_V$. The experimental energy of such roton mode is about 4.4 times larger than what we find; so it is unclear the connection between our mode and experimental data. A larger vacancy roton energy might arise in presence of clusters of vacancies. By analyzing the contributions to $f(\tau) = \langle e^{\hat{H}_\tau \hat{A}} e^{-\hat{H}_\tau \hat{A}} \rangle$ with $\hat{A} = e^{-i\vec{q}\cdot\vec{x}_v}$, one can see that the vacancy–roton mode is connected to motions of the vacancy between different basal planes. The fundamental difference between in–basal–plane and inter–basal–plane motions is that the lattice position in the first case is a centre of inversion whereas this is not so in the second case. The fact that hcp is not a Bravais lattice is fundamental in this respect. We have verified that in bcc crystal and in a two dimensional triangular lattice, both Bravais lattices, no such vacancy roton mode is present.

IV. TESTS ON KNOWN SPECTRAL MODELS

In this section we show several tests of application of the GIFT method on known analytical spectral models suitably discretized and “dirtied” with random noise to “simulate” actual data. It will appear evident what we have already pointed out in the introduction: only some features of the exact solution can be consistently reproduced; we have no possibility to reconstruct exactly the shape of $s(\omega)$; on the other hand, access is granted to the identification of the presence of peaks and to their positions, to some integral properties involving $s(\omega)$ and to its support.

The most natural test for the reliability of the GIFT approach we have developed is provided by a systematic study of Laplace inversion problems whose analytical solution is known. Our idea is to focus our attention on model functions of the form:

$$s(\omega) = \theta(\omega) \sum_{j=1}^{N_p} p_j e^{-\frac{(\omega-\mu_j)^2}{2\sigma_j^2}} \sum_{j=1}^{N_p} p_j = 1 \quad (15)$$

linear combinations of Gaussians multiplied by $\theta(\omega)$, the Heaviside distribution, resembling qualitatively the experimental results for spectral functions in condensed matter physics at $T = 0$. We may perform several tests varying the parameters $N_p$, number of maxima, $\{\mu_1,...,\mu_{N_p}\}$, positions of the maxima, $\{\alpha_1,...,\alpha_{N_p}\}$, widths of the peaks and $\{p_1,...,p_{N_p}\}$, the areas under the peaks. The Laplace transform $f(\tau)$ of (15) may be expressed in terms of the standard complementary error
function:
\[ \text{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_{z}^{+\infty} dt e^{-t^2}, \]
whose values are tabulated, in the following form:
\[ f(\tau) = \frac{1}{N} \sum_{j=1}^{N} p_j e^{-\mu_j + \tau^2 \sigma_j^2} \text{erfc} \left( \frac{\tau \alpha_j - \mu_j / \alpha_j}{\sqrt{2}} \right) \]
In order to simulate the output of a typical QMC calculation, we define the measured imaginary time data \( F = \{f_0, ... f_l\} \) as:
\[ f_j = f(j\delta\tau) + \varepsilon_j \]
where \( f(j\delta\tau) \) is evaluated from (17), and \( \varepsilon_j \) are random numbers, mimicking the error bars affecting QMC data, following Gaussian distributions with zero mean and variances, \( \sigma_j^2 \), comparable with the ones typically occurring in our QMC results (\( \sigma_j / f_j \) in the range 0.1–4 %). \( f_j \) play the role of the output of QMC simulation; GIFT falsification uses \( N_c \) random sets \( F^* = \{f^*_0, ..., f^*_l\} \) defined by
\[ f^*_j = f_j + \varepsilon^*_j \]
\( \varepsilon^*_j \) being Gaussian random variables with zero mean and variances which here, to be coherent with the applications we have presented, we assume to be equal to \( \sigma_j^2 \).

Our aim is to compare (15) with the GIFT result we obtain pretending that our knowledge about the imaginary time correlation function is limited to the discretized and noisy data \( F \) in (18), and to other available information about the moments \( c_n \) which, inside these tests on analytically solvable models, can be evaluated from (15); we will neglect now the error bars affecting the values of the \( c_n \). The parameters we have employed in our GIFT reconstructions are listed in Table I. Obviously, the choices of the interval of the frequency space, of the resolution \( \Delta \omega \) (which fixes \( N_\omega \)), of the discretization \( \Delta \tau \) and of the number of points in imaginary time \( l \) are crucial for a specific spectral function one is trying to reconstruct and should be chosen consistently with the considered model; the other parameters are not crucial for a correct functioning of the GIFT method and they have been chosen in order to falsify a wide variety of models leaving the computational cost of the algorithm at a reasonable level.

Also in the reconstruction of known models of spectral functions one can compare GIFT results with those based on the strategy of MEM by adding in the fitness function an entropic term, as we did with the dynamical structure factors in superfluid \(^4\)He from QMC imaginary time correlation functions.

### A. Single peak reconstruction

The simplest test–case is provided by the attempt of reconstructing spectral functions displaying only one peak at a given point \( \mu \) with a width \( \alpha \). The upper panel of Fig. 7 makes evident the difficulty of the inverse problem: two functions with the same parameter \( \mu_a = \mu_b = 10 \) but different values of the widths, respectively \( \alpha_a = 0.1 \) and \( \alpha_b = 1.0 \), in imaginary time domain differ by about 0.5%, of the same order as the typical QMC error bars. It is clear then that the information about the width of the peak is always strongly obscured by the noise. However, from the middle and lower panel of Fig. 7 it is manifest that GIFT reconstruction, obtained using in the fitness \( \Phi_{T\Phi} \), only the first moment \( c_1 \) (i.e. \( \gamma_n = 0 \forall n \neq 1 \)); green and blue lines represent MEM-like reconstructions with different values of the \( \eta \) parameter in the fitness (see legend). Lower panel: \( s_0(\omega) \) (dotted line) and reconstructed \( S_{GIFT}(\omega) \) using in the fitness \( \Phi_{T\Phi} \) only the first moment \( c_1 \) (i.e. \( \gamma_n = 0 \forall n \neq 1 \)).
In order to get closer to realistic physical applications, we try to reconstruct also spectral functions displaying a double peak. Inside such a double peak reconstruction, we may check also the estimation of the integrated

\[ I_0(\omega) = \int_0^\omega d\omega' s(\omega') \]  

\[ I_{-1}(\omega) = \int_0^\omega d\omega' \frac{s(\omega')}{\omega'} \]  

spectral functions:

Figure 8: (Color online) Double peak reconstruction for well separated peaks. Upper panel: Noisy imaginary time correlation function obtained via (18) from \( f(\tau) \) (dotted line) which is the Laplace transform of \( s(\omega) \) (dotted line in the lower panel, see text for parameters). Lower panel: \( s(\omega) \) (dotted line) and reconstructed \( S_{\text{GIFT}}(\omega) \) (red line) from \( f(\tau) \) using in the fitness \( \Phi_D \), only the first moment \( c_1 \) (i.e. \( \gamma_n = 0 \) \( \forall n \neq 1 \)); green and blue lines represent MEM-like reconstructions with different values of the \( \eta \) parameter in the fitness (see legend).

**B. Double peak reconstruction**

In order to get closer to realistic physical applications, we try to reconstruct also spectral functions displaying a double peak. Inside such a double peak reconstruction, we may check also the estimation of the integrated

\[ I_0(\omega) \]  

\[ I_{-1}(\omega) \]  

\( I_0(\omega) \) provides information about the spectral weight under the peaks in \( s(\omega) \); in particular in the \( \omega \) range between the two peaks \( I_0(\omega) \) gives the information from which we have derived the strength of the single quasi–particle peak, \( Z(q) \), in our GIFT study of superfluid \( ^4\text{He} \), as we will show in the following section. On the other hand, the asymptotic value of \( I_{-1}(\omega) \) for large \( \omega \) provides the key to estimate the static response function \( \chi(q) \).

In Fig. 8 we show a reconstruction of a spectral function \( s(\omega) \) for two well separated peaks \( (p_1 = 0.5, p_2 = 0.5, \mu_1 = 10, \mu_2 = 21, \alpha_1 = 0.1 \text{ and } \alpha_2 = 2.0) \) using in the fitness \( \Phi_D \), only the first moment \( c_1 \) (i.e. \( \gamma_n = 0 \) \( \forall n \neq 1 \)); this is the typical fitness used in our reconstruction of spectral functions of superfluid \( ^4\text{He} \). The corresponding \( I_0(\omega) \) and \( I_{-1}(\omega) \) are plotted in Fig. 8 compared with the analytic results from [15]. We observe that no appreciable difference emerges, with respect to the exact results, as far as the determination of the positions of the peaks, of the areas under the peaks, and of the \( c_{-1} \) moment (see Fig. 9) are concerned: the accuracy is very good; on the other hand, the shape of the reconstructed \( s(\omega) \) has not to be taken too seriously because it be-
Figure 10: Double peak reconstruction for overlapping peaks. Upper panel: Two noisy imaginary time correlation functions obtained via (18) from $f^{(0)}(\tau)$ (open circles) and $f^{(1)}(\tau)$ (x symbols), which are the Laplace transforms of $s_a(\omega)$ (dotted line in the middle panel) and $s_b(\omega)$ (dotted line in the lower panel); see text for parameters. The inset is a zoom on one imaginary time instant. Middle panel: $s_a(\omega)$ (dotted line) and reconstructed $S_{\text{GIFT}}(\omega)$ using in the fitness $\Phi_{D^*}$ only the first moment $c_1$ (i.e. $\gamma_n = 0 \ \forall n \neq 1$). Lower panel: $s_b(\omega)$ (dotted line) and reconstructed $S_{\text{GIFT}}(\omega)$ using in the fitness $\Phi_{D^*}$ only the first moment $c_1$ (i.e. $\gamma_n = 0 \ \forall n \neq 1$).

Figure 11: Multiple peak reconstruction. Upper panel: Noisy imaginary time correlation function obtained via (18) from $f(\tau)$ which is the Laplace transform of $s(\omega)$ (dotted line in the lower panel). Lower panel: $s(\omega)$ (dotted line) and reconstructed $S_{\text{GIFT}}(\omega)$ from $f(\tau)$ using in the fitness $\Phi_{D^*}$ only the first moment $c_1$ (i.e. $\gamma_n = 0 \ \forall n \neq 1$).

C. Multiple peak reconstruction

Finally, we devise the following test: we try to reconstruct a spectral function $s(\omega)$ ($p_1 = 0.5$, $p_2 = 0.1$, $p_3 = 0.2$, $p_4 = 0.2$, $\mu_1 = 10$, $\mu_2 = 21$, $\mu_3 = 27$, $\mu_4 = 35$, $\alpha_1 = 0.1$, $\alpha_2 = 2$, $\alpha_3 = 4$, $\alpha_4 = 6$), displaying a main peak and a broad contribution at higher $\omega$, made of a superposition of three Gaussians, resembling qualitatively the shape of the multiphononic contribution in the dynamical structure factor of superfluid $^4$He. We have tested our method using the usual fitness function $\Phi_{D^*}$ with only the first moment $c_1$ included (i.e. $\gamma_n = 0 \ \forall n \neq 1$): the results are plotted in Fig. 11. In Fig. 12 the integrated spectral functions are plotted; from the comparison between the exact $I_0(\omega)$ and the one obtained from the reconstructed $S_{\text{GIFT}}(\omega)$ one can observe that the spectral weights under the main peak and the broad contribution are well reproduced. Also the large $\omega$ limit of $I_{-1}(\omega)$ is in good agreement with the exact value.

One can also study the effect of the noise in $f(\tau)$ in order to check the GIFT ability in recovering correct information on the true $s(\omega)$. In Fig. 13 we show two $S_{\text{GIFT}}(\omega)$ reconstructed from a noisy $f(\tau)$ with $\sigma_\gamma$, 10 times and 50 times greater than in the test shown in Fig. 11. Only in the second case, which represents a situation of very high relative noise ($\sigma_\gamma/f_\gamma$ in the range 5–200 %), information on the correct spectral function is sensi-
f - ruling out the necessity of more accurate observations of GIFT performance. By maintaining the noise level in information by using imaginary time with $\delta \tau$ is possible to see that the two constructions are shown in the upper panel of Fig. 14. By adding noise, the result of such GIFT multi-peak reconstruction is shown in the middle panel of Fig. 14. No substantial improvement can be observed with respect to the previous case in spite of an increased computational cost of GIFT. The computational cost of the GIFT algorithm with this parameters we have only averaged over $N' = 160$ random sets. Also in this case we found no substantial improvement in $S_{GIFT}(\omega)$ as compared to the standard case.

In the previous tests we have not explored different variants of GIFT as, for instance, a basis set different from step functions; one cannot exclude the possibility that by using different variants of this method more information could be obtained.

V. CONCLUSIONS

We have built up a new strategy to attack inverse problems which has been used to study dynamics in quantum many-body systems from QMC simulations; we have obtained very accurate results in the $^4$He case, in the liquid and in the solid phase, even in presence of disorder, providing major improvements with respect to previous studies appeared in literature on this case. We have stressed the important point that the problem we have faced belongs to the huge class of inverse problems, a deep topic also from a fundamental epistemological point of view. The basic idea of the falsification principle guided us in our particular implementation of analytic continuation, but, of course, may provide important implications in many fields of scientific research. Moreover, every problem emerging in Physics or applied Mathematics that could be cast in the form of equation (2), independently of the specific kernel in equation (2), can be attacked with GIFT. The method can be extended to in-
include different kinds of constraints on the spectral function or additional information like cross correlations between the statistical noise of $f(\tau)$ at different imaginary times. Many variants of GIFT can be devised depending on the problem, for instance a basis set different from step functions (5) can be used or non uniform discretization in presence of problems with multiple time scales, or distribution of noise that is not Gaussian.

VI. ACKNOWLEDGMENTS

We acknowledge useful discussions with S. Moroni, A. Motta and M. Nava. This work was supported by the Supercomputing facilities of CILEA.

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