LECTURE 4

§7. POOR MAN'S TRUNCATION: BORN-OPPENHEIMER

Let's now take a first pass at the really crucial question of how one derives an accurate low-energy Hamiltonian or Lagrangian for a complex system, by truncating/integrating out the high-energy degrees of freedom. Note that there is nothing field-theoretical or even quantum-mechanical about this procedure - physicists have been doing it for a very long time, in order to simplify the description of complex systems to those coordinates that interest them. Older and very instructive examples are, eg.,

The Rayleigh description of frictional forces
The Navier-Stokes eqtn. (hydrodynamics).
Gas kinetics (Boltzmann eqtn)
Maxwell's eqtns. (classical Electrodynamics).

It was of course the quantisation of classical EM that gave us the first workable Quantum field theory (QED) and led ultimately to the development of the RNG as a tool for doing this truncation in a more systematic way - note that the development of RNG theory also received an essential stimulus from classical hydrodynamics.

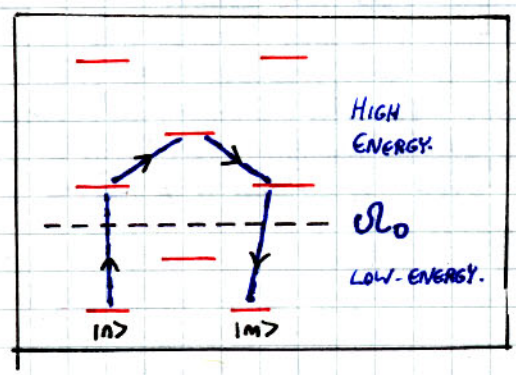
The simplest way to truncate is perturbatively - let's begin with this, and then develop it a little further in the form of the Born-Oppenheimer approximation - which also serves the useful purpose of making a connection to "dynamical" Berry phases.

7(a) TRUNCATION IN 2ND-ORDER PERTURBATION THEORY

This is easy - we simply expand the perturbation in the basis states of the unperturbed Hamiltonian, and then truncate directly. Suppose we have

$$\mathcal{H} = \mathcal{H}_0 + V \qquad (7.1)$$

$$\mathcal{H}_0 = \sum_n |n\rangle \epsilon_n^0 \langle n| \qquad (7.2)$$



with states in a Hilbert space defined up to an energy cut-off E_c. What we want to do is write down a new Hamiltonian, operating only in the restricted Hilbert space with UV cut-off Ω_0. Thus we "truncate out" the high-energy states. In general this is a complicated operation. We begin here by assuming a set of discrete states in both Hilbert spaces. Then, the operation

can be done perturbatively in a straightforward way.

Note first that if $\mathcal{H}$ is diagonal in the basis states chosen (ie., the states $\{|n\rangle\}$ can be treated as non-degenerate eigenstates), then this operation is utterly trivial - the new Hamiltonian has exactly the same form as the old one, the only difference being in their 2 Hilbert spaces.

However the more usual case is one in which we work with an approximate set of eigenstates, between which transitions occur due to a term V in the effective Hamiltonian. What we wish to achieve is the operation

$$\hat{\mathcal{H}}^{\text{eff}}_{E_c} \xrightarrow{\text{2nd-order pert.}} \hat{\mathcal{H}}^{\text{eff}}_{\Omega_0} \qquad \mathcal{H}(E_c) \to \mathcal{H}(\Omega_0) \tag{7.3}$$

where the $\mathcal{H}(\epsilon_0)$ denote Hilbert spaces with a UV cut-off E_0, and $\mathcal{H}^{\text{eff}}_{E_0}$ is the effective Hamiltonian operating in this space. As noted in (7.1), we have

$$\hat{\mathcal{H}}^{\text{eff}}_{E_c} = \sum_{n,m}^{\mathcal{H}(E_c)} |n\rangle \left[\epsilon^0_n \delta_{nm} + V_{nm} \right] \langle m| \tag{7.4}$$

and we perform the truncation to 2nd order in $\hat{V}$. This is a standard problem. Notice first what is happening physically - by reducing the UV cut-off to Ω_0, we are actually excluding processes, mediated by $\hat{V}$, in which the system goes from $|n\rangle$ to $|m\rangle$ via a level $|\ell\rangle$ which lies in the energy range $E_c \geq \epsilon^0_\ell \geq \Omega_0$. From (7.4), dropping these transitions would give the wrong form for $\mathcal{H}$, so we must somehow put their effects back again. In higher-order perturbation theory many such processes contribute (see figure on last page, showing a 4-th order process). From this it is obvious that we must have

$$\hat{\mathcal{H}}^{\text{eff}}_{\Omega_0} = \sum_{n\,m}^{\mathcal{H}(\Omega_0)} |n\rangle \Big\{ \epsilon^0_n \delta_{nm} + V_{nm} \Big] \langle m| + \sum_{\ell}^{\delta\mathcal{H}} V_{n\ell} V_{\ell m} \left(\frac{1}{\epsilon^0_n - \epsilon^0_\ell} + \frac{1}{\epsilon^0_m - \epsilon^0_\ell} \right) \Big\} \langle m| \tag{7.5}$$

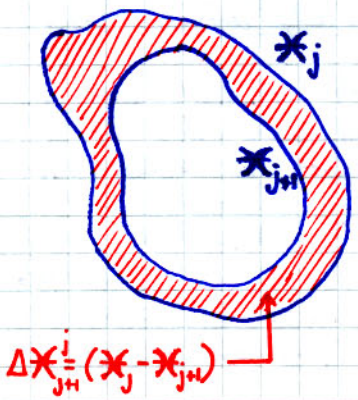
In both (7.4) and (7.5) the restrictions on states $|n\rangle, |m\rangle$ are made explicit in the sums (eg., the sum in (7.4) is over states $|n\rangle, |m\rangle$ in the Hilbert space $\mathcal{H}(E_c)$). The sum over ℓ in (7.5) is in the "difference space" $\delta\mathcal{H} = \mathcal{H}(E_c) - \mathcal{H}(\Omega_0)$. Note also that (7.5) assumes that $|m\rangle$ and $|n\rangle$ are not degenerate - if they are, there is the obvious replacement of the 2nd term by

$$|n\rangle \sum_{\ell}^{\delta\mathcal{H}} |V_{n\ell}|^2 / (\epsilon^0_n - \epsilon^0_\ell) \langle m| \tag{7.6}$$

Forms like (7.5) and (7.6) are trivially derived from the standard results

for matrix elements of an operator in perturbation theory (see, eg., ref. LL3, sections §38, 39).

We can do this more formally and more generally as follows. Imagine that we wish to truncate the range of operation of a Hamiltonian $\hat{H}$ from a Hilbert space $\mathcal{H}_j$ to a more restricted space $\mathcal{H}_{j+1}$, whilst at the same time making sure it is still accurate. We define the effective Hamiltonian $\hat{H}_{\mathcal{H}}$, whose operation is restricted to the Hilbert space $\mathcal{H}$. In general this Hamiltonian is a function of energy E, as we shall see (this is a "retardation effect").



Then it is fairly easy to see that the truncation to 2nd-order is going to have the form

$$\hat{H}_{\mathcal{H}_{j+1}}(E) = \hat{H}_{\mathcal{H}_j}(E) + \Delta\hat{H}_{\mathcal{H}^j_{j+1}} \frac{1}{E - \hat{H}_{\mathcal{H}_j}} \Delta\hat{H}_{\Delta\mathcal{H}^j_{j+1}} \qquad (7.7)$$

which is really a short-hand for

$$\hat{P}_{\mathcal{H}_{j+1}} \hat{H}_{\mathcal{H}_{j+1}} \hat{P}_{\mathcal{H}_{j+1}} = \hat{P}_{\mathcal{H}_{j+1}} \hat{H}_{\mathcal{H}_j}(E) \hat{P}_{\mathcal{H}_{j+1}} + \Delta\hat{H}_{\Delta\mathcal{H}^j_{j+1}} \hat{P}_{\mathcal{H}_{j+1}} \frac{1}{E - \hat{H}_{\mathcal{H}_j}} \hat{P}_{\mathcal{H}_{j+1}} \Delta\hat{H}_{\Delta\mathcal{H}^j_{j+1}} \qquad (7.8)$$

where the $\hat{P}_{\mathcal{H}}$ is a projection operator - if we write $\hat{P}_{\mathcal{H}_j} \hat{O} \hat{P}_{\mathcal{H}_j}$, then the projection operators restrict the action of the operator, on both left and right, to the Hilbert space $\mathcal{H}_j$. As indicated in the diagram, the Hilbert space $\Delta\mathcal{H}^j_{j+1}$ is the difference between $\mathcal{H}_j$ and $\mathcal{H}_{j+1}$; and the "perturbation" is now

$$\Delta\hat{H}_{\Delta\mathcal{H}^j_{j+1}} \equiv \hat{H}_{(\mathcal{H}_j - \mathcal{H}_{j+1})} \qquad (7.9)$$

ie.,
$$\equiv (\hat{P}_{\mathcal{H}_j} - \hat{P}_{\mathcal{H}_{j+1}}) \hat{H}_{\mathcal{H}_j} (\hat{P}_{\mathcal{H}_j} - \hat{P}_{\mathcal{H}_{j+1}}) \qquad (7.10)$$

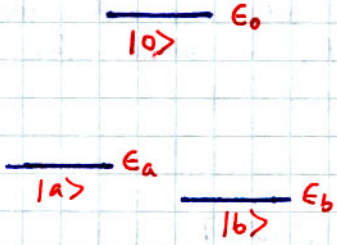
ie., the operator is $\hat{H}_{\mathcal{H}_j}$, but restricted to act only in the small part of Hilbert space between $\mathcal{H}_j$ and $\mathcal{H}_{j+1}$.

All of this can be used as the starting point for the renormalisation group method of truncation, which is one method I will discuss. But we will first cover simpler methods.

EXAMPLE: 3-LEVEL SYSTEM

This is a very simple example - we will truncate out one of the levels to produce a 2-level Hamiltonian,

using 2nd-order perturbation theory. The stucture of the Hamiltonian is, in the unperturbed basis, given as



$$\mathcal{H}^{(3)}_{nm} = \begin{pmatrix} \epsilon_0 & V_{0a} & V_{0b} \\ V_{a0} & \xi & \Delta \\ V_{b0} & \Delta & -\xi \end{pmatrix} \qquad (7.11)$$

where we have < direct matrix element Δ linking states $|a\rangle$ and $|b\rangle$, as well as a bias field ξ acting - this is just the usual TLS we are already familiar with. But one can also make transitions via the high-energy state $|0\rangle$. It is fairly easy to see that to 2nd-order in these transitions, the system truncates to the 2-level form

$$\mathcal{H}^{(2)}_{nm} = \begin{pmatrix} \tilde{\epsilon}_a & \tilde{\Delta} \\ \tilde{\Delta} & \tilde{\epsilon}_b \end{pmatrix} \qquad (7.12)$$

where

$$\left.\begin{aligned} \tilde{\Delta} &= \Delta - V_{a0}V_{0b}\left(\frac{1}{\epsilon_0-\epsilon_b} + \frac{1}{\epsilon_0-\epsilon_a}\right) \\ \tilde{\epsilon}_a &= \epsilon_a - |V_{0a}|^2/(\epsilon_0-\epsilon_a) \\ \tilde{\epsilon}_b &= \epsilon_b - |V_{0b}|^2/(\epsilon_0-\epsilon_b) \end{aligned}\right\} \qquad (7.13)$$

and where

$$\left.\begin{aligned} \epsilon_a &= (\xi^2+\Delta^2)^{1/2} \\ \epsilon_b &= -(\xi^2+\Delta^2)^{1/2} \end{aligned}\right\} \qquad (7.14)$$

I have cheated slightly here, by using as basis states $|a\rangle$ and $|b\rangle$ the eigenstates of the problem in the absence of $|0\rangle$. Notice the effect of the transitions through $|0\rangle$; they push levels $|a\rangle$ and $|b\rangle$ down ("level repulsion") and they renormalise Δ (by adding an extra channel for transitions).

EXAMPLE : SPIN-BOSON MODEL

Now, instead of just one degree of freedom to be truncated, let's do it for a very large number. Suppose we start from a Hamiltonian of type

$$\mathcal{H}_{E_c} = \Delta\hat{\tau}_x + \tfrac{1}{2}\sum_q\left[\theta(E_c-\omega_q)\left(m_q\dot{x}_q^2 + \omega_q^2 x_q^2 + 2C_q'' x_q \hat{\tau}_z\right)\right]. \qquad (7.15)$$

ie., a spin-boson Hamiltonian of type (2.12), but with zero bias ($\xi = 0$) and no transverse couplings ($C_q^\perp = 0$). What happens now if we truncate to a lower UV cut-off? We can

answer s question most easily in the language of eqtns. (7.7) - (7.10); the key is to find the form of $\Delta\hat{H}$ in (7.9). Since we are truncating out energies between E_c and a lower cut-off Ω_0, energies which are both assumed to be high compared to Δ, we are simply truncating out bosons. Thus we see that

$$\Delta\mathcal{H}_{\Delta\omega} = \sum_{q}^{E_c > \omega_k > \Omega_0} \left[\tfrac{1}{2} m_k (\dot{x}_q^2 + \omega_q^2 x_q^2) + C_q x_q \hat{\tau}_z \right] \tag{7.16}$$

$$\equiv \sum_{q}^{E_c > \omega_k > \Omega_0} \left[\omega_q (b_q^+ b_q + \tfrac{1}{2}) + \frac{C_q}{\sqrt{2\omega_q}} (b_q + b_q^+) \hat{\tau}_z \right]$$

$$\equiv \int_{\Omega_0}^{E_c} d\omega_q \left[\omega_q (b_q^+ b_q + \tfrac{1}{2}) + \frac{C_q}{\sqrt{2\omega_q}} (b_q + b_q^+) \tau_z \right] N(\omega_q) \tag{7.17}$$

where we define the bath operators b_q, b_q^+ in terms of the bath coordinate operators via

$$\left.\begin{aligned} \hat{x}_q &= \frac{1}{\sqrt{2 m_q \omega_q}} (b_q + b_q^+) \\ \hat{p}_q &= i \left(\frac{m_q \omega_q}{2} \right)^{1/2} (b_q^+ - b_q) \end{aligned}\right\} \tag{7.18}$$

and define the density of states $N(\omega) = dk/d\omega$. The first term is uninteresting, because we are going to work here at low T, such that $kT \ll \Omega_0$. In this case we can assume that

$$\left.\begin{aligned} n_q &= \langle b_q^+ b_q \rangle \backsim 0. \\ b_q b_{q'}^+ &\backsim \delta_{qq'} \end{aligned}\right\} \quad (kT \ll \Omega_0). \tag{7.19}$$

and one then easily sees that, from (7.7)

$$\hat{\mathcal{H}}_{\Omega_0}(\epsilon) = \hat{\mathcal{H}}_{E_c}(\epsilon) - \int_{\Omega_0}^{E_c} d\omega_q N(\omega_q) \left\{ C_q x_q \hat{\tau}_z \frac{1}{\omega_q + \hat{\mathcal{H}}_0 - \epsilon} C_q x_q \hat{\tau}_z \right\} \tag{7.20}$$

where

$$\hat{\mathcal{H}}_0 = \Delta \hat{\tau}_x + \sum_{q}^{\omega_q < \Omega_0} C_q x_q \hat{\tau}_z \tag{7.21}$$

What we will be interested in here, both from a methodological point of view and for comparison with later results, is the change this causes in the tunneling splitting. Let's see how this works out. We will assume that $\epsilon \ll \Omega_0$, so that we can expand (recall $E_c > \omega_q > \Omega_0$):

$$\frac{1}{\omega_q + \hat{\mathcal{H}}_0 - \epsilon} \backsim \frac{1}{\omega_q} \left[1 + \frac{\epsilon - \hat{\mathcal{H}}_0}{\omega_q} + \cdots \right] \tag{7.22}$$

and then we have an expression for the change in the Hamiltonian

$$\delta\hat{H}_{eff} \equiv \hat{H}_{\Omega_0}(\epsilon) - \hat{H}_{E_c}(\epsilon)$$

$$= -\int_{\Omega_0}^{E_c} d\omega_q\, N(\omega_q)\left\{ c_q^2 x_q^2 \left[\frac{1}{\omega_q} + \frac{\epsilon}{\omega_q^2} + \frac{\Delta}{\omega_q^2}\hat{\tau}_x + \sum_{q}^{\omega_q<\Omega_0} c_q x_q \hat{\tau}_z\right]\right\} \qquad (7.23)$$

We drop the last term, which is irrelevant to the renormalization of Δ. Using $\hat{\tau}_z\hat{\tau}_x\hat{\tau}_z = -\hat{\tau}_x$, we find, using (7.19) to deal with x_q^2, that

$$\delta\hat{H}_{eff} = -\int_{\Omega_0}^{E_c} d\omega_q\, N(\omega_q)\, c_q^2 x_q^2 \left(\frac{1}{\omega_q} + \frac{1}{\omega_q^2}(\epsilon + \Delta\hat{\tau}_x)\right) + \cdots$$

$$\equiv -\int_{\Omega_0}^{E_c} d\omega\, N(\omega)\, \frac{C^2(\omega)}{2m_\omega\omega}\left(\frac{1}{\omega} + \frac{1}{\omega^2}(\epsilon + \Delta\hat{\tau}_x)\right) + \cdots$$

$$\equiv -\int_{\Omega_0}^{E_c} \frac{d\omega}{\pi}\, J_{\parallel}(\omega)\left[\frac{1}{\omega} + \frac{1}{\omega^2}(\epsilon + \Delta\hat{\tau}_x)\right] + \cdots \qquad (7.24)$$

where in the last form we use the definition

$$\left.\begin{aligned} J_{\parallel}(\omega) &= \frac{\pi}{2}\sum_q \frac{(C_q^{\parallel})^2}{m_q\omega_q}\,\delta(\omega-\omega_q) \\ &\equiv \frac{\pi}{2}\,N(\omega)\,\frac{C_{\parallel}^2(\omega)}{m_\omega\omega} \end{aligned}\right\} \qquad (7.25)$$

(this function $J_{\parallel}(\omega)$ is sometimes called the "Caldeira-Leggett" spectral function). From (7.24) we immediately see that Δ has changed; we now have

$$\Delta(\Omega_0) = \Delta(E_c)\left[1 - \int_{\Omega_0}^{E_c} d\omega\, \frac{J_{\parallel}(\omega)}{\pi\omega^2}\right] \qquad (7.29)$$

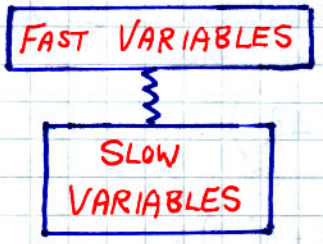
The other terms in (7.24) will not be discussed here. The notation in (7.29) is that Δ is now seen as a function of the upper cut-off in the effective Hamiltonian.

It is crucial to remember that results like (7.12) and (7.29) are PERTURBATIVE - they are only meaningful under the usual conditions of applicability of perturbation theory (viz., that in (7.8), $\Delta\hat{H} \ll (E - \hat{H})$, in obvious notation).

Now physically, this means we are truncating out terms that are coming from very "fast" virtual processes (high-energy) compared to the ones we are interested in. This means we are really making a kind of adiabatic approx., which leads us directly to the Born-Oppenheimer approximation...

7(b) BORN-OPPENHEIMER APPROXIMATION

We consider the following problem. Suppose we have a system whose degrees of freedom can be divided into "slow" and "fast" degrees of freedom. We are only interested in the slow degrees of freedom, and we wish to take account of the effect of the fast coordinates on the dynamics of the slow ones. Formally we can imagine the situation as shown schematically at left; we have a set of high energy degrees of freedom which we wish to truncate out, and our problem is the same as before.



We can also think of the fast variables as an "environment" which is coupled to the slow variables - we are going to "average over", or "integrate out" the effect of the environment.

The Born-Oppenheimer (BO) approximation is usually developed as follows. Let us suppose we can write the Hamiltonian for the combined system as

$$\mathcal{H}_{E_c}(\underline{Q}, \{x_k\}) \equiv \mathcal{H}_{E_c}(\underline{Q}, \underline{x}) = \mathcal{H}_0(\underline{Q}) + \mathcal{H}_1(\underline{x}) + V(\underline{Q}, \underline{x}) \qquad (7.30)$$

where the vector $\underline{Q}$ labels the slow variables, $\underline{x} = \{x_k\}$ the fast variables. It is clear that some UV cut-off (here called E_c) is implicit in this form.

The next step is to introduce a wave-function ansatz for this Hamiltonian, based on the idea that the fast variables adapt their dynamics relatively smoothly to the slowly-varying $\underline{Q}$. Thus one writes

$$\hat{\mathcal{H}}_{E_c} \Psi(\underline{Q}, \underline{x}) = E \Psi(\underline{Q}, \underline{x}) \qquad (7.31)$$

where

$$\Psi(\underline{Q}, \underline{x}) = \sum_m \Phi_m(\underline{Q}) \varphi_m(\underline{Q}, \underline{x}) \qquad (7.32)$$

and the fast variable w.fns. satisfy

$$(\mathcal{H}_1(\underline{x}) + V(\underline{Q}, \underline{x})) \varphi_m(\underline{Q}, \underline{x}) = \epsilon_m(\underline{Q}) \varphi_m(\underline{Q}, \underline{x}) \qquad (7.33)$$

ie., $\underline{Q}$ is just a parameter in Hamiltonian (7.33). All of this you should recognize from our previous discussion of the adiabatic approx. (section 4(a)).

If we now substitute (7.32) into (7.31) we get

$$\sum_m [\mathcal{H}_0(\underline{Q}) + \epsilon_m(\underline{Q})] \Phi_m(\underline{Q}) \varphi_m(\underline{Q}, \underline{x}) = E \sum_m \Phi_m(\underline{Q}) \varphi_m(\underline{Q}, \underline{x}) \qquad (7.34)$$

To go a little further we must specify the form of $\mathcal{H}_0(\underline{Q})$:

$$\hat{\mathcal{H}}_0(\underline{Q}) = \left[\underline{P}^2/2M + U(\underline{Q})\right] \equiv \left[-\hbar^2 \nabla_{\underline{Q}}^2/2M + U(\underline{Q})\right] \qquad (7.35)$$

What we now wish to demonstrate is that if the levels of interest are at energies well below the "fast" energy levels, we can write the following BO effective Hamiltonian, for the low levels:

$$\mathcal{H}^{\text{eff}}_{nm} = \left\{ \frac{-\hbar^2}{2M} \sum_{\ell} \left(\delta_{n\ell}\nabla_Q - iA_{n\ell}(\underline{Q})\right)\left(\delta_{\ell m}\nabla_Q - iA_{\ell m}(\underline{Q})\right) + \delta_{nm}\left(\epsilon_n(Q) + \mathcal{U}(Q)\right)\right\} \tag{7.36}$$

where the non-Abelian gauge potential is

$$A_{nm}(\underline{Q}) = i\langle \varphi_n | \nabla_Q | \varphi_m \rangle \tag{7.37}$$

This effective Hamiltonian satisfies

$$\mathcal{H}^{\text{eff}}_{nm}\, \Phi_m(Q) = E\, \Phi_n(Q) \tag{7.38}$$

and is thus the correct low-energy Hamiltonian for the dynamics of the slow variable Q, under the BO approximation. Actually the form of the BO approximation only includes the diagonal part of $A_{nm}(\underline{Q})$, ie., one has

$$\mathcal{H}^{BO}_n = \frac{-\hbar^2}{2M}\left(\nabla_Q - iA_n(\underline{Q})\right)^2 + \left(\epsilon_n(Q) + \mathcal{U}(Q)\right) \tag{7.39}$$

$$\text{with} \qquad A_n(\underline{Q}) = \delta_{nm} A_{nm}(Q) \equiv A_{nn}(\underline{Q}) \tag{7.40}$$

Now lets go to the derivation of these forms. Formally this is very simple. If we start from the kinetic part of $\mathcal{H}_0(Q)$ in (7.34), we see immediately that we get the appropriate matrix element by computing

$$\langle n | \nabla_Q^2 \Phi_m | m \rangle \equiv \langle \phi_n | \nabla_Q^2 \Phi_m | \phi_m \rangle = \sum_{\ell} \left(\delta_{n\ell}\nabla_Q - iA_{n\ell}(\underline{Q})\right)\left(\delta_{\ell m}\nabla_Q - iA_{\ell m}(Q)\right)\Phi_m \tag{7.41}$$

and the rest follows immediately. The Born-Oppenheimer result then follows by realising that

$$A_{nm}(Q) = i\langle n | \nabla_Q | m \rangle \equiv i\,\frac{\langle n | \nabla_Q \mathcal{H}(Q) | m \rangle}{E_m(Q) - E_n(Q)} \tag{7.42}$$

(cf. eqtn (4.32) and surroundings), where $\mathcal{H}(Q)$ is just the Hamiltonian in the form given in (7.30), viz.,

$$\mathcal{H}(\underline{Q}) \qquad \mathcal{H}_0(\underline{Q}) + \left(\mathcal{H}_1(x) + V(\underline{Q},x)\right). \tag{7.43}$$

The BO approximation then consists in the argument that if the energy level $E_n(\underline{Q})$ of interest are widely separated from higher energy levels, then off-diagonal terms in (7.42) will be negligible. Whether this is true or not is another question - corrections are obviously corrections to an adiabatic approximation, and can be studied in ways analogous to the discussion in section §4(a).

The connection of this approximation to the idea of chopping out high-energy parts of the Hilbert space to produce a renormalized Hamiltonian is not completely clear (at least formally) in what we've done so far. You can't see it completely without a discussion in terms of renormalization group theory, and even there it is rather complex - so I defer it for the moment.

However to give a taste of what is coming, let's go back to the spin-boson example:

EXAMPLE: SPIN-BOSON MODEL

We go back to the diagonal spin-boson model of (7.13), and now ask how to implement a BO approximation. This is a very well-known problem - it is in fact the lattice polaron problem.

According to the BO approximation, the high energy bosons ($\omega_q \gg \Delta$) in the spin-boson system adjust very quickly to the dynamics of the spin - this adjustment is thus to first approximation instantaneous. So let us again look at oscillators in the range $E_c > \omega_q > \Omega_0$, and write a BO ansatz for the low-energy states of the spin coupled to these high-frequency oscillators. In line with (7.32) we write, for the 2 spin states

$$\left.\begin{aligned} \underline{\Psi}_\uparrow(\{\phi_q^0\}) &= |\uparrow\rangle \overset{E_c>\omega_q>\Omega_0}{\prod_q} \phi_q^0(\uparrow) \\ \underline{\Psi}_\downarrow(\{\phi_q^0\}) &= |\downarrow\rangle \prod_q \phi_q^0(\downarrow) \end{aligned}\right\} \tag{7.44}$$

We now ask what is the separation between the 2 lowest energy states, in which the ground state oscillator wave-functions $|\phi_q^0(6)\rangle$ are incorporated also into the wave-function. These oscillator states are

$$\left.\begin{aligned} \phi_q^0(6) &= e^{i6A_q\hat{P}_q}\,\phi_q^0(0) \\ A_q &= C_q''/\hbar m_q \omega_q^2 \end{aligned}\right\} \tag{7.45}$$

where $\phi_q^0(0)$ is the oscillator ground-state wave-function in the absence of any coupling to the central spin, and $\hat{p}_q$ is the operator in (7.18); we define $6 = \pm 1$ for spin $\uparrow, \downarrow$.

We are interested in the splitting between levels $\underline{\Psi}_+$ and $\underline{\Psi}_-$, where

$$\underline{\Psi}_\pm(\{\phi_q^0\}) = \frac{1}{\sqrt{2}}\left[\underline{\Psi}_\uparrow(\{\phi_q^0\}) \pm \underline{\Psi}_\downarrow(\{\phi_q^0\})\right] \tag{7.46}$$

This renormalized splitting $\Delta(\Omega_0)$ is then just given in terms of $\Delta(E_c)$ by

$$\Delta(\Omega_0) = \Delta(E_c) \prod_q^{E_c > \omega_q > \Omega_0} \langle \phi_q^0(\uparrow) | \phi_q^0(\downarrow) \rangle$$

$$= \Delta(E_c) \prod_q^{E_c > \omega_q > \Omega_0} e^{-C_q^2/2m_q\omega_q^3}$$

$$\equiv \Delta(E_c) \exp\left\{ - \int_{\Omega_0}^{E_c} \frac{d\omega}{\pi} \frac{J_{\perp}(\omega)}{\omega^2} \right\} \qquad (7.47)$$

which we compare with (7.29); the perturbative result is just the first term in the expansion of this exponential. We shall understand all this better in a later more detailed look at truncation / renormalization techniques.

REFERENCES for LECTURE 4

** For a paper which is reasonably close in spirit to the present discussion of renormalization in 2nd-order pert. theory, see A.C. Hewson, J. Phys C14, 2747 (1981). An illuminating discussion, in simple terms, of the connection to scaling appears in P. Nozières, J. de Physique 39, 1117 (1978), and in P. Nozières & A. Blandin, J. de Physique 41, 193 (1980); see also P.W. Anderson, J. Phys. C3, 2346 (1970).

** For a good discussion of the Born-Oppenheimer approx., see various articles in Wilc. For the application to the spin-boson problem, see AJ Leggett et al., Rev. Mod. Phys 59, 1 (1987).