Static Response from Quantum Monte Carlo Calculations

Saverio Moroni,[1],[a] David M. Ceperley,[1] and Gaetano Senatore[2]
[1] *National Center for Supercomputing Applications and Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801*
[2] *Dipartimento di Fisica Teorica, Università di Trieste, Strada Costiera 11, I-34014 Trieste, Italy*
(Received 18 June 1992)

We have evaluated the density-density static response of a many-body system by calculating with the quantum Monte Carlo method the energy and density change caused by an external potential. Our results for the linear response function of liquid ^{4}He at zero pressure and temperature are in excellent agreement with the available experimental data. The results for the response function of 2D electrons also at zero temperature, obtained within the fixed-node approximation, constitute the most accurate information available to date for this system.

PACS numbers: 05.30.–d, 02.50.+s

The quantum Monte Carlo method (QMC) provides a systematic route to the calculation of exact properties of many-body systems [1]. For bosons, in particular, stable algorithms exist that yield virtually exact results [2, 3]. This is not the case with fermions, which suffer from the so-called sign problem. However, very accurate results have been obtained for a number of systems, ranging from the homogeneous electron fluid [4, 5], to light molecules [6], and to solid hydrogen [7], using the fixed-node approximation. The vast majority of calculations to date have been for equilibrium properties such as energy, one-particle-orbital occupation numbers, and static correlation functions. Calculations of time-dependent correlation functions and of the related response functions [8] have been lacking for continuum systems. With the exception of some recent progress [9] for lattice models, the same lack of results holds for the static response functions which are properties of the many-body system that, apart from their intrinsic interest, are of importance to density functional developments beyond LDA [10] and crucial to the recently developed theory of quantum freezing [11].

We show that the static density-density response function is directly calculable by QMC with little increase in technical complexity as compared with other properties. We directly use the definition of static response function, rather than evaluate it in terms of the time-dependent correlations, via the fluctuation-dissipation theorem [8]. We apply a static external potential,

$$v_{\rm ext}(\mathbf{r}) = 2v_{\mathbf{q}}\cos(\mathbf{q}\cdot\mathbf{r}), \tag{1}$$

which induces a modulation of the density with respect to its mean value, n_0. Such a modulation contains periodic components at all wave vectors that are nonvanishing integer multiples of $\mathbf{q}$. In particular, one finds a modulation with wave vector $\mathbf{q}$, $n_1(\mathbf{r}) = 2n_{\mathbf{q}}\cos(\mathbf{q}\cdot\mathbf{r})$, where

$$n_{\mathbf{q}} = \chi(q)v_{\mathbf{q}} + C_3 v_{\mathbf{q}}^3 + \cdots \tag{2}$$

only contains odd powers of $v_{\mathbf{q}}$. Here $\chi(q)$ denotes the static density-density linear response function in Fourier space. Similarly the ground-state energy (per particle) can be expanded in even powers of $v_{\mathbf{q}}$:

$$E_v = E_0 + \frac{\chi(q)}{n_0}v_{\mathbf{q}}^2 + C_4 v_{\mathbf{q}}^4 + \cdots. \tag{3}$$

The coefficients C_3 and C_4 in the above equations are determined by the cubic response function [12]. QMC allows the direct evaluation of both $n_{\mathbf{q}}$ and E_v, for given $\mathbf{q}$ and $v_{\mathbf{q}}$. We perform simulations at a few coupling strengths $v_{\mathbf{q}}$ and then extract $\chi(q)$ as well as the higher-order response functions from the calculated $n_{\mathbf{q}}$ or E_v, by fitting in powers of $v_{\mathbf{q}}$. As an illustration, we have chosen to study superfluid ^{4}He and the two-dimensional (2D) electron fluid in a uniform background, both at zero temperature. These systems are prototype quantum Bose and Fermi fluids.

For a given potential, QMC provides a means to numerically sample the ground-state wave function Ψ_0 of the many-body system. In practice, this is achieved by means of random walk algorithms, which propagate the wave function from a suitable starting guess Ψ_T to the exact (for bosons) ground-state function. In the diffusion Monte Carlo method (DMC) [6] one evolves the wave function in imaginary time to project out higher energy components of the trial function. To guide the diffusion process efficiently and to apply fermion antisymmetry for many-body systems one needs an accurate trial function. This is optimized by the variational Monte Carlo technique (VMC) [1] before using it in DMC.

To study superfluid ^{4}He we have chosen the Aziz two-body model potential [13], which gives results for both thermodynamic and structural properties in very good agreement with the available experimental evidence [14]. As a check of our DMC algorithm we have performed preliminary calculations without an external potential, verifying the equivalence of our results with those of previous calculations [14] with a Jastrow trial wave function,

$$\Psi_T^0(\mathbf{R}) = \prod_{i<j}\exp[-u(r_{ij})], \tag{4}$$

and a McMillan pseudopotential $u(r) = ar^{-5}$, with a a

variational parameter. For the system in external field we used the trial function

$$\Psi_T^v(\mathbf{R}) = \Psi_T^0(\mathbf{R}) \prod_i \exp[\alpha \cos(\mathbf{q}\cdot\mathbf{r}_i)], \quad (5)$$

with α a new variational parameter, related to the external potential strength $v_\mathbf{q}$, and Ψ_T^0 given by Eq. (4). One can easily show that $\Psi_T^v(\mathbf{R})$, to leading order in α, correctly yields $n(\mathbf{r}) = n_0 + 2\alpha\gamma\cos(\mathbf{q}\cdot\mathbf{r})$, with γ a function of the density n_0. To determine the relationship between the amplitude of the external potential $v_\mathbf{q}$, and the variational wave-function parameter α, we have found it convenient to fix the wave-function parameter α and determine the corresponding potential $v_\mathbf{q}$ which satisfies the minimum condition $\partial E_v/\partial\alpha = 0$. Once the trial function Ψ_T has been optimized, we perform diffusion runs to sample the exact ground-state wave function Ψ_0, and then we evaluate the total energy and the Fourier component $n_\mathbf{q}$ of the density. One should keep in mind that while the estimate of the energy is exact, within statistical errors, the *extrapolated estimate* [1] yielding $n_\mathbf{q}$ is approximate. In fact its accuracy depends quadratically on the difference $\delta\Psi = \Psi_0 - \Psi_T$. Therefore we shall generally evaluate $\chi(q)$ from the energy, using Eq. (3).

We have studied in detail superfluid ^{4}He at zero temperature and at a number density $n_0 = 0.021\,86$ Å^{-3} which experimentally corresponds to zero pressure. Figure 1 shows a typical result of the total energy E_v versus the strength $v_\mathbf{q}$ of the modulating potential for a wave vector $q = 1.91$ Å^{-1}. The fit to the polynomial in $v_\mathbf{q}$ of Eq. (3) reproduces the calculated energies perfectly, the error bars being not discernible on this scale, and yields $\chi(q)/n_0 = -0.215(8)$ K^{-1}. From similar fits at different periodicities, with $v_\mathbf{q}$'s such that generally $n_\mathbf{q}/n_0 \lesssim 0.1$, we obtain other values of $\chi(q)$ which are collected in Fig. 2. In the same figure we also show the available experimental data [15] and the Feynman approximation [16], which relates the static response to the static structure factor $S(q)$, $\chi_F(q) = -S^2(q)/(\hbar^2 q^2/4Mn_0)$. Here, M is the mass of the ^{4}He atom. Our choice of density was especially motivated by the existence of experimental data, which—to our knowledge—are the only ones available for the static response of a fully degenerate simple quantum liquid. Clearly, our results are in excellent agreement with experiment. It is evident that at this low density the Feynman approximation severely underestimates the true response, for which [16] it is a lower bound. The results of Figs. 1 and 2 were on a system of 64 atoms. These results were checked in a few cases by comparing with those of 125 atoms.

The 2D electron system is of importance in practical situations [17], and receives continuing attention due to its peculiar behavior in the presence of a magnetic field [18]. A fundamental model in many-body theory, to us this system has the great advantage of being less demanding computationally than its three-dimensional counterpart. This is of some importance in the present case, considering that fermions are anyway slower to simulate than bosons. Thus, we have studied unpolarized electrons at $T = 0$, interacting with the potential $1/r$, at a few densities of practical interest [17, 18]. We use the standard units of length where $n_0 = 1/\pi r_s^2 a_B^2$, and r_s—the radius of the Wigner disk in units of the Bohr radius a_B—gives a measure of the coupling strength. We have performed our DMC simulations within the fixed-node approximation, which is known to be both quite accurate and variational in character [6]. To simulate the unperturbed system we take a standard trial function [1] Φ_T^0 which is the product of two plane-wave Slater determinants D_s (one for each spin projection s) times a Jastrow function Ψ_T^0 of the form given in Eq. (4). Explicitly,

$$\Phi_T^0 = D_\uparrow D_\downarrow \Psi_T^0, \quad (6)$$

with the pseudopotential entering Ψ_T^0 of a suitable form [5]. Although the nodal structure of Φ_T^0 is thought to be accurate enough for the unperturbed system [5] we have

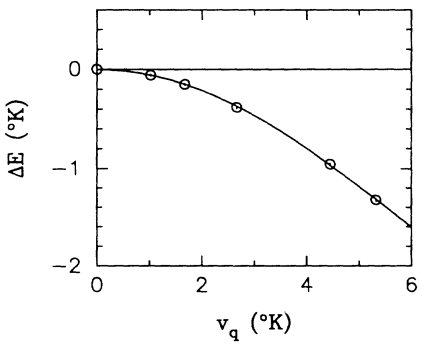

FIG. 1. The energy of liquid ^{4}He at $T = 0$ and $n_0 = 0.021\,86$ Å^{-3} vs the strength $v_\mathbf{q}$ of the applied potential measured with respect to that of the uniform fluid, $\Delta E = E_v - E_0$. The circles are the calculated MC energies and the curve gives a fit in powers of $v_\mathbf{q}$ (see text).

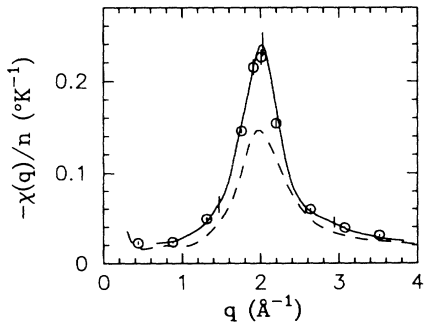

FIG. 2. Linear static response function $\chi(q)$ of liquid ^{4}He at the state specified in Fig. 1. The circles give the present MC results, while the full curve reports experimental data [15]. Error bars are reported on each MC point and few typical error bars are shown also for the experimental data. The dashed curve gives the Feynman approximation (see text).

no experience on its accuracy after the perturbation has been applied. Therefore, we have considered two alternative trial functions for the perturbed system. The wave function denoted by $\Phi^v_{T,1}$ is obtained by multiplying Φ^0_T by a simple modulating factor in exactly the same way as Ψ^v_T is obtained from Ψ^0_T [cf. Eqs. (4) and (5)]. This means that $\Phi^v_{T,1}$ and $\Phi^0_{T,1}$ have identical nodes which one knows is incorrect for noninteracting particles. A second trial function is instead obtained retaining the form of Eq. (6), i.e.,

$$\Phi^v_{T,2} = D^v_\uparrow D^v_\downarrow \Psi^0_T, \tag{7}$$

and constructing the determinants D^v_s in terms of one-particle orbitals (Mathieu functions) for noninteracting electrons in a new external field, $v'(\mathbf{r}) = \alpha\cos(\mathbf{q}\cdot\mathbf{r})$, with α a variational parameter. In general, $\Phi^v_{T,2}$ will possess a different nodal structure than Φ^0_T and $\Phi^v_{T,1}$, while still yielding a modulated density. We have compared the VMC and DMC energies obtained starting with either $\Phi^v_{T,1}$ or $\Phi^v_{T,2}$, and systematically found the energy of $\Phi^v_{T,2}$ lower. Hence we have performed all subsequent calculations with trial wave functions of the form given in Eq. (7). Note that the effective potential should be weak enough that the filling of the single particle orbitals is not altered. Similar to the boson case, we evaluate $\chi(q)$ from a fit of our calculated total energies, according to Eq. (3), since this route is more accurate than looking at the density response from Eq. (2).

Our fixed-node static response $\chi(q)$ for the 2D electron gas is shown in Figs. 3 and 4, at two values of the coupling strength, i.e., $r_s = 1$ and $r_s = 5$. These results were obtained from simulations with 26, 58, and 90 electrons. We correct the static response functions for the finite systems by assuming that the interacting and the noninteracting response functions have the same scaling with the electron number N. This procedure correctly makes the results with different N closer to each other, and closer to the known exact behavior at small q. In the same figures we also report, for comparison, the response function of noninteracting electrons $\chi_0(q)$ [17] and the mean-field RPA approximation, which is simply given by $\chi_{\rm RPA}(q) = \chi_0(q)/[1 - (2\pi e^2/q)\chi_0(q)]$. Already at $r_s = 1$ the differences between the RPA and the fixed-node response are appreciable. Clearly they increase with the coupling, as is seen from Fig. 4. We also report in the figures a number of approximate schemes [19–22]. While interpolating between χ_0 and $\chi_{\rm RPA}$, they all show quantitative differences with respect to our results in the important region around $2q_F$, $q_F = (2\pi n_0)^{1/2}$ being the Fermi wave vector. Similar calculations on the spin response function are in progress.

It will not have escaped the reader that our method of evaluating the static response functions is computationally demanding. In fact to obtain $\chi(q)$, at a given thermodynamic state, requires a few simulations for each wave vector q—thus involving of the order of tens of simulations to construct $\chi(q)$ over the range of relevant wave vectors. Though the use of the fluctuation-dissipation theorem could in principle require less computer time, since the entire response function would be calculated at once, estimation of the systematic errors for the convergence of the time integral is problematical and the formula is not appropriate with fixed-node DMC. In fact the direct method used here has the advantage of giving insight into the structure of both the perturbed wave function and the higher-order response functions. The calculations were performed on a network of IBM RS-6000 workstations.

In summary, we have presented calculations of the static linear response in quantum liquids, based on diffusion Monte Carlo simulations. Our results for bosons, which are exact within the statistical uncertainty and the assumption of the Aziz pair interaction [13], are in perfect agreement with the available experimental data,

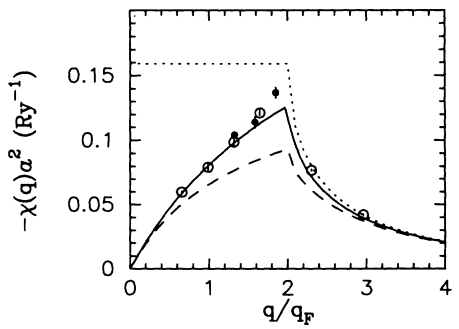

FIG. 3. Linear static response function $\chi(q)$ of the 2D electron fluid at $r_s = 1$. The empty and full circles give fixed-node MC results obtained from simulations with 58 and 90 particles, respectively. Dotted and dashed curves show the response of noninteracting particles and the RPA approximation (see text), while the full curve gives an approximation due to Sato and Ichimaru [19].

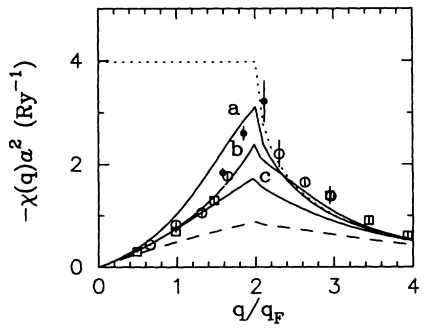

FIG. 4. Linear static response function $\chi(q)$ of the 2D electron fluid at $r_s = 5$. The squares, empty circles, and full circles give fixed-node MC results obtained from simulations with 26, 58, and 90 particles, respectively. Dotted and dashed curves show the response of noninteracting particles and the RPA approximation (see text). The full curves labeled a, b, c give other approximations [20–22].

thus giving further confidence in the interparticle potential. In the absence of experimental results for the static response of 2D electrons, our results for this system, obtained within the accurate fixed-node approximation, provide the best information available to date. In both cases we are confident that our results will stimulate developments in the area of density functional formalism [10] and, more in general, in that of many-body theory.

This work has been supported in part by the MURST and by NSF Grant No. DMR 88-08126 and computational facilities at the NCSA.

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[a] Present address: International School for Advanced Studies (SISSA), Strada Costiera 11, 34014 Trieste, Italy.

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