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Exercise Set 3
(Due date: Tuesday, November. 10, 2009)

Exercise 7 (**Cubic symmetry and electrical conductivity**) (15 points)

All physical observables must be invariant under all elements of the crystal symmetries. Consider the electrical conductivity tensor $\hat{\sigma}(\vec{q})$

$$j_i(\vec{q}) = \sum_j \sigma_{ij}(\vec{q}) E_j(\vec{q})$$

with wave vector $\vec{q}$ (i, j label directions in space, for a cubic lattice $i, j = x, y, z$). The usual conductivity is measured for $\vec{q} = 0$. $\hat{\sigma}(\vec{q})$ has the symmetry of the space group, $\hat{\sigma}(\vec{q} = 0)$ the symmetry of the point group:

$$D^{-1}\hat{\sigma}D = \hat{\sigma}$$

Show that for cubic symmetry, the nine different entries σ_{ij} are given by a single electrical conductivity value σ:

$$\hat{\sigma} = \sigma \mathbb{1} \tag{1}$$

Hint: Use some of the 48 point group symmetry elements, starting with rotations around 2-fold axes that lead to simple matrices D and D^{-1}.

Exercise 8 (**Born-Oppenheimer approximation**) (20 points)

Consider the following Hamiltonian for two coupled one dimensional harmonic oscillators:

$$H = \frac{p^2}{2m} + \frac{P^2}{2M} + \frac{kx^2}{2} + \frac{KX^2}{2} + \lambda x X \tag{2}$$

with $[x, p] = i\hbar$, $[X, P] = i\hbar$ and $M \gg m$.

a) Show that the stationary Schrödinger equation

$$H\psi(x, X) = E\psi(x, X)$$

has the following eigenvalues,

$$E_{n,N} = \hbar\omega_+\left(n + \frac{1}{2}\right) + \hbar\omega_-\left(N + \frac{1}{2}\right),$$

where $n, N = 0, 1, 2, \ldots$ and

$$\omega_\pm^2 = \frac{1}{2}\left(\frac{k}{m} + \frac{K}{M}\right) \pm \sqrt{\frac{1}{4}\left(\frac{k}{m} - \frac{K}{M}\right)^2 + \frac{\lambda^2}{mM}}\,.$$

What happens for $\lambda = 0$?

Hint: Use a coordinate transform $p_1 = \frac{p}{\sqrt{m}}$, $p_2 = \frac{P}{\sqrt{M}}$, $y_1 = \sqrt{m}x$, $y_2 = \sqrt{M}X$ to obtain an equation

$$H = \frac{1}{2}(\vec{p}^2 + \vec{y}^T D \vec{y})$$

in terms of $\vec{p} = \begin{pmatrix} p_1 \\ p_2 \end{pmatrix}$ and $\vec{y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$, then do a coordinate rotation that diagonalizes D to obtain two independent oscillators.

b) Calculate $E_{n,N}$ also in Born-Oppenheimer (or adiabatic) approximation. Write the eigenvalues in adiabatic approximation as

$$E_{n,N}^{\text{adiabatic}} = \hbar\omega_0\left(n + \frac{1}{2}\right) + \hbar\Omega_0\left(N + \frac{1}{2}\right),$$

and compare with the exact solution.