Dynamical Properties

1 Treating a Perturbing Potential

For a perturbing potential $A$, the free energy is given by

$$ e^{-\beta F(\lambda)} = \int dR e^{-\beta V_{\lambda} - \beta \lambda A} $$

(1)

$$ F(\lambda) = F(0) + \lambda \langle A \rangle_0 - \frac{\beta \lambda^2}{2} [\langle A^2 \rangle_0 - \langle A \rangle_0^2] + O(\lambda^3) $$

(2)

$$ F(\lambda) = F(0) + \int_0^\lambda d\lambda' \langle A \rangle_{\lambda'}' $$

(3)

If $B$ is a property of the system,

$$ B(\lambda) = B(0) - \beta \lambda [\langle AB \rangle_0 - \langle A \rangle_0 \langle B \rangle_0] + O(\lambda^2) $$

(4)

For example, let $A = \rho_k$ and $B = \rho_{-k}$ (density-density response). Then

$$ \frac{dp_{-k}}{d\lambda} = -\beta |\langle \rho_k \rangle|^2 = -\beta NS_k $$

(5)

2 Diffusion and velocity-velocity correlation.

The diffusion equation is

$$ \frac{\partial \rho}{\partial t} = D \nabla^2 \rho(\mathbf{r}, t) $$

(6)

$D$ can be determined from the mean-square displacement, or, equivalently, the velocity-velocity correlation time.

$$ D = \lim_{t \to \infty} \frac{1}{6t} \langle [\mathbf{r}(t) - \mathbf{r}(0)]^2 \rangle $$

(7)

$$ = \frac{1}{3} \int_0^\infty dt \mathbf{v}(t) \cdot \mathbf{v}(0) $$

(8)

3 Treating a Dynamic Perturbing Potential

For an external field $A e^{-i\omega t}$, denote the response of $B$ as $\chi_{BA}(\omega)e^{-i\omega t}$. The fluctuation-dissipation theorem says

$$ \chi_{BA}(\omega) = \beta \int_0^\infty dt e^{i\omega t} \langle B(t) \frac{d\langle A \rangle}{dt} \rangle $$

(9)

The energy absorption of the system is

$$ \frac{dE}{dt} = \beta \frac{\omega^2}{2} \int_0^\infty dt \cos(\omega t) \langle A(0)A(t) \rangle $$

(10)

The dynamic structure factor (density-density response) is given by

$$ S_k(\omega) = \frac{1}{2\pi} \int_0^\infty dt F_k(t) e^{i\omega t}, \quad \text{where} \quad F_k(t) = \frac{1}{2} \langle \rho_k(t) \rho_{-k}(0) \rangle $$

(11)

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