Physics 581 **Quantum Mechanics II** P. M. Goldbart, 3135 ESB
Handout 16 `webusers.physics.illinois.edu/~goldbart` University of Illinois
13 April 2010 HOMEWORK 11 `goldbart@illinois.edu`

1) Angular momentum operators – optional: Introduce the angular momentum operators $\{L_i\}_{i=1}^{3}$, which satisfy $[L_i, L_j] = i\hbar\epsilon_{ijk}L_k$. Carefully solve the angular momentum eigenproblem by using the operator method described in *Baym*, pp. 155-159.

2) Addition of spin-1/2 angular momenta: Consider the addition of two spin-1/2 angular momenta, $\mathbf{S}^{(1)}$ and $\mathbf{S}^{(2)}$.

a) How many states are there in the product basis?

b) If $\mathbf{J} = \mathbf{S}^{(1)} + \mathbf{S}^{(2)}$, what are the possible eigenvalues of $\mathbf{J} \cdot \mathbf{J}$?

c) By using the recursive algorithm construct all the Clebsch-Gordan coefficients for this problem

d) Consider the general problem of adding together two angular momenta, $\mathbf{J} = \mathbf{L}^{(1)} + \mathbf{L}^{(2)}$, with $\mathbf{L}^{(1)} \cdot \mathbf{L}^{(1)} = \hbar^2 l_1(l_1 + 1)$ and $\mathbf{L}^{(2)} \cdot \mathbf{L}^{(2)} = \hbar^2 l_2(l_2 + 1)$. List the possible eigenvalues of $\mathbf{J} \cdot \mathbf{J}$ that can arise?

e) Consider the addition of *three* spin-1 angular momenta, $\mathbf{L}^{(1)}$, $\mathbf{L}^{(2)}$ and $\mathbf{L}^{(3)}$. How many basis states are there?

f) If $\mathbf{J} = \mathbf{L}^{(1)} + \mathbf{L}^{(2)} + \mathbf{L}^{(3)}$, what eigenvalues can $\mathbf{J} \cdot \mathbf{J}$ have? What are the degeneracies of these eigenvalues?

3) Basis of angular momentum eigenstates:

a) What is the dimension of the basis of angular momentum eigenstates for which $\mathbf{J} \cdot \mathbf{J} = \hbar^2 j(j + 1)$? We shall refer to the space spanned by this basis as $\mathcal{V}_j$.

b) What is the dimension of the space $\mathcal{V}_{j_1} \otimes \mathcal{V}_{j_2}$?

c) What is the dimension of the space ${}^{\oplus}\sum_{l=|j_1-j_2|}^{j_1+j_2} \mathcal{V}_l$?

d) Reconcile these two answers by showing that

$$(2j_1 + 1)(2j_2 + 1) = \sum_{l=|j_1-j_2|}^{j_1+j_2} (2l + 1).$$

4) Rotation operators and Euler angles – optional: Euler angles $\{\phi, \theta, \psi\}$ parametrise an arbitrary rotation. In terms of these angles, the rotation operator R may be written as $R_{\phi,\theta,\psi} = \exp(-i\phi J_z)\exp(-i\theta J_y)\exp(-i\psi J_z)$.

a) Give the angles that describe the inverse to this rotation.

The d-functions are matrix elements of R:

$$d^{(j)}_{m,m'}(\phi,\theta,\psi) = \langle jm|R_{\phi\theta\psi}|jm'\rangle.$$

b) Show that $d^{(j)}_{m,m'}(\phi,\theta,\psi) = \mathrm{e}^{-im\phi}\, d^{(j)}_{m,m'}(\theta)\,\mathrm{e}^{-im'\psi}$, where $d^{(j)}_{m,m'}(\theta)$ corresponds to a rotation about the y-axis only.

c) Show that $d^{(j)}_{m,m'}(\theta)$ is a real matrix.

5) Spherical tensor operators: The set of operators $\{T^{(k)}_q\}$ with $q = -k, \ldots, k$ are the components of a spherical tensor operator.

a) State the transformation law for rotations through a finite angle.

b) Derive the infinitesimal version of part (a) in terms of a commutator.

c) A spinless particle has angular momentum $\mathbf{J} = \mathbf{R}\times\mathbf{P}$, where $\mathbf{R}$ is the position operator and $\mathbf{P}$ is the momentum operator. Show that $\mathbf{P}\cdot\mathbf{P}$ is a rank-zero spherical tensor operator.

d) State the Wigner-Eckart theorem for $\{T^{(k)}_q\}$.

e) Deduce the selection rules for the matrix elements of rank-zero, rank-one, and rank-two spherical tensor operators. In each case, sketch the region of the j-j' plane corresponding to non-vanishing matrix elements.

f) A perturbation is applied to a nondegenerate system the hamiltonian, H_0, of which commutes with $\mathbf{J}\cdot\mathbf{J}$ and J_z. To first order in perturbation theory, discuss which energy eigenvalues are shifted by the perturbation, and which are not, for the cases of rank-zero, rank-one, and rank-two spherical tensor operators. Give a physical situation which provides a perturbation of each of these three types.

g) Consider the operator

$$\Lambda \equiv [J_x,[J_x,T^{(k)}_q]] + [J_y,[J_y,T^{(k)}_q]] + [J_z,[J_z,T^{(k)}_q]],$$

which is built from the angular momentum operator $\mathbf{J}$ and a component $T^{(k)}_q$ of a rank-k irreducible spherical tensor operator. Show that $\Lambda = k(k+1)\,T^{(k)}_q$.

h) $U^{(k)}_q$ and $V^{(k)}_q$ are components of two rank-k irreducible spherical tensor operators. Show that the operator

$$\Gamma \equiv \sum_{q=-k}^{k} (-1)^q\, U^{(k)}_q\, V^{(k)}_{-q}$$

is a scalar operator.

6) Fluctuation dissipation theorem: The purpose of this problem set is to explore the *fluctuation-dissipation theorem*, due to H.B Callen and T.A. Welton and set forth in their 1951 paper: *Irreversibility and Generalized Noise*, Physical Review **83**, 34-40 (1951). This theorem relates:

(i) the efficacy with which a large, dissipative system absorbs energy irreversibly from an external source system that perturbs it in a time-dependent manner, to

(ii) the internal equilibrium fluctuations characteristic of the dissipative system.

The fluctuation dissipation theorem generalizes Nyquist's 1928 result relating the resistance of an electrical conductor to equilibrium fluctuations of the voltage across (or electrical current through) the conductor. In Nyquist's example, the dissipative system is the conductor and the source system is the device that creates an external electric field that drives the current according to the dissipative system's resistance. The interplay between equilibrium fluctuations and the nonequilibrium, entropy-creating process of Ohmic electrical transport is a striking feature that should be noted.

The Callen-Welton exposition is an outstanding example of scientific writing; I especially value the *Conclusion* section, which, in a pair of succinct paragraphs (the second and third), provides the intuitive ideas underlying the theorem. I also value the clear and logically economical presentation of the fluctuation-dissipation theorem given by L.D. Landau and E.M. Lifshitz in *Statistical Physics* I, Sec. 124.

We now address the theorem itself. Consider a large quantum system—our *dissipative* system—that has fundamental collections of coordinates and momenta that we shall respectively denote by q and p. We suppose that this system is governed by a time-independent Hamiltonian $H_0(q,p)$, and that H_0 has a complete set of eigenstates $\{|E_n\rangle\}$ and corresponding eigenvalues $\{E_n\}$, indexed by the quantum number n. The dissipative system can be coupled to a *source* system, which perturbs the dissipative system through a term $H_1(q,p;t) = -F(t)\,D(q,p)$ that augments the Hamiltonian H_0. We shall refer to the time-dependent c-number $F(t)$ as the *force* and the conjugate, dissipative-system-dependent physical observable $D(q,p)$ as the *displacement*, although they need not have these physical interpretations. For convenience, we shall suppose that the quantum mechanical mean value of D vanishes in any eigenstate $\{|E_n\rangle\}$ of H_0.

At time t, the internal energy $\mathcal{E}(t)$ of the dissipative system in any (normalised) quantum state $|\Psi(t)\rangle$ is given by $\langle\Psi(t)|H_0(q,p) + H_1(q,p;t)|\Psi(t)\rangle$.

a) Show that the rate $\frac{d}{dt}\mathcal{E}(t)$ at which the dissipative system absorbs energy from the source system is given exactly by

$$-\langle\Psi(t)|D(q,p)|\Psi(t)\rangle\,\frac{d}{dt}F(t).$$

In the presence of the force F, the quantum statistical mechanical mean value of the displacement $\langle D\rangle$ (defined below) is driven away from zero. We suppose that the force is sufficiently small that, to a good approximation, the response of $\langle D\rangle$ to F is given, phenomenologically, by

$$\langle D\rangle(t) = -\int_0^\infty dt'\, A(t')\, F(t-t'),$$

i.e., the linear response regime holds. Here, $A(\tau)$ is called the response function, and the limits and argument structure of the relationship between $\langle D\rangle$ and F reflect (i) causality (i.e., that future values of the force cannot influence past values of the displacement), and (ii) the time-homogeneity (i.e., time translation invariance) of the unperturbed dissipative system.

b) By taking Fourier transforms, show that $\langle D\rangle(\omega) = -A(\omega)\, F(\omega)$, where the Fourier transform and its inverse are, respectively, defined via

$$\begin{aligned} K(\omega) &= \int_{-\infty}^{\infty} dt\, \mathrm{e}^{-i\omega t} K(t), \\ K(t) &= \int_{-\infty}^{\infty} \hat{d}\omega\, \mathrm{e}^{i\omega t} K(\omega), \end{aligned}$$

in which $\hat{d}\omega := d\omega/2\pi$. [Note that $A(\tau)$ can be taken to vanish for negative argument, and therefore that its Fourier transform is defined by a semi-infinite integral. This consequence of causality is of significance for the analytic structure of $A(\tau)$.]

c) Assume that $F(t)$ is perfectly harmonic, i.e., that $F(t) = F_0 \sin(\Omega t)$. Show that, provided one averages over a period of the applied force, the energy absorbtion rate is given by $\frac{1}{2}\Omega\, A''(\Omega)\, F_0^2$, where $A''(\Omega)$ is the imaginary part of the Fourier transform of the response function.

We now turn to the issue of the intrinsic fluctuations of the dissipative system.

d) Show that in the energy eigenstate $|E_n\rangle$ the *quantal* fluctuation of the displacement, $\langle E_n|(D - \langle E_n|D|E_n\rangle)^2|E_n\rangle$, is given by

$$\sum_m |\langle E_n|D|E_m\rangle|^2.$$

e) Next, introduce the density of states of the dissipative system, $\rho(E) := \sum_m \delta(E - E_m)$, and use it to express the quantal fluctuation of the displacement as

$$\hbar \int_0^\infty d\omega\, \{\rho(E_n + \hbar\omega)\, |\langle E_n|D|E_n + \hbar\omega\rangle|^2 + \rho(E_n - \hbar\omega)\, |\langle E_n|D|E_n - \hbar\omega\rangle|^2\}.$$

Now allow for *thermal* fluctuations by averaging over the states $|E_n\rangle$, weighted by the canonical distribution $f(E)$ [i.e., $f(E) := \mathcal{Z}^{-1}\exp(-E/T)$, normalized by the canonical partition function $\mathcal{Z} := \int dE\, \rho(E)\, \exp(-E/T)$] to obtain the quantum statistical mechanical average $\langle\cdots\rangle$ in the equilibrium state associated with H_0 and temperature T. Note that we have set Boltzmann's constant k_{B} to unity.

f) Hence show that

$$\langle D^2 \rangle = \hbar \int_0^\infty d\omega \, \{1 + \exp(-\hbar\omega/T)\} \int dE \, f(E) \, \rho(E) \, \rho(E + \hbar\omega) \, |\langle E + \hbar\omega|D|E\rangle|^2,$$

where the mean value $\langle \cdots \rangle$ is defined as the thermal equilibrium average $\sum_n f(E_n) \cdots$ of the quantal average $\langle E_n| \cdots |E_n\rangle$.

We now return to the issue of the response function A and, in particular, its imaginary (i.e., dissipative) part A''. To determine this microscopically, we account for the perturbation H_1 using time-dependent perturbation theory.

g) By recalling that the partial transition rate from state n to state m is given by

$$\frac{2\pi}{\hbar} \frac{F_0^2}{4} |\langle E_m|D|E_n\rangle|^2 \{\delta(\hbar\Omega - (E_m - E_n)) + \delta(\hbar\Omega + (E_m - E_n))\},$$

explain why the the rate at which the dissipative system absorbs energy from the source system is given, to leading order in perturbation theory, by

$$\frac{\pi}{2} F_0^2 \, \Omega \sum_m |\langle E_m|D|E_n\rangle|^2 \{\delta(\hbar\Omega - (E_m - E_n)) - \delta(\hbar\Omega + (E_m - E_n))\}.$$

h) Hence, by introducing the density of states, thermally averaging over the initial state n, and using the specific form of the canonical distribution function $f(E)$, show that the energy absorption rate becomes

$$\frac{\pi}{2} F_0^2 \, \Omega \int dE \, \rho(E) \, f(E) \{|\langle E + \hbar\omega|D|E\rangle|^2 \rho(E + \hbar\omega) - |\langle E - \hbar\omega|D|E\rangle|^2 \rho(E - \hbar\omega)\}.$$

i) By comparing the results of parts (c) and (h), show that the dissipative part A'' of the response function A is given by

$$A''(\omega) = \pi\{1 - \exp(-\hbar\omega/T)\} \int dE \, \rho(E) \, \rho(E + \hbar\omega) \, f(E) \, |\langle E + \hbar\omega|D|E\rangle|^2.$$

j) By using the result for the dissipative part of the response function A'' from part (i), together with the result for the equilibrium fluctuation $\langle D^2 \rangle$ from part (f), show that the fluctuation and the response function are precisely correlated via the *fluctuation-dissipation theorem*:

$$\langle D^2 \rangle = \frac{2}{\pi} \int_0^\infty \frac{d\omega}{\omega} \, A''(\omega) \, E(\omega, T) = \frac{\hbar}{\pi} \int_0^\infty d\omega \, A''(\omega) \, \coth(\hbar\omega/2T),$$

where $E(\omega, T)$ is the mean value of internal energy of a harmonic oscillator of natural frequency ω in equilibrium at temperature T. It can readily be shown (but you need not do it now) that this result also holds at the level of individual frequencies: $\langle \frac{1}{2} (D(\omega) \, D(\omega')^\dagger + D(\omega')^\dagger \, D(\omega)) \rangle = 2\pi\hbar \, \delta(\omega - \omega') \, A''(\omega) \, \coth(\hbar\omega/2T)$.

k) Show that when the classical limit holds [i.e., if $A''(\omega)$ is appreciably large only for $\omega \ll T/\hbar$] the the fluctuation-dissipation theorem reduces to

$$\langle D^2 \rangle = \frac{2}{\pi} T \int_0^\infty d\omega \, A''(\omega) \, \frac{1}{\omega}.$$

l) Read and think about the *Conclusion* section of the Callen-Welton paper.