# Monte Carlo Studies of the Dynamics of Quantum Many-Body Systems

H.-B. Schüttler and D. J. Scalapino
*Department of Physics, University of California, Santa Barbara, California 93106*
(Received 3 May 1985)

We propose a least-squares-fit method to extract real-frequency correlation functions from imaginary-time Monte Carlo data of a many-particle system. We apply it to the density correlation function in a one-dimensional model of spinless fermions. The spectral functions thus obtained reflect accurately the particle-hole and the soliton-antisoliton excitations of the system in the respective limits of noninteracting and strongly coupled fermions. They are in qualitative agreement with the available analytical results.

PACS numbers: 75.10.Jm, 71.10.+x

In recent years, Monte Carlo (MC) methods have become a powerful tool for the investigation of the thermodynamics and static correlations of quantum many-body systems.[1] However, little progress has been made so far in the development of MC techniques that would allow the study of the real-time dynamics of such systems. Recent attempts to simulate real-frequency[2] or real-time[3] correlation functions directly have dealt only with the simplest (one degree of freedom) model systems and have given reasonable results only after an exceedingly large number of MC steps. Also, Padé approximants have been used to analytically continue imaginary-time MC data for single-degree-of-freedom models.[4] Considering the enormous amounts of computation time required, it is difficult to use these methods for many-particle systems.

In the present work, we propose a method to extract real-frequency self-correlation functions from the corresponding imaginary-time Green's functions of many-particle systems that can be simulated by standard quantum MC techniques. The starting point of our approach is the integral equation,[5]

$$G(\tau)=\pi^{-1}\int d\omega(1+e^{-\beta\omega})^{-1}e^{-\tau\omega}\phi''(\omega), \quad (1)$$

which relates the imaginary-time Green's function of two operators, $A$ and $B$, at temperature $T$,

$$G(\tau)\equiv\langle A(-i\tau)B(0)\rangle, \quad (2)$$

$$0\leq\tau\leq\beta\equiv 1/k_{\mathrm{B}}T,$$

to the spectral function

$$\phi''(\omega)\equiv\tfrac{1}{2}\int dt\, e^{i\omega t}\langle A(t)B(0)+B(0)A(t)\rangle. \quad (3)$$

Here, $A(t)\equiv\exp(iHt)A\exp(-iHt)$, $H$ is the Hamiltonian of the system, and

$$\langle\ldots\rangle\equiv\mathrm{Tr}[\exp(-\beta H)\ldots]/\mathrm{Tr}[\exp(-\beta H)]$$

denotes the thermal average. Although (3) itself is not of physical interest, it is directly related to the physically relevant linear response functions. For example, the time Fourier transform of $S(t)\equiv\langle A(t)B(0)\rangle$ is given by

$$S(\omega)=2(1+e^{-\beta\omega})^{-1}\phi''(\omega). \quad (4)$$

Thus the dynamics can be obtained from $\phi''(\omega)$ if Eq. (1) can be inverted to give $\phi''(\omega)$ in terms of the Monte Carlo calculation of $G(\tau)$. Unfortunately, the kernel in Eq. (1) is such that $G$ is insensitive to the detailed structure of $\phi''$. Small statistical errors in the MC data for $G$ lead to large errors in $\phi''$. Here, we suggest a method to overcome this difficulty in the case of a self-correlation function (i.e., for $B=A^{\dagger}$) for which $\phi''(\omega)\geq 0$.

First of all, in order to increase the sensitivity, we simulate not only $G(\tau)$ itself, but also, *independently*, its $\tau$ derivatives, $G^{(m)}(\tau)(m=1,2,\ldots)$, using relations like

$$G^{(1)}(\tau)=\langle[H,A(-i\tau)]B(0)\rangle \quad (5)$$

and so on. Note that the $G^{(m)}$ $(m\geq 1)$, as given by (1), contain under the integral the same spectral function $\phi''$ as $G$, weighted, however, with additional factors $(-\omega)^m$.

To extract $\phi''$ from such a set of MC data, $G^{(m)}(\tau_i)$ (where $i=0,1,\ldots,L$, say, and $m=0,1,\ldots,M$), we then use a *least-squares-fit* procedure: Starting from an approximate trial function for $\phi''(\omega)$, $\phi_F(\omega,a_1,\ldots,a_F)$, with adjustable parameters $a_1,\ldots,a_F$, we define a sum of squared deviations,

$$D(a_1,\ldots,a_F)=\sum_{i,m}\{[G^{(m)}(\tau_i)-G_F^{(m)}(\tau_i,a_1,\ldots,a_F)]/\Delta G_i^{(m)}\}^2, \quad (6)$$

where $\Delta G_i^{(m)}$ is the standard deviation of $G^{(m)}(\tau_i)$ and $G_F(m)(\tau_i,a_1,\ldots,a_F)$ is (the $m$th derivative of) the "fitted" imaginary-time Green's function $(m=0,1,\ldots,M)$, obtained by inserting $\phi_F(\omega,a_1,\ldots,a_F)$ into the integral (1). We then determine the "best" trial function $\phi_F$ by minimizing $D(a_1,\ldots,a_F)$ with respect to


© 1985 The American Physical Society

$a_1, \ldots, a_F$ under the *constraint* that

$$\phi_F(\omega, a_1, \ldots, a_F) \geq 0 \tag{7}$$

for all values of $\omega$, thereby taking the positivity of $\phi''(\omega)$ explicitly into account. In carrying out the model calculations presented below, we have found that this constraint is essential in stabilizing the fit against large, unphysical fluctuations.

To test this method, we consider a simple one-dimensional model of spinless fermions. The Hamiltonian[6] is

$$H = \sum_{j=1}^{N} [-t(c_j^\dagger c_{j+1} + \text{H.c.}) + V n_j n_{j+1}], \tag{8}$$

where $c_j$ annihilates a fermion at lattice site $j$, $n_j = c_j^\dagger c_j$, and we assume periodic boundary conditions. Using the "world-line" algorithm,[7] we have simulated the zeroth, first, and second derivative of the density correlation function, $G(\tau, k)$, i.e., the self-correlation function of the operator

$$\tilde{n}_k \equiv N^{-1/2} \sum_j e^{-ikj}(n_j - \langle n_j \rangle). \tag{9}$$

All results shown below pertain to an $N = 16$ site lattice at a temperature $k_B T = 0.2t$ and a Trotter number $L = 25$, which corresponds to an imaginary time "slice" $\Delta\tau \equiv \beta/L = 0.2/t$.[7] For each of the two runs shown in Figs. 1 and 2, 2000 fermion configurations[7] were sampled which took of the order of 10 h of CPU time per run on a VAX 750 using a standard FORTRAN program. The statistical errors ($\Delta G_i^{(m)}$) in our $G(\tau)$ data were of the same order of magnitude at all $\tau_i$, typically 0.5%–1.0% of the value of $G^{(m)}(\tau = 0)$. The relative error $\Delta G_i^{(m)}/G^{(m)}(\tau_i)$ was therefore quite small near $\tau = 0$ and $\tau = \beta$ (0.5%–1.0%), but substantially larger (10%–100%) at intermediate values of $\tau$ ($\tau \sim \beta/2$), since, for the cases considered, $G^{(m)}(\tau)$ becomes very small in this region [typically $G(\tau = \beta/2)/G(\tau = 0) \sim 10^{-2}$–$10^{-3}$].

As a trial function $\phi_F$, we choose a histogram representation with a certain "block" width $\Delta W$, i.e., for $\omega \geq 0$

$$\phi_F(\omega, a_1, \ldots, a_F) = \sum_{l=1}^{F} a_l \phi_l(\omega), \tag{10}$$

where $\phi_l(\omega)$ is unity when $(l-1)\Delta W < \omega < l\Delta W$ and zero otherwise. Because of time and space inversion symmetry, the exact spectral function satisfies $\phi''(-\omega, k) = \phi''(\omega, k) = \phi''(\omega, -k)$. Therefore, we set

$$\phi_F(\omega, a_1, \ldots, a_F) = \phi_F(-\omega, a_1, \ldots, a_F)$$

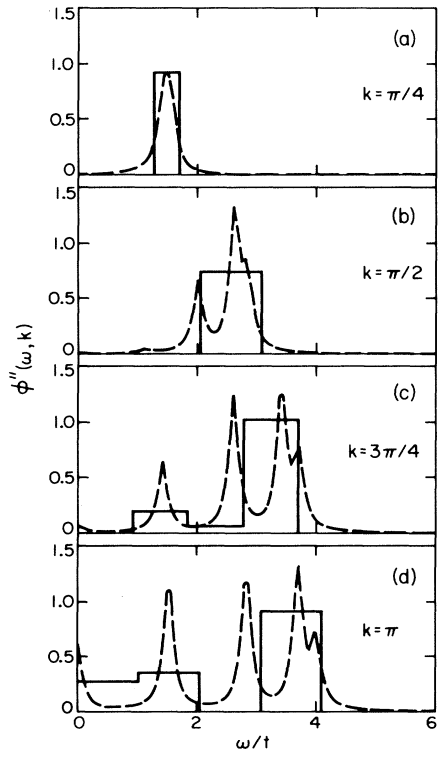


FIG. 1. Real-frequency density correlation function of a noninteracting half-filled sixteen-site chain ($V = 0$, $k_B T = 0.2t$). Full line, fit to MC data; dashed line, exact result.

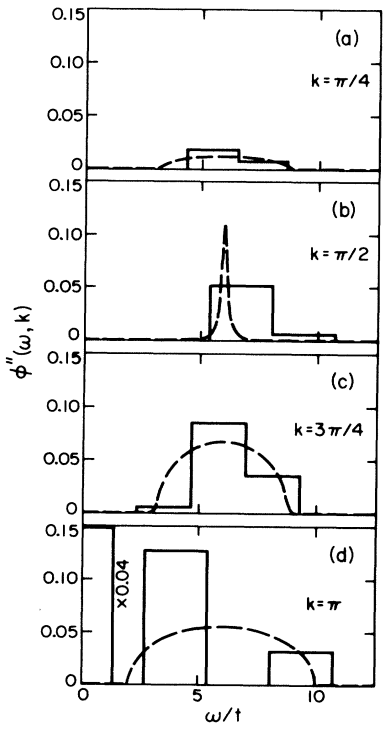


FIG. 2. Real-frequency density correlation function of a strongly interacting half-filled sixteen-site chain ($V = 6t$, $k_B T = 0.2t$). Full line, fit to MC data; dashed line, analytical strong-coupling result for the infinite system.

for $\omega \leq 0$. The advantage of this trial function is that the absolute minimum of (6) under the constraint (7) can be found very easily: After we have set $a_l \equiv b_l^2$ (so that $\phi_F \geq 0$), the search for the absolute minimum of $D(b_1^2, \ldots, b_F^2)$ reduces to a series of linear equations. To determine the block width $\Delta W$ or, equivalently, the total width of the spectrum, $W = F\Delta W$ was used as an additional fit parameter which was varied to minimize $D$.

In Fig. 1, we show $\phi_F$ obtained in this way for a noninteracting ($V=0$), half-filled (eight-fermion) system using a trial function with $F=4$ blocks. Also shown is the exact $\phi''(\omega,k)$ which, in this case, is a superposition of $\delta$ functions of the form $\delta(\epsilon_{p+k} - \epsilon_p - \omega)$, broadened into Lorentzians for purposes of display. Here, $\epsilon_p = -2t\cos p$, $-\pi < p \leq \pi$, is the single-particle energy at wave vector $p$. At our relatively low temperature ($k_B T/4t = 0.05$), and for small momentum transfer, $k \ll \pi$, $\phi''(\omega,k)$ exhibits a narrow structure around $\omega = v_F k = 2tk$, corresponding to the creation of particle-hole excitations across the Fermi "surface," $p_F = \pm\pi/2$. With increasing momentum transfer $k$, this peak structure is shifted to higher frequencies (up to the full band width $\omega \sim 4t$) and "broadened" asymmetrically, as more and more lines appear in the spectrum. Notice that the fit result follows this behavior of the exact spectral function quite systematically.

Also note that in general, because of the noise in the input data, the individual $\delta$ functions in $\phi''(\omega,k)$ cannot be resolved by the fit procedure. Let us emphasize, however, that in the infinite-system limit, this detailed $\delta$-function structure is not of physical interest. As we increase the system size, an increasing number of more and more densely spaced $\delta$-function peaks appears in the spectrum, each of them carrying less and less weight. What is physically relevant is then only some "smeared out" average of $\phi''(\omega,k)$ over a frequency width of the order of or larger than the typical level spacing. The finite width of our rectangular blocks, $\Delta W$, in (10) takes this "infinite system smearing," at least crudely, into account.

In Fig. 2, we show the fit result for a strongly interacting, half-filled system with $V/t = 6$, again with $F=4$. If $V \geq 2t$, the half-filled (infinite) system exhibits a charge-density wave ground state.[6,8] For $t=0$, it would correspond to a configuration of alternatingly occupied and empty sites. There are two such configurations ($A$ and $B$, say), energetically degenerate. The lowest excited state with an excitation energy $V$ consists then of a pair of domain walls (or a "soliton-antisoliton" pair) separating segments of $A$- and $B$-type ground-state configurations.[6] Analogously, two-pair, three-pair, . . . states can be created with excitation energies $2V$, $3V$, . . . , respectively. A small but finite intersite transfer $t \ll V$ broadens these highly degenerate states into bands of a width of the order $t$.[6] The one- and two-pair band is clearly visible in our fit result. Also shown in Fig. 2 is the result of the lowest-order strong-coupling calculation[9] for the one-pair contribution to the spectral function of an infinite system. Since, for our model parameters, the bandwidth is of the same order as the interband spacing, this strong-coupling calculation is certainly of doubtful validity as it completely neglects interband mixing of states. Its lack of agreement with our fit result, namely the difference in the bandwidth, should therefore not be too surprising. We should also mention that, in fitting the strong-coupling data, we have allowed for an additional contribution of the form $a_0\delta(\omega)$ in the trial function (10) in order to account for elastic (Bragg) scattering off the charge-density-wave superlattice. Notice that, as expected, this Bragg peak occurs at $k=\pi$ (represented as an extra block of width $\Delta W/2$, centered around $\omega = 0$).

We have also carried out simulations for a strongly interacting system, again with $V/t = 6$, which is one fermion short of being half filled (seven fermions per sixteen sites). In this case, the system exhibits a soliton pair already in its ground state. As a result of inelastic scattering off this pair, we would expect to see (at least for small wave vector $k$) low-frequency excitations below $\omega \sim V$,[9] which are not present in the exactly half-filled case. Indeed, this behavior is borne out in the fit results.

Considering the lack of detailed quantitative agreement between our fit results and the exact solution (e.g., for the noninteracting fermion case), the question arises as to how to improve these results. First of all, one should, of course, try to enhance the resolution of the trial function $\phi_F$, by increasing the number of blocks $F$. Using the MC data described above, we have carried out such fits with block numbers up to $F=8$. The results for the intensity distribution $\phi_F(\omega)$ are very similar to those shown in Figs. 1 and 2 (where $F=4$). However, they do not show substantial improvement in their quantitative agreement with the exact results. Also, the minimized value of the sum of the squared deviations Eq. (6) decreases only by a few more percent as we increase the number of blocks from $F=4$ to $F=8$. This indicates that most of the information about $\phi''(\omega)$ contained in the given set of $G(\tau)$ data has been exhausted by the "$F=4$" fit. Nevertheless, it is encouraging to see that the results with different $F$ values are at least stable, i.e., qualitatively in agreement with each other. We therefore believe that better fit results for the spectral function $\phi''(\omega)$ will necessarily require an improved statistical accuracy of the input data $G(\tau)$, in addition to an enhanced resolution of the trial function $\phi_F$. For example, we have applied our method to $G(\tau)$ data that were obtained by randomly superimposing a certain

noise level on the exact $G(\tau)$ values that are readily available for the noninteracting system. Indeed, we find a significant improvement of the fit results if the noise level $\Delta G_i^{(m)}$ is reduced by factors of 3–10 from that present in our MC data. It is not unrealistic to assume that such an improved accuracy of the MC data can be achieved within reasonable time by use of faster computation facilities. Nevertheless, we feel that even with the given level of accuracy, our method can provide useful insights.

In conclusion, we have demonstrated that our method allows one to extract qualitatively, and in certain quantitatively, real-frequency spectra of many-particle systems from imaginary-time data, simulated within reasonable amounts of computation time.

We would like to thank Dr. M. Imada for many helpful discussions. This material is based upon work supported by the National Science Foundation under Grant No. DMR83-20481. We are grateful to E.I. du Pont de Nemours and Company and the Xerox Corporation for their support.

[1]*Applications of the Monte Carlo Method in Statistical Physics,* edited by K. Binder (Springer-Verlag, Berlin, 1984); *Monte Carlo Methods in Quantum Problems,* NATO Advanced Study Institute Series, edited by M. H. Kalos (Reidel, Dordrecht, 1984).

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

[3]E. C. Behrman, G. A. Jongeward, and P. G. Wolynes, J. Chem. Phys. **79**, 6277 (1983).

[4]D. Thirumvalai and B. Berne, J. Chem. Phys. **79**, 5029 (1983).

[5]H.-B. Schüttler and D. J. Scalapino, to be published; Eq. (1) can be proved, for example, by insertion of complete sets of energy eigenstates between the operators $\exp(-\beta H)$, $A$, and $B$ that enter into (2) and (3), respectively. Factoring the respective $t$ and $\tau$ dependences out of the resulting matrix elements, inserting (3) into the left-hand side of (1), and carrying out the $t$ and $\omega$ integration, one arrives at an expression for the left-hand side of (1) that is identical with that of (2).

[6]J. Hubbard, Phys. Rev. B **17**, 494 (1978), and references cited therein.

[7]J. E. Hirsch, D. J. Scalapino, R. L. Sugar, and R. Blankenbecler, Phys. Rev. Lett. **47**, 1628 (1981), and Phys. Rev. B **26**, 5033 (1982).

[8]A. Luther and I. Peschel, Phys. Rev. B **12**, 3908 (1975).

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