Conventions concerning Riccati - Bessel fns:

$$e^{irx} = \sum_{l=0}^{\infty} (2l+1) i^l \frac{j_l(r)}{r} P_l(x)$$

Use this to define j_l. Then as $\int_{-1}^{1} P_l P_{l'} dx = \frac{2}{2l+1} \delta_{ll'}$

$$j_l(r) = \frac{i^{-l}}{2} \int_{-1}^{1} r e^{irx} P_l(x)\, dx$$

$$= \frac{i^{-l}}{2} r \left[\frac{e^{irx}}{ir} P_l \right]_{-1}^{1} + O\left(\frac{1}{r}\right)$$

$$= \frac{i^{-l} e^{ir} - i^l e^{-ir}}{2i} + O\left(\frac{1}{r}\right)$$

so

$$\boxed{j_l(r) = \sin\left(r - l\frac{\pi}{2}\right) + O\left(\frac{1}{r}\right) \qquad \text{as } r \to \infty}$$

Also from leading coefficient $\frac{(2l)!}{2^l (l!)^2}$ of P_l one gets

$$j_l(r) = \frac{r^{l+1}}{(2l+1)!!} \left(1 + O(r^2)\right) \qquad r \to 0$$

Let's use notation for Hankel functions which gives

$$h_l^{+}(r) \sim i^{-l} e^{ir}$$

so that

$$j_l(r) = \frac{h_l^{+} - h_l^{-}}{2i}$$

Let's begin with free wave function of momentum $\underline{p} = p\hat{p}$ with $p = |\underline{p}|$ and expand it is spherical harmonics:

$$\varphi_{\mathbf{p}} = e^{i\mathbf{p}\cdot\mathbf{x}} = \sum_{\ell=0}^{\infty} (2\ell+1) i^\ell \varphi_\ell(r) P_\ell(\hat{p}\cdot\hat{x}) \qquad r = |\mathbf{x}|$$

and

$$\varphi_\ell = \frac{j_\ell(pr)}{pr} \sim \frac{\sin(pr - \ell\pi/2)}{pr}$$

The honest wave function $\psi_{\mathbf{p}}^+$ obtained by solving the Lipmann-Schwinger equation also has an expansion

$$\psi_{\mathbf{p}}^+(\mathbf{x}) = \sum_{\ell=0}^{\infty} (2\ell+1) i^\ell \psi_\ell^+(r) P_\ell(\hat{p}\cdot\hat{x})$$

where ψ_ℓ^+ satisfies the radial equation

$$(*) \qquad \left[\frac{1}{r^2}\frac{d}{dr} r^2 \frac{d}{dr} - \frac{\ell(\ell+1)}{r^2} - V(r) + p^2\right]\psi_\ell^+ = 0$$

and the boundary condition at 0

$$\psi_\ell^+(r) = \text{const}\cdot r^\ell \qquad \text{as } r \to 0$$

and the boundary condition at ∞

$$\psi_\ell^+ - \varphi_\ell \quad \text{contains only outgoing waves.}$$

Suppose for simplicity $V = 0$ for $r > a$. Then in this range any solution of the radial equation $(*)$ has the form

$$\psi_\ell = \text{const.}\,\frac{h_\ell^+(pr)}{r} + \text{const.}\,\frac{h_\ell^-(pr)}{r}$$

so we conclude that

$$\psi_\ell^+(r) = \frac{S_\ell(p)\, h_\ell^+(pr) - h_\ell^-(pr)}{2ipr} \qquad \text{for } r > a$$

Similarly

$$\psi_{k}^-(\mathbf{x}) = \sum_{\ell=0}^{\infty} (2\ell+1) i^\ell \psi_\ell^-(r,k) P_\ell(\hat{k}\cdot\hat{x})$$

where

$$\psi_\ell^-(r,k) = \left(h_\ell^+(kr) - S_\ell(k)^{-1} h_\ell^-(kr)\right)/2ikr \qquad \text{for } r > a$$

Now the scattering matrix expresses ψ_p^+ in terms of ψ_k^- for different k, and by energy conservation only k with $|k| = p$ occur. In general (V not rotationally invariant), one expects a formula of the form

$$\psi_p^+ = \int_{|k|=p} f(\hat{k}, \hat{p})\, \psi_k^-$$

where f is a function on the 2-sphere. In the rotationally invariant case, f should be invariant under rotations and hence it should depend only on the angle between $\hat{k}$ and $\hat{p}$. Thus we can expand it

$$f(\hat{k}, \hat{p}) = \sum{}' f_\ell P_\ell(\hat{p}\cdot\hat{k}).$$

Now what I need to know is how to evaluate the effect of this kernel on the functions $P_\ell(\hat{k}\cdot\hat{x})$. So I need to know

$$\int_{\hat{k}} P_\ell(\hat{p}\cdot\hat{k})\, P_\ell(\hat{k}\cdot x)$$

As this is an invariant function of $\hat{p}, \hat{x}$ it depends only on the angle so

$$\int_{\hat{k}} P_\ell(\hat{p}\cdot\hat{k})\, P_\ell(\hat{k}\cdot\hat{x}) = \sum_{\ell'} a_{\ell'} P_{\ell'}(\hat{p}\cdot\hat{x})$$

but the left side is an eigenfunction for $\Delta_{\hat{p}}$ with eigenvalue $-\ell(\ell+1)$, so the sum on the right is $\text{const.}\, P_\ell(\hat{p}\cdot\hat{x})$

To evaluate the constant take $\hat{x} = \hat{p}$

$$\int_0^{2\pi}\int_0^{\pi} P_\ell(\cos\theta)^2 \underbrace{\sin\theta\, d\theta\, d\varphi}_{\substack{\text{usual vol.}\\ \text{on } S^2}} \cdot \underset{\substack{\uparrow \\ \text{average} \\ \text{over } S^2}}{\frac{1}{4\pi}} = \frac{1}{2}\int_0^{\pi} P_\ell(\cos\theta)^2 \sin\theta\, d\theta$$

$$= \frac{1}{2}\int_{-1}^{1} P_\ell^2\, dx = \frac{1}{2\ell+1}$$

Thus

$$\boxed{\int_{\hat{k}\in S^2} P_\ell(\hat{p}\cdot\hat{k})\, P_{\ell'}(\hat{k}\cdot\hat{x}) = \frac{1}{2\ell+1} P_\ell(\hat{p}\cdot\hat{x})\,\delta_{\ell\ell'}}$$

$\hat{k}\in S^2$ ← total volume normalized to 1

It follows that if we put

$$f(\hat{p},\hat{k}) = \sum_\ell (2\ell+1)\, S_\ell(k)\, P_\ell(\hat{p}\cdot\hat{k})$$

then we have

$$\psi_p^+ = \int_{\hat{k}\in S^2} f(\hat{p},\hat{k})\cdot\psi_k^-$$

Notice that one has on S^2 the expansion

$$\boxed{\sum_{\ell=0}^{\infty}(2\ell+1)\, P_\ell(\hat{p}\cdot\hat{x}) = \delta(\hat{p},\hat{x})}$$

for the δ-function. (To continue further in this direction will lead us into the theory of spherical functions)

Let's return the Lippmann-Schwinger eqn:

$$\psi_p^+(x) = e^{ip\cdot x} + \int\left(-\frac{1}{4\pi}\right)\frac{e^{ik|x-x'|}}{|x-x'|}\, V(x')\,\psi_p^+(x')\, d^3x'$$

$k = |p|$

Assume V has compact support, and use that as $x\to\infty$ we have

$$\frac{e^{ik|x-x'|}}{|x-x'|} = \frac{e^{ikr - ik\hat{x}\cdot x'}}{r}\left(1 + O\left(\tfrac{1}{r}\right)\right)$$

uniformly for x' bounded. This shows

$$\psi_p^+(x) - e^{ip\cdot x} = \frac{e^{ikr}}{r}\left(-\frac{1}{4\pi}\right)\int e^{-ik\hat{x}\cdot x'}\, V(x')\psi_p(x')\, d^3x' + O\left(\tfrac{1}{r^2}\right)$$

Denote the coefficient of $\frac{e^{ikr}}{r}$ by $\tilde{f}(k\hat{x}, p)$, so that we have

1) $\boxed{\psi_p^+ \text{[redacted]} = e^{ip\cdot x} + \frac{e^{ikr}}{r}\tilde{f}(k, p) + O\left(\tfrac{1}{r^2}\right)}$

if $x \to \infty$ with [redacted] direction $\hat{x} = \hat{k}$.

Now in the rotationally symmetric case

$$\psi_p^+(x) = \sum (2l+1)\, i^l\, \frac{S_l(p)\, h_l^+(pr) - h_l^-(pr)}{2i\text{[redacted]}pr} P_l(\hat{p}\cdot\hat{x})$$

$$e^{ip\cdot x} = \sum \quad " \quad " \quad \frac{h_l^+(pr) - h_l^-(pr)}{2ipr} P_l(\hat{p}\cdot\hat{x})$$

so

$$\psi_p^+(x) - e^{ip\cdot x} = \sum_l (2l+1)\frac{S_l(p)-1}{2ip}\underbrace{\frac{i^l h_l^+(pr)}{r}}_{\sim \frac{e^{ipr}}{r}} P_l(\hat{p}\cdot\hat{x})$$

hence

2) $\boxed{\tilde{f}(k, p) = \sum_l (2l+1)\frac{S_l(p)-1}{2ip} P_l(\hat{k}\cdot\hat{p})}$

Terminology: $\tilde{f}(k, p)$, [redacted] which gives the coefficient of the spherical way part of ψ_p^+, is called the <u>full scattering amplitude</u>. 2) gives its partial wave expansion so $\frac{S_l(p)-1}{2ip}$ = l-th partial amplitude. The differential cross-section is given by

$$\frac{d\sigma}{d\Omega} = \left|\tilde{f}(\mathbb{k},\mathbb{p})\right|^2$$

Here $d\Omega$ is a solid angle piece in the direction of $\mathbb{k}$ and $d\sigma$ denotes the part of the incident beam which gets scattered into $d\Omega$.

July 7, 1979

Understand T-matrix.

Let's consider a standard stationary scattering situation:

$$H = H_0 + V$$

where the Møller wave operators intertwining H_0 and the scattering states of H exist. Denote by $\{\varphi_a\}$ a complete set of eigenstates for H_0 with

$$H_0\varphi_a = E_a\varphi_a$$

$$\langle\varphi_b|\varphi_a\rangle = \delta(a-b).$$

We are assuming that for φ square-integrable there is a $\psi = \Omega^+\varphi$ in the scattering subspace for H such that

$$U(t)\Omega^+\varphi \sim U_0(t)\varphi \qquad t \to -\infty$$

i.e.

$$\Omega^+\varphi = \lim_{t\to-\infty} e^{iHt}e^{-iH_0t}\varphi$$

But

$$\frac{d}{dt}\left(e^{iHt}e^{-iH_0t}\right) = e^{iHt}\underbrace{(iH-iH_0)}_{iV}e^{-iH_0t}$$

so $$\varphi - \Omega^+\varphi = i\int_{-\infty}^{0} e^{iHt} V e^{-iH_0 t}\varphi \, dt$$

or $$\Omega^+\varphi = \varphi + \frac{1}{i}\int_{-\infty}^{0} e^{iHt} V e^{-iH_0 t}\varphi \, dt$$

The integral is nicely convergent because $e^{-iH_0 t}$ transports φ outside the support of V, hence we can also write

$$\Omega^+\varphi = \varphi + \lim_{\varepsilon\to 0^+} \frac{1}{i}\int_{-\infty}^{0} e^{\varepsilon t} e^{iHt} V e^{-iH_0 t}\varphi \, dt$$

The reason for doing this is that the integral becomes convergent for the eigenfunctions φ_a and so we have

$$\Omega^+\varphi_a = \varphi_a + \lim_{\varepsilon \downarrow 0} \frac{1}{i} \underbrace{\int_{-\infty}^{0} e^{(\varepsilon - iE_a + iH)t}}_{(\varepsilon - iE_a + iH)^{-1}} V\varphi_a \, dt$$

or

$$\boxed{\Omega^+\varphi_a = \varphi_a + \lim_{\varepsilon\downarrow 0} \underbrace{(E_a + i\varepsilon - H)^{-1}}_{[redacted]\; G^+_{[redacted]}(E_a)} V\varphi_a}$$

[redacted] (The above holds in the sense of distributions, i.e. after integrating against a test function, say $\langle \varphi_a | \varphi \rangle$ with $\varphi \in L^2$.) Note the above formula contains the Green's function for H:

$$G^+(E) = \frac{1}{E - H} \quad \text{continued from UHP,}$$

and it is not the Lipmann-Schwinger equation which one uses to compute $\Omega^+ \varphi_a = \psi_a^+$:

$$\varphi_a = \psi_a^+ - G_0^+(E_a) V \psi_a^+$$

July 9, 1979

$$H = H_0 + \varepsilon V \qquad H_0 \varphi_n = E_n \varphi_n \quad , \quad |\varphi_n| = 1$$

Assume the ground state φ_0 is non-degenerate and construct its change:

$$\psi = \varphi_0 + \varepsilon \psi_1 + \varepsilon^2 \psi_2 + \cdots$$
$$\lambda = E_0 + \varepsilon \lambda_1 + \cdots\cdots$$

$$(H - \lambda)\psi = 0$$

$$(H_0 - E_0)\psi_1 + (\overset{V}{\overset{\shortparallel}{H_1}} - \lambda_1)\varphi_0 = 0. \quad \text{Take } \langle \varphi_0 | \text{ to}$$

get

$$\langle \varphi_0 | V - \lambda_1 | \varphi_0 \rangle = 0 \quad \text{or} \quad \lambda_1 = \langle \varphi_0 | V | \varphi_0 \rangle.$$

Then

$$(E_0 - H_0)\psi_1 = (V - \lambda_1)\varphi_0$$

and so if ψ_1 is required to be $\perp$ to φ_0 we get

$$\psi_1 = (E_0 - H_0)^{-1}(V - \lambda_1)\varphi_0$$

$$= \sum_{n \geq 1} \varphi_n \frac{1}{E_0 - E_n} \langle \varphi_n | V | \varphi_0 \rangle$$

Then from

$$(H_0 - E_0)\psi_2 + (V - \lambda_1)\psi_1 - \lambda_2 \varphi_0 = 0$$

we get

$$\lambda_2 = \langle \varphi_0 | V | \psi_1 \rangle = \sum_{n \geq 1} \frac{\langle \varphi_0 | V | \varphi_n \rangle \langle \varphi_n | V | \varphi_0 \rangle}{E_0 - E_n}$$

Also

$$\psi_2 = (E_0 - H_0)^{-1} P (V - \lambda_1)\psi_1 \qquad P = \sum_{n \geq 1} |\varphi_n \rangle \langle \varphi_n| = \text{proj} \perp \text{to } \varphi_0.$$

$$\psi_2 = (E_0 - H_0)^{-1} P(V\psi_1) - (E_0 - H_0)^{-1}(\lambda_1 \psi_1)$$

$$= \sum_{\substack{n \geq 1 \\ m \geq 1}}' \varphi_n \frac{1}{E_0 - E_n} \langle \varphi_n | V | \varphi_m \rangle \frac{1}{E_0 - E_m} \langle \varphi_m | V | \varphi_0 \rangle$$

$$- \sum_{n \geq 1}' \varphi_n \frac{1}{(E_0 - E_n)^2} \langle \varphi_n | V | \varphi_0 \rangle \langle \varphi_0 | V | \varphi_0 \rangle$$

As

$$(H_0 - \lambda_0)\psi_3 + (V - \lambda_1)\psi_2 + (-\lambda_2)\psi_1 - \lambda_3 \varphi_0 = 0$$

we have

$$\lambda_3 = \langle \varphi_0 | V | \psi_2 \rangle$$

so

$$\lambda_3 = \sum_{\substack{n \geq 1 \\ m \geq 1}} \frac{\langle \varphi_0 | V | \varphi_n \rangle \langle \varphi_n | V | \varphi_m \rangle \langle \varphi_m | V | \varphi_0 \rangle}{(E_0 - E_n)\ (E_0 - E_m)}$$

$$- \sum_{n \geq 1} \frac{\langle \varphi_0 | V | \varphi_n \rangle \langle \varphi_n | V | \varphi_0 \rangle \langle \varphi_0 | V | \varphi_0 \rangle}{(E_0 - E_n)^2}$$

So the formulas get increasingly complicated, and the beautiful point of the Feynman diagrams is that they explain all the higher terms, so it seems.

July 13, 1979

Let's consider phonons again. The simplest case consists of the lattice $\mathbb{Z}$, which we can think of inside $\mathbb{R}$, and where we have longitudinal displacements. Assume only nearest neighbor interactions

Each spring has equilibrium length 1 and spring constant k. Potential energy is

$$\sum_n \frac{k}{2}(u_n - u_{n-1})^2$$

so total energy is

$$H = \frac{1}{2m}\sum_n p_n^2 + \frac{1}{2}k\sum_n (u_n - u_{n-1})^2$$

$$= \underbrace{\frac{1}{2m}\sum_n p_n^2 + k\sum_n u_n^2}_{H_0} \underbrace{- k\sum_n u_n u_{n-1}}_{H_1}$$

Suppose $m = 1$, $k = \frac{\omega_0^2}{2}$, so that ω_0 is the vibration frequency supposing no interaction.

Now following RDMattuck's book, the idea will be to look at the above as a many body problem. The point is that any harm. oscillator, such as H_0, looks like the Fock space belonging to another system. Let's review this. Take a general harmonic oscillator

$$H_0 = \frac{1}{2}p\cdot p + \frac{1}{2}q\cdot \omega^2 q$$

where ω is positive definite. Then there is a ground state represented in the coordinate repn. by

$$|0\rangle = e^{-\frac{1}{2}q\cdot\omega q} / \text{normalization}$$

This is killed by

$$a = ip + \omega q \qquad (\text{really } a_n = ip_n + (\omega q)_n)$$

so these operators span the space of annihilation ops. Their adjoints

$$a^* = -ip + \omega q$$

span the space of creation operators. One knows that if you operate by n-creation ops on $|0\rangle$ you get n-particle states. The whole space of states is the symmetric algebra on the space W of 1-particle states.

When the oscillator describes the vibrations in a crystal lattice, the 1-particle states are called phonons, or rather phonon is the name for the fictitious particle whose states are the lines in $W = a^*|0\rangle$. The terminology comes from the situation where one constructs Fock space, describing many particles, out a 1-particle Hilbert space situation. For example one takes the 1-particle space describing an electron in a Coulomb potential and then Fock space describes n-independent electrons.

Next we need a basis for the 1-phonon states, which should be eigenfunctions for H_0.

Notice that it might not be convenient to describe 1-phonon states in either the coordinate or momentum representations. For example, suppose one has a simple harmonic oscillator: $H = \frac{1}{2}p^2 + \frac{1}{2}u^2$. The ground state is $e^{-\frac{1}{2}u^2}$ up to a constant and the 1-phonon state is $u\,e^{-\frac{1}{2}u^2}$. This suggests that for the lattice the space of 1-particle states contains wave functions of the form

$$f(\cdot\, u_{n-1}, u_n, \ldots\ldots)\, e^{-\frac{1}{2}u\cdot\omega u}$$

where f is linear (homogeneous). Let's see when this is an eigenfunction

$$\left[-\frac{d^2}{du^2} + (\omega u)^2\right] f e^{-\frac{1}{2}u\cdot\omega u} = f\left[-\frac{d^2}{du^2} + (\omega u)^2\right] e^{-\frac{1}{2}u\cdot\omega u}$$

$$-2\frac{df}{du}(-\omega u)\, e^{-\frac{1}{2}u\cdot\omega u}$$

$$= \left\{f\cdot(\operatorname{tr}\omega) + 2\nabla f\cdot\omega u\right\} e^{-\frac{1}{2}u\cdot\omega u} = 2\lambda f\cdot e^{-\frac{1}{2}u\cdot\omega u}$$

So if remove the ground energy $\frac{1}{2}\operatorname{tr}\omega$, then the condition is that

$$\nabla f\cdot\omega u = \lambda f \overset{\text{since } f \text{ is linear}}{=} \lambda\, \nabla f\cdot u$$

Hence ∇f is an eigenvector for ω and λ is the associated eigenvalue. Since ω^2, hence ω, is real these eigenvectors ∇f can be taken to be real, however it is nicer to realize the eigenvectors as plane waves propagating through the lattice. In this way we get a basis for the one-particle states described by a wave vector k. Actually these waves are classical motions, so one should look at the classical equations of motion

$$\ddot{u} = -\omega^2 u .$$

Written out this is

$$\ddot{u}_n = -\sum_{n'} \omega^2(n-n')u_{n'}$$

so if we take $\quad u_n = e^{-i\nu t} e^{ikn} \quad$ (this is a wave with frequency ν and wave number k), then

$$-\nu^2 e^{ikn} = -\sum_{n'} \omega^2(n-n') e^{ikn'}$$

or

$$\nu^2 = \sum \omega^2(n) e^{-ikn}$$

Hence

$$\omega^2(n) = \sum_{n'} \omega(n-n')\,\omega(n')$$

so that $\quad \nu^2 = (\hat{\omega}(k))^2$, and since we are assuming $\omega \geq 0$, we have

$$\nu = \hat{\omega}(k) = \sum \omega(n) e^{-ikn}$$

In this way we get one eigenfunction for each k mod 2π, and both k and $-k$ yield the same frequency ν.

In the linear chain example

$$u \cdot \omega^2 u = \frac{\omega_0^2}{4} \sum (u_n - u_{n-1})^2 = \frac{\omega_0^2}{2}\left(\sum u_n^2 - \sum u_n u_{n-1}\right)$$

we get the equation of motion

$$\ddot{u}_n = -\frac{\omega_0^2}{2}\left(2u_n - u_{n-1} - u_{n+1}\right)$$

$$\ddot{u}_n = \frac{\omega_0^2}{2}\left(u_{n+1} - 2u_n + u_{n-1}\right)$$

and $$\widehat{\omega^2}(k) = -\frac{\omega_0^2}{2}\left(e^{ik} - 2 + e^{-ik}\right) = \omega_0^2\left(1 - \cos k\right)$$

so $\hat{\omega}(k) = \omega_0\sqrt{1-\cos k}$ gives the frequency for <u>the phonon of wave</u> number k.

Summary: A harmonic oscillator has a many particle interpretation: The state space of the oscillator has a canonical interpretation as a boson Fock space over a one-particle space. Suppose that the oscillator comes from vibrations of a lattice. Then the particles are called phonons and a basis for the one-phonon states is given by characters on the lattice. Be more specific:

Suppose the Hamiltonian is

$$H_0 = \frac{1}{2}p\cdot p + \frac{1}{2}q\cdot\omega^2 q$$

$$= \frac{1}{2}\sum p_n^2 + \frac{1}{2}\sum (\omega^2)(n-n')\, q_n q_{n'}$$

where n runs over the lattice and we assume that there is only a 1-dimensional vibration allowed at each lattice site. ω^2 is a positive-definite real matrix with positive square root ω. I've seen that the ground state in the coord. repn. is

$$e^{-\frac{1}{2}q\cdot\omega q}\cdot\text{const.}$$

and that the space of 1-phonon states consists of

$$f e^{-\frac{1}{2} q \cdot \omega q}$$

where $f(q) = \sum_i c_n q_n$ is linear in the q_n. The good basis for the 1-phonon states is given by

$$\left(\sum_n{}' q_n e^{ikn}\right) e^{-\frac{1}{2} q \cdot \omega q}$$

where k ranges over the first Brillouin zone, i.e. representatives for the characters on the lattice.

But this coordinate description is not what one really wants to work with. What one wants is to associate to each k, creation + annihilation operators satisfying the usual commutation relations, so the whole Hilbert space has the natural basis called the occupation number representation.

Put

$$Q_k = \frac{1}{\sqrt{N}} \sum{}' q_n e^{+ikn}$$

$$P_k = \frac{1}{\sqrt{N}} \sum{}' p_n e^{+ikn}$$

where N = number of elements in the lattice (Here we put periodic boundary conditions on a genuine lattice.). Then

$$Q_k^* = Q_{-k} \qquad P_k^* = P_{-k}$$

$$[P_k, Q_{k'}] = \frac{1}{N} \sum_{n,n'} \underbrace{[p_n, q_{n'}]}_{\frac{1}{i}\delta_{nn'}} e^{+(ikn + ik'n')}$$

$$= \frac{1}{iN} \sum_n{}' e^{+i(k+k')n} = \frac{1}{i} \delta_{k+k'}$$

The annihilation operators are spanned by the operators

$$ip_n + (\omega q)_n$$

which commute. So put

$$\tilde{a}_k = \sum \left[ip_n + (\omega q)_n \right] e^{+ikn}$$

$$\tilde{a}_k = i P_k + \omega_k Q_k$$

$$\Big(\sum_n (\omega q)_n e^{-ikn} = \sum_n \Big(\sum_{n'} \omega(n-n') q_{n'} \Big) e^{+ikn}$$

$$= \sum_{n'} \sum_n \omega(\overset{n+n'}{n - n'}) q_{n'} e^{+ik\overset{n+n'}{n}}$$

$$= \Big(\sum' \omega(n) e^{ikn} \Big) \Big(\sum q_{n'} e^{ikn'} \Big)$$

$$= \omega(k) Q_k . \Big)$$

Then

$$\tilde{a}_k^* = -iP_{-k} + \omega_{-k} Q_{-k} .$$

Note that $\omega_k = \omega_{-k}$ because $\omega(n-n')$ is real and symmetric, hence

$$\omega_k = \sum \omega(n) e^{ink} = \sum \omega(-n) e^{ink} = \sum \omega(n) e^{-ink} = \omega_{-k}$$

Then

$$[\tilde{a}_k, \tilde{a}^*_{k'}] = \left[iP_k + \omega_k Q_k, -iP_{-k'} + \omega_{k'} Q_{-k'} \right]$$

$$= \cancel{i}\frac{1}{i} \omega_{k'} \delta_{k-k'} + \omega_k \delta_{k-k'} = 2\omega_k \delta_{k-k'}$$

So we get the desired creation + annihilation ops. by setting

$$a_k = \frac{1}{\sqrt{2\omega_k}} (iP_k + \omega_k Q_k)$$

$$a_k^* = \frac{1}{\sqrt{2\omega_k}} (-iP_{-k} + \omega_k Q_{-k})$$

The Hamiltonian is found to be

$$H = \sum{}' \omega_k a_k^* a_k^{\text{[redacted]}} + \frac{1}{2}\sum_k{}' \omega_k$$

Check: $\omega_k a_k^* a_k^{\text{[redacted]}} = \frac{1}{2}\left(P_{-k}P_k + \omega_k^2 Q_{-k}Q_k - \omega_k\right)$ ← not correct but it becomes correct when added to $\omega_{-k} a^*_{-k} a_{-k}$

and $$\sum_k P_{-k}P_k = \frac{1}{N}\sum_k \Big(\sum_n p_n e^{-ikn}\Big)\Big(\sum_{n'} p_{n'} e^{ikn'}\Big)$$

$$= \sum{}' p_n^2$$

$$\sum_k \omega_k^2 Q_{-k}Q_k = \frac{1}{N}\sum_k \omega_k^2 \Big(\sum_n q_n e^{-ikn}\Big)\Big(\sum_{n'} q_{n'} e^{ikn'}\Big)$$

$$= \sum_{n,n'} \underbrace{\Big(\frac{1}{N}\sum_k \omega_k^2 e^{-ik(n-n')}\Big)}_{=(\omega^2)(n-n')} q_n q_{n'}$$

by Fourier inversion

So now you have reached the point where you have a very nice description of the states of the [redacted] oscillator.

$$\omega_k a_k^* a_k = \frac{1}{2}\left(-iP_{-k} + \omega_k Q_{-k}\right)\left(iP_k + \omega_k Q_k\right)$$

$$= \frac{1}{2}\left[P_{-k}P_k + \omega_k^2 Q_{-k}Q_k - i\,\omega_k\left(P_{-k}Q_k - Q_{-k}P_k\right)\right]$$

July 14, 1979

Yesterday we reviewed how the space of states for a harmonic oscillator could be identified with a Fock space, and hence given an occupation number representation. For a lattice the 1-particle states were identified with classical waves propagating through the lattice.

Now I want to perturb the potential energy term of the oscillator. For example, I want to go from the Einstein oscillator to the honest one.

<u>Question:</u> What is it that you want to compute?

The phonon case is built out of simple harmonic oscillators each of which get perturbed separately, so I ought to be able to see what's going on for a simple harmonic oscillator. So suppose

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}(\omega_0^2 + \varepsilon)q^2$$

where ε is the perturbation. Both H, H_0 work on the same Hilbert spase and p, q do not change. The ground state and one-particle states change because of the interaction. In this situation what is the one-particle Green's function? It is up to an i-factor

$$\langle \psi_G | T q(t)\, q(0) | \psi_G \rangle$$

where ψ_G is the ground state for H and

$$q(t) = e^{iHt} q\, e^{-iHt}$$

In the case of the lattice vibrations one looks at the matrix

$$\langle \psi_G | T\, q_n(t) q_{n'}(0) | \psi_G \rangle .$$

This is a perfectly nice gadget, but my problem seems to be to understand this as the amplitude of a particle created at n' at time 0 being found at n at time t.

Lets consider a simple harmonic oscillator

$$H = \tfrac{1}{2} p^2 + \tfrac{1}{2} \underbrace{(\omega_0^2 + \varepsilon)}_{\omega^2} q^2$$

and try to calculate the Green's function

$$\langle \psi_G | q(t) q(0) | \psi_G \rangle \qquad t \geq 0$$

by a perturbation series. It might be easier to do a finite temperature Green's function

$$\frac{\mathrm{tr}\,(e^{-\beta H}\, e^{\sigma H} q\, e^{-\sigma H} q)}{\mathrm{tr}(e^{-\beta H})}$$

The numerator can be expressed

$$\mathrm{tr}(e^{-\beta H_0}\, \underbrace{e^{\beta H_0} e^{-\beta H} e^{\sigma H} e^{-\sigma H_0}}_{U(\beta,\sigma)}\, \underbrace{e^{\sigma H_0} q\, e^{-\sigma H_0}}_{q(\sigma)}\, \underbrace{e^{\sigma H_0} e^{-\sigma H}}_{U(\sigma,0)}\, q)$$

in the interaction picture

The denominator is $\mathrm{tr}(e^{-\beta H_0}\, U(\beta,0))$.

Hence the Green's function is

$$\frac{\mathrm{tr}\left(e^{-\beta H_0}\, U(\beta,\sigma)\, q(\sigma)\, U(\sigma,0)\, q\right)}{\mathrm{tr}\left(e^{-\beta H_0}\, U(\beta,0)\right)}$$

Let's concentrate on the partition function

$$\mathrm{tr}\left(e^{-\beta H}\right) = \mathrm{tr}\left(e^{-\beta H_0}\, U(\beta,0)\right)$$

whose logarithm gives the free energy, and on

$$\frac{\mathrm{tr}\left(e^{-\beta H}\right)}{\mathrm{tr}\left(e^{-\beta H_0}\right)} = \langle U(\beta,0)\rangle_0$$

whose logarithm gives thes shift in free energy.

$$\begin{aligned}\frac{d}{d\sigma} U(\sigma,0) &= \frac{d}{d\sigma} e^{\sigma H_0} e^{-\sigma H}\\ &= e^{\sigma H_0}(H_0 - H)\, e^{-\sigma H}\\ &= -e^{\sigma H_0}\, V\, e^{-\sigma H}\\ &= -H_I(\sigma)\, U(\sigma,0)\end{aligned}$$

$$U(\sigma,0) = I - \int_0^\sigma H_I(\sigma_1)\, U(\sigma_1,0)\, d\sigma_1$$

Simplify $U(\sigma,0)$ to $U(\sigma)$.
Then iterating yields Dyson's series

$$U(\sigma) = I - \int_0^\sigma H_I(\sigma_1)\, d\sigma_1 + \frac{1}{2!}\int_0^\sigma\!\!\int_0^\sigma d\sigma_1\, d\sigma_2\, T\left(H_I(\sigma_1) H_I(\sigma_2)\right) - \cdots$$

In order to use this one needs to evaluate

$$\langle T\, H_I(\sigma_1) \cdots H_I(\sigma_n)\rangle$$

via Wick's theorem in order to get diagrams.

Perhaps a simpler approach to Feynman diagrams is via Feynman path integrals. Let's review this in the case of one-dimensional motion. The goal is to compute $e^{-\beta H}$ where $H = \frac{1}{2}p^2 + V(q)$. Note that $\langle x|e^{-\beta H}|x'\rangle / Z$, where $Z =$ [redacted] partition function $= tr(e^{-\beta H})$, is the density matrix. One obtains an expression for $e^{-\beta H}$ as a path integral by dividing $[0,\beta]$ up into n parts of length $\varepsilon = \beta/n$, and using matrix multiplication

$$e^{-\beta H} = e^{-\varepsilon H} \cdots\cdots e^{-\varepsilon H} \qquad n \text{ times.}$$

$$\langle x|e^{-\beta H}|x'\rangle = \int \langle x|e^{-\varepsilon H}|q_{n-1}\rangle dq_{n-1}\langle q_{n-1}|e^{-\varepsilon H}|q_{n-2}\rangle \cdots dq_1 \langle q_1|e^{-\varepsilon H}|x'\rangle$$

The point is that $e^{-\varepsilon H} = e^{-\varepsilon \frac{p^2}{2}} e^{-\varepsilon V} = e^{-\varepsilon V} e^{-\varepsilon \frac{p^2}{2}}$ to the first order and so

$$\langle q|e^{-\varepsilon H}|q'\rangle = e^{-\varepsilon V(q)} \int \frac{dp}{2\pi} e^{ipq} e^{-\varepsilon \frac{p^2}{2}} e^{-ipq'}$$

$$= e^{-\varepsilon V(q)} \int \frac{dp}{2\pi} e^{-\frac{\varepsilon}{2}\left(p^2 - 2ip\left(\frac{q-q'}{\varepsilon}\right) - \left(\frac{q-q'}{\varepsilon}\right)^2\right) - \frac{\varepsilon}{2}\left(\frac{q-q'}{\varepsilon}\right)^2}$$

$$= \frac{1}{\sqrt{2\pi\varepsilon}} e^{-\left[\frac{1}{2}\left(\frac{q-q'}{\varepsilon}\right)^2 + V(q)\right]\varepsilon}$$

Thus we have

$$\langle x|e^{-\beta H}|x'\rangle = \iint\limits_{\substack{\text{paths } q \text{ on } [0,\beta] \\ q(0)=x',\ q(\beta)=x}} e^{\int_0^\beta \left[\frac{1}{2}\dot{q}^2 + V(q)\right] dt} \Big/ \text{norm. const}$$

and the partition function is

$$\mathrm{tr}(e^{-\beta H}) = \iint\limits_{q(0)=q(\beta)} e^{-\int_0^\beta \left[\frac{1}{2}\dot{q}^2 + V(q)\right] dt} \Big/ \text{norm. const.}$$

Let's use this to "evaluate" the partition function for the simple harmonic oscillator with $V = \frac{1}{2}\omega^2 q^2$. We shall use Fourier series to describe paths

$$q(t) = \frac{A_0}{2} + \sum_{n=1}^{\infty} A_n \cos\frac{2\pi n}{\beta}t + B_n \sin\frac{2\pi n}{\beta}t$$

$$\frac{1}{2}\omega^2 \int_0^\beta q^2\, dt = \frac{\beta\omega^2}{2}\left[A_0^2 + \sum_1^\infty A_n^2 + B_n^2\right]$$

$$\dot{q} = \sum_{n=1}^{\infty} -\frac{2\pi n}{\beta} A_n \sin\frac{2\pi n t}{\beta} + \frac{2\pi n}{\beta} B_n \cos\frac{2\pi n t}{\beta}$$

$$\int_0^\beta \frac{1}{2}\dot{q}^2\, dt = \frac{1}{2}\beta\left(\frac{2\pi}{\beta}\right)^2 \sum_1^\infty n^2\left(A_n^2 + B_n^2\right)$$

$$\therefore \int_0^\beta \left(\frac{1}{2}\dot{q}^2 + \frac{1}{2}\omega^2 q^2\right) dt =$$

2 $$= \frac{\beta\omega^2}{2} A_0^2 + \sum_1^\infty \left(\frac{\beta\omega^2}{2} + \frac{1}{2}\frac{4\pi^2}{\beta}n^2\right)\left(A_n^2 + B_n^2\right)$$

So it's clear we have a bunch of independent Gaussian integrals. Since

$$\int e^{-\frac{1}{2}kA^2}\, dA = \frac{1}{\sqrt{2\pi A}}$$

the answer to the path integral will be

$$\frac{1}{\sqrt{\frac{\beta^2\omega^2}{4\pi^2}}} \prod_{n=1}^{\infty}\left(1 + \frac{\beta^2\omega^2}{4\pi^2 n^2}\right)^{-1} \cdot \text{const ind. of } \beta, \omega$$

or inverse of $\frac{\beta\omega}{2\pi}\prod_{n=1}^{\infty}\left(1+\frac{\left(\frac{\beta\omega}{2}\right)^2}{\pi^2 n^2}\right)$

which is something like $\sinh\left(\frac{\beta\omega}{2}\right)$, so it checks. (Recall

$$\mathrm{tr}(e^{-\beta H}) = \sum_{n\geq 0} e^{-\beta(n+\frac{1}{2})\omega} = \frac{e^{-\frac{1}{2}\beta\omega}}{1-e^{-\beta\omega}} = \frac{1}{e^{\frac{1}{2}\beta\omega}-e^{-\frac{1}{2}\beta\omega}} = \frac{1}{2\sinh\left(\frac{\beta\omega}{2}\right)}$$

Next let's turn to a perturbation calculation of the partition function.

July 15, 1979

Let's suppose $H = H_0 + V$. The partition function $\mathrm{tr}(e^{-\beta H})$ is the integral over all closed paths $q : [0,\beta] \to \mathbb{R}$ of the amplitude:

$$e^{-\int_0^\beta H\,dt}$$

Better notation $H_0 = \frac{1}{2}p^2 + V(q)$, $H = H_0 + \delta V$. Then the amplitude is

$$e^{-\int_0^\beta \left(\frac{1}{2}\dot{q}^2 + V + \delta V\right)dt}$$

$$= e^{-\int_0^\beta \left[\frac{1}{2}\dot{q}^2 + V(q)\right]dt}\left[\sum_{n\geq 0}\frac{(-1)^n}{n!}\left(\int_0^\beta (\delta V)(q(t))\,dt\right)^n\right]$$

Consider the first order contribution to the path integral. It is the integral over all paths weighted by the unperturbed amplitude $e^{-\int H_0 dt}$ of the function

$$q(t) \longmapsto \int_0^\beta \delta V(q(t))\,dt$$

Think of doing an infinite integral with independent variables $q(t)$ for each t. What we have is an analogue of

$$\int \sum_{i=1}^{N} f(x_i)\, dx^N = \sum_{i=1}^{N} \int f(x_i)\,dx_i \int \frac{dx^N}{dx_i}.$$

So our first order contribution is

$$-\int_0^\beta dt \int dq\, \delta V(q) \iint_{\substack{\text{paths with } q(t)=q \\ \text{still } q(0)=q(\beta)}} e^{-\int H_0 dt}$$

Similarly our 2nd order contribution is

$$\frac{(-1)^2}{2!}\int_0^\beta\int_0^\beta dt_1\, dt_2 \int dq_1\, dq_2\, \delta V(q_1)\delta V(q_2) \iint_{\substack{\text{paths with } q(t_1)=q_1,\, q(t_2)=q_2 \\ \text{still } q(0)=q(\beta).}} e^{-\int H_0 dt}$$

Notice the last integral is symmetric in t_1, t_2. Since we know that for $t_1 > t_2$

$$\langle q_1 | e^{-(t_1-t_2)H_0} | q_2 \rangle = \iint_{\substack{\text{paths on } [t_2, t_1] \text{ with} \\ q(t_2)=q_2,\ q(t_1)=q_1}} e^{-\int H_0 dt}$$

it follows that the 2nd order contribution is

$$\int_0^\beta dt_1 \int_0^{t_1} dt_2\ \mathrm{tr}\left(e^{-(\beta-t_1)H_0}\,\delta V\, e^{-(t_1-t_2)H_0}\,\delta V\, e^{-t_2 H_0}\right)$$

Hence it is clear that the path integral gives back the Dyson series, and nothing new seems to have been gained.

So next let's turn to the oscillator

$$H = \frac{1}{2}p^2 + \frac{1}{2}\underbrace{(\omega_0^2+\varepsilon)}_{\omega^2}q^2$$

In this case $\delta V = \frac{\varepsilon}{2}q^2$ so that the terms in the Dyson series involve Green's functions:

$$\frac{tr\left(e^{-(\beta-t_1)H_0}\, q\, e^{-(t_1-t_2)H_0}\, q \cdots\cdots q\, e^{-t_nH_0}\right)}{tr\left(e^{-\beta H_0}\right)}$$

(here $\beta \geq t_1 \geq t_2 \geq \cdots \geq t_n \geq 0$ and we extend these quantities to other time values by symmetry). To get at these expectation values of time ordered products

$$\langle T q(t_1)\cdots q(t_n)\rangle$$

we use Schwinger's idea that they are generated by, or better have as generating function, the partition function for the Hamiltonian perturbed by a source, which is time-dependent. This requires explanation.

So let us take

$$H_0 = \frac{1}{2}p^2 + \frac{1}{2}\omega_0^2 q^2$$

and the time-dependent Hamiltonian

$$H = H_0 - J(t)q$$

where $J(t)$ is defined on $[0,\beta]$. Instead of e^{-tH} we now deal with $U(t,t')$ solving

$$\frac{d}{dt}U(t,t') = -H(t)U(t,t') \qquad U(t',t') = I$$

and then the "partition function" is

$$\operatorname{tr}\left(U(\beta,0)\right).$$

Let's see how this varies when J is subjected to an infinitesimal variation δJ. One has

$$\delta U(\beta,0) = -\int_0^\beta dt \; U(\beta,t)\underbrace{\delta H(t)}_{-\delta J(t)\,q} U(t,0)$$

so

$$\delta\log(\operatorname{tr}U(\beta,0)) = \frac{\operatorname{tr}(\delta U(\beta,0))}{\operatorname{tr}(U(\beta,0))} = \int_0^\beta dt \; \delta J(t) \underbrace{\frac{\operatorname{tr}\left(U(\beta,t)\,q\,U(t,0)\right)}{\operatorname{tr}(U(\beta,0))}}_{\text{denote this by } \langle q(t)\rangle .}$$

Then

$$\frac{d}{dt}\, U(\beta,t)\,q\,U(t,0) = U(\beta,t)\underbrace{\left(H(t)q - qH(t)\right)}_{[\frac{1}{2}p^2,\,q] = \frac{1}{i}p} U(t,0)$$

$$[H(t), \tfrac{1}{i}p] = \tfrac{1}{i}[\tfrac{1}{2}\omega_0^2 q^2 - J(t)q, p]$$

$$= \tfrac{1}{i}\left(\omega_0^2 q - J(t)\right)[q,p] = \omega_0^2 q - J(t)$$

Thus

$$\frac{d}{dt}\langle q(t)\rangle = \frac{1}{i}\langle p(t)\rangle$$

$$\frac{d^2}{dt^2}\langle q(t)\rangle = \omega_0^2\langle q(t)\rangle - J(t)$$

Notice that

$$\underbrace{\frac{\operatorname{tr}\left(U(\beta,0)\,q\right)}{\operatorname{tr}U(\beta,0)}}_{\langle q(0)\rangle} = \underbrace{\frac{\operatorname{tr}\left(q\,U(\beta,0)\right)}{\operatorname{tr}U(\beta,0)}}_{\langle q(\beta)\rangle}$$

so we have to solve the DE with periodic boundary conditions on the interval $[0,\beta]$. Let's denote the solution by

$$\langle q(t)\rangle = \int_0^\beta G(t,t')\,J(t')\,dt'$$

where G is the periodic Green's function:

$$\left(-\frac{d^2}{dt^2} + \omega_0^2\right) G(t,t') = \delta(t,t')$$

Since

$$\delta(t-t') = \frac{1}{\beta}\sum_{n\in\mathbb{Z}} e^{i\frac{2\pi n}{\beta}(t-t')}$$

one has

$$G(t,t') = \frac{1}{\beta}\sum_{n\in\mathbb{Z}} \frac{e^{i\frac{2\pi n}{\beta}(t-t')}}{\left(\frac{2\pi n}{\beta}\right)^2 + \omega_0^2}$$

Then

$$\delta \log\left(\operatorname{tr} U(\beta,0)\right) = \int_0^\beta dt\, \delta J(t) \int_0^\beta G(t,t')\,J(t')\,dt'$$

so integrating both sides we get

$$\log \frac{\operatorname{tr}(U(\beta,0))}{\operatorname{tr}(U_0(\beta,0))} = \frac{1}{2}\int_0^\beta\!\!\int_0^\beta dt\,dt' \quad J(t)\,G(t,t')\,J(t')$$

Now we want to obtain the expectation values of time-ordered products using the formula

$$\left.\frac{\delta^n}{\delta J(t_1)\cdots\delta J(t_n)}\left(\frac{\operatorname{tr} U(\beta,0)}{\operatorname{tr} U_0(\beta,0)}\right)\right|_{J=0} = \langle T(q(t_1)\cdots q(t_n))\rangle$$

which results from the Dyson expansion

$$\frac{\operatorname{tr} U(\beta,0)}{\operatorname{tr} U_0(\beta,0)} = 1 + \int_0^\beta \frac{\operatorname{tr}\left(U_0(\beta,t)\,J(t)\,q\,U_0(t,0)\right)}{\operatorname{tr}\left(U_0(\beta,0)\right)}\,dt + \cdots\cdots$$

$$\int_0^\beta dt_1 \int_0^{t_1} dt_2 \; \frac{\operatorname{tr}\left(U_0(\beta,t_1)J(t_1)\,q\,U(t_2,t_1)J(t_2)\,q\,U(t_2,0)\right)}{\operatorname{tr}\left(U_0(\beta,0)\right)}$$

$$= 1 + \int_0^\beta dt\, J(t) \langle q(t) \rangle + \int_0^\beta dt_1 \int_0^{t_1} dt_2\, J(t_1) J(t_2) \langle q(t_1) q(t_2) \rangle + \cdots$$

(Note that it is not immediately clear how to make sense out of $\dfrac{\delta^2}{\delta J(t_1)^2}$ although for the present purposes we get by with continuity.)

So we reach the problem of computing

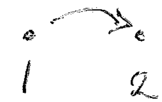
$$\frac{d}{dx_1} \cdots \frac{d}{dx_n}\, e^{Q(x)} \Big|_{x=0} \qquad Q(x) = \tfrac{1}{2} \sum a_{ij} x_i x_j$$

It is

$$e^{Q} \left(\frac{d}{dx_1} + \frac{\partial Q}{\partial x_1} \right) \cdots \left(\frac{d}{dx_n} + \frac{\partial Q}{\partial x_n} \right) 1 \Big|_{x=0}$$

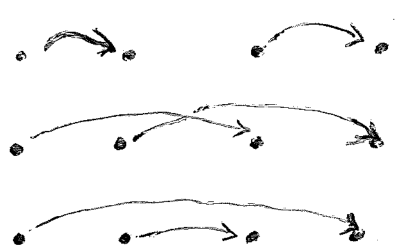
and this is a sum of terms one for each possible way of contracting a $\frac{d}{dx_i}$ against a $\frac{\partial Q}{\partial x_j}$ for $j > i$ $\neq 0$ get an a_{ij}. Such a term is represented by a graph, e.g.

$n = 1$ get 0

$n = 2$ get 

$n = 3$ get 0

$n = 4$. get three possibilities



The idea is that an arrow leaving a point i means you use $\frac{d}{dx_i}$ and entering j means you use $\frac{\partial Q}{\partial x_j}$.

Now when I compute the effect of a change in the potential energy $\frac{1}{2}(\omega_0^2+\varepsilon)q^2$, then I am interested in time-ordered products

$$\langle T(q(t_1)^2\, q(t_2)^2 \cdots q(t_n)^2)\rangle$$

and here your graphs take the familiar form

$n = 1$ 

$n = 2$  ??

It seems we have to be carefuls about multiplicities.

Summary: In general for a perturbation

$$H = H_0 + H_1$$

we would like to compute the change in free energy

$$\Delta \mathcal{F} = -\frac{1}{\beta}\log\left(\frac{tr(e^{-\beta H})}{tr(e^{-\beta H_0})}\right)$$

Now $\dfrac{tr(e^{-\beta H})}{tr(e^{-\beta H_0})} = \langle e^{\beta H_0}e^{-\beta H}\rangle_0$ = thermal average value of $e^{\beta H_0}e^{-\beta H}$

and $e^{\beta H_0}e^{-\beta H}$ has Dyson expansion yielding

$$\frac{tr(e^{-\beta H})}{tr(e^{-\beta H_0})} = 1 - \int_0^\beta dt\,\langle H_1(t)\rangle_0 + \frac{1}{2!}\int_0^\beta dt_1\int_0^\beta dt_2\,\langle T\, H_1(t_1)H_1(t_2)\rangle_0 - \cdots$$

where $H_1(t) = e^{tH_0}H_1e^{-tH_0}$.

In the cases where this gets applied H_0 is the Hamiltonian of an oscillator $H_0 = \frac{1}{2}p^2 + \frac{1}{2}\omega_0^2 q^2$ and H_1 is a polynomial in q, for example

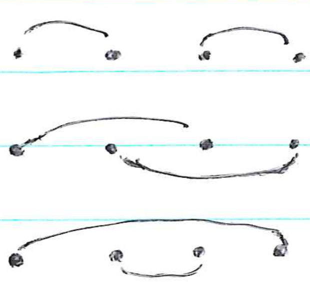
$$H_1 = \frac{1}{2}\varepsilon q^2$$

Then what we need to know is how to compute the [redacted] expectation values

$$\langle T(q(t_1)q(t_2)\cdots q(t_n))\rangle$$

for an oscillator. For this there is a Feynman diagram recipe which goes as follows. [redacted]

First of all the expectation value is zero unless there are an even number of t's, say t_n becomes t_{2n}. Next form a diagram consisting of $2n$ points in a line and lines connecting them in pairs: e.g. for $n=2$ one gets the following diagrams



It seems like we get [redacted] $\frac{2n!}{n!\,2^n} = 1\cdot 3\cdots(2n-1)$ such diagrams. Given a diagram in which t_i is connected to t_j we get the factor $G(t_i, t_j)$. Thus

$$\langle T(q(t_1)\cdots q(t_{2n}))\rangle = \sum_{\substack{\text{diagrams} \\ \text{i.e. } (2,\dots,2) \text{ part.}}} \prod_{\text{edge}} G(\text{edge})$$

The problem is to understand how diagrams label the terms in the perturbation expansion for the ground state energy. What I want to reconcile is the Rayleigh-Schrödinger series

$$\Delta E_0 = \langle \varphi_0 | V | \varphi_0 \rangle + \sum_{n \neq 0} \frac{|\langle \varphi_0 | V | \varphi_n \rangle|^2}{E_0 - E_n} + \cdots$$

which is valid when E_0 is a non-degenerate energy level (not necessarily the ground state), with the diagram version which uses the fact E_0 is the ground state.

$H\varphi_n = E_n \varphi_n, \quad H\psi_n = E_n' \psi_n$

The basic formula is

$$\underset{R(t)}{\;} \langle \varphi_0 | e^{itH_0} e^{-itH} | \varphi_0 \rangle = e^{itE_0} \sum_n \langle \varphi_0 | \psi_n \rangle e^{-itE_n'} \langle \psi_n | \varphi_0 \rangle$$

$$= \sum_n e^{-it(E_0 - E_n')} |\langle \psi_n | \varphi_0 \rangle|^2$$

~~Hence R(t) is the amplitude The quotient~~

$$\cancel{\langle \varphi_0 | e^{-itH} | \varphi_0 \rangle = \frac{\langle \varphi_0 | e^{itH_0} e^{-itH} | \varphi_0 \rangle}{\langle \varphi_0 | e^{-itH_0} | \varphi_0 \rangle} = \sum_n e^{-itE_n'} |\langle \psi_n | \varphi_0 \rangle|^2}$$

~~is the amplitude of finding the system in the ground~~

$R(t)$ is the amplitude for finding the system in the ground state when its starts in the ground state at $t=0$ and the perturbation is turned on for a time t.

Notice that when $E_0' < E_n'$ for $n \geq 1$ and t is pushed in imaginary direction (so that $\mathrm{Re}(it) = \mathrm{Re}(\beta) \to +\infty$, then one has

$$R(t) \sim e^{-it(E_0 - E_0')} |\langle \psi_0 | \varphi_0 \rangle|^2$$

and so we can determine the ground state shift $E_0 - E_0'$. It's clear that what one is doing is the same thing as working with $\langle \varphi_0 | e^{\beta H_0} e^{-\beta H} | \varphi_0 \rangle$ as $\beta \to +\infty$.

So we want to look at

$$\langle \varphi_0 | e^{\beta H_0} e^{-\beta H} | \varphi_0 \rangle = 1 - \int_0^\beta \langle \varphi_0 | e^{\sigma H_0} V e^{-\sigma H_0} | \varphi_0 \rangle \, d\sigma$$

$$+ \int_0^\beta d\sigma_1 \int_0^{\sigma_1} d\sigma_2 \, \langle \varphi_0 | V(\sigma_1) V(\sigma_2) | \varphi_0 \rangle .$$

— . . . .

It might be easier to use

$$\langle \varphi_0 | e^{-\beta H} | \varphi_0 \rangle = \sum_n e^{-\beta E_n'} |\langle \varphi_0 | \psi_n \rangle|^2$$

which is just a matrix element for the density operator. The idea now is that the expansion of $\langle \varphi_0 | e^{-\beta H} | \varphi_0 \rangle$ in diagrams, by the linked cluster theorem, is exp of linked diagrams. This has to be a pure formality.

Now

$$\langle \varphi_0 | V(\sigma) | \varphi_0 \rangle = \langle \varphi_0 | e^{\sigma H_0} V e^{-\sigma H_0} | \varphi_0 \rangle$$

$$= e^{\sigma H_0} \langle \varphi_0 | V | \varphi_0 \rangle e^{-\sigma H_0} \quad = \langle \varphi_0 | V | \varphi_0 \rangle$$

$$= V_{00}$$

where $V_{\ell m} = \langle \varphi_\ell | V | \varphi_m \rangle$. Also

$$\langle \varphi_0 | V(\sigma_1) V(\sigma_2) | \varphi_0 \rangle = \sum_n \langle \varphi_0 | V(\sigma_1) | \varphi_n \rangle \langle \varphi_n | V(\sigma_2) | \varphi_0 \rangle$$

$$= \sum_n e^{\sigma_1(E_0 - E_n)} V_{0n} \, e^{\sigma_2(E_n - E_0)} V_{n0}$$

$$= \sum_n e^{(\sigma_1 - \sigma_2)(E_0 - E_n)} V_{0n} V_{n0}$$

In general

$$V(\sigma) = \sum_{m,n} |m\rangle \langle m | V(\sigma) | n \rangle \langle n|$$

$$= \sum_{m,n} |m\rangle e^{\sigma(E_m - E_n)} V_{mn} \langle n|$$

so the real problem is to compute the terms

$$\int_0^\beta d\sigma_1 \int_0^{\sigma_1} d\sigma_2 \cdots \int_0^{\sigma_{k-1}} d\sigma_k \; e^{\sigma_1(E_{m_0} - E_{m_1})} e^{\sigma_2(E_{m_1} - E_{m_2})} \cdots e^{\sigma_k(E_{m_{k-1}} - E_{m_k})}$$

Let's calculate carefully

$$f_\beta(a_1, a_2, \ldots, a_k) = \int_0^\beta d\sigma_1 \int_0^{\sigma_1} d\sigma_2 \cdots \int_0^{\sigma_{k-1}} d\sigma_k \; e^{a_1\sigma_1 + \cdots + a_k \sigma_k}$$

For $k = 1$

$$f_\beta(a) = \int_0^\beta d\sigma \, e^{a\sigma} = \frac{e^{a\beta} - 1}{a}$$

$k=2$

$$f_\beta(a_1, a_2) = \int_0^\beta d\sigma\, e^{\sigma a_1} f_\sigma(a_2)$$

$$= \int_0^\beta d\sigma \quad e^{\sigma a_1}\left(\frac{e^{a_2\sigma}-1}{a_2}\right)$$

$$= \frac{1}{a_2}\left[\frac{e^{(a_1+a_2)\sigma}}{a_1+a_2} - \frac{e^{\sigma a_1}}{a_1}\right]_0^\beta$$

$$= \frac{e^{(a_1+a_2)\beta}}{(a_1+a_2)a_2} - \frac{e^{a_1\beta}}{a_1 a_2} - \frac{1}{(a_1+a_2)a_2} + \frac{1}{a_1 a_2}$$

$$f_\beta(a_1,a_2,a_3) = \int_0^\beta d\sigma\, e^{a_1\sigma}\left[\frac{e^{(a_2+a_3)\sigma}}{(a_2+a_3)a_3} - \frac{e^{a_2\sigma}}{a_2 a_3} - \frac{1}{(a_2+a_3)a_3} + \frac{1}{a_2 a_3}\right]$$

$$= \frac{e^{(a_1+a_2+a_3)\beta}-1}{(a_1+a_2+a_3)(a_2+a_3)a_3} - \frac{e^{(a_1+a_2)\beta}-1}{(a_1+a_2)a_2a_3} - \frac{e^{a_1\beta}-1}{a_1(a_2+a_3)a_3} + \frac{e^{a_1\beta}-1}{a_2a_3}$$

One sees that $f_\beta(a_1,\ldots,a_k)$ involves 2^k terms

Wait.

$$-\frac{1}{a_1+a_2} + \frac{1}{a_1} = \frac{-a_1+a_1+a_2}{(a_1+a_2)a_1} = \frac{a_2}{(a_1+a_2)a_1}$$

so

$$f_\beta(a_1,a_2) = \frac{e^{(a_1+a_2)\beta}}{(a_1+a_2)a_2} - \frac{e^{a_1\beta}}{a_1a_2} + \frac{1}{(a_1+a_2)a_1}$$

$$f_\beta(a_1,a_2,a_3) = \frac{e^{(a_1+a_2+a_3)\beta}-1}{(a_1+a_2+a_3)(a_2+a_3)a_3} - \frac{e^{(a_1+a_2)\beta}-1}{(a_1+a_2)a_2a_3} + \frac{e^{a_1\beta}-1}{a_1(a_2+a_3)a_2}$$

$$= \frac{e^{(a_1+a_2+a_3)\beta}}{(a_1+a_2+a_3)(a_2+a_3)a_3} - \frac{e^{(a_1+a_2)\beta}}{(a_1+a_2)a_2a_3} + \frac{e^{a_1\beta}}{a_1(a_2+a_3)a_2} + \frac{1}{a_1(a_1+a_2)(a_1+a_2+a_3)}$$

Another idea: Take Laplace transform of

$$(*)\quad \int_0^\beta d\sigma_1 \int_0^{\sigma_1} d\sigma_2 \cdots \int_0^{\sigma_{k-1}} d\sigma_k \; e^{\sigma_1 E_0}\, e^{E_1(-\sigma_1+\sigma_2)}\, e^{E_2(-\sigma_2+\sigma_3)} \cdots e^{E_k(-\sigma_k+0)}$$

with respect to β:

$$\int_0^\infty e^{-s\beta}\, d\beta \int_0^\beta d\sigma_1 \cdots \int_0^{\sigma_{k-1}} d\sigma_k\, e^{\sigma_1 E_0}\, e^{-E_1(\sigma_1-\sigma_2)} \cdots\cdots e^{-E_k(\sigma_k)}$$

$$= \int_0^\infty d\sigma_k \int_{\sigma_k}^\infty d\sigma_{k-1} \cdots \int_{\sigma_1}^\infty d\beta\; e^{-s\beta + \sigma_1 E_0 - E_1(\sigma_1-\sigma_2) - \cdots - E_k(\sigma_k)}$$

so now let $\sigma_k + t_{k-1} = \sigma_{k-1}$ etc.

$$0 \le \underbrace{\sigma_k}_{t_k} \le \underbrace{\sigma_{k-1}}_{t_{k-1}} \le \cdots \le \underbrace{\sigma_1 \le \beta}_{t_0}$$

$$= \int_0^\infty dt_k \int_0^\infty dt_{k-1} \cdots \int_0^\infty dt_0\; e^{-s(t_0+t_1+\cdots+t_k) + (t_1+\cdots+t_k)E_0 - E_1 t_1 - \cdots - E_k t_k}$$

$$= \int_0^\infty e^{-st_k + E_0 t_k - E_k t_k}\, dt_k \cdots\cdots \int_0^\infty dt_1\, e^{-(s-E_0+E_1)t_1} \int_0^\infty dt_0\, e^{-st_0}$$

$$= \frac{1}{s} \prod_{n=1}^{k} \frac{1}{s-E_0+E_n} = \prod_{n=0}^{k} \frac{1}{s-E_0+E_n}$$

Inversion formula then gives for the integral $(*)$

$$\frac{1}{2\pi i}\int_{a-i\infty}^{a+i\infty} \frac{e^{s\beta}}{\prod_{n=0}^{k}(s-E_0+E_n)}$$

which is a sum of $n+1$ terms involving the exponentials $e^{(E_0-E_n)\beta}$

So what's going on seems to be the following: To compute $e^{-\beta H}$ we use the Laplace transform:

$$\int_0^\infty e^{-\beta s} e^{-\beta H}\, d\beta = \frac{1}{s+H}$$

$$e^{-\beta H} = \frac{1}{2\pi i}\int_{a-i\infty}^{a+i\infty} \frac{e^{s\beta}}{s+H}\, ds$$

can take $a=0$ if $H>0$.

and the expansion

$$\frac{1}{s+H} = \frac{1}{s+H_0} - \frac{1}{s+H_0} V \frac{1}{s+H_0} + \cdots\cdots\cdots .$$

This result becomes simpler if one puts in the H_0 eigenvectors:

$$\frac{1}{s+H_0} V \frac{1}{s+H_0} V \cdots V \frac{1}{s+H_0} = |n_0\rangle \frac{1}{s+E_{n_0}} V_{n_0 n_1} \frac{1}{s+E_{n_1}} \cdots V_{n_{k-1} n_k} \frac{1}{s+E_{n_k}} \langle n_k|$$

where the summation convention holds. Thus $e^{-\beta H}$ involves a sum of terms

$$\frac{1}{2\pi i}\int_{-i\infty}^{i\infty} |n_0\rangle\langle n_k| \left(\prod_{i=0}^{k} \frac{1}{s+E_{n_i}}\right) V_{n_0 n_1} V_{n_1 n_2} \cdots V_{n_{k-1} n_k}\; e^{s\beta}\, ds .$$

More precisely to get a matrix element of $e^{-\beta H}$, say $\langle n|e^{-\beta H}|m\rangle$, you fix $n_0 = n$ and $n_k = m$. So the only problem is how to evaluate the terms

$$\frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \frac{e^{s\beta}}{\prod_{i=0}^{k}(s+E_{n_i})}\, ds .$$

This is a simple residue calculation, but the answer depends on the multiplicity of each of E_{n_i}. If the E_{n_i}

are distinct, this integral is

$$\sum_{i=0}^{k} \frac{e^{-E_{n_i}\beta}}{\prod_{j\neq i}(E_{n_j}-E_{n_i})}$$

July 18, 1979

Review: $H = H_0 + V$, $\quad Id = \sum |n\rangle\langle n|$

where $H_0|n\rangle = E_n|n\rangle$. Use Laplace transform

$$\int_0^\infty e^{-s\beta}e^{-\beta H}\,d\beta = \frac{1}{s+H} = \frac{1}{s+H_0} - \frac{1}{s+H_0}V\frac{1}{s+H_0} + \cdots$$

so

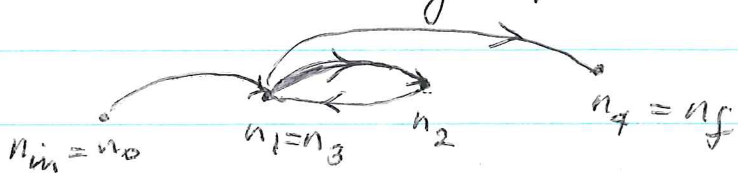
$$e^{-\beta H} = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\left[\frac{1}{s+H_0} - \frac{1}{s+H_0}V\frac{1}{s+H_0} + \cdots\right]e^{\beta s}\,ds$$

$$= e^{-\beta H_0} - \frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\left[\sum_{n_0,n_1}|n_0\rangle\frac{1}{s+E_{n_0}}V_{n_0n_1}\frac{1}{s+E_{n_1}}\langle n_1|\right]e^{\beta s}\,ds + \cdots$$

Hence a matrix element $\langle n_f|e^{-\beta H}|n_{in}\rangle$ is a sum of terms as follows. A k-th order term is given by a sequence $n_{in}=n_0, n_1, n_2, \ldots, n_k=n_f$ and the contribution is

$$(-1)^k V_{n_kn_{k-1}}\cdots\cdots V_{n_2n_1}V_{n_1n_0}\cdot\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}\frac{e^{\beta s}}{\prod_{i=0}^{k}(s+E_{n_i})}\,ds$$

Let's draw a graph having $\{n\}$ for vertices and a directed edge from n_{i-1} to n_i: e.g.



Thus a k-th order graph, has k directed edges and every vertex except n_{in} and n_f have an even number of edges, the same number entering as leaving. n_{in} has an extra edge leaving while n_f has an extra extra entering. It clear that the sign $(-1)^k$ and the V-product can be read off the graph and does not depend on the order one traverses the graph. Notice that such a graph is always connected. The last factor depends only on the vertices of the graph and their multiplicities. Basically it is a sum exponential polys in β with the exponential factor $e^{-\beta E_{n_i}}$ for each vertex n_i and polynomial factor of degree = multiplicity of the vertex minus 1.

Suppose we are interested in the ground state energy E_G and assume that the perturbation is small enough that E_G is very close to E_0 = ground energy for H_0. We let $\beta \to \infty$ and look at leading terms in $\langle 0 | e^{-\beta H} | 0 \rangle$. It's clear that we only have to worry about the residue of $e^{\beta s} / \prod (s + E_{n_i})$ at $s = -E_0$, hence we only have to consider graphs which pass thru 0. Then it might be possible to obtain disconnected graphs by removing the basepoint 0.

$$e^{-\beta H} = e^{-\beta H_0} - \int_0^\beta dt_1\, e^{-(\beta - t_1)H_0} V e^{-t_1 H_0}$$

$$+ \int_0^\beta dt_1 \int_0^{t_1} dt_2\; e^{-(\beta - t_1)H_0} V e^{-(t_1 - t_2)H} V e^{-t_2 H} - \cdots$$

The integrals are convolutions, hence the above is obvious the inverse Laplace transform of

$$\frac{1}{s+H} = \frac{1}{s+H_0} - \frac{1}{s+H_0} V \frac{1}{s+H_0} + \cdots$$

July 19, 1979 (Erica is 1)

Review the problem: I small perturbation $H = H_0 + V$ of Hamiltonian H_0 with a non-degenerate ground state, and I want to compute the ground state energy shift. The answer is given by the Rayleigh-Schroedinger series, however there seems to be a Feynman diagram method explaining the terms of the series, and therefore giving all the terms of the series at once. So far Feynman diagrams seem to be connected to the machinery of Fock space, so it wasn't clear how to handle a general H_0 with a machine based on the oscillator.

The answer is to form the fermion Fock space for independent fermions governed by H and then work in dimension 1. In other words, if H operates on $\mathcal{H}$, then we extend it as a derivation to $\Lambda\mathcal{H}$ and look at what goes on in $\Lambda^1\mathcal{H}$.

Recall that the ground state of H_0 on $\Lambda^N\mathcal{H}$ is $\varphi_0 \wedge \varphi_1 \wedge \cdots \wedge \varphi_{N-1}$ where $H_0\varphi_n = E_n\varphi_n$ are orthonormal eigenfunctions and we arrange them in order of energy: $E_0 \leq E_1 \leq \cdots\cdots$. In other words the Fermi energy is

$$E_F = E_0 + \cdots + E_{N-1}$$

and you see the "Fermi sea".

We use the occupation number repn. for $\Lambda\mathcal{H}$, i.e. the orthonormal basis $\varphi_{i_1} \wedge \cdots \wedge \varphi_{i_N}$, and annihilation and creation operators $a_n = i(\langle\varphi_n|)$, $a_n^* = e(\varphi_n)$. Then the Hamiltonian is

$$H_0 = \sum E_n a_n^* a_n$$

$$V = \sum V_{mn} a_m^* a_n$$

We also need $\quad a_n^*(\sigma) = e^{\sigma H_0} c(\varphi_n) e^{-\sigma H_0} = e^{\sigma E_n} a_n^*$

$$a_n(\sigma) = e^{-\sigma E_n} a_n$$

so

$$V(\sigma) = \sum_{m,n} e^{\sigma(E_m - E_n)} V_{mn} \, a_m^* a_n$$

(Check: $\langle \varphi_m | V(\sigma) | \varphi_n \rangle = \langle \varphi_m | e^{\sigma H_0} V e^{-\sigma H_0} | \varphi_n \rangle = e^{\sigma(E_m - E_n)} V_{mn}$)

Next we compute $\langle 0 | e^{-\beta H} | 0 \rangle$.

$$e^{-\beta H} = e^{-\beta H_0} - \int_0^\beta e^{-(\beta - t)H_0} V e^{-tH_0} dt$$

$$+ \int_0^\beta dt_2 \int_0^{t_2} dt_1 \; e^{-(\beta - t_2)H_0} V e^{-(t_2 - t_1)H_0} V e^{-t_1 H_0} - \cdots$$

so

$$\langle 0 | e^{-\beta H} | 0 \rangle = e^{-\beta E_0} - \int_0^\beta dt \, e^{-(\beta - t)E_0} V_{00} e^{-tE_0}$$

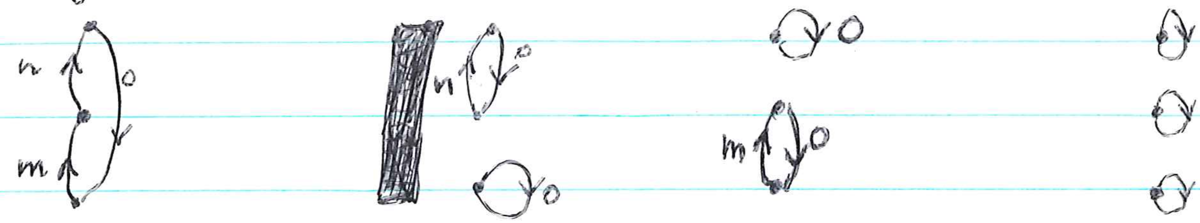
$$+ \sum_n \int_0^\beta dt_2 \int_0^{t_1} dt_1 \, e^{-(\beta - t_2)E_0} V_{0n} e^{-(t_2 - t_1)E_n} V_{n0} e^{-t_2 E_0}$$

$$- \sum_{n,m} \int_0^\beta dt_3 \int_0^{t_3} dt_2 \int_0^{t_2} dt_1 \, e^{-(\beta - t_3)E_0} V_{0n} e^{-(t_3 - t_2)E_n} V_{nm} e^{-(t_2 - t_1)E_m}$$

$$\times V_{m0} e^{-t_1 E_0}.$$

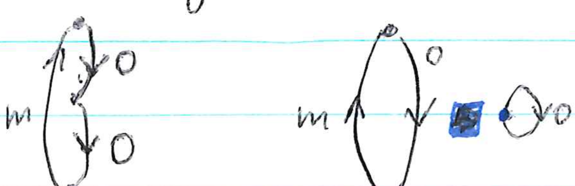
Each of the terms in the above sum can be represented by a diagram as I did yesterday (vertices were energies E_n and edges were V_{mn}), but this approach isn't the good one. Instead we want the edges to [redacted] be labelled by the energies. Thus the third order term corresponding to the path $0 \to m \to n \to 0$ [redacted] belongs to the diagram,

It's clear that in this way we still only get connected graphs, so there is no possibility of a linked cluster theorem. What has to be done still is to require that the 0-state be interpreted as a hole, so its arrow must go backwards in time. This means we have the following third order diagrams.



$m, n \geq 1$ $\quad$ $m = 0,\ n \geq 1$ $\quad$ $m \geq 1,\ n = 0$ $\quad$ $m = n = 0$

Somehow the general theory says you want to include the diagrams



in third order if you want a linked cluster theorem to hold.

So to see what's happening, let's return to the general theory, where one works in the exterior algebra. Let's review what was learned in March.

Look at $H = H_0 + V$ a hermitian operator acting on W, where $V = V(t)$ has compact support. Extend H, H_0 to Fock space ΛW as derivations. Fix p and let $|0\rangle$ be the ground state for H_0 acting on $\Lambda^p W$. Thus if φ_n, $n \geq 1$ is an orth. basis of eigenfns for H_0: $H_0 \varphi_n = E_n \varphi_n$ with $E_1 \leq E_2 \leq \cdots\cdots$, we have $|0\rangle = \varphi_1 \wedge \cdots \wedge \varphi_p$, and we suppose $E_p < E_{p+1}$ so that the ground state is non-degenerate. Then we want to compute

$$\langle 0|S|0\rangle = \frac{\langle 0|U(t_f, t_{in})|0\rangle}{\langle 0|U_0(t_f, t_{in})|0\rangle}$$

where $U(t,t')$ is the time evolution operator for H and $t_f > \mathrm{Supp}\, V > t_{in}$. Following Schwinger we consider an infinitesimal variation δV of V and calculate

$$\delta \log \langle 0|S|0\rangle = \frac{\langle 0|\delta U(t_f, t_{in})|0\rangle}{\langle 0|U(t_f, t_{in})|0\rangle}$$

using Bloch evolution: $\frac{d}{dt} U(t,t') = -HU(t,t')$

$$= -\int_{t_{in}}^{t_f} \frac{\langle 0|U(t_f, t)\,\delta V(t)\, U(t, t_{in})|0\rangle}{\langle 0|U(t_f, t_{in})|0\rangle}\, dt$$

We compute the integrand as follows: We have

$$|0\rangle = \varphi_1 \wedge \cdots \wedge \varphi_p \in \Lambda^p W \quad\Big|\quad \langle 0| = \varphi_1^* \wedge \cdots \wedge \varphi_p^* \in \Lambda^p W^*$$

and
$$\langle 0 | U(t_f, t_{in}) | 0 \rangle = \det \langle \varphi_i | U(t_f, t_{in}) | \varphi_j \rangle$$

is assumed to be $\neq 0$. The elements $\varphi_1^*, \ldots, \varphi_p^*$ span $(W/W^+)^* = (W^+)^\perp$, where $W = \underbrace{\mathrm{span}(\varphi_1, \ldots, \varphi_p)}_{W^-} \oplus \underbrace{\mathrm{span}(\varphi_{p+1}, \ldots)}_{W^+}$. Since the determinant is $\neq 0$, the elements $U(t_f, t_{in})\varphi_j$, $1 \leq j \leq p$, form a basis for the linear functions on $\mathrm{span}(\varphi_1^*, \ldots, \varphi_p^*)$, so we find another basis $\lambda_1, \ldots, \lambda_p$ with $\lambda_i(U(t_f, t_{in})\varphi_j) = \delta_{ij}$. Then it follows that

$$\lambda_1 \wedge \cdots \wedge \lambda_p = \frac{\langle 0 |}{\langle 0 | U(t_f, t_{in}) | 0 \rangle} .$$

But $\delta V(t)$ is a derivation on the exterior algebra, so

$$\delta V(t)\, U(t, t_{in})\, \varphi_1 \wedge \cdots \wedge \varphi_p = \sum_{j=1}^{p} (-1)^{j+1} \varphi_1^t \cdots \varphi_{j-1}^t \;\delta V(t) \varphi_j^t \;\varphi_{j+1}^t \cdots \varphi_p^t$$

where $\varphi_j^t = U(t, t_{in})\varphi_j$. So now taking the inner product with $\lambda_1^t \wedge \cdots \wedge \lambda_p^t$, where $\lambda_j^t = \lambda_j U(t_f, t)$ and using $\lambda_i^t \varphi_j^t = \delta_{ij}$, we find the integrand is

$$\sum_{j=1}^{p} \lambda_j^t \, \delta V(t) \varphi_j^t = \mathrm{tr}\Big(\delta V(t) \underbrace{\sum_{j=1}^{p} \varphi_j^t \otimes \lambda_j^t}_{P^-(t)} \Big)$$

where $P^-(t)$ is the projection onto $U(t, t_{in}) W^-$ with kernel $U(t, t_f) W^+$.

So our formula is

$$\delta \log \langle 0|S|0\rangle = -\int_{-\infty}^{\infty} \operatorname{tr}\left(\delta V(t)\, P^-(t)\right) dt$$

On the other the Green's function for H on W with the boundary conditions $\frac{d}{dt} + H$

$$\begin{aligned} \operatorname{Im} G(t,t') &\subset W^+ \qquad & t = t_f \\ &\subset W^- \qquad & t = t_{in} \end{aligned}$$

is given by

$$G(t,t') = \begin{cases} u(t,t')P^+(t') & t > t' \\ -u(t,t')P^-(t') & t < t' \end{cases}$$

where $P^\pm(t)$ again are the projections relative to

$$W = \underbrace{u(t,t_{in})W^-}_{P^-} \oplus \underbrace{u(t,t_f)W^+}_{P^+}$$

So we can also write

$$\delta \log \langle 0|S|0\rangle = \int_{-\infty}^{\infty} \operatorname{tr}\left(\delta V(t)\, G(t^-,t)\right) dt$$

This last formula suggests that in some sense one has

$$\langle 0|S|0\rangle = \det(1 + G_0 V)$$

the only problem being that $G(t,t')$ is discontinuous on the diagonal and we have used the value $G(t^-,t)$ for the diagonal value. If this formula holds one has

$$\log\langle 0|S|0\rangle = \log\det(1+G_0V) = \operatorname{tr}\left(\log(1+G_0V)\right)$$

and the logarithm can be evaluated as a series. Anyway this would explain why $\log\langle 0|S|0\rangle$ might have a linked diagram expansion.

So our next project must be to understand the diagrams belonging to $\langle 0|S|0\rangle$. Recall

$$\langle 0|S|0\rangle = 1 - \int_{-\infty}^{\infty} \langle 0|\hat{V}(t)|0\rangle\, dt + \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{t_2} dt_1 \langle 0|\hat{V}(t_2)\hat{V}(t_1)|0\rangle - $$

where

$$\hat{V}(t) = e^{tH_0} V(t) e^{-tH_0}$$

and $|0\rangle = \varphi_1 \wedge \cdots \wedge \varphi_p$ in $\Lambda^p W$. Now

$$H_0 = \sum_k{}' E_k a_k^* a_k \qquad V(t) = \sum{}' V_{kl}(t) a_k^* a_l$$

where $a_k = i(\varphi_k^*)$ and $a_k^* = e(\varphi_k)$. Check:

$$V_{mn} = \langle \varphi_m | V | \varphi_n\rangle = \sum{}' V_{kl} \langle \underbrace{\varphi_m | a_k^*}_{\delta_{km}} \underbrace{a_l | \varphi_n}_{\delta_{ln}} \rangle = V_{mn}.$$

If we want to use Wick's theorem we want to replace a_k for $k \le p$ (destroys a particle below Fermi level) by a hole creation operator b_k^*. So we put

$$b_k = a_k^* \qquad k \le p$$

whence $\{b_k, b_l^*\} = \{a_k^*, a_l\} = \{a_l, a_k^*\} = \delta_{lk}$ still holds. H_0 becomes

$$H_0 = \sum_{k \le p} E_k b_k b_k^* + \sum_{k>p}{}' E_k a_k^* a_k$$

$$= \sum_{k \le p} E_k - \sum_{k \le p} E_k b_k^* b_k + \sum_{k > p} E_k a_k^* a_k$$

July 20, 1979

Recall we have a 1-particle Hamiltonian on W

$$H = H_0 + V(t)$$

where V has compact support and H_0 has non-degenerate discrete spectrum $H_0\varphi_n = E_n\varphi_n$ with $E_1 < E_2 < \cdots\cdots$. Extend H to fermion Fock space and look at a system of p particles, i.e. at the action on $\Lambda^p W$. The ground state is $|0\rangle = \varphi_1 \wedge \cdots \wedge \varphi_p$ and the Fermi energy is $E_1 + \cdots + E_p$. We have

$$H = \sum_k E_k a_k^* a_k + \sum_{k,l}{}' V_{kl}\, a_k^* a_l$$

where $a_k = i(\varphi_k^*)$, $a_k^* = e(\varphi_k)$. The goal is to compute

$$\langle 0|S|0\rangle = 1 - \int_{-\infty}^{\infty} \langle 0|\hat{V}(t)|0\rangle dt + \int_{-\infty}^{\infty} dt_2 \int_{-\infty}^{t_2} dt_1 \langle 0|\hat{V}(t_2)\hat{V}(t_1)|0\rangle - \cdots$$

where

$$\hat{V}(t) = e^{tH_0} V e^{-tH_0} \qquad\qquad e^{tH_0} a_k^* e^{-tH_0} = e^{tE_k} a_k^*$$

So the first order term is $\qquad e^{tH_0} a_k e^{-tH_0} = e^{-tE_k} a_k$

$$\sum_{k,l} \int_{-\infty}^{\infty} V_{kl} \langle 0| e^{t(E_k - E_l)} a_k^* a_l |0\rangle dt = \sum_{k \le p} \int_{-\infty}^{\infty} V_{kk}\, dt$$

because

$$\langle 0|a_k^* a_l|0\rangle = \delta_{kl} \qquad k,l \le p$$
$$= 0 \qquad \text{if either } k,l > p.$$

These terms can be described by the diagrams

meaning that a hole is created and immediatelly filled.

The next thing is to compute 2nd order terms:

$$+\int_{-\infty}^{\infty}dt_2\int_{-\infty}^{t_2}dt_1\sum_{klmn}V_{kl}V_{mn}\,e^{t_2(E_k-E_l)+t_1(E_m-E_n)}\langle 0|a_k^* a_l\, a_m^* a_n|0\rangle$$

In order to evaluate the $\langle\ \rangle$ factor it is convenient to introduce hole creators & annihilators:

$$b_k = a_k^* \qquad k \le p$$

But proceed directly first. In order to have a non-zero term we must have $n \le p$, $k \le p$. Then we create [redacted] a hole in state n at time t_1. Also $a_m^* a_n|0\rangle = 0$ if $m \le p$ [redacted] $m \ne n$, so assuming $m \ne n$, we also create a particle in state m. So from the part $a_m^* a_n|0\rangle$, in order to get something $\ne 0$ we have the diagrams

t_1 

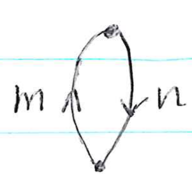
here $a_m^* a_n|0\rangle = (-1)^{n-1}\varphi_m \wedge \varphi_1 \wedge \cdots \wedge \hat{\varphi}_n \wedge \cdots \wedge \varphi_p$

[redacted]

or t_1 

here $m=n$ and $a_m^* a_n|0\rangle = |0\rangle$

So the only [redacted] way for [redacted] $a_k^* a_l$ to bring this to $|0\rangle$ is to have the diagrams

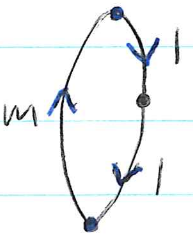


here $l=m>p$, $k=n\le p$ and $a_n^* a_m a_m^* a_n|0\rangle = |0\rangle$

or 

here $m=n\le p$, $k=l\le p$ and $a_k^* a_k a_n^* a_n|0\rangle = |0\rangle$.

When we come to the third order we are going to have trobble getting the diagram



for $p=1$. In effect the only way to get this ~~to~~ be $\neq 0$ is:

$$\varphi_1 \xmapsto{a_m^* a_1} \varphi_m \xmapsto{a_1 a_1^*} \varphi_m \xmapsto{a_1^* a_m} \varphi_1$$

and notice that the $a_1 a_1^*$ is in the wrong order. If we leave it in the form $a_1^* a_1$ then it kills φ_m and doesn't contribute.

So maybe what we should do is the following. The diagrams do not correspond to terms in the expansion, but rather to the terms you get after putting things in normal product form. So for example the term involving

$$a_1^* a_m a_1^* a_1 a_m^* a_1 \qquad m > 1$$

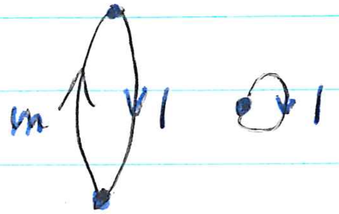
when written out in normal product forms

$$b_1 a_m b_1 b_1^* a_m^* b_1^*$$

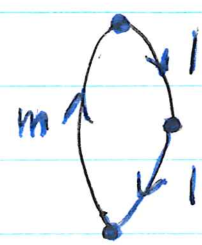
involves two possible contractions

$$b_1 a_m b_1 b_1^* a_m^* b_1^* \qquad \text{and} \qquad \overbrace{b_1 a_m}^{t_3} \overbrace{b_1 b_1^*}^{t_2} \overbrace{a_m^* b_1^*}^{t_1}$$

which belong to the diagrams



and



whose contributions cancel.

The problem appears to compute expectation values

$$\langle 0 | T (a^*_{k_1} a_{l_1})(t_1) \cdots (a^*_{k_n} a_{l_n})(t_n) | 0 \rangle .$$

Let's try to use Schwinger's source method for computing these. This means we consider

$$H = H_0 + H_1$$

$$= \sum' E_k a^*_k a_k + \sum_n J_k a_k + \sum_n \tilde{J}_k a^*_k$$

where $J_k, \tilde{J}_k$ are time-dependent of compact support. Unfortunately this choice of H_1 doesn't preserve the number of particles, so something is missing.

It seems that in order to make sense out of the source concept one wants $J_k(t)$ to belong to the space of operators a^*_l and $\tilde{J}_k(t)$ to belong to the space of operators a_l, but then it seems like a perturbation $\sum'_{k,l} V_{kl} a^*_k a_l$ is much simpler.

July 22, 1979

$$H = \underbrace{\sum{}' E_k a_k^* a_k}_{H_0} + \underbrace{\sum{}' V_{k\ell} a_k^* a_\ell}_{V}$$

operating on $\Lambda^* \mathcal{H}$ where $a_k = i(\varphi_k^*)$, $a_k^* = e(\varphi_k)$ and φ_k is an orth. basis for $\mathcal{H}$ with

$$H_0 \varphi_k = E_k \varphi_k.$$

Assume $E_1 < E_2 < \cdots\cdots$ and let $|0\rangle = \varphi_1 \wedge \cdots \wedge \varphi_p \in \Lambda^p \mathcal{H}$ be the ground state for H_0 on $\Lambda^p \mathcal{H}$. Now the idea is to calculate the ground-ground amplitude $\langle 0|S|0\rangle$ assuming $V = V(t)$ has compact support. One has

$$\langle 0|S|0\rangle = 1 - \int \langle 0|\hat{V}(t)|0\rangle dt + \frac{1}{2!}\iint \langle 0|T\,\hat{V}(t_1)\hat{V}(t_2)|0\rangle dt_1 dt_2$$

where $\hat{V}(t) = e^{tH_0} V(t) e^{-tH_0}$. Introduce hole creation + destruction operators

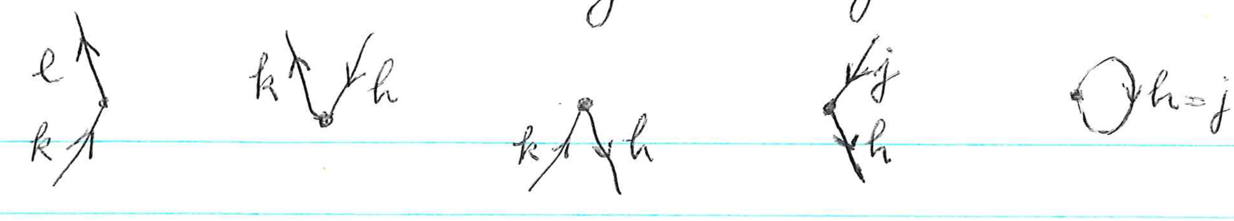
$$b_k = a_k^* \qquad k \leq p.$$

Then the interaction V can be written as a sum of 5 kinds of terms

$$V = \sum_{k,\ell > p} V_{k\ell} a_k^* a_\ell + \sum_{\substack{k>p \\ h\leq p}} V_{kh} a_k^* b_h^* + \sum_{\substack{h\leq p \\ k>p}} V_{hk} b_h a_k$$

$$+ \sum_{h,j \leq p} V_{hj} \underbrace{b_h b_j^*}_{(-b_j^* b_h + \delta_{hj})}$$

which can be described by the diagrams



suppose we want to evaluate the nth order term

$$(-1)^n \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{t_1} dt_2 \cdots \int_{-\infty}^{t_{n-1}} dt_n \ \langle 0 | \hat{V}(t_1) \cdots \hat{V}(t_n) | 0 \rangle$$

Then you express each V as the sum of the terms as on the bottom of page 94. This means we have to evaluate elements of the form

$$\langle 0 | c_1 c_2 \cdots c_{2n} | 0 \rangle$$

where each c_i is one of the creation or annihilation operators. (Actually c_{2n} should be c_{2m} where $n-m$ is the number of V_{hh} summands which occur. To simplify suppose we might suppose this scalar part $\sum_{h \le p} V_{hh}$ of the Hamiltonian has been removed. Then we won't have to worry about loops .)

I think from the point of view of the operators

$$b_k = \begin{cases} a_k^* & k \le p \\ a_k & k > p \end{cases}$$

the exterior alg $\Lambda^* \mathcal{H}$ together with $|0\rangle = \varphi_1 \wedge \cdots \wedge \varphi_p$ is just isomorphic to $\Lambda^* \mathcal{H}$ with $|0\rangle = 1$. This is clear because the b_k annihilate $|0\rangle = \varphi_1 \wedge \cdots \wedge \varphi_p$ and the commutation relations remain the same.

So when it comes to evaluating $\langle 0 | c_1 c_2 \cdots c_{2n} | 0 \rangle$

I can suppose $|0\rangle = 1$. This element is ± 1 or 0. Up to sign we can rearrange the c_i so that all b_1^*, b_1 factors occur to the right of the others. Then the only way to get something non-zero is to have the product

$$(b_1 b_1^*) \cdots (b_1 b_1^*)$$

because one is essentially working with an exterior algebra on one generator tensored with something else. So the only way $\langle 0 | c_1 \cdots c_{2n} | 0 \rangle \neq 0$ is such that when we look at any index k and ignore the rest, then we find

$$b_1 \cdots b_1^* \cdots\cdots b_1 \cdots b_1^* \cdots\cdots\cdots b_1 \cdots b_1^*$$

So we end up with the same problem as before, namely we are permitted

but not

This probably means that this method for evaluating the terms of the Feynman-Dyson expansion will not give enough terms for the linked cluster theorem.

Therefore it seems necessary to go back to a more basic viewpoint. Let us return to the Clifford algebra viewpoint. Recall that the Clifford algebra C

is the algebra of operators on ΛW generated by a_k, a_k^* and that it splits into $C = C^{ev} \oplus C^{odd}$ and that it has a natural increasing filtration with $gr \simeq \Lambda W \otimes \Lambda W^*$. What concerns me is the space $F_2 C^{ev}$ spanned by quadratic products $a_k^* a_\ell$, $a_k a_\ell$, $a_k^* a_\ell^*$, and scalars (better $a_k a_\ell^*$). This is a Lie algebra, [redacted] direct sum of an orthogonal Lie alg. and the scalars. The problem is to evaluate

$$\langle 0 | A_1 \cdots A_n | 0 \rangle$$

where $A_i \in F_2 C^{ev}$