RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 28, NUMBER 9 1 NOVEMBER 1983

Dynamic correlation functions in quantum systems: A Monte Carlo algorithm

J. E. Hirsch
Department of Physics, University of California, San Diego, La Jolla, California 92093

J. R. Schrieffer
Department of Physics and Institute for Theoretical Physics, University of California, Santa Barbara, California 93106

(Received 2 May 1983; revised manuscript received 15 August 1983)

We propose a new algorithm to compute dynamic correlation functions in quantum systems at zero temperature using Monte Carlo techniques. The method, which avoids inverse-Laplace transforms, is based on a representation of the Dirac δ function as the limit of a Gaussian. We illustrate the method on the one-dimensional harmonic oscillator.

I. INTRODUCTION

The linear response $A(t)$ of a many-body system to an externally applied force $F(t')$ can be expressed in terms of the correlation function

$$C_{AB}(t-t') = \langle A(t)B(t')\rangle \ , \tag{1}$$

where $B(t')$ is conjugate to $F(t')$. At zero temperature $\langle\ \rangle$ denotes the ground-state expectation value and as usual

$$A(t) = e^{iHt}Ae^{-iHt} \ . \tag{2}$$

Experiments such as inelastic neutron scattering measure the time Fourier transform of C_{AB} with t and t' real,

$$C_{AB}(\omega) = \sum_n \langle 0|A|n\rangle\langle n|B|0\rangle \delta(\omega-(E_n-E_0)) \ , \tag{3}$$

where the summation extends over all the eigenstates $|n\rangle$ of H with energy E_n.

There has been recently considerable interest in the application of Monte Carlo techniques to the study of interacting quantum systems.[1] Since these methods deal with real quantities, one can compute directly correlation functions in *imaginary time*

$$C_{AB}(\tau) = \langle 0|e^{H\tau}Ae^{-H\tau}B|0\rangle \ . \tag{4}$$

However, it is well known that the inverse-Laplace transform required to obtain $C_{AB}(\omega)$ is highly unstable to the statistical error in $C_{AB}(\tau)$.

We propose here an alternative scheme which deals directly with the correlation functions in real frequency. It is based on the Gaussian representation of the δ function

$$\delta(\omega-\epsilon) = \lim_{\bar\beta\to\infty} \sqrt{\bar\beta/\pi}\, e^{-\bar\beta(\omega-\epsilon)^2} \ , \tag{5}$$

and the correlation function Eq. (3) becomes

$$C_{AB}(\omega) = \lim_{\bar\beta\to\infty} \sqrt{\bar\beta/\pi}\,\langle 0|A\exp[-\bar\beta(H-E_0-\omega)^2]B|0\rangle \ . \tag{6}$$

We generate the ground state by the conventional imaginary time filtering procedure[1]

$$C_{AB}(\omega) = \lim_{\bar\beta\to\infty}\lim_{\beta\to\infty}\left(\frac{\bar\beta}{\pi}\right)^{1/2} \frac{\langle\chi|e^{-\beta H}A\exp[-\bar\beta(H-E_0-\omega)^2]Be^{-\beta H}|\zeta\rangle}{\langle\chi|e^{-2\beta H}|\zeta\rangle} \ , \tag{7}$$

where $|\zeta\rangle$ and $|\chi\rangle$ are arbitrary states that have nonvanishing overlap with the ground state of the system. The denominator cancels the unknown overlap matrix elements of $|\zeta\rangle$ and $|\chi\rangle$ with the ground state. Equation (7) constitutes the basic equation in our approach. Note that we need to perform an independent evaluation of E_0, which can be done by standard Monte Carlo methods.[1]

We evaluate (7) numerically using a stochastic technique. First, divide both the β and $\bar\beta$ axis in small slices of size $\Delta\tau$ and $\Delta\bar\tau$, respectively,

$$\begin{aligned} e^{-\beta H} &= (e^{-\Delta\tau H})^L \ , \\ \exp[-\bar\beta(H-\lambda)^2] &= [\exp[-\Delta\bar\tau(H-\lambda)^2]]^{\bar L} \ , \end{aligned} \tag{8}$$

where $L=\beta/\Delta\tau$, $\bar L=\bar\beta/\Delta\bar\tau$, and $\lambda=E_0+\omega$. Next, evaluate the matrix elements V_1 and V_2 of $e^{-\Delta\tau H}$ and $\exp[-\Delta\bar\tau(H-\lambda)^2]$ approximately, with errors proportional to $\Delta\tau^2$ and $\Delta\bar\tau^2$. For fermions on a lattice, for example, an efficient method is the checkerboard breakup.[2] One obtains

$$\bar C_{AB}(\omega) = \left(\frac{\bar\beta}{\pi}\right)^{1/2} \frac{\langle\chi|V_1^L A V_2^{\bar L} B V_1^L|\zeta\rangle}{\langle\chi|V_1^{2L}|\zeta\rangle} \ . \tag{9}$$

For large β,L and $\bar\beta,\bar L$, $\bar C_{AB}(\omega)$ converges to the desired correlation function. To compute Eq. (9), we propose to use a random walk method, originating with von Neumann and Ulam[3] and developed recently by several authors.[4-6] Following the recent work of Kuti,[5] we write for the matrix elements of V_i $(i=1,2)$

$$\langle i|V_i|j\rangle = P_{ij}^i R_{ij}^i \ , \tag{10}$$

where the transition probability P_{ij}^i satisfies

$$P_{ij}^i \geq 0, \quad \sum_i P_{ij}^i = 1 \tag{11}$$

and R_{ij}^i is the residue. There is considerable freedom in the

decomposition (10), which can be used to optimize convergence. The stochastic procedure consists of generating random walks for the numerator and denominator of Eq. (9), governed by the transition probabilities defined above, and computing for each walk a score as the product of the residues. The average of the scores converges to the expressions in Eq. (9) for a large number of walks.[5,6]

II. HARMONIC OSCILLATOR

We consider the Hamiltonian

$$H=\tfrac{1}{2}p^2+\tfrac{1}{2}\omega_0^2x^2 \tag{12}$$

and scale H, p, and x so that these operators are dimensionless, with $\omega_0=1$, and $[p,x]=-i$. We consider the correlation functions Eq. (3),

$$C_{xx}(\omega)=\frac{1}{2\omega_0}\delta(\omega-\omega_0) \tag{13}$$

and

$$C_{x^2x^2}(\omega)=\frac{1}{4\omega_0^2}[\delta(\omega)+2\delta(\omega-2\omega_0)]\ . \tag{14}$$

Approximants for these functions for finite $\bar{\beta}$ are shown in Fig. 1. A finite $\bar{\beta}$ can be interpreted as a finite Gaussian "experimental" resolution.

We construct the matrix elements of the time-evolution operator as

$$V_1(x,x')=\langle xe^{-\Delta\tau H}|x'\rangle\cong\langle x|e^{-(\Delta\tau/4)x^2}e^{-(\Delta\tau/2)p^2}e^{-(\Delta\tau/4)x'^2}|x'\rangle=\left(\frac{1}{2\pi\Delta\tau}\right)^{1/2}\exp\left[-\frac{\Delta\tau}{4}(x^2+x'^2)\right]\exp\left[-\frac{(x-x')^2}{2\Delta\tau}\right] \tag{15}$$

which is correct to order $\Delta\tau^3$. For the Gaussian operator, we write

$$V_2(xx')=\left\langle x\left|\exp\left[-\overline{\Delta\tau}\left(\frac{p^2}{2}+\frac{1}{2}x^2-\lambda\right)^2\right]\right|x'\right\rangle\cong\exp\left[-\frac{\overline{\Delta\tau}}{2}\left(\frac{1}{2}x^2-\lambda\right)^2\right]F(x,x')\exp\left[-\frac{\overline{\Delta\tau}}{2}\left(\frac{1}{2}x'^2-\lambda\right)^2\right]\ , \tag{16}$$

where $F(x,x')$ is given, to lowest order in $\overline{\Delta\tau}$, by

$$F(x,x')=\frac{1}{\pi}\int_0^\infty dp\,\cos p(x-x')\exp\left[-\overline{\Delta\tau}\left(\frac{p^4}{4}+\frac{p^2}{2}\left[\frac{1}{2}(x^2+x'^2)-2\lambda\right]\right)\right]\ . \tag{17}$$

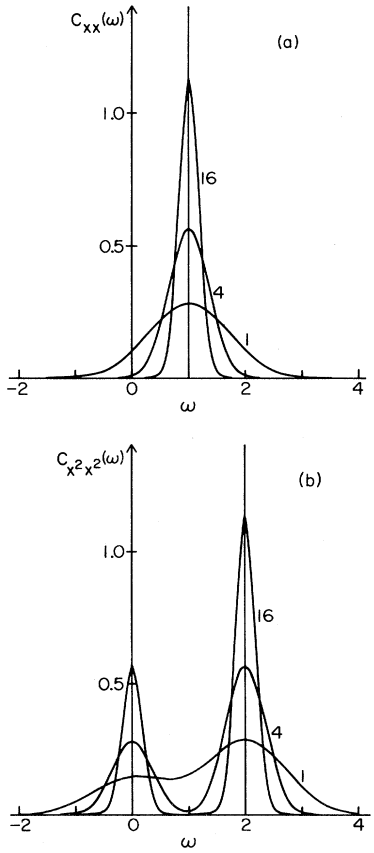

FIG. 1. Approximants for the harmonic oscillator dynamic correlation functions for the position and position squared operators, for $\bar{\beta}=1$, 4, and 16.

Unfortunately, we were unable to find a closed analytic form for Eq. (17) so that this integral was computed numerically.

Figure 2 shows the matrix elements $V_2(x,x')$ for fixed x' as a function of x for the case $\omega=0$. Unlike V_1, $V_2(x,x')$ is negative in a small region and this leads to certain difficulties in the numerical computations. We define

$$f_2(x')\cong\int dx\,|V_2(x,x')| \tag{18}$$

and the transition probability and residues as

$$P_2(x,x')\cong\frac{|V_2(x,x')|}{f_2(x')}\ , \tag{19}$$

$$R_2(x,x')\cong f_2(x')\,\mathrm{sgn}\,V_2(x,x')\ , \tag{20}$$

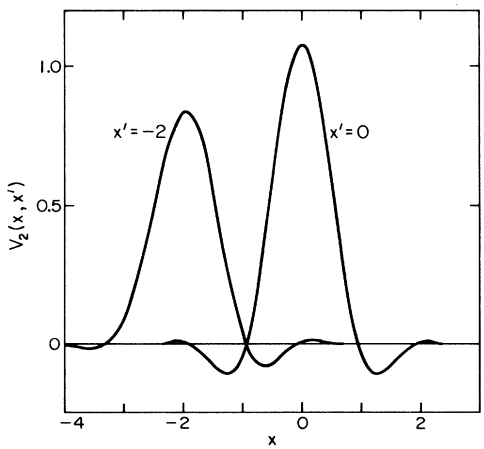

FIG. 2. Matrix elements of the Gaussian operator $V_2(x,x')$ vs x for $x'=0$ and -2. $\Delta\bar{\tau}=0.1$.

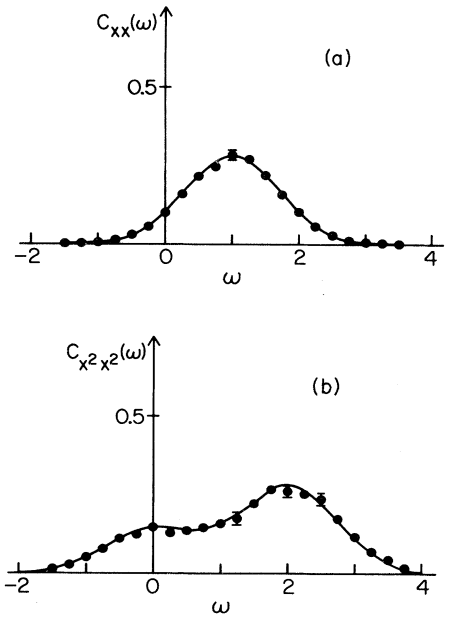

FIG. 3. Numerical results of the stochastic evaluation of the correlation function for $\bar{\beta}=1$. Fifty states were propagated simultaneously and the procedure repeated 250 times. The smooth lines are the exact results for $\bar{\beta}=1$.

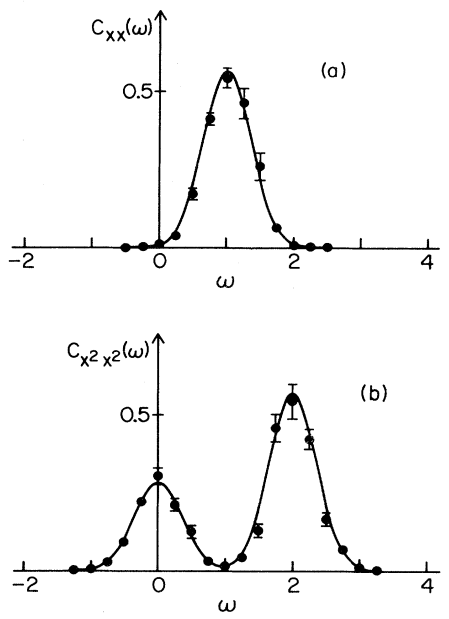

FIG. 4. Same as Fig. 3 for $\bar{\beta}=4$. Here, 100 states were propagated 600 times.

so that Eqs. (10) and (11) are satisfied. The matrices for the usual time-evolution operator are constructed in the same way.

The convergence of the matrix elements $V_1(x,x')$ with $\Delta\tau$ is very fast, and we find that $\Delta\tau=0.1$ gives negligible errors (less than 0.01%). The convergence of V_2 is slower, and we find errors for the matrix elements of about 2%, 0.6%, and 0.2% with $\overline{\Delta\tau}-0.1$, 0.05, and 0.025, respectively. In the numerical computations, we have taken $\overline{\Delta\tau}=0.025$.

To compute C_{xx} and $C_{x^2x^2}$, we use a discrete mesh of 21 values for $-4<x<4$, and choose the initial and final states $|\zeta\rangle=|\chi\rangle$ as the uniform wave function in that interval. Taking $\beta=4$ ensured that the ground state was accurately projected out. To compute Eq. (9) stochastically, one can use two slightly different procedures. In one,[6] one propagates only one state at a time and calculates the average over numerator and denominator many times. This procedure fails for the present case because of the negative matrix elements (Fig. 2): the convergence becomes very poor for $\bar{L}\gtrsim 10$. Thus, we follow a different procedure.[4] We propagate a population of many states at the same time. Instead of carrying separate residues, we add or delete states at each $\overline{\Delta\tau}$ step according to their statistical weight. The only residue that is carried is the sign. However, the crucial step is that after each step we collect together the weights (positive and negative) of each state $|\chi\rangle$ and reproduce the net weight of $|\chi\rangle$, as input to the next $\Delta\tau$ step. In this way we are able to overcome the negative matrix elements of V_2.

In Fig. 3, we show results for the correlation functions for the case $\bar{\beta}=1$, where we have propagated 50 states repeating the procedure 250 times. In Fig. 4, we propagated 100 states 600 times for the case $\bar{\beta}=4$. As $\bar{\beta}$ gets larger, the cancellations become more important and more states have to be taken to obtain reasonable results.

Finally, we remark that the procedure of inverse-Laplace transforming would be difficult even for this simple problem. For example, the Laplace transform of the sum of three δ functions at $\omega=0$, ω_0, and $3\omega_0$ differs by less than 2% from the Laplace transform of $C_{x^2x^2}(\omega)$ [Eq. (14)] over the range $0\leq\tau\leq 2$, if the weight of the δ functions is appropriately chosen. The same applies to the Laplace transform of a δ function at the origin plus a flat response from $\omega=0$ to $3.75\omega_0$. Thus, a Monte Carlo simulation of $C_{x^2x^2}(\tau)$ for $\beta=4$ with statistical error of about 2% would be unable to distinguish between these widely different spectral functions. In contrast, our results [Fig. 4(b)] clearly indicate that the largest response occurs at $\omega=0$ and $2\omega_0$.

III. CONCLUSIONS

We have discussed a new algorithm to compute dynamic correlation functions in quantum systems using Monte Carlo techniques, which eliminates the difficult problem of inverse-Laplace transform of noisy data. We have applied our approach to the harmonic oscillator and found promising results. To get accurate results it is necessary to take a time step $\overline{\Delta\tau}$ in the Gaussian propagation which is small compared to $\Delta\tau$ in the ground-state filtering. Possibly this can be avoided by using the Green's-function Monte Carlo method.[4] A complication found was that the Gaussian propagator had some negative matrix elements which could be handled by propagating the net weights of many states at each time step. We are presently attempting to apply this algorithm to the calculation of dynamic correlation functions in one-dimensional many-body problems.

ACKNOWLEDGMENTS

J.H. is grateful to J. Kuti for helpful discussions on methodology, and to D. Fredkin for conversations on the inverse-Laplace-transform problem. This work was supported in part by NSF Grants No. DMR82-17881, No. DMR82-16285, and No. PHY77-27084. In addition, we acknowledge the support of the University of California Regents Fund.

---

[1]See *Monte Carlo Methods in Quantum Problems,* edited by M. Kalos (D. Reidel, Dordrecht, The Netherlands, in press), and references therein.

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

[3]J. Hammersley and D. Handscomb, *Monte Carlo Methods* (Wiley, New York, 1964), p. 85.

[4]See D. M. Ceperley and M. H. Kalos, in *Monte Carlo Methods in Statistical Physics,* edited by K. Binder (Springer, Berlin, 1979), and references therein.

[5]J. Kuti, Phys. Rev. Lett. 49, 183 (1982); J. Kuti and J. Polonyi, in Proceedings of the John Hopkins Workshop on Current Problems and Particle Theory, 1982 (unpublished), Vol. 6, p. 15.

[6]R. Blankenbecler and R. L. Sugar, Phys. Rev. D 27, 1304 (1983).