Zeros of the Frequency-Dependent Linear Density Response

In a recent Letter, Ng and Singwi\textsuperscript{1} present a theorem stating that the linear density response,

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

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

Mears and Kohn\textsuperscript{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 eigenvalues of $\chi$, determined by

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

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\textsuperscript{3} by

$$\chi(r, r'; \omega) = \sum_n e^{i m E_n + \mu N} \chi_n(r, r'; \omega),$$

where $\chi_n$ is the response function of state $n$. This is the conventional\textsuperscript{1} definition, in which dynamical effects of the coupling to the bath are neglected. The eigenvalues of the finite temperature $\chi$ for the ring also exhibit zeros at isolated frequencies:

$$\lambda_n(\omega) = \frac{1}{2\pi m} \sum_m \int \frac{1}{\omega - (l^2 + 2l m) + i\eta} \frac{1}{\omega + (l^2 - 2l m) + i\eta},$$

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., $v(r, t) = f(t) e^{-i\omega t} \chi(r)$. We choose $\chi(r)$ as an eigenfunction of $\chi$ whose eigenvalues vanish at frequency $\omega$. With the Fourier transform $\tilde{f}$ of $f$, the time-dependent linear density response is then given by

$$n(r, t) = \int \omega d\omega e^{-i\omega t} \tilde{f}(\omega) \int d^3 r' \chi(r, r'; \omega) \tilde{\chi}(r').$$

If the perturbation is switched on with the adiabatic switching function $f(t) = e^{-i\eta t}$, the Fourier transform is a Lorentzian, $\tilde{f}(\omega - \omega_0) = \eta/\pi(\omega - \omega_0)^2 + \eta^2$, which reduces to $\delta(\omega - \omega)$ in the limit $\eta \rightarrow 0$. Thus, the adiabatic density response vanishes:

$$n(r, t)_{\text{adiabatic}} = e^{-i\omega t} \int d^3 r' \chi(r, r'; \omega) \chi(r') = 0.\text{ (3)}$$

We emphasize that Eq. (3) applies only to adiabatically switched-on perturbations [i.e., to perturbations whose Fourier transform tends to $\delta(\omega - \omega_0)$. 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 $\tilde{f}$ 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 $t_0$, $n_2$ is obtained directly from Eq. (6) of the work of Runge and Gross.\textsuperscript{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 $\Delta W$ 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 $\omega$. In fact, Eq. (3) implies that, to second order in the perturbation, $\Delta W = 0$ at $\omega = \omega_0$ [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\textsuperscript{2} 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 $\delta v(r) - v'(r)$; the difference between $n(r)$ and $n'(r)$ might show up only in higher perturbative orders. The statement that the linear mapping $\delta n = \chi \delta v$ 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.

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