Phys 507A - Solid State Physics I

Assignment 4: Quantum waves: Phonons and photons. *Due Mar. 16th*

1. *Coherent states.*

   A coherent state is defined as the eigenstate of the anihilation operator $\hat{a}$,

   $$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle, \tag{1}$$

   with eigenvalue given by the complex number α (Note, $\hat{a}$ is not Hermitian, so it can have complex eigenvalues).

   (a) Prove that the state

   $$|\alpha\rangle = \mathrm{e}^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle \tag{2}$$

   is a coherent state, i.e., it satisfies Eq. (1).

   (b) Prove that the coherent state [Eq. (2)] is normalized.

   (c) Note that the probability of measuring n phonons (or n photons) in the coherent state is Poisson. What is the mean number of phonons in this state and what is its root-mean-square deviation?

2. *Specific heat due to lattice vibrations.*

   (a) Show that the low temperature specific heat of a crystal is proportional to T^d, where T is the temperature and d is the dimension of the crystal.

   (b) How does the high temperature specific heat scales with temperature?

3. *van Hove singularities.*

   (a) In a linear harmonic chain with only nearest-neighbor interactions, the normal-mode dispersion relation has the form $\omega(k) = \omega_0|\sin(ka/2)|$, where the constant ω_0 is the maximum frequency and a is the distance between the atoms. Show that the density of normal modes in this case is given by

   $$g(\omega) = \frac{2}{\pi a\sqrt{\omega_0^2 - \omega^2}}. \tag{3}$$

   The singularity at $\omega = \omega_0$ is a van Hove singularity. The van Hove singularity in the phonon density of states appears whenever $|\nabla_k \omega| = 0$.

(b) In three dimensions the van Hove singularities are infinities not in the normal mode density itself, but in its derivative. Show that the normal modes in the neighborhood of a maximum of $\omega(\boldsymbol{k})$, for example, lead to a term in the phonon density of states that varies as $(\omega_0 - \omega)^{1/2}$.*Hint: Assume the dispersion for* $\boldsymbol{k}$ *in the neighborhood of* $\boldsymbol{k}_0$ *can be approximated by* $\omega \approx \omega_0 - \alpha(\boldsymbol{k} - \boldsymbol{k}_0)^2$.

The phonon density of states can be measured using neutron scattering. A typical phonon density of states is shown in p. 465 of Ashcroft & Mermin. Note the presence of kinks as a function of ω; each of these kinks are van Hove singularities.

4. *Second quantization.*

When dealing with quantum mechanics of many-particle systems, it is convenient to reformulate the Schröedinger equation in the language of creation and destruction operators, a procedure denoted second quantization.

In the language of first quantization, the Hamiltonian takes the form

$$H = \sum_{i=1}^{N} T(x_i) + \frac{1}{2} \sum_{i \neq j = 1}^{N} V(x_i, x_j), \tag{4}$$

where T is the kinetic energy and V is the potential energy of interaction between two particles. For example, $T(\boldsymbol{x}) = -\frac{\hbar^2}{2m}\nabla^2$, and $V = \frac{e^2}{|\boldsymbol{x}_i - \boldsymbol{x}_j|}$ is the Coulomb interaction between electrons.

Now consider a complete set of single-particle wave functions $\langle \boldsymbol{x} | \phi_k \rangle \equiv \phi_k(\boldsymbol{x})$. These satisfy the completeness relation, $\sum_k |\phi_k\rangle\langle\phi_k| = 1$. For example, consider plane waves, $\phi_k(x) = \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{x}}$.

A complete set of many-particle states may be built by constructing all antisymmetric (for fermions) or symmetric (for bosons) combinations of single-particle states. This procedure is quite cumbersome. A much more convenient way is to seek a completely different quantum mechanical basis that describes the number of particles occuppying each state.

Denote $|n_1\, n_2\, n_3\, \cdots\rangle$ as the state with n_1 particles in state ϕ_1, n_2 particles in state ϕ_2, etc. We can make this basis more concrete by introducing creation operators $a_k^\dagger$ and destruction operators a_k that act on this Hilbert space. For example, if $|0\rangle$ denotes the vacuum (state with no particles), then $a_k^\dagger|0\rangle = |\phi_k\rangle$, and $a_k|\phi_k\rangle = |0\rangle$. We may write

$$|n_1\, n_2\, \cdots\, n_\infty\rangle = (a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}\cdots(a_\infty^\dagger)^{n_\infty}|0\rangle. \tag{5}$$

The key point of second quantization is that this occupation state will be *antisymmetric* under particle interchange if we assume the operators satisfy the following anticommutation rules:

$$\{a_k, a_{k'}^\dagger\} = \delta_{k,k'} \quad ; \quad \{a_k, a_{k'}\} = \{a_k^\dagger, a_{k'}^\dagger\} = 0. \tag{6}$$

Here $\{A, B\} = AB + BA$ is the anticommutator of operators A, B. Similarly, the occupation state will be *symmetric* under particle interchange if we assume the operators satisfy

$$[a_k, a_{k'}^\dagger] = \delta_{k,k'} \quad ; \quad [a_k, a_{k'}] = [a_k^\dagger, a_{k'}^\dagger] = 0, \tag{7}$$

where $[A, B] = AB - BA$ is the usual commutator. For convenience, we write $[A, B]_\pm = AB \pm BA$, keeping in mind that fermions anticommute, and bosons commute.

(a) Define the field operator

$$\hat{\psi}(\boldsymbol{x}) = \sum_k \phi_k(\boldsymbol{x}) a_k \quad ; \quad \hat{\psi}^\dagger(\boldsymbol{x}) = \sum_k \phi_k^*(\boldsymbol{x}) a_k^\dagger. \tag{8}$$

Show that $[\hat{\psi}(\boldsymbol{x}), \hat{\psi}^\dagger(\boldsymbol{x'})]_\pm = \delta(\boldsymbol{x} - \boldsymbol{x'})$, and $[\hat{\psi}(\boldsymbol{x}), \hat{\psi}(\boldsymbol{x'})]_\pm = [\hat{\psi}^\dagger(\boldsymbol{x}), \hat{\psi}^\dagger(\boldsymbol{x'})]_\pm = 0$.

(b) Show that $\hat{\psi}^\dagger|0\rangle = |\boldsymbol{x}\rangle$, i.e., the field operator creates a particle localized at the point $\boldsymbol{x}$ in space. Similarly, $\hat{\psi}(\boldsymbol{x})$ destroys a localized particle at $\boldsymbol{x}$ (in other words, $\hat{\psi}(\boldsymbol{x})$ creates a hole at $\boldsymbol{x}$).

(c) The quantity $\hat{\psi}^\dagger(\boldsymbol{x}) T(\boldsymbol{x}) \hat{\psi}(\boldsymbol{x})$ is interpreted as a kinetic energy density. Similarly, $\hat{\psi}^\dagger(\boldsymbol{x}) \hat{\psi}^\dagger(\boldsymbol{x'}) V(\boldsymbol{x}, \boldsymbol{x'}) \hat{\psi}(\boldsymbol{x'}) \hat{\psi}(\boldsymbol{x})$ is the interaction energy density for a pair of particles at $(\boldsymbol{x}, \boldsymbol{x'})$. Therefore the complete Hamiltonian of the many-particle system may be written as

$$H = \int d^3x \hat{\psi}^\dagger(\boldsymbol{x}) T(\boldsymbol{x}) \hat{\psi}(\boldsymbol{x}) + \int d^3x \int d^3x' \frac{1}{2} \hat{\psi}^\dagger(\boldsymbol{x}) \hat{\psi}^\dagger(\boldsymbol{x'}) V(\boldsymbol{x}, \boldsymbol{x'}) \hat{\psi}(\boldsymbol{x'}) \hat{\psi}(\boldsymbol{x}). \tag{9}$$

Note the ordering of the last two operators. Using this prescription, show that

$$H = \sum_{k,k'} a_k^\dagger \langle k|T|k'\rangle a_{k'} + \frac{1}{2} \sum_{k,k',k'',k'''} a_k^\dagger a_{k'}^\dagger \langle kk'|V|k''k'''\rangle a_{k'''} a_{k''}. \tag{10}$$

This Hamiltonian is a convenient sum over state quantum numbers (Compare to first quantization, where the Hamiltonian is expressed as a sum over the N particle labels).