Dynamical Properties of Quantum Many-Body Systems at Zero Temperature

E. R. Gagliano and C. A. Balseiro
Centro Atómico Bariloche, Instituto Balseiro, Comisión Nacional de Energía Atómica, 8400 San Carlos de Bariloche, Río Negro, Argentina
(Received 16 June 1987)

We present a method to compute dynamical correlation functions in quantum many-body systems at zero temperature. The ground state of a finite system is evaluated exactly by a modified Lanczos method and from it the real-frequency correlation functions are obtained by a projective technique for the memory-function formalism. We apply the method to the density-density correlation function of a one-dimensional spinless fermion system. Exact results are recovered in the noninteracting limit; in the strong-coupling limit our results are compared with Monte Carlo simulation and analytical approximations.

PACS numbers: 75.10.Jm, 05.30.Ch, 71.10.+x, 71.45.Gm

In recent years, numerical simulation has proved to be a powerful tool for the study of the thermodynamic and ground-state properties of many-body systems. However, evaluation of dynamical properties is still an open problem despite the effort devoted to the development of appropriate Monte Carlo techniques to study such properties. In most many-body problems, strong- and weak-coupling limits can be described by analytical approximations. However, frequently we are interested in the crossover between these two regimes where many real systems lie. Numerical methods are a powerful tool for the study of these situations which give rise to the most interesting physics. Recently, Hirsch and Schrieffer[1] proposed an algorithm to compute correlation functions of quantum systems. The method gives excellent results only when used to evaluate real-frequency correlation functions of simple, one-degree-of-freedom, systems. Alternative methods[2] have been developed to evaluate real-time correlation functions directly and to make analytic continuation of the imaginary-time results for these simple systems. The extension of all these methods to the study of many-particle systems seems very difficult mainly because of the enormous amount of computational time required.

Schüttler and Scalapino[3] developed a least-squares-fit method to evaluate real-frequency correlation functions of many-particle systems. The results obtained with this method are only qualitatively correct. Use of this technique to evaluate correlation functions quantitatively would again imply prohibitive amounts of computational time.

We present here an alternative method to calculate real-frequency correlation functions of finite many-body systems at zero temperature. This method is ideal to study the dynamics of finite systems such as spin systems and fermions in a lattice. It allows us to calculate precisely real-frequency correlation functions of moderately large systems.

A self-correlation function at zero temperature is defined by

$$C_A(t-t') = \langle \psi_0 | A^\dagger(t) A(t') | \psi_0 \rangle, \tag{1}$$

where $A^\dagger$ is the Hermitean conjugate of the operator A, $A(t)$ is the Heisenberg representation of A, and $|\psi_0\rangle$ is the ground state of the system. Many experiments measure directly the Fourier transform $C_A(\omega)$ of $C_A(t-t')$ which is given by

$$C_A(\omega) = \sum_n \langle \psi_0 | A^\dagger | \psi_n \rangle \langle \psi_n | A | \psi_0 \rangle \times \delta(\omega - (E_n - E_0)), \tag{2}$$

where the summation is taken over all the eigenstates $|\psi_n\rangle$ of H with energy E_n, E_0 being the ground-state energy.

We start by evaluating the ground-state energy E_0 and wave function $|\psi_0\rangle$ of the system. With these quantities known, the correlation functions can be easily calculated with very good precision.

The ground-state properties are obtained by a modified Lanczos method.[4,5] The method consists of the following steps: (i) Take a first approximation ϕ_0 to the exact ground-state wave function ψ_0, such that $\langle \phi_0 | \psi_0 \rangle \neq 0$; (ii) by operating with H on ϕ_0, generate an orthogonal state $\tilde{\phi}_0$; (iii) take a linear combination ϕ_1 of ϕ_0 and $\tilde{\phi}_0$ as a variational state and minimize the energy; and (iv) repeat steps (i)–(iii) with use of the improved state ϕ_1 until convergence is obtained. This method has been used to evaluate the exact energy and wave function of an anisotropic spin-$\frac{1}{2}$ Heisenberg chain with 24 sites, which shows the power of the algorithm.[5]

To obtain the dynamical correlation functions, we define

$$G_A(Z) = \langle \psi_0 | A^\dagger (Z - H)^{-1} A | \psi_0 \rangle. \tag{3}$$

The correlation function $C_A(\omega)$ is obtained as

$$C_A(\omega) = \pi^{-1} \mathrm{Im} G_A(\omega + i\eta + E_0). \tag{4}$$

The real part of the dynamical susceptibilities can also be obtained directly from $G_A(Z)$ without use of the tedious procedure given by the Kramers-Kronig relation. The resolvant $G_A(Z)$ is written in the form of a continued fraction:

$$G_A(Z)=\cfrac{\langle\psi_0|A^\dagger A|\psi_0\rangle}{Z-a_0-\cfrac{b_1^2}{Z-a_1-\cfrac{b_2^2}{Z-\cdots}}}. \tag{5}$$

The coefficients a_n and b_n can be evaluated from the moments $\mu_n=\langle\psi_0|A^\dagger H^n A|\psi_0\rangle$.[6,7] However, for large systems the moments increase rapidly with n, and the method is very sensitive to numerical errors. We found it convenient to evaluate the coefficients by a projective technique developed for the memory-function formalism.[7] The advantage of this method is that it avoids the use of recursion relations for the moments. The method can be summarized as follows: (1) Define the state $|f_0\rangle=A|\psi_0\rangle$; (2) generate a set of orthogonal states with the relation

$$|f_{n+1}\rangle=H|f_n\rangle-a_n|f_n\rangle-b_n^2|f_{n-1}\rangle; \tag{6}$$

and (3) evaluate the coefficients a_n and b_n:

$$a_n=\langle f_n|H|f_n\rangle/\langle f_n|f_n\rangle, \tag{7a}$$

$$b_{n+1}^2=\langle f_{n+1}|f_{n+1}\rangle/\langle f_n|f_n\rangle,\quad b_0=0. \tag{7b}$$

With this procedure we can evaluate a large number of coefficients a_n and b_n and construct the continued-fraction expression for $G_A(Z)$. Since we are dealing with large but finite systems the Green's function $G_A(Z)$ has a finite number of poles, and the procedure described above allows us to evaluate all the poles accurately.

To test the method, we have calculated the density-density correlation function for a one-dimensional model of spinless fermions. The Hamiltonian is given by

$$H=\sum_{i=1}^{N}-t(C_i^\dagger C_{i+1}+C_{i+1}^\dagger C_i)+Gn_in_{i+1}, \tag{8}$$

where $C_i^\dagger$ creates an electron at site i, and $n_i=C_i^\dagger C_i$ is the number operator. We consider a half-filled band and assume periodic boundary conditions. This model can be mapped into an anisotropic spin-$\frac{1}{2}$ Heisenberg model.[8]

In this system we can distinguish two opposed regimes: (a) When $G/2t<1$, the system is conducting and, for $N\to\infty$, the excitation spectrum is a gapless continuum. (b) When $G/2t>1$, the system exhibits a charge-density-wave ground state. There are two sublattices A and B such that $\langle n_i\rangle<\frac{1}{2}$ in A and $\langle n_i\rangle>\frac{1}{2}$ in B. For $N\to\infty$, the ground state is doubly degenerate and separated by a gap from a continuum. In this strong-coupling regime, the two degenerate ground states differ in the phase of the charge-density wave. The lowest excited states correspond to a soliton-antisoliton pair. Each pair increases the energy by an amount of the order of G, and so the spectrum consists of bands centered at G, $2G$, $3G$, ...

We have calculated the correlation function $C_n(k,\omega)$ defined as the Fourier transform of

$$C_n(k,t-t')=\langle n_k(t)n_k(t')\rangle, \tag{9}$$

with

$$n_k=N^{-1/2}\textstyle\sum_l e^{-ikl}(n_l-\frac{1}{2}). \tag{10}$$

For $G=0$ the model is easily solvable and the correlation function is given by a superposition of δ functions of the form $\delta(\epsilon_{k+p}-\epsilon_p-\omega)$, where $\epsilon_p=-2t\cos p$, with $p=2\pi n/N$. We have evaluated the correlation function in this limit with the method proposed above for systems of different sizes ($N\le 18$). The numerical errors depend on the value of k and on the number of sites N. However, the largest error, obtained for $N=18$, is smaller than 2%. For $G\neq 0$ we have performed direct diagonalization of systems with $N\le 10$ and used the spectral representation of Eq. (2) to compare results.

In Table I the positions and residues of the poles for $N\le 10$ and $G=2t$ obtained with our method are compared with the results obtained by direct diagonalization (for $N=10$, see Müller *et al.*[9]). We found that our result and the exact one coincide within the first five significant digits (see Table I). We have tested the

TABLE I. Poles and weights for different chain lengths. ω_i is the energy of the particle-hole excitation. A_i is the weight of the ω_i excitation. Except for the figures denoted with an asterisk, our results coincide at least within the first five significant digits with the exact ones. The largest error is obtained for the pole with very small weight; direct diagonalization results for this pole are $\omega=6.948\,34$ and $A=0.004\,78$.

N		Poles and weights				
6	ω	1.3695	5.8416	...	...	...
	A	4.6298	0.2544	...	...	...
8	ω	0	2.6021	4.5057	5.7314	6.9476*
	A	3.4392	2.1132	0.1652	0.1152	0.0049*
10	ω	0.8465	4.1533	6.1266	...	...
	A	5.0676	0.6924	0.0650	...	...

method for other values of G and the errors are of the same order (smaller than 0.07% for $N \leq 10$). We also calculated, for comparison purposes,[9] the first frequency moment of $C_n(k,\omega)$ obtaining an excellent agreement with the exact result.

In Figs. 1 and 2 we present the results for a system of sixteen sites in the noninteracting ($G=0$) and strongly interacting ($G=6t$) limits. In the figures, the peaks have been broadened by the inclusion of a finite η [see Eq. (4)] for display purposes.

In Fig. 1 the exact result is not included since in the scale used it could not be distinguished from the numerical result. For the sake of comparison we display the Monte Carlo histograms of Ref. 3. The results of Fig. 1 ($G=0$) clearly show the electron-hole excitations of the system. For small values of k, a single peak at low frequency is obtained that corresponds to an electron-hole excitation across the "Fermi surface." As k increases, more structure is obtained since there are more ways of promoting one electron to increase its crystal momentum by k. For $k=\pi$, a line at $\omega=0$ is obtained which corresponds to the promotion of one particle from $-k_F$ to k_F ($k_F=\pi/2$).

In the strong-coupling limit ($G=6t$) the soliton-antisoliton excitations are clearly observed. All the structure shown in Fig. 2, obtained for $\omega \neq 0$, corresponds to a single soliton-antisoliton pair. Excitations with two soliton-antisoliton pairs are also observed, but their in-

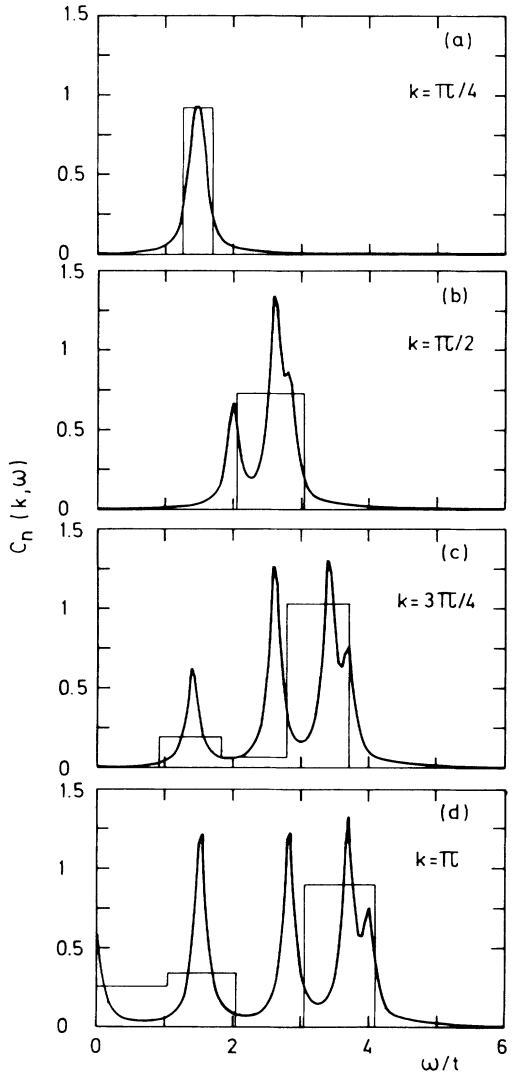

FIG. 1. Real-frequency density correlation function of a noninteracting half-filled sixteen-site chain. ($G=0$, $\eta=0.1t$). Thin line, Monte Carlo results (Ref. 3); heavy line, present approach.

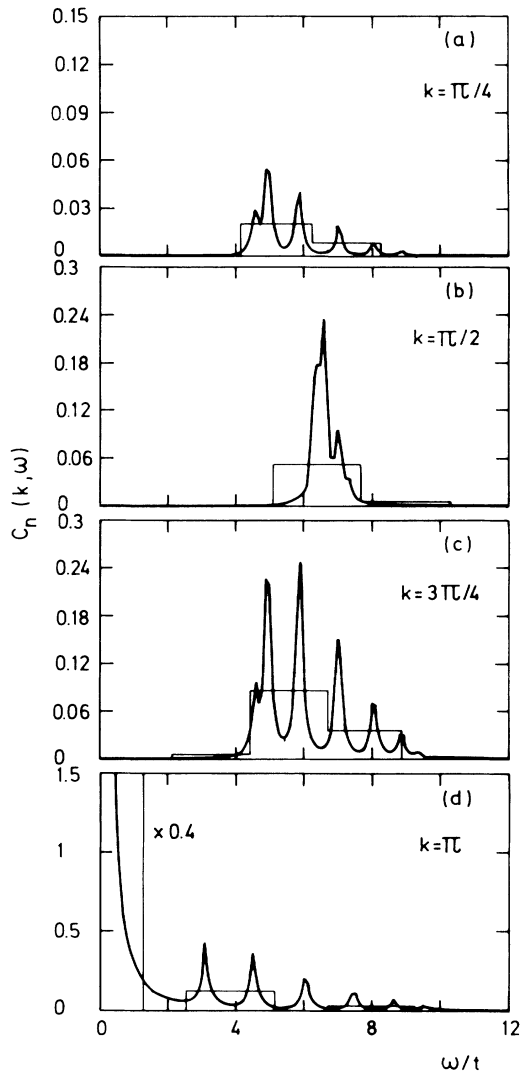

FIG. 2. Real-frequency density correlation function of a strongly interacting half-filled sixteen-site chain ($G=6t$, $\eta=0.1t$). Thin line, Monte Carlo results (Ref. 3); heavy line, present approach.

tensities are very small and cannot be appreciated on the scale used in the figure. The results show that there is a "band" of excitations centered at G. This band is narrower for $k=\pi/2$ in agreement with analytical approximations obtained in the strong-coupling limit of infinite systems.[10] In agreement with the obtained results, the analytical strong-coupling approximation predicts absorption peaks around $\omega \simeq nG$, $n=1,2,\ldots$, whose intensity decreases as n increases. For $k=\pi$ a line is obtained for $\omega=0$ since the operator n_k with $k=\pi$ connects the two degenerate ground states.

The results shown in Figs. 1 and 2 are calculated with use of 25 coefficients a_n and b_n. In the frequency region of the figures ($\omega/t \leq 12$) the results are not sensitive to the number of coefficients used for $n \geq 20$. Similar results are obtained for $N=18$.

All the results presented in Figs. 1 and 2 were obtained after $\simeq 5$ h of central processing unit (CPU) time on a VAX 11/780. The method presented here requires only a fraction of the time needed for the Monte Carlo simulation and gives essentially exact results. We should mention that most of the CPU time is used to construct the ground state. Once the ground-state wave function is obtained with good accuracy ($\simeq 10^{-6}$) all correlation functions can be easily calculated with moderate computational time.

In summary, we have presented a method to compute real-frequency correlation functions in finite systems at zero temperature. The method allows us to compute exact numerical results and is appropriate for the study of the dynamics of spin systems and fermions in a lattice. We have demonstrated that explicit calculation of the coefficients of the memory function provides a computationally efficient method of evaluating correlation functions.

Reasonably large systems can be studied. With our computing facilities, the dynamical properties of spin-$\frac{1}{2}$ Heisenberg systems with $N \leq 24$ can be evaluated in moderate computing time. For larger systems, larger and faster computing facilities would be required. However, in strong-coupling limits, good approximations can be obtained by a pruning of the Hilbert space. This approximation would allow us to study larger systems with a good accuracy in the dynamical properties at low frequencies.

The method is easily generalized to calculate correlations $\langle A^{\dagger}(t)B(t')\rangle$ for any pair of observables $A^{\dagger}$ and B and, once the ground-state properties ($|\psi_0\rangle$ and E_0) are known, all correlations can be obtained with a small computational effort.

Finally, as a side conclusion, we may say that Monte Carlo simulation[3] gives quite good qualitative results in the strong-coupling limit of the spinless model of Eq. (8). However, the method presented here provides a way to obtain exact numerical results in less computing time.

Now that we have achieved an accurate method for the evaluation of the dynamical properties of finite systems, the next goal in the numerical studies of quantum many-body systems would be development of a theory for the finite-size scaling of such properties.

We are indebted to R. Barrachina and C. Wiecko for bringing Refs. 6 and 7 to our attention. One of us (E.R.G.) is supported by the Consejo Nacionale de Investigaciones Científicas y Técnicas, Argentina.

[1]J. E. Hirsch and J. R. Schrieffer, Phys. Rev. B **28**, 5353 (1983).

[2]E. C. Behrmann, G. A. Jongeward, and P. G. Wolynes, J. Chem. Phys. **79**, 6277 (1983); D. Thirumvalai and B. Berne, J. Chem. Phys. **79**, 5029 (1983).

[3]H. B. Schütter and D. J. Scalapino, Phys. Rev. Lett. **55**, 1204 (1985), and Phys. Rev. B **34**, 4744 (1986).

[4]E. Dagotto and A. Moreo, Phys. Rev. D **31**, 865 (1985); E. R. Gagliano and S. Bacci, Phys. Rev. D **36**, 546 (1987).

[5]E. R. Gagliano, E. Dagotto, A. Moreo, and F. Alcaraz, Phys. Rev. B **34**, 1677 (1987).

[6]R. G. Gordon, J. Math. Phys. **9**, 655 (1968).

[7]G. Grosso and G. Pastori Parravicini, in *Memory Function Approaches to Stochastic Problems in Condensed Matter,* edited by M. W. Evans, P. Grigolini, and G. Pastori Parravicini, Advances in Chemical Physics, Vol. 62 (Wiley, New York, 1985), p. 133.

[8]J. des Cloizeaux and M. Gaudin, J. Math. Phys. **7**, 1384 (1966).

[9]G. Müller, H. Thomas, M. W. Puga, and H. Beck, J. Phys. C **14**, 3399 (1981).

[10]N. Ishimura and H. Shiba, Prog. Theor. Phys. **63**, 743 (1980), and references therein.