Tutorial sheet 12

Discussion topic: linear response

24. Linear response function of a system of identical particles

Let $\hat{\mathsf{A}}$, $\hat{\mathsf{B}}$ be two observables of a many-body system, which are sums of single-particle observables:

$$\hat{\mathsf{A}} = \sum_i \hat{\mathsf{a}}^{(i)}, \qquad \hat{\mathsf{B}} = \sum_i \hat{\mathsf{b}}^{(i)},$$

and $\{|\varphi_\alpha\rangle\}$ be a basis of the single-particle Hamiltonian $\hat{\mathsf{h}}$ and ϵ_α the corresponding energy eigenvalues. Matrix elements in this basis are denoted as $a_{\alpha\gamma} \equiv \langle\varphi_\alpha|\,\hat{\mathsf{a}}\,|\varphi_\gamma\rangle$. The Bose–Einstein and Fermi–Dirac distributions are collectively denoted as f, with $f_\alpha \equiv f(\epsilon_\alpha) = [\,\mathrm{e}^{\beta(\epsilon_\alpha-\mu)} \mp 1]^{-1}$, where the upper resp. lower sign is for bosons resp. fermions.

i. Single-particle operators in second quantization
Convince yourself (check your QM II lecture!) that $\hat{\mathsf{A}}$ can be expressed as

$$\hat{\mathsf{A}} = \sum_{\alpha,\gamma} a_{\alpha\gamma}\hat{\mathsf{c}}_\alpha^\dagger\hat{\mathsf{c}}_\gamma,$$

with $\hat{\mathsf{c}}_\alpha^\dagger$ resp. $\hat{\mathsf{c}}_\alpha$ the creation resp. annihilation operator (for particles with energy ϵ_α) in Fock space.

ii. Show that

$$\Big\langle \big[\hat{\mathsf{B}},\hat{\mathsf{A}}\big] \Big\rangle_{\mathrm{eq.}} = \mathrm{tr}\big(f(\hat{\mathsf{h}})\,[\hat{\mathsf{b}},\hat{\mathsf{a}}]\big)$$

where $\langle\cdots\rangle_{\mathrm{eq.}}$ denotes the grand canonical expectation value—which involves a trace $\mathrm{Tr}\,(\cdots)$ in Fock space—while $\mathrm{tr}\,(\cdots)$ stands for the trace in the single-particle Hilbert space.

iii. Deduce from the previous result that the generalized susceptibility for the linear response of $\hat{\mathsf{B}}$ to an excitation coupling to $\hat{\mathsf{A}}$ is given by

$$\tilde{\chi}_{\mathsf{BA}}(\omega) = \lim_{\varepsilon\to 0^+}\sum_{\alpha,\gamma}(f_\alpha - f_\gamma)\frac{b_{\alpha\gamma}a_{\gamma\alpha}}{\epsilon_\gamma - \epsilon_\alpha - \hbar\omega - \mathrm{i}\varepsilon}.$$

Hint: One may use the useful relations $\langle\hat{\mathsf{c}}_\alpha^\dagger\hat{\mathsf{c}}_\gamma\rangle = \delta_{\alpha\gamma}f_\alpha$ and $\langle\hat{\mathsf{c}}_\alpha^\dagger\hat{\mathsf{c}}_\gamma\hat{\mathsf{c}}_\zeta^\dagger\hat{\mathsf{c}}_\eta\rangle = \delta_{\alpha\gamma}\delta_{\zeta\eta}f_\alpha f_\zeta + \delta_{\alpha\eta}\delta_{\gamma\zeta}f_\alpha(1 \pm f_\zeta)$ (check them!).
Alternatively, one may use the (physically less enlightening) identity

$$\big[\hat{\mathsf{A}}\,\hat{\mathsf{B}},\hat{\mathsf{C}}\,\hat{\mathsf{D}}\big] = \hat{\mathsf{A}}\big[\hat{\mathsf{B}},\hat{\mathsf{C}}\big]_\mp\hat{\mathsf{D}} \pm \big[\hat{\mathsf{A}},\hat{\mathsf{C}}\big]_\mp\hat{\mathsf{B}}\,\hat{\mathsf{D}} + \hat{\mathsf{C}}\,\hat{\mathsf{A}}\big[\hat{\mathsf{B}},\hat{\mathsf{D}}\big]_\mp \pm \hat{\mathsf{C}}\big[\hat{\mathsf{A}},\hat{\mathsf{D}}\big]_\mp\hat{\mathsf{B}},$$

where $[\,\cdot\,,\,\cdot\,]_-$ denotes the commutator and $[\,\cdot\,,\,\cdot\,]_+$ the anticommutator.