Zeros of the Frequency-Dependent Linear Density Response

In a recent Letter, Ng and Singwi[1] present a theorem stating that the linear density response,

$$n(r,\omega) = \int d^3r' \chi(r,r';\omega) v(r',\omega),$$

of a many-body system in equilibrium has no zeros under very general thermodynamical conditions. We do not agree with this result.

Mearns and Kohn[2] have examined the linear density response of the ground state of noninteracting particles confined to a one-dimensional ring or a box with zero external potential. At isolated frequencies, the eigenval-

ues of χ, determined by

$$\int d^3r' \chi(r,r';\omega)\zeta_l(r',\omega) = \lambda_l(\omega)\zeta_l(r,\omega),$$

were found to be zero. These are counterexamples to the theorem of Ng and Singwi at zero temperature. At finite temperature, the response function is defined[3] by

$$\chi(r,r';\omega) = \sum_n e^{\beta[\Omega - E_n + \mu N_n]}\chi_n(r,r';\omega),$$

where χ_n is the response function of state n. This is the *conventional*[3] definition, in which dynamical effects of the coupling to the bath are neglected. The eigenvalues of the finite temperature χ for the ring also exhibit zeros at isolated frequencies:

$$\lambda_l(\omega) = \frac{1}{2\pi}\sum_{m=-\infty}^{\infty} f_m \left[\frac{1}{\omega - (l^2 + 2lk_m) + i\eta} - \frac{1}{\omega + (l^2 - 2lk_m) + i\eta} \right]. \tag{1}$$

Here $f_m = \{\exp[\beta(k_m^2 - \mu)] + 1\}^{-1}$ is the Fermi occupation for state m, and $k_m = m + \frac{1}{2}$. We believe this counterexample is typical of *finite-size* systems in thermal equilibrium.

To examine these counterexamples in more detail, we consider a monochromatic perturbation multiplied by a switching function $f(t)$, i.e., $v(r,t) = f(t)e^{-i\bar{\omega}t}\zeta(r)$. We choose $\zeta(r)$ as an eigenfunction of χ whose eigenvalue vanishes at frequency $\bar{\omega}$. With the Fourier transform $\bar{f}$ of f, the *time-dependent* linear density response is then given by

$$n(r,t) = \int_{-\infty}^{\infty} d\omega\, e^{-i\omega t}\bar{f}(\omega - \bar{\omega})\left[\int d^3r' \chi(r,r';\omega)\zeta(r')\right]. \tag{2}$$

If the perturbation is switched on with the adiabatic switching function $f(t) = e^{-\eta|t|}$, the Fourier transform is a Lorentzian, $\bar{f}(\omega - \bar{\omega}) = \eta/\pi[(\omega - \bar{\omega})^2 + \eta^2]$, which reduces to $\delta(\omega - \bar{\omega})$ in the limit $\eta \to 0$. Thus, the adiabatic density response vanishes:

$$n(r,t)_{\text{adiabatic}} = e^{-i\bar{\omega}t}\left[\int d^3r' \chi(r,r';\bar{\omega})\zeta(r')\right] = 0. \tag{3}$$

We emphasize that Eq. (3) applies only to adiabatically switched-on perturbations [i.e., to perturbations whose Fourier transform tends to $\delta(\omega - \bar{\omega})$]. If the perturbation is switched on at a *finite* time t_0 [e.g., with a sudden switching function, $f(t) = \theta(t - t_0)$], then $\bar{f}$ does not reduce to a delta function (or a sum of delta functions), so that vanishing of the square bracket in (2) at *isolated* frequencies does not imply a vanishing density response $n(r,t)$. Moreover, for two potentials $v_1(r,t)$ and $v_2(r,t)$ switched on at *finite* t_0, it has been shown that the corresponding linear density shifts $n_1(r,t)$ and $n_2(r,t)$ are different, provided the potentials differ by more than an r-independent function of time. For potentials expandable in a Taylor series around t_0, this follows directly from Eq. (6) of the work of Runge and Gross.[4] For more general potentials acting on the system for a short time, this follows from the first part of Ref. 1.

The proof given by Ng and Singwi is based on the statement that the energy transfer ΔW satisfies the strict

inequality $\Delta W > 0$ for nonquasistatic ($\omega > 0$) processes. However, this does not imply that $\Delta W > 0$ to *second order* in v. In fact, Eq. (3) implies that, to second order in the perturbation, $\Delta W = 0$ at $\omega = \bar{\omega}$ [cf. Eq. (18) of Ng and Singwi].

Finally, we comment on the argument given by Ng and Singwi for the static limit ($\omega = 0$): The Hohenberg-Kohn theorem[5] guarantees that two ground-state densities, $n(r)$ and $n'(r)$, are different if the associated external potentials, $v(r)$ and $v'(r)$, differ by more than a constant. However, this does not imply a nonvanishing density change $\delta n(r) = n(r) - n'(r)$ to *first order* in $\delta v(r) = v(r) - v'(r)$; the difference between $n(r)$ and $n'(r)$ might show up only in higher perturbative orders. The statement that the *linear* mapping $\delta n = \hat{\chi}\delta v$ has no zeros (at $\omega = 0$) requires a separate proof. Such a proof is given in Ref. 2, where it is demonstrated that the ground-state response function has no vanishing eigenvalues below the first resonant frequency.

E. K. U. Gross, D. Mearns, and L. N. Oliveira
Department of Physics
University of California, Santa Barbara
Santa Barbara, California 93106

[1]T. K. Ng and K. S. Singwi, Phys. Rev. Lett. **59**, 2627 (1987).

[2]D. Mearns and W. Kohn, Phys. Rev. A **35**, 4796 (1987).

[3]A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971), p. 299.

[4]E. Runge and E. K. U. Gross, Phys. Rev. Lett. **52**, 997 (1984).

[5]P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).