Scattering from Atoms Bound to Lattice [nln94]

Consider array of atoms harmonically bound to sites of rigid lattice. We set $\hbar = 1$ and atomic mass $M = 1$:

Hamiltonian: $\mathcal{H} = \frac{1}{2}\big(p^2 + \omega_0^2 u^2\big) = \omega_0 \left(a^\dagger a + \frac{1}{2}\right)$.

Displacement of atom from equilibrium position:[1] $u(t) = \frac{1}{\sqrt{2\omega_0}}\big(ae^{-\imath\omega_0 t} + a^\dagger e^{\imath\omega_0 t}\big)$.

Dynamical variable: $A(q,t) = e^{\imath q u(t)}$.

Correlation function: $\tilde{S}_{AA}(q,t) \doteq \langle A^\dagger(q,0)A(q,-t)\rangle$.

Use Baker-Hausdorff expansion:[2] $e^A e^B = \exp\left(A + B + \frac{1}{2}[A,B] + \ldots\right)$.

$$\begin{aligned}\Rightarrow\ \tilde{S}_{AA}(q,t) &= \langle e^{-\imath q u} e^{\imath q u(-t)}\rangle = \langle e^{\imath q[u(-t)-u]}\rangle e^{q^2[u,u(-t)]/2} \\ &= e^{-q^2\langle [u(-t)-u]^2/2\rangle} e^{q^2[uu(-t)-u(-t)u]/2} = e^{-q^2[\langle u^2\rangle - \langle uu(-t)\rangle]}. \end{aligned} \tag{1}$$

Boson distribution: $\langle a^\dagger a\rangle = n_\mathrm{B} = \frac{1}{e^{\beta\omega_0} - 1} \quad \Rightarrow\ \langle aa^\dagger\rangle = 1 + n_\mathrm{B}$.

Debye-Waller factor: $W = \frac{1}{2}q^2\langle u^2\rangle = \frac{q^2}{4\omega_0}\underbrace{\coth\frac{\beta\omega_0}{2}}_{1+2n_\mathrm{B}}, \quad \Rightarrow\ e^{-q^2\langle u^2\rangle} \doteq e^{-2W}$.

$$\begin{aligned}\langle uu(-t)\rangle &= \frac{1}{2\omega_0}\left[\langle a^\dagger a\rangle e^{\imath\omega_0 t} + \langle aa^\dagger\rangle e^{-\imath\omega_0 t}\right] \\ &= \frac{1}{4\omega_0}\mathrm{cosech}\frac{\beta\omega_0}{2}\left[e^{-\imath\omega_0 t + \beta\omega_0/2} + e^{\imath\omega_0 t - \beta\omega_0/2}\right]. \end{aligned} \tag{2}$$

Use[3] $e^{y(s+1/s)/2} = \sum_{n=-\infty}^{+\infty} s^n \mathrm{I}_n(y)$ with $y \doteq \frac{q^2}{2\omega_0}\mathrm{cosech}\frac{\beta\omega_0}{2},\ s \doteq e^{-\imath\omega_0 t + \beta\omega_0/2}$.

$$\tilde{S}_{AA}(q,t) = e^{-2W}\sum_{n=-\infty}^{+\infty} \mathrm{I}_n\left(\frac{q^2}{2\omega_0}\mathrm{cosech}\frac{\beta\omega_0}{2}\right)\exp\left(\frac{1}{2}\beta n\omega_0 - \imath n\omega_0 t\right). \tag{3}$$

$$S_{AA}(q,\omega) = e^{\beta\omega/2 - 2W}\sum_{n=-\infty}^{+\infty} \mathrm{I}_n\left(\frac{q^2}{2\omega_0}\mathrm{cosech}\frac{\beta\omega_0}{2}\right)\delta(\omega - n\omega_0) \tag{4}$$

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[1] We consider component of displacement parallel to $\mathbf{q} \doteq \mathbf{k}_\mathrm{f} - \mathbf{k}_\mathrm{i}$ only.

[2] Use also $\langle e^A\rangle = e^{\langle A^2\rangle/2}$ for linear combinations of boson operators.

[3] $\mathrm{I}_n(y)$ are modified Bessel functions of the first kind. Note that $\mathrm{I}_{-n}(y) = \mathrm{I}_n(y)$.