Quasielastic response with a real-time path-integral Monte Carlo method

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We formulate the quasielastic response of a nonrelativistic many-body system at zero temperature in terms of ground-state density-matrix elements and real-time path integrals that embody the final-state interactions. While the former provide the weight for a conventional Monte Carlo calculation, the latter require a more sophisticated treatment. We argue that the stationary-phase Monte Carlo technique recently developed by Doll *et al.* can be used to study the approach to "Y scaling." We perform calculations for a particle in a potential well in one and three dimensions and compare them with the exact results available for these models.

I. INTRODUCTION

Inelastic scattering is a very useful experimental tool in many-body physics. This is because, in Born approximation, the inelastic cross section is proportional to the dynamic structure factor (or dynamic response) of the many-body system, $S(\mathbf{q},\omega)$. Different probes (e.g., electrons, neutrons, x rays) can be used to study a variety of systems, from solids to liquids, from atoms to nucleons. A suitable choice of energy and momentum transfers $\omega\mathbf{q}$ allows the experimenter to focus on one of several different aspects of the many-body system, such as collective modes or single-particle properties.

This paper deals with quasielastic (QE) scattering, which involves energy and momentum transfers much higher than the characteristic scale of the collective modes. QE scattering can be viewed as a two-body collision between the probe and one of the constituents of the many-body system. Many-body effects come into play because the initial momentum of the struck constituent is determined by a probability $n(k)$ (the one-body momentum distribution) and because the struck particle can interact with the other particles during its recoil (final-state interaction).

At high momentum transfers, if the recoil kinetic energy can be assumed to be much larger than the interparticle potential, final-state interactions (FSI's) are expected to become negligible, thus making QE scattering an effective means of probing the single-particle momentum distribution of the many-body system. This assumption is called the impulse approximation (IA) and leads to the phenomenon of Y scaling;[1] i.e., the fact that $qS(\mathbf{q},\omega)$ depends solely upon the "scaling" variable $Y \equiv M\omega/q - q/2$, M being the mass of the struck particle, and not separately upon q and ω (we assume nonrelativistic kinematics throughout). Remarkably, in the IA, the momentum distribution $n(k)$ can be extracted from the QE cross section in a completely model-independent fashion. This fact is of obvious interest to the theorist. Fundamental ideas such as Bose condensation in liquid ^{4}He can be tested,[2] and our ability to calculate equilibrium properties of many-body systems can be checked, together with our knowledge of the interaction potential between the constituents. For example, powerful computational techniques, such as Green's function Monte Carlo[3] or path-integral Monte Carlo[4] (PIMC), have been used to calculate the ground state of quantum liquids. The situation in nuclear physics is less satisfactory, as the short-range behavior of the internucleon force is still not understood completely.

What do we learn from the abundant experimental data available for both quantum liquids[5] and atomic nuclei?[6] Unfortunately, the connection between data and theory is less straightforward than the naive IA suggests. Indeed, interatomic forces (and nuclear forces to a lesser extent) are characterized by a short-range, highly repulsive component—almost a hard core—which undermines the picture of free particle recoil.[7] Consider a particle initially sitting in the long-range, weakly attractive potential well because of its neighbors. After being struck by the probe, it will recoil with high momentum (i.e., essentially free) until it bounces from the "hard wall" presented by one of its neighbors' short-range repulsive potential. This will happen even at high recoil momenta. Furthermore, in real experiments, only a finite range of momentum transfers is available, and it may well be that even the long-range attractive part of the potential has to be taken into account in trying to unravel the effects of the FSI's.

This problem is particularly severe in nuclear physics.[8] Here QE scattering is limited to the region of negative Y, where the energy transfer is low enough that inelastic processes (such as Δ-resonance excitation) are unimportant. Therefore, the nuclear recoil energy is at best about ten times its binding energy. For comparison, momentum transfers as high as 24 Å^{-1} have been achieved in QE scattering from liquid ^{4}He, yielding typical recoil energies about 100 times the binding energy. One can observe significant differences between the response at such high momentum transfers and that at lower ones (e.g., $q = 7$ Å^{-1}), corresponding to those available in nuclear physics experiments.

Several calculations of FSI's have been performed for both neutron scattering from quantum liquids and electron scattering from nuclei. The first appeared in the

work of Hohenberg and Platzman[2] (HP) on QE neutron scattering and the IA for liquid ^{4}He and was based on the following simple considerations. The response at high q is dominated by the pole at the single-particle recoil energy, $E_r=\omega+Y^2/2M$. The effect of collisions during the recoil results in a mean free path, or lifetime, of the recoiling particle, which gives the energy E_r an imaginary part. This shows up as a broadening of the QE peak. In this ansatz, the effect of FSI's can be accounted for by convolving the IA structure factor with a Lorentzian broadening function. More relevant to the present work is the calculation by Gersch *et al.*,[9] who were able to expand the structure factor as a sum of integrals of many-body correlation functions, the expansion parameter being the inverse of the momentum transfer q. At $q\rightarrow\infty$, the response is given by the lowest-order term, which they found to be exactly the IA. In this way they could calculate not only the broadening of the QE peak, but also its shift toward lower Y due to FSI's at finite q. However, their theory is not applicable to strong two-body interactions. The reason can be understood qualitatively for hard-core (HC) interactions, where the scattering amplitude, which can be regarded as a renormalized potential, grows linearly with q. Therefore, $O(V/q)$ corrections to the IA cannot be expected to vanish at high q. Indeed, as shown by Weinstein and Negele[7] with a perturbative calculation of the HC Bose gas, although Y scaling is still observed asymptotically, the scaling function is not related in an obvious way to the momentum distribution. The persistence of correlation effects in the infinite-q limit is also a feature of Silver's theory of FSI's.[10] Like HP, he predicts a convolution form for the QE response, but the broadening function he derives, largely from semiclassical arguments, is not a Lorentzian. This theory is in excellent agreement with neutron-scattering data from liquid ^{4}He; it is expected to be successful at very high momentum transfers, which have been attained in neutron scattering, but its relevance to QE electron scattering is not clear.[11]

This brief (and by no means exhaustive) review of theories of FSI's indicates that they generally suffer from one or more of the following limitations: low-order truncation of the perturbation expansion, inconsistent treatment of the static (ground-state) and dynamic (final-state) properties, and unrealistic (e.g., pure hard-core) potentials. Therefore, it would be desirable to develop a first-principles calculation of the dynamic response given a realistic potential to provide a link between the observed quasielastic cross sections and the inferred momentum distributions.

In view of the success of stochastic methods[12] in calculating many-body equilibrium properties, such as ground-state wave functions and static correlation functions, it is natural to ask whether analogous methods can be applied to the calculation of a dynamic property such as the QE response. An important ingredient in the success of these static calculations is a well-chosen trial function embodying much of the physics. Fortunately, for the QE response, the IA can provide an analogous zeroth-order approximation to guide the calculation. Although there are no conceptual obstacles toward this end, there is an as yet insurmounted practical difficulty when one tries to develop a stochastic method to perform quantum-dynamics calculations. The evaluation of a static property can be reduced to averaging an observable over a sampling weight function in a rather straightforward way, at least for Bose systems. For instance, matrix elements of the imaginary time evolution operator provide such a weight in the PIMC method. Quantum dynamics, on the other hand, requires that the evolution operator matrix elements be evaluated in real time. This turns Boltzmann-like factors into oscillatory exponentials, for which stochastic sampling methods have long looked hopeless. Recently, however, Doll, Freeman, and co-workers[13–15] have devised a new technique, the stationary-phase Monte Carlo (SPMC) method, to evaluate oscillatory integrals by sampling the integrand more densely near the points of constructive interference.

Although SPMC is still far from being a general purpose quantum-dynamics technique, it is a good candidate for a first-principles nonrelativistic calculation of the QE response, formulated in terms of path integrals. Our reasoning is as follows: The problems introduced by the evaluation of path integrals in real time become obviously less and less severe the shorter the time scale involved, as long as the potential remains finite. An estimate of the important time scale in QE scattering is given by the ratio of the characteristic length scale of the problem, set by the equilibrium density matrix, to the velocity of the recoiling particle, determined by the momentum transfer $\mathbf{q}$. Thus only short times are important at high-momentum transfers and one legitimately expects the SPMC method to give a satisfactory answer. This is the same argument that led Gersch *et al.* to develop a $1/q$ expansion for the FSI.[9]

There are two goals for this paper. First, we develop a formulation of the QE response in which the IA is multiplicatively corrected by a real-time path integral between two ground-state configurations of the many-body system. We propose to evaluate the path integral, which embodies the FSI, by the SPMC method. Second, we test the principle of this method by applying it to a one-body system in an external potential well. This problem is exactly soluble in one dimension and easily treated numerically in three dimensions. We limit our treatment here to finite interactions; strong (e.g., hard-core) potentials require a further treatment, which will be given elsewhere.

Our paper is organized as follows: In Sec. II we set up the QE response formalism and derive the path-integral formulation, which allows us to establish Y scaling. In Sec. III we review the SPMC technique and develop it in a way that is best suited to our problem. In Sec. IV we present our numerical methods and results, both for the Monte Carlo (MC) and for the exact calculations, and we also compare the SPMC method to the stationary-phase method when possible. Finally, our conclusions are given in Sec. V.

II. PATH-INTEGRAL REPRESENTATION OF THE QE RESPONSE

Consider a system of N particles interacting via a finite two-body potential V (which we assume to be spin and

isospin independent for simplicity) and an external probe, interacting with the constituents of the system through a potential v that is weak compared to V. We are interested in the rate of the inclusive process in which the probe scatters from the system transferring momentum $\mathbf{q}$ and energy ω:

$$\sigma(\mathbf{q},\omega)=2\pi|v(q)|^2NS(\mathbf{q},\omega) .$$

The dynamic response, or structure factor, $S(\mathbf{q},\omega)$, is given

by the Fourier transform of the time-dependent density-density correlation function:

$$S(\mathbf{q},\omega)=\frac{1}{2\pi N}\int dt\, e^{i\omega t}\langle \rho_{-\mathbf{q}}(t)\rho_{\mathbf{q}}(0)\rangle , \tag{1}$$

where $\langle\ \rangle$ indicates the average over a statistical density matrix describing the state of the target and the Heisenberg operators $\rho_{\mathbf{q}}(0)$ and $\rho_{-\mathbf{q}}(t)$, respectively, inject momentum $\mathbf{q}$ into the system at time 0 and remove it at time t,

$$\rho_{\mathbf{q}}(t)=\sum_{i=1}^{N} e^{i\mathbf{q}\cdot\mathbf{r}_i(t)} .$$

We set $\hbar=1$ throughout this paper.

It is convenient to split the response into two parts, according to whether the particle absorbing momentum $\mathbf{q}$ is or is not the same one to give it up after time t. We thus define the incoherent response

$$S^i(\mathbf{q},\omega)=\frac{1}{2\pi N}\int dt\, e^{i\omega t}\left\langle \sum_i e^{-i\mathbf{q}\cdot\mathbf{r}_i(t)} e^{i\mathbf{q}\cdot\mathbf{r}_i(0)}\right\rangle , \tag{2a}$$

and the coherent response

$$S^c(\mathbf{q},\omega)=\frac{1}{2\pi N}\int dt\, e^{i\omega t}\left\langle \sum_{i\neq j} e^{-i\mathbf{q}\cdot\mathbf{r}_i(t)} e^{i\mathbf{q}\cdot\mathbf{r}_j(0)}\right\rangle . \tag{2b}$$

In the IA, as we discussed in Sec. I, FSI's are neglected, and one can write

$$e^{-i\mathbf{q}\cdot\mathbf{r}_i(t)} e^{i\mathbf{q}\cdot\mathbf{r}_i(0)}|\mathbf{k}_1,\ldots,\mathbf{k}_N\rangle = e^{-i(\mathbf{q}\cdot\mathbf{k}_i+q^2/2)t}|\mathbf{k}_1,\ldots,\mathbf{k}_N\rangle ,$$

whereupon the incoherent response scales to a function of the single variable $Y\equiv\omega/q-q/2$ (we set the mass of the constituents equal to 1):

$$S^i_{\mathrm{IA}}(\mathbf{q},\omega)=\frac{1}{4\pi^2 q}\int_{|Y|}^{\infty} dp\, pn(p) ,$$

where $n(p)$ is the one-body momentum distribution. Therefore, in the IA, the QE cross section can be calculated from the static properties of the ground state or thermal ensemble of the many-body system. A similar treatment of S^c leads to an expression that falls off very rapidly with q compared to S^i. This happens because the coherent response probes the ground-state density matrix at momenta of order q (typically much larger than Y).

Experimentally, one defines the functions

$$F^{i(c)}(q,Y)\equiv qS^{i(c)}(\mathbf{q},\omega)$$

and looks for scaling by considering the behavior of qS at fixed Y as q increases. In the IA, one expects F^c to vanish at high q, while F^i approaches the q-independent function

$$F^i_{\mathrm{IA}}(Y)=\frac{1}{4\pi^2}\int_{|Y|}^{\infty} dp\, pn(p) , \tag{3}$$

from which the momentum distribution can be obtained simply by differentiating with respect to Y. However, sizable deviations from the IA are observed in real experiments; to account for them properly, one must carry out a more complete calculation of the dynamic response.

We start by inserting complete sets of position eigenstates into Eq. (1):

$$qS(\mathbf{q},\omega)=\int dx\, dx' \rho(x,x')\Omega(x',x) . \tag{4}$$

Here x denotes the ensemble of all the particle coordinates; these are $n=N\times d$ in number for N particles in d dimensions. $\rho(x,x')$ is the density-matrix element, and

$$\Omega(x',x)=q\int \frac{dt}{2\pi N} e^{i\omega t}\sum_{i,j}\int dx_0 \langle x'|e^{iHt}|x_0\rangle\langle x_0|e^{-iHt}|x\rangle e^{i\mathbf{q}\cdot(\mathbf{x}_i-\mathbf{x}_j^0)} \tag{5a}$$

is the "response operator." We now introduce path-integral representations of the propagators forward and backward in time:

$$\begin{aligned}\langle x_0|e^{-iHt}|x\rangle &= \int_x^{x_0}\mathcal{D}[x_+(\tau)]\exp\left\{i\int_0^t d\tau\left[\frac{1}{2}\left[\frac{dx_+}{d\tau}\right]^2-V(x_+)\right]\right\},\\ \langle x'|e^{iHt}|x_0\rangle &= \int_{x_0}^{x'}\mathcal{D}[x_-(\tau)]\exp\left\{-i\int_0^t\left[\frac{1}{2}\left[\frac{dx_-}{d\tau}\right]^2-V(x_-)\right]\right\} .\end{aligned} \tag{5b}$$

Consider the incoherent response first. For a finite interaction potential V, we expect that the main contribution to S comes from the IA, Eq. (3) (in fact, this is a rigorous result[16]). As discussed in Sec. I, this corresponds to consider a free-particle recoil. Therefore, a good starting point will be to shift to new path-integration variables $z_\pm(\tau)$ centered around the path of the freely recoiling particle

$$x_+(\tau)=z_+(\tau)+(x_0-x)\frac{\tau}{t}+x ,$$

$$x_-(\tau)=z_-(\tau)+(x_0-x')\frac{\tau}{t}+x'$$

[so that $z_{\pm}(0)=z_{\pm}(t)=0$], and to substitute $x_0 \rightarrow x_0(x+x')/2$, thus obtaining

$$\Omega^i(x',x)=q\int\frac{dt}{2\pi}e^{i\omega t}\int\frac{dx_0}{(2\pi|t|)^n}\exp\left[-iqx_{0\parallel}+iq\frac{(x-x')_{\parallel}}{2}-ix_0\frac{(x-x')}{t}\right]$$
$$\times\int_0^0\mathcal{D}z_+\mathcal{D}z_-\exp\left\{i\int_0^t d\tau\left[\tfrac{1}{2}\left[\frac{dz_+}{d\tau}\right]^2-V_+\right]\right\}\exp\left\{-i\int_0^t d\tau\left[\tfrac{1}{2}\left[\frac{dz_-}{d\tau}\right]^2-V_-\right]\right\}.$$

The subscript $\parallel$ denotes the coordinate of the recoiling particle along the momentum transfer vector $\mathbf{q}$; we will use the subscript $\perp$ to indicate all the remaining $n-1$ coordinates (the "spectators"). $V_{\pm}$ is the potential evaluated along the paths $x_{\pm}(\tau)$. The first line of the preceding formula depicts a particle receiving momentum $\mathbf{q}$ at time zero, propagating in a straight line between x and x_0 forward in time t, and then backward to x' after giving up momentum $\mathbf{q}$. The path integrals in the second line describe the quantum fluctuations around this classical picture, as well as the interactions within the many-body system. The IA and the approach to scaling, however, are not yet evident. A few more algebraic steps are needed, which again are suggested by the physics.

As we argued at the end of Sec. I, we expect shorter and shorter time scales to be relevant to QE scattering as the momentum transfer grows larger and larger. In such a short time, the struck particle will propagate a finite distance along the direction of its high-speed recoil (i.e., parallel to $\mathbf{q}$), while the motion in the other directions (and that of the particles in the system) will tend to be frozen. Incidentally, we note that this picture isn't justified in the presence of strong interactions, when "billiard ball" collisions can take place. As we are dealing here with finite interactions, we choose new sets of coordinates in line with our reasoning. We introduce velocities by defining $x_0\equiv vt$ and explicitly scale time by the inverse of the momentum transfer, $t\equiv(\xi-1)(x-x')_{\parallel}/q$. Notice that now particles moving at finite velocity will travel only distances $\sim 1/q$. The recoil velocity $v_{\parallel}$ has to be proportional to q, so we set $v_{\parallel}\equiv(\kappa+1)\omega/q$. Upon introducing these changes of variables, we arrive at

$$\Omega^i(x',x)=\frac{1}{2\pi}e^{-iY(x-x')_{\parallel}}\int\frac{d\kappa\,d\xi}{2\pi}e^{-i\kappa\xi}\int\frac{d^{n-1}v_{\perp}}{(2\pi)^{n-1}}e^{iv(x-x')_{\perp}}\int_0^0\mathcal{D}\zeta_+\mathcal{D}\zeta_-e^{i(S_+-S_-)}, \tag{6a}$$

$$S_{\pm}=\tfrac{1}{2}\int_0^1 d\sigma\left[\frac{d\zeta_{\pm}}{d\sigma}\right]^2-\frac{(x-x')_{\parallel}}{q}(\tilde{\xi}-1)\int_0^1 d\sigma\,V_{\pm}(z_{\pm};\tilde{\xi},\tilde{\kappa};x,x';\sigma), \tag{6b}$$

where $\sigma\equiv\tau/t$ is the scaled time,

$$\tilde{\xi}\equiv\xi/[(\omega|x-x'|_{\parallel})/q]^{1/2},$$
$$\tilde{\kappa}\equiv\kappa/[(\omega|x-x'|_{\parallel})/q]^{1/2},$$

and

$$z_{\pm}\equiv\zeta_{\pm}\sqrt{|t|}.$$

Notice that $\tilde{\xi}$, $\tilde{\kappa}$, and $z_{\pm}$ are all suppressed as $1/\sqrt{q}$ at high q; i.e., at high-momentum transfers, the argument of the potential becomes independent of the fluctuations around the free-particle recoil. We emphasize that Eq. (6), although derived largely from intuitive arguments, is formally exact.

Before we discuss the result we have just derived, we rewrite Eq. (6) using a Fourier representation of the path,[17] which makes the kinetic energy diagonal (i.e., local) in the path coordinates. This will prove convenient in the next sections, as well as for computational purposes. Because the end points of the paths are fixed [$\zeta_{\pm}(\sigma=0)=\zeta_{\pm}(\sigma=1)=0$], we can write

$$\zeta_{\pm}(\sigma)=\frac{\sqrt{2}}{\pi}\sum_{m=1}^{\infty}\frac{1}{m}\eta_{m\pm}\sin(m\pi\sigma),$$

so that the action becomes

$$S_{\pm}=\sum_{m=1}^{\infty}\eta_{m\pm}^2/2-\frac{(x-x')_{\parallel}}{q}(\tilde{\xi}-1)\int_0^1 d\sigma\,V_{\pm}.$$

The argument of the potential will be written down explicitly later.

Equation (6) reveals that we have succeeded in separating the IA contribution from terms that are of order $1/q$ or higher. Indeed, since we are considering finite two-body interactions, if we let $q\rightarrow\infty$, we easily recover the IA, Eq. (3), as all integrals in Eq. (6a) become trivial, yielding

$$\Omega^i_{\mathrm{IA}}(x',x)=\frac{1}{2\pi}e^{-iY(x-x')_{\parallel}}\delta^{(n-1)}(x-x')_{\perp}.$$

It has long been known that the $O(1/q)$ correction to the IA can be written down in a rather straightforward fashion. This is also easily derived from Eq. (6). We simply expand

$$\exp\left[-i\frac{(x-x')_{\parallel}}{q}(\tilde{\xi}-1)\int_0^1 d\sigma\,V_{\pm}\right]$$
$$\simeq 1+i\frac{(x-x')_{\parallel}}{q}\int_0^1 d\sigma\,V_{\pm}$$

and evaluate the potential at the zeroth-order path in $1/q$ ($z_{\pm}=0$), to obtain

$$\Omega^i_1(x',x)=\frac{i}{2\pi q}e^{-iY(x-x')_{\parallel}}\delta^{(n-1)}(x-x')_{\perp}(x-x')_{\parallel}$$
$$\times\int_0^1 d\sigma[V(x-(x-x')_{\parallel}\sigma)-V(x')]. \tag{7}$$

Upon substituting Eq. (7) into Eq. (4), we recover Eq. (31) of Ref. 9.

We turn now to the coherent response. We rewrite the matrix elements of the density operator in Eq. (5) as fol-

$$e^{i\mathbf{q}\cdot(\mathbf{x}_i-\mathbf{x}_j^0)}=e^{i\mathbf{q}\cdot(\mathbf{x}_j-\mathbf{x}_j^0)}e^{i\mathbf{q}\cdot(\mathbf{x}_i-\mathbf{x}_j)} .$$

Therefore, grouping the identical contributions from all pairs, we obtain

$$qS^c(\mathbf{q},\omega)=(N-1)\int dx\,dx'\rho(x,x')e^{i\mathbf{q}\cdot(\mathbf{x}_1-\mathbf{x}_2)}\Omega^i(x',x) , \tag{8}$$

i.e., our discussion of the matrix elements $\Omega^i(x',x)$ remains unchanged, the only difference being a "coherence" factor multiplying the density matrix. This factor is responsible for the rapid decay of the coherent response at high q, where it measures the probability of finding two particles with very high momenta in the equilibrium density matrix of the system.

Now that we have set up the path-integral formalism in a way that makes the approach to scaling quite transparent, we are left with the problem of carrying out the integrations. These are of two different kinds: Equations (4) and (8) are the average of the response operator $\Omega(x',x)$ weighted by the density-matrix elements $\rho(x,x')$; we expect standard MC techniques to be suitable for this calculation. However, Eq. (6) is a high-dimensional oscillatory integral, which we propose to evaluate by the SPMC method.

III. THE STATIONARY-PHASE MONTE CARLO METHOD

We now summarize the principles of the SPMC method. Many of the results reported in this section were originally derived by Doll, Freeman, and coworkers (DF), who were motivated by the need of calculating dynamic correlations at finite temperature,[18] i.e., functions of the type

$$C_{AB}(t)=\mathrm{tr}[\exp(-\beta H)A\exp(iHt)B \times\exp(-iHt)]/\mathrm{tr}[\exp(-\beta H)] .$$

This bears a strong resemblance to our problem, which nonetheless is complicated by the fact that we work in frequency space and, above all, that we formulate the correlation function in a way [see Eq. (4)] that forces us to work with integrals of pure phase factors. Thus, while DF have studied extensively the model problem

$$\int dx\,\rho(x)\exp[if(x)]\Big/\int dx\,\rho(x) , \tag{9a}$$

where $\rho(x)$ is a smooth probability distribution stemming from the Boltzmann factor, we have to face integrals of the type [see Eq. (6)]

$$\int dx\,\exp[if(x)] . \tag{9b}$$

In any case, the strategy is to follow DF's basic idea: to generate a weight for a MC calculation that samples the integrand more densely in the regions where the phase interference is constructive, i.e., near the stationary points. Let us consider the following one-dimensional (1D) example, for which generalization to arbitrary dimension is straightforward.

Starting from the identity

$$I\equiv\int dx\,e^{if(x)} =\int dx\,e^{if(x)}\int dy\,P(y)e^{i[f(x-y)-f(x)]} , \tag{10}$$

where $P(y)$ is a normalized "probability" function, peaked around this origin, we write

$$D(x)\equiv\int dy\,P(y)e^{i[f(x-y)-f(x)]} \simeq\int dy\,P(y)e^{-iyf'(x)}\equiv D_1(x) , \tag{11}$$

whereupon

$$I=\int dx\,D_1(x)e^{if(x)}\left[1+\frac{D(x)-D_1(x)}{D_1(x)}\right] . \tag{12}$$

This is convenient if the right-hand side (rhs) integral in (11) can be done easily. This is the case if $P(y)$ is a Gaussian, $P(y)=e^{-y^2/2\epsilon^2}/(2\pi\epsilon^2)^{1/2}$, as we will assume hereafter. The function

$$D_1(x)=e^{-[\epsilon f'(x)]^2/2}$$

is called the SPMC filter. If ϵ is small enough, $D_1(x)$ is a good approximation for $D(x)$, and one can hope to be able to evaluate the difference $\delta D(x)\equiv D(x)-D_1(x)\ll D(x)$ with a few-point MC calculation.

The integral (12) has the pleasant feature that the function $D_1(x)$ now provides a good weight for a stochastic evaluation of I:

$$I=\mathcal{N}\left\langle e^{if(x)}\left[1+\frac{\delta D(x)}{D_1(x)}\right]\right\rangle_{D_1(x)} , \tag{13}$$

where $\mathcal{N}=\int dx\,D_1(x)$ denotes the normalization of D_1 and we use the notation $\langle\cdots\rangle_{D_1}$ to denote average with the weight function D_1. This weight samples preferentially around the stationary points of the original integral (10) (where f' is small), helping to filter the signal from the noise. An obvious complication is that one has to normalize the sampling weight (i.e., calculate $\mathcal{N}$). This is in general much harder at zero temperature [see Eq. (9b)] than it is at finite temperature [Eq. (9a)], where one can cautiously seek help in the identity

$$I=\left\langle e^{if(x)}\left[1+\frac{\delta D(x)}{D_1(x)}\right]\right\rangle_{D_1(x)\rho(x)}\langle D_1(x)\rangle_{\rho(x)} .$$

Fortunately, in the application of (13) to our problem, we need not worry about the normalization of the weight, which turns out to be straightforward, as we will see.

Instead, a more serious problem is encountered in applying this method to evaluating a real-time path integral such as that given in Eq. (6). Indeed, the main contribution to the phase (i.e., to the action) comes from the kinetic energy, which is a quadratic form in the integration variables. Let us consider the trivial integral

$I=\int dx\, e^{ix^2/2}$ (this integral has also been considered by DF,[13] though still in the context of "finite temperatures"). The SPMC filter is a Gaussian, $e^{-\epsilon^2 x^2/2}$, decaying too slowly to filter the noise coming from the oscillations of the integral. However, quadratic phases offer the advantage that the function $D(x)$ can be evaluated *exactly:*

$$D(x)=(1-i\epsilon^2)^{-1/2}\exp\left[-\frac{\epsilon^2}{1+\epsilon^4}\frac{x^2}{2}\right]\times\exp\left[-i\frac{\epsilon^4}{1+\epsilon^4}\frac{x^2}{2}\right]. \quad (14)$$

Now, since $\delta D(x)\equiv 0$, ϵ can be chosen arbitrarily, and the integral becomes

$$I=\frac{1}{\sqrt{1-i\epsilon^2}}\int dx\,\exp\left[i\frac{x^2}{2}\frac{1}{(1+\epsilon^4)}\right]\times\exp\left[-\frac{x^2}{2}\frac{\epsilon^2}{(1+\epsilon^4)}\right].$$

The second exponential provides the weight for a MC calculation of the oscillatory integral. Furthermore, a good choice for ϵ ($\epsilon\geq 1$) will suppress the oscillations, as the phase has acquired a factor $1/(1+\epsilon^4)$.

If the phase in I is of the type $f(x)=[x^2/2-V(x)]$, we simply replace x in Eq. (14) by $x-V'(x)$, thus obtaining an approximation for $D(x), D_2(x)$ that is correct up to terms $O(V'')$:

$$D_2(x)=(1-i\epsilon^2)^{-1/2}\exp\left[-\frac{\epsilon^2}{1+\epsilon^4}\frac{[x-V'(x)]^2}{2}\right]\times\exp\left[-i\frac{\epsilon^4}{1+\epsilon^4}\frac{[x-V'(x)]^2}{2}\right]. \quad (15)$$

In this case, however, the choice of ϵ is less obvious than for a quadratic phase. One has to compromise between high values of ϵ, which dramatically improve the signal-to-noise ratio but make a MC calculation of $\delta D\equiv D-D_2$ impractical, and low values of ϵ, which yield the correct result but with extremely large variance. We shall be content with choosing $\epsilon\sim 1$ and ignoring δD.[19] We observe that $\delta D\sim O(V'')$ and thus expect it to be reasonably small because we are working with finite, smooth potentials; this can be checked by estimating δD with Gaussian approximations.

In this way we can write

$$I\simeq I_2=\int dx\, w(x)\left[\frac{D_2(x)}{w(x)}\right]\exp[if(x)]\Big/\int dx\, w(x)\,, \quad (16)$$

and the only problem left is the choice of the normalized weight $w(x)$ to be used in the MC evaluation of I_2. For this, we propose to take the normalized probability distribution

$$w(x)=\exp\left[-\frac{\epsilon^2}{1+\epsilon^4}\frac{x^2}{2}\right]\Big/\left[2\pi\frac{(1+\epsilon^4)}{\epsilon^2}\right]^{1/2}. \quad (17)$$

Once again, we expect this choice to be appropriate whenever the phase is largely a quadratic function of the coordinates.

Finally, we would like to point out that the method we have presented is similar to the stationary-phase approximation because it is not exact (if we ignore δD), but it relies on the "smoothness" of the potential. However, its application is much more straightforward, since it requires neither evaluation of determinants nor searches for stationary points, which may become prohibitive for high-dimensional integrals.

IV. NUMERICAL METHODS AND RESULTS

In the preceding sections we have derived an exact expression for the dynamic response of a nonrelativistic many-body system. We have used a path-integral representation of the time evolution operator and have chosen a reference path as suggested by the physics of the problem we want to address, namely, the approach to scaling. Indeed, we were able to derive, in a straightforward way, the scaling form of the structure factor at high-momentum transfers and the $O(1/q)$ correction to scaling; both expressions are well known and have been derived by different means by other authors.

In view of the generality of the path-integral method, one expects it to be of some help in those cases in which the nature of the interactions or the experimental data available requires more than simple perturbative expansions. However, while there exist well-established techniques for computing with path integrals in imaginary time, only recently have people turned to dynamics problems requiring the evaluation of path integrals in real time.[20] We have seen that the SPMC method offers some promise, especially when the relevant time scales in the problem are small; however, more work is clearly needed in that direction. In fact, not only do we lack a general technique, but we are not even aware of any attempt made at solving realistic problems.[21]

Therefore, we set out to solve model problems, for which an exact solution is available either analytically or by numerical quadrature. We calculate the dynamic response for a particle in a potential well in one and three dimensions. As we simply want to test the principles of our method, we choose a finite attractive well $V(r)=-V_0\cosh^{-2}(r)$. Such a potential lacks an important feature, displayed by atomic and nuclear potentials, namely, a strong short-distance repulsive component. We shall address this problem in the following. In the meanwhile, we shall make contact with physical situations when appropriate.

We are now ready to look at the details of the computation. The eigenstates of the potential are known analytically in 1D,[22] while they are easily calculable numerically in 3D.[23] Thus, from the ground-state wave function ψ_0, we obtain the density matrix $\rho(x,x')=\psi_0(x)\psi_0(x')$. Hence, using the Metropolis algorithm, we can generate the ground-state configurations needed to do the integrals in Eq. (4).

Next we consider Eq. (6). The path integrals are carried out as usual, by keeping a finite number of modes in the Fourier representation of the paths and discretizing commensurately the time integrals of the potential:

$$\int_0^0 \mathcal{D}\xi_+ \mathcal{D}\xi_- e^{i[S_+(\xi_+,\dot{\xi}_+,t)-S_-(\xi_-,\dot{\xi}_-,t)]} = \int \frac{d^M\eta_+ d^M\eta_-}{(2\pi)^M} \exp\left\{ i\,\mathrm{sgn}(t) \sum_{m=1}^{M} (\eta_m^+)^2/2 - it/(M+1) \sum_{j=1}^{M+1} V_{+j} \right.$$
$$\left. - i\,\mathrm{sgn}(t) \sum_{m=1}^{M} (\eta_m^-)^2/2 + it/(M+1) \sum_{j=1}^{M+1} V_{-j} \right\}$$

where $\zeta_0=\zeta_{M+1}=0$. M modes are needed for $M+1$ time slices; m numbers the modes, and j the time slices. Otherwise, the notation is that used in Sec. II. We write down the argument of the potential explicitly, for the 3D case,

$$V_{+j}=V\{\mathbf{z}_j^+(\{\eta^+\})+[(\omega/q^2)(x-x')_\parallel(\tilde{\kappa}+1)(\tilde{\xi}-1)-(x-x')_\parallel/2]\sigma\hat{q}+\mathbf{x}-(\mathbf{x}-\mathbf{x}')_\perp\sigma/2+\mathbf{v}_\perp(x-x')_\parallel/q(\tilde{\xi}-1)\sigma\}\ ,$$
$$V_{-j}=V\{\mathbf{z}_j^-(\{\eta^-\})+[(\omega/q^2)(x-x')_\parallel(\tilde{\kappa}+1)(\tilde{\xi}-1)+(x-x')_\parallel/2]\sigma\hat{q}+\mathbf{x}+(\mathbf{x}-\mathbf{x}')_\perp\sigma/2+\mathbf{v}_\perp(x-x')_\parallel/q(\tilde{\xi}-1)\sigma\}\ ,$$

with $\hat{q}\equiv\mathbf{q}/q$, $\mathbf{z}=\zeta\sqrt{|t|}$, and ζ and η are related by a sine transform.

These expressions, together with the κ,ξ integrals, result in a $(6M+2)$-dimensional oscillatory integral, whose phase reduces to a quadratic form as $t\to 0$. We treat it by SPMC, as explained in Sec. III. To make the correspondence with the formulas derived in that section more straightforward, we chose to use a Fourier representation of the path. As for the choice of the SPMC parameter ϵ, we have used different values for the integrals over the "light-cone" variables κ,ξ than for the path integral. We will denote these using ϵ_l and ϵ_x, respectively.

A different treatment is required by carrying out the integral over the transverse velocities $\mathbf{v}_\perp$, which arises whenever there is more than one particle in the system or the spatial dimension is greater than 1. The $t\to 0$ limit of the phase is linear in $\mathbf{v}_\perp$: This indicates that the SPMC method is not suitable for this case. However, in the same limit, the integral yields a δ function in the transverse coordinates of the density matrix. This suggests that a good way of proceeding is to expand the potential through second order in $\mathbf{v}_\perp$ and do the resulting Gaussian integral analytically, thus obtaining a quadratic phase in $(\mathbf{x}-\mathbf{x}')_\perp$. Note that, in doing so, we are neglecting terms of order $1/q^4$ in the phase; therefore, we expect the resulting approximation to be very accurate.

At this stage we have gained some insight in the calculation. Only very small values of $(\mathbf{x}-\mathbf{x}')_\perp$ contribute constructively to the integral, i.e., $|(\mathbf{x}-\mathbf{x}')_\perp| \ll (x-x')_\parallel$. This means that it would be inefficient to generate $\mathbf{x},\mathbf{x}'$ from the density matrix, which is isotropic. Instead, we take advantage of the new quadratic phase in $(\mathbf{x}-\mathbf{x}')_\perp$ and generate values of $(\mathbf{x}-\mathbf{x}')_\perp$ by SPMC, obtaining a narrow Gaussian distribution around zero at high q. The density matrix is used to generate $(\mathbf{x}+\mathbf{x}')$ as well as $(x-x')_\parallel$ via the metropolis algorithm. It is amusing to note that the normalization of this weight is now $2\pi q S_{\mathrm{IA}}$ $(Y=0)$.

We have calculated the QE response for a particle in the 1D well, $V(x)=0.8\cosh^{-2}(x)$, and in the 3D spherical well, $V(r)=21\cosh^{-2}(r)$. The potential sets the length scale, and hence the momentum scale. The ground-state energies are, respectively, $E_0=-0.36$ and -12.5. For any given Y, the requirement that the struck particle be excited to the continuum (i.e., that $\omega>-E_0$) fixes a minimum value for the momentum transfer:

$$q>q_0=-Y+(Y^2-2E_0)^{1/2}\ .$$

The time scale of the problem is set by the ratio $\langle|x-x'|\rangle_\parallel/q$. If the product of this number and the average value of the potential is smaller than 1, one can regard the time scale as "small," and the intuitive arguments at the end of Sec. I apply. However, as the product approaches 1, we expect the SPMC method, as formulated in the present paper, to break down. This will clearly happen for very strong potentials at any q and for weak potentials near $q\simeq q_0$. For our potentials, this happens around $q\lesssim 2$ in 1D and $q<10$ in 3D. For nuclear interactions, considering the attractive part of the potential only, one estimates that SPMC breaks down at momentum transfers smaller than 1 GeV/c.

For the particle in one dimension, we have calculated the QE response at fixed $Y=-0.5$ for all the allowed values of q. In Fig. 1 we plot $F^i(q,Y)$ versus q and compare it to the exact result (solid line) as well as to the IA [Eq. (3)], which is a constant. We have also performed the real-time integrals (6) by the stationary-phase (SP) method[24] and plot the results for comparison. The time integrals were carried out on a 16-point grid (i.e., we keep

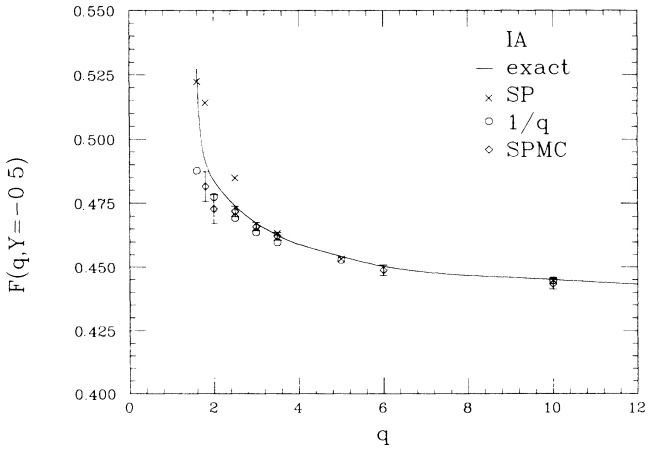

FIG. 1. $F(q,Y)$ as a function of q at fixed $Y=-0.5$ for a particle in the 1D potential well $V(x)=-0.8\cosh^{-2}x$. In our units, $\hbar=m=1$. The ground-state energy is $E_0=-0.37$; the minimum allowed momentum transfer is $q_0=1.5$. Here and in the remaining figures we plot $\pm\sigma$ error bars.

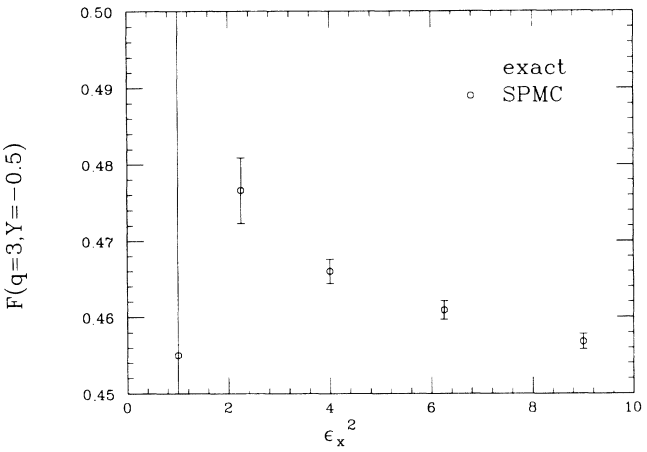

FIG. 2. $F(q=3, Y=-0.5)$ as a function of the SPMC parameter ϵ_x^2 ($\epsilon_l=1$). The potential is the same as in Fig. 1.

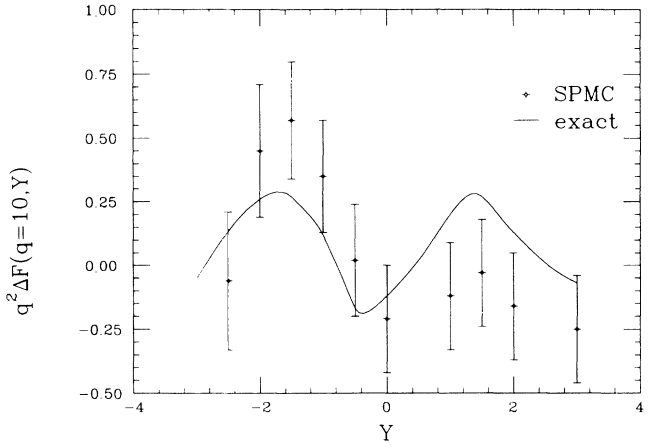

FIG. 4. Contributions $O(1/q^2)$ and higher to $F(q,Y)$ as a function of Y at fixed $q=10$ (same potential as Fig. 3). The q dependence was eliminated in lowest order by subtracting the IA and the $O(1/q)$ contribution [see Eq. (7)] and multiplying through by $q^2=100$.

15 Fourier modes). The SPMC parameters were chosen to be $\epsilon_l=1$ and $\epsilon_x=2$. We have checked the ϵ dependence of the results by calculating at different ϵ_x and ϵ_l. In Fig. 2 we plot the scaled response $F(q=3,\ Y=-0.5)$ with $\epsilon_l=1$ for different values of ϵ_x. We can see how the statistical errors decrease dramatically moving up from $\epsilon_x=1$. At higher values (i.e., $\epsilon_x\simeq 2.5$), a systematic error sets in that should be attributed to the fact that we are ignoring the correction δD in our calculation.

Next we present results for the particle in the 3D potential well. In Fig. 3 we plot $F^i(q,Y)$ at fixed $q=10$ as a function of Y. We kept 15 Fourier modes and checked for convergence with 23 modes at $Y=-0.5$. The dimension of the oscillatory integral, in this case, was 140. The SPMC parameters were chosen to be $\epsilon_l=1$ and $\epsilon_x=2.2$. We notice that the peak of the curve is shifted towards negative Y, with respect to the IA. It is known that this is the case when we are dealing with smooth, attractive interactions, because the deviations from the IA are best described by the $O(1/q)$ correction [Eq. (7)], which is odd in Y. Exact calculations show that the coherent response,[25] $F^c(q,Y)$, is suppressed by about a factor $10^2\sim 10^3$ with respect to $F^i(q,Y)$, which makes it impossible to carry out a meaningful SPMC calculation, given our error bars.

In Fig. 4 we plot the difference between the scaled response function $F(q,Y)$ and its value through order $1/q$, which can be calculated reliably (i.e., without the complications introduced by the real-time dynamics) using Eq. (7). It is no surprise that this quantity is very small. Indeed, as we pointed out before, Eq. (7) works remarkably well for smooth interactions. The results are multiplied by $q^2=100$, since they are expected to be $O(1/q^2)$.

In Fig. 5 we plot $F(q,Y)$ at fixed $Y=-1.5$. Again we

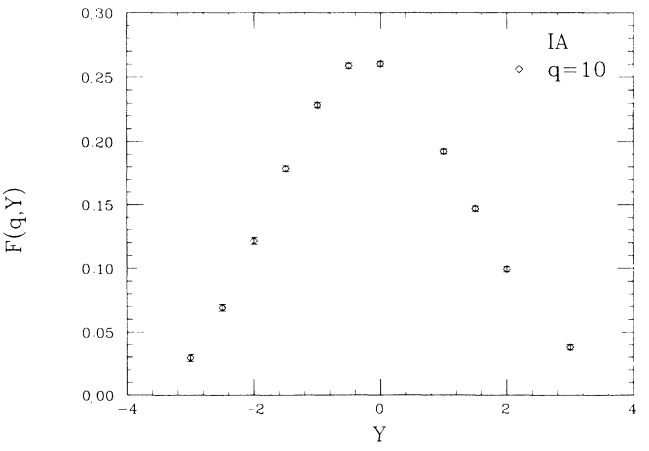

FIG. 3. $F(q,Y)$ as a function of Y at fixed $q=10$ for a particle in the 3D spherical well $V(r)=-21\cosh^{-2}r$. The ground-state energy is $E_0=-12.5$. The scaling limit (which for our potential coincides with the IA) is reached at about $q=40$, within our error bars (see also Fig. 5).

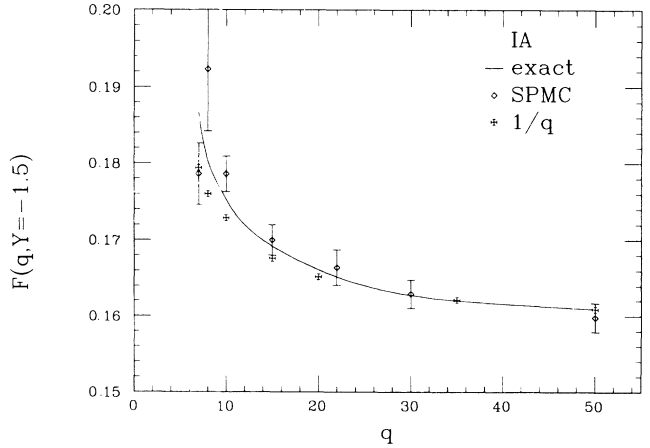

FIG. 5. $F(q,Y)$ as a function of q at fixed $Y=-1.5$. The potential is the same as in Fig. 3. The minimum allowed momentum transfer is $q_0=6.72$.

performed the calculation with 15 modes and checked the result at $q=15$ with 23 modes. The SPMC parameters are the same as those we chose for Fig. 3. We can see that the SPMC gives a satisfactory answer down to $q\sim 10$. Below that, the errors become large. The reason is that we are not including the derivatives of the potential in our sampling weight [i.e., our weight is given by Eq. (7) instead of Eq. (15)]; this works satisfactorily at high q, because the derivatives of the potential are all suppressed by $1/\sqrt{q}$. The lowest q for which we calculate, $q=7$, is very close to the lowest allowed momentum transfer $q_0=6.72$. We also point out that, although the strength of the potential V_0 is much smaller in the 1D case than in three dimensions, the SPMC method in the latter case breaks down at relatively much lower values of q; we attribute this to the role played by the centrifugal force in three dimensions.

V. CONCLUSIONS

We have discussed the QE response of a nonrelativistic many-body system in the high-momentum transfer limit. We have formulated the response in a way that separates the final-state (dynamic) properties from those of the initial state (static). This has allowed us to establish Y scaling for finite many-body interactions, where the short-time propagator tends to the free propagator as $t\rightarrow 0$.

We were able to recover the simple expression of the $O(1/q)$ scaling violations first obtained by Gersch *et al.* using a different approach. Although Gersch's theory is not suitable for calculations involving strong interactions, the path-integral method clearly suggests how to proceed in this case. Indeed, we recall that the potential was explicitly introduced in Eq. (5b), but one need not do so. Instead, the propagators in Eq. (5a) can be rewritten exactly as a convolution of short-time propagators:

$$\langle x'|e^{-iHt}|x\rangle=\int dx_1\cdots dx_{N-1}\langle x'|e^{-iHt/N}|x_1\rangle\cdots\langle x_{N-1}|e^{-iHt/N}|x\rangle\ .$$

If N is chosen large enough that in the time interval t/N only binary interactions are important, then the short-time propagators can be written as products of two-body terms, which are the Fourier transform of the two-body Green's function for the strong potential. These can be renormalized in a number of ways (e.g., summing ladder diagrams) to yield a well-behaved result, whence a smooth time-dependent effective potential can be derived in a straightforward way. We leave this subject to be taken up in future work.

In this paper we have considered finite interactions. We have argued that the SPMC technique can be used to evaluate path integrals in real time, provided that the important time scale is not too large. This is the case when one is interested in the QE response near the scaling limit. We have shown that an appropriate choice of the reference path allows us to extract the IA in a trivial way. We emphasize that the $O(1/q)$ corrections to the IA are not built in our formulation explicitly, so that the agreement between SPMC and exact result beyond the IA is to be taken as a confirmation that the technique is suitable for the real-time dynamics calculations we are interested in. Of course, if we only needed to deal with weak potentials, we would not regard the SPMC method as very practical because in that case Eq. (7) would be an excellent approximation to the exact result (as we showed in Sec. IV). Our hope is that the path-integral method, combined with SPMC, can be extended to treat strong interactions in the way we have outlined. If this proves possible, the results will be of great relevance to many physical situations that are accessible to experiments.

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