ground energy shift
Goldstone diagrams 600

I am considering $\mathcal{H} = \Lambda \mathcal{H}_1$ with $H = H_0 + H'$ given on $\mathcal{H}_1$ extended as a derivation of $\mathcal{H}$. I want to compute

$$\frac{\operatorname{tr} e^{-\beta H}}{\operatorname{tr} e^{-\beta H_0}} = \langle \underbrace{e^{\beta H_0} e^{-\beta H}}_{S} \rangle = 1 - \int_0^\beta dt \langle H'(t) \rangle + \cdots\cdots$$

By using Wick's theorem I saw that this Dyson expansion could be expressed [redacted] using fermion integration as

$$\langle S \rangle = \frac{\int e^{-\int_0^\beta \tilde{\psi}(\frac{d}{dt} + H_0)\psi\, dt - \int_0^\beta \tilde{\psi} H' \psi\, dt}}{\int e^{-\int_0^\beta \tilde{\psi}(\frac{d}{dt} + H_0)\psi\, dt}}$$

Here $\tilde{\psi}(t), \psi(t)$ are independent anti-commuting variables given on $[0,\beta]$ such that they are anti-periodic in t: $\tilde{\psi}(\beta) = -\tilde{\beta}(0)$ etc. Also [redacted] there is a renormalization problem in the above formula which one solves by interpreting

$$\int_0^\beta \tilde{\psi} H' \psi\, dt \quad \text{as} \quad \int_0^\beta \tilde{\psi}(t+\varepsilon) H' \psi(t)\, dt$$

and then letting $\varepsilon \downarrow 0$.

Yesterday we went through the diagram expansion for $\langle S \rangle$. First transform to [redacted] momentum repn:

$$\psi(t) = \sum \psi(k) \frac{e^{ikt}}{\sqrt{\beta}} \qquad k \in \frac{2\pi}{\beta}\left(\frac{1}{2} + \mathbb{Z}\right)$$

$$\tilde{\psi}(t) = -\tilde{\psi}(k) \text{ ---}$$

whence

$$\int_0^\beta \tilde{\psi}\left(\frac{d}{dt} + H_0 + H'\right)\psi\, dt = \sum_k \tilde{\psi}(-k)\left(ik + H_0 + e^{-ik\varepsilon} H'\right)\psi(k).$$

a vertex in the diagram will have an arrow coming in with momentum k and an arrow going out with the same momentum

The connected diagrams are loops and we saw they give the expansion:

$$\log\left(\frac{\mathrm{tr}\, e^{-\beta H}}{\mathrm{tr}\, e^{-\beta H_0}}\right) = \mathrm{tr}\,(G_0 H') - \frac{1}{2}\mathrm{tr}((G_0 H')^2) + \frac{1}{3}\mathrm{tr}((G_0 H')^3) - \cdots$$

which agrees with the expected formula

$$\langle S \rangle = \det(1 + G_0 H') = \text{``}\left(\frac{\det\left(\frac{d}{dt} + H\right)}{\det\left(\frac{d}{dt} + H_0\right)}\right)\text{''}$$

Now to get the ground energy shift you let $\beta \to \infty$. But first describe how to calculate $\mathrm{tr}\,(G_0 H')^p$. These are operators on the space of anti-periodic functions $\psi(t)$ on $[0,\beta]$ with values in $\mathcal{H}_1$ and $G_0 = \left(\frac{d}{dt} + H_0\right)^{-1}$, whereas H_0 is independent of t. If we use the Fourier transform we get the space of functions $k \mapsto \psi(k)$ from $\frac{2\pi}{\beta}\left(\frac{1}{2} + \mathbb{Z}\right)$ to $\mathcal{H}_1$ and $G_0 = \frac{1}{ik + H_0}$. Therefore

$$\mathrm{tr}(G_0 H')^p = \sum_k \mathrm{tr}_{\mathcal{H}_1}\left(\frac{1}{ik + H_0} H' \cdots\cdots \frac{1}{ik + H_0} H'\right)$$

$$\sim \beta \int \frac{dk}{2\pi}\, \mathrm{tr}_{\mathcal{H}_1}\left(\left(\frac{1}{ik + H_0} H'\right)^p\right).$$

Let's look at this when $H_0 = \sum \mu_n a_n^* a_n$ and $H' = \sum V_{mn} a_m^* a_n$ but remember that the interaction $\int \tilde{\psi} H' \psi$ is interpreted as $\int \tilde{\psi}(t+\varepsilon) H' \psi(t) = \sum_k \tilde{\psi}(-k) e^{-ik\varepsilon} H' \psi(k)$ where $\varepsilon \downarrow 0$.

Then $\operatorname{tr}(G_0 H')^p = \sum_k \sum_{n_1 \cdots n_p} \frac{e^{-ik\varepsilon}}{ik+\mu_{n_1}} V_{n_1 n_2} \frac{e^{-ik\varepsilon}}{ik+\mu_{n_2}} \cdots \frac{e^{-ik\varepsilon}}{ik+\mu_{n_p}} V_{n_p n_1}$

So

$$\frac{1}{\beta} \operatorname{tr}(G_0 H') \longrightarrow \sum_n \int \frac{dk}{2\pi} \frac{e^{-ik\varepsilon}}{ik+\mu_n} V_{nn}$$

Because $\varepsilon > 0$ the exponential $e^{-ik\varepsilon}$ decays in the LHP, hence

$$\int \frac{dk}{2\pi} \frac{e^{-ik\varepsilon}}{ik+\mu_n} = \begin{cases} -e^{\mu_n \varepsilon} & \mu_n < 0 \\ 0 & \mu_n > 0 \end{cases}$$

because the pole occurs at $k = i\mu_n$. So one gets

$$\frac{1}{\beta} \operatorname{tr}(G_0 H') \longrightarrow -\sum_{\mu_n < 0} V_{nn}$$

For $p \geq 2$ the denominator in

$$\frac{1}{\beta} \operatorname{tr}(G_0 H')^p = \sum_{n_1 \cdots n_p} \int \frac{dk}{2\pi} \frac{e^{-(ik\varepsilon)p}}{\prod (ik+\mu_{n_i})} V_{n_1 n_2} \cdots V_{n_p n_1}$$

is of degree p, so there are no convergence problems, and so we can put $\varepsilon = 0$. This probably means that $(G_0 H')^p$ has a good trace for $p \geq 2$.

Now let's consider the case where $\mu_0 < 0$ but $\mu_n > 0$ for $n \neq 0$. The ground state for H_0 on $\Lambda \mathcal{H}_1$ is just $|0\rangle \in \mathcal{H}_1 = \Lambda \mathcal{H}_1$. If the perturbation H' is small enough, then the ground state for H on $\Lambda \mathcal{H}_1$ is also the ground state of H on $\mathcal{H}_1$, so the above series for the ground shift should be the RS series.

$$-\Delta E = \lim_{\beta \to \infty} \frac{1}{\beta} \log\left(\frac{\operatorname{tr} e^{-\beta H}}{\operatorname{tr} e^{-\beta H_0}}\right) = \sum_{p \geq 1} \frac{(-1)^{p-1}}{p} \int \frac{dk}{2\pi} \operatorname{tr}\left(\frac{1}{ik+H_0} V\right)^p$$

$$= \int \frac{dk}{2\pi} \log \underbrace{\det\left(1 + \frac{1}{ik+H_0} V\right)}_{\frac{\det(ik + H_0 + V)}{\det(ik + H_0)}}$$

So what we want to evaluate is

$$\int \frac{dk}{2\pi} \log\left(\frac{ik+\mu'}{ik+\mu}\right)$$

where μ, μ' are in the same half-plane. Except we have forgotten the problem with the trace term $\mathrm{tr}\left(\frac{1}{ik+H_0}V\right)$. One takes care of this by deforming the integral into a circle in the lower half-plane around μ, μ'. A better way of saying this is that the integral is to replaced by the integral over $\mathbb{R}$ completed by a large circle in the LHP. It's clear then that one gets zero if μ, μ' are in the UHP.

Finally to evaluate the integral use integration by parts

$$\oint \frac{dk}{2\pi} \log\left(\frac{ik+\mu'}{ik+\mu}\right) = -\oint \frac{dk}{2\pi} k \frac{d}{dk} \log\left(\frac{ik+\mu'}{ik+\mu}\right)$$

$$= +\oint \frac{dk}{2\pi} k\left(\frac{i}{ik+\mu'} - \frac{i}{ik+\mu}\right)$$

$$= \frac{1}{2\pi i}\oint dk\ ik\left(\frac{1}{k-i\mu'} - \frac{1}{k-i\mu}\right)$$

$$= -\mu' + \mu$$

Hence you end up with

$$\Delta E = \mu_0' - \mu_0$$

and more generally $\Delta E = \sum_{i=1}^{h} (\mu_i' - \mu_i)$ where one sums over the negative eigenvalues.

January 30, 1980

Review: We have on $\Lambda \mathcal{H}_1$ a 1-particle operator $H = H_0 + H'$ and we compute

$$\frac{tr(e^{-\beta H})}{tr(e^{-\beta H_0})} = \frac{\prod(1+e^{-\beta\tilde{\mu}_n})}{\prod(1+e^{-\beta\mu_n})} \sim e^{-\beta\left(\sum_{\tilde{\mu}_n<0}\tilde{\mu}_n - \sum_{\mu_n<0}\mu_n\right)} \qquad \text{as } \beta\to\infty$$

where the $\tilde{\mu}_n$ (resp μ_n) are the eigenvalues of H (resp. H_0) on $\mathcal{H}_1$. Use

$$\frac{tr(e^{-\beta H})}{tr(e^{-\beta H_0})} = \langle \underbrace{e^{\beta H_0}e^{-\beta H}}_{S} \rangle = 1 - \int_0^\beta \langle H'(t)\rangle dt + \cdots$$

(Dyson exp.)

You apply Wick's thm. to convert the Dyson expansion into a sum over diagrams, then

$$\begin{aligned} \log\langle S\rangle &= \textstyle\sum \text{ over connected diagrams} \\ &= tr(G_0H') - \tfrac{1}{2}tr(G_0H')^2 + \cdots \\ &= \log\det(1+G_0H') \end{aligned}$$

where G_0 is the inverse of $\frac{d}{dt}+H_0$ on $\mathcal{H}_1\otimes L^2([0,\beta])$ with anti-periodic boundary conditions. Formally we have

$$\frac{tr(e^{-\beta H})}{tr(e^{-\beta H_0})} = \frac{\det\left(\frac{d}{dt}+H\right)}{\det\left(\frac{d}{dt}+H_0\right)}$$

and we always have

$$tr(e^{-\beta H}) = \det\left(1+e^{-\beta(H|\mathcal{H}_1)}\right).$$

which suggests $\quad \det\left(1+e^{-\beta H|\mathcal{H}_1}\right) = \det\left(\frac{d}{dt}+H_0\right)\cdot \text{const}.$

Let's take a simple case where $H = \mu a^* a$. The eigenfunctions for $\frac{d}{dt}+H_0$ with anti-periodic b.c. on $\mathcal{H}_1\otimes L^2[0,\beta]$ are

$\frac{e^{ikt}}{\sqrt{\beta}}$ where $k \in \frac{2\pi}{\beta}(\frac{1}{2}+\mathbb{Z})$, so $(d/dt)+H_0$ has the eigenvalues $ik+\mu$. Thus formally:

$$\det\left(\frac{d}{dt}+H_0\right) = \prod_{k\in\frac{2\pi}{\beta}(\frac{1}{2}+\mathbb{Z})} (ik+\mu)$$

so we get

$$1+e^{-\beta\mu} = \prod_{k\in\frac{2\pi}{\beta}(\frac{1}{2}+\mathbb{Z})} (ik+\mu)$$

which is not complete non-sense.

Return to the formula

$$\log\langle S\rangle = \operatorname{tr}(G_0H') - \frac{1}{2}\operatorname{tr}(G_0H')^2 + \cdots$$
$$= \log\det(1+G_0H')$$

and let $\beta\to\infty$. We saw that we get an expression for the ground energy shift

$$-\Delta E = \int\frac{dk}{2\pi}\log\det\left(1+\frac{1}{ik+H_0}H'\right)$$
$$= \sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n}\int\frac{dk}{2\pi}\operatorname{tr}_{\mathcal{H}_1}\left(\left(\frac{1}{ik+H_0}H'\right)^n\right)$$

where for $n=1$ the integral is regularized by completing the contour by a large circle in the lower half-plane.

A simpler way to obtain the above formula goes as follows: To be precise $H=H_0+H'$ is given on $\mathcal{H}^1$ and it is assumed that H' is small. The quantity to be computed is the sum of negative eigenvalues of H minus the same sum for H_0. H' is assumed small so that the number of negative eigenvalues for H and H_0 is the same. One has

$$\sum_{\tilde{\mu}_n<0}' \tilde{\mu}_n = \operatorname{tr}(P_H^- H)$$

where P_H^- projects on the negative eigenspaces:

$$P_H^- = \frac{1}{2\pi i}\oint \frac{1}{s-H}\,ds$$

the contour enclosed negative eigenvalues. Thus

$$\sum_{\tilde{\mu}_n<0} \tilde{\mu}_n = \frac{1}{2\pi i}\oint \operatorname{tr}\left(\frac{s}{s-H}\right) ds$$

same contour because H' is small

so

$$\Delta E = \sum_{\tilde{\mu}_n<0} \tilde{\mu}_n - \sum_{\mu_n<0}\mu_n = \frac{1}{2\pi i}\oint \operatorname{tr}\left(\frac{s}{s-H} - \frac{s}{s-H_0}\right) ds$$

$$= \frac{1}{2\pi i}\oint s \, d\log\left(\det \frac{s-H}{s-H_0}\right)$$

so integrating by parts:

$$-\Delta E = \frac{1}{2\pi i}\oint \log\left(\det\left(1-\frac{1}{s-H_0}H'\right)\right) ds$$

Here's another derivation: Put $H_\lambda = H_0 + \lambda H'$ and let $P_\lambda = P_{H_\lambda}^-$ = orth. projection on the negative space for H_λ. Then $P_\lambda = \frac{1}{2\pi i}\oint \frac{1}{s-H_\lambda}ds$. Now

$$E_\lambda = \operatorname{tr}(H_\lambda P_\lambda)$$

$$\frac{dE_\lambda}{d\lambda} = \operatorname{tr}(H' P_\lambda) + \operatorname{tr}\left(H_\lambda \frac{dP_\lambda}{d\lambda}\right)$$

The last term is 0: From $P_\lambda^2 = P_\lambda$ get $P_\lambda \frac{dP_\lambda}{d\lambda} + \frac{dP_\lambda}{d\lambda}P_\lambda = \frac{dP_\lambda}{d\lambda}$

$$(1-P_\lambda)\frac{dP_\lambda}{d\lambda} = \frac{dP_\lambda}{d\lambda}P_\lambda \qquad P_\lambda \frac{dP_\lambda}{d\lambda} = \frac{dP_\lambda}{d\lambda}(1-P_\lambda)$$

Thus relative to the decomposition $\mathcal{H}_1 = P_\lambda \mathcal{H}_1 \oplus (1-P_\lambda)\mathcal{H}_1$ the operator $\frac{dP_\lambda}{d\lambda}$ has zero diagonal components and H_λ has only diagonal components. Hence $H_\lambda \frac{dP_\lambda}{d\lambda}$ has zero diagonal components, so $\operatorname{tr}\left(H_\lambda \frac{dP_\lambda}{d\lambda}\right) = 0$. Alternatively

$$\operatorname{tr}\left(H_\lambda \frac{dP_\lambda}{d\lambda}\right) = \operatorname{tr}\left(P_\lambda H_\lambda \frac{dP_\lambda}{d\lambda}\right) + \operatorname{tr}\left((1-P_\lambda)H_\lambda \frac{dP_\lambda}{d\lambda}\right)$$

$$= \operatorname{tr}\Big(H_\lambda \underbrace{\frac{dP_\lambda}{d\lambda} P_\lambda}\Big) + \quad ''$$

$$\frac{dP_\lambda}{d\lambda} P_\lambda^2 = (1-P_\lambda)\frac{dP_\lambda}{d\lambda} P_\lambda$$

$$= \operatorname{tr}\left(P_\lambda H_\lambda (1-P_\lambda)\frac{dP_\lambda}{d\lambda}\right) + \quad ''$$

$$= 0$$

Thus

$$\frac{dE_\lambda}{d\lambda} = \operatorname{tr}(H' P_\lambda) = \frac{1}{2\pi i}\oint \operatorname{tr}\left(\frac{1}{s-H_\lambda} H'\right) ds$$

$$= \frac{-1}{2\pi i}\oint \operatorname{tr} \frac{d}{d\lambda}\log(s-H_\lambda)\, ds$$

$$= -\frac{1}{2\pi i}\oint \frac{d}{d\lambda}\log\det(s-H_\lambda)\, ds$$

so integrating from $\lambda = 0$ to 1.

$$-\Delta E = \frac{1}{2\pi i}\oint \log\det\left(\frac{s-H}{s-H_0}\right) ds$$

One of the virtues of the above proof is that it works with the Green's function $\frac{1}{s-H_\lambda}$ thru the expression

$$\operatorname{tr}\left(\frac{1}{s-H_\lambda} H'\right)$$

since

$$\operatorname{tr}\left(\frac{1}{s-H_\lambda} H'\right) = \operatorname{tr}\left(\frac{1}{s-H_0} H' + \frac{1}{s-H_0}\lambda H' \frac{1}{s-H_0} H' + \cdots\right)$$

the answer is still given as a series with coefficients involving $\frac{1}{2\pi i}\oint \mathrm{tr}\left(\frac{1}{s-H_0}H'\right)^n ds \qquad n \geq 1$

so the problem is to calculate these iterated traces. Rather the problem is to compute the residue, the point being that one has repeated poles inside the contour.

January 31, 1980

We've seen that the shift ΔE in the ground eigenvalue of H_0 due to a small perturbation H' is given by

$$\Delta E = \frac{1}{2\pi i}\oint \operatorname{tr}\left(\frac{s}{s-H} - \frac{s}{s-H_0}\right) ds \underset{\substack{\uparrow \\ \text{int by} \\ \text{parts}}}{=} -\frac{1}{2\pi i}\oint \operatorname{tr}\log\frac{s-H}{s-H_0}\, ds$$

small circle containing μ_0, μ_0

$$= -\frac{1}{2\pi i}\oint \operatorname{tr}\log(1-G_0H')\,ds \qquad G_0 = \frac{1}{s-H_0}$$

$$= \sum_{p\geq 1}\frac{1}{p}\underbrace{\frac{1}{2\pi i}\oint \operatorname{tr}[(G_0H')^p]\,ds}_{\text{denote this } R_p}$$

The problem is therefore to compute the residues, and the important thing is the poles inside the contour of integration.

Let $P =$ projection onto ground eigenspace of H_0; $P = \frac{1}{2\pi i}\oint \frac{1}{s-H_0}ds$, and let $Q = I - P$. Then

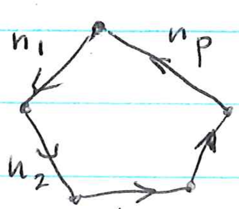
$$G_0 = \frac{1}{s-H_0} = P\frac{1}{s-H_0}P + Q\frac{1}{s-H_0}Q$$

and if this is inserted in the expression for R_n we find R_p is a sum of 2^p terms.

To simplify suppose the ground state of H_0 is non-degenerate, and let's suppose $H_0 = \sum_n \mu_n |n\rangle\langle n|$. Then

$$(1) \qquad \operatorname{tr}(G_0H')^p = \sum_{n_1,\dots,n_p} \frac{1}{s-\mu_{n_1}}V_{n_1n_2}\cdots\frac{1}{s-\mu_{n_{p-1}}}V_{n_{p-1}n_p}\frac{1}{s-\mu_{n_p}}V_{n_pn_1}$$

and we can visualize this as a sum over diagrams



From the viewpoint of taking the residue at $s = \mu_0$ the big sum (1) breaks into 2^p sums indexed by the subset of $i \in \{1, \ldots, p\}$ such that $n_i = 0$. Some of these 2^p terms will be the same by cyclic symmetry and others will be zero because of analyticity at $s = \mu_0$ or other considerations. So the 2^p terms effectively reduce to fewer ones. Compute:

p=1:  terms $\frac{1}{s-\mu_n} V_{nn}$, and only $n=0$

is non-analytic at $s = \mu_0$. So

$$\Delta E^{(1)} = \frac{1}{2\pi i} \oint \operatorname{tr} G_0 H' = V_{00}$$

p=2:  The case n_1, n_2 both $\neq 0$ doesn't occur

$n_1 = n_2 = 0$ " "

because $\frac{1}{(s-\mu_0)^2}$ has zero residue.

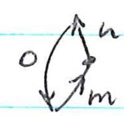
Key case is  contribution

$$\frac{1}{2\pi i} \int \frac{1}{s-\mu_n} V_{0n} \frac{1}{s-\mu_0} V_{n0} = \frac{V_{0n} V_{n0}}{\mu_0 - \mu_n}$$

so

$$\Delta E^{(2)} = -\sum_{n \neq 0}{}' \frac{V_{0n} V_{n0}}{\mu_n - \mu_0}$$

p=3: all $n_i \neq 0$ or all $n_i = 0$ don't occur

 one zero, symm. factor = 1.

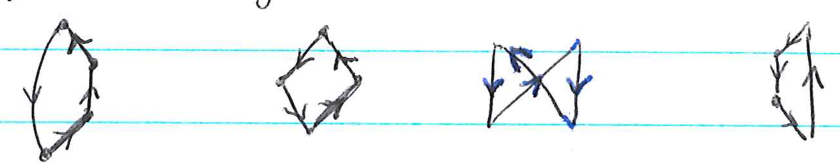
$$\sum_{m,n \neq 0}{}' \frac{V_{0n} V_{nm} V_{m0}}{(\mu_n - \mu_0)(\mu_m - \mu_0)}$$

two zeros symm. factor = 1  $\sum_{n \neq 0}{}' V_{n0} V_{n0} V_{00} \underbrace{\frac{1}{2\pi i} \int \frac{1}{(s-\mu_n)(s-\mu_0)^2} ds}_{\frac{-1}{(\mu_n - \mu_0)^2}}$

so we get

$$\Delta E^{(3)} = \sum_{m,n\neq 0}' \frac{V_{0n}V_{nm}V_{m0}}{(\mu_n-\mu_0)(\mu_m-\mu_0)} - \sum_{n\neq 0}' \frac{V_{0n}V_{n0}V_{00}}{(\mu_n-\mu_0)^2}$$

Finally RD Mattuck has a way of visualizing the different diagrams contributing to ΔE which is derived from diagrams using time instead of the energy s. He thinks of $|0\rangle$ as a hole, and the point is that it must go backward in time, whereas the states $|n\rangle$ for $n\neq 0$ go forward in time. Thus in fourth order the different diagrams are



It seems that "backwards in time" $\longleftrightarrow$ "analytic outside contour"
forwards in time $\longleftrightarrow$ "analytic inside contour"

The Gell-Mann Low theorem gives another way to obtain the ground energy shift. Let's review this method (Aug 26, 1979).

Start with an eigenvector φ_a of H_0: $H_0\varphi_a = E_a\varphi_a$. Let $\psi_\varepsilon(t)$ denote the solution of

$$i\frac{\partial}{\partial t}\psi_\varepsilon = (H_0 + e^{\varepsilon t}V)\psi_\varepsilon \qquad \varepsilon > 0$$

such that $\psi_\varepsilon(t) \sim e^{-iE_a t}\varphi_a$ as $t\to -\infty$.

It is assumed such a solution exists because $e^{\varepsilon t}$ decays at

$t \to -\infty$. Write the Schroedinger DE in the form

$$\left(i\frac{\partial}{\partial t} - H_0\right)\psi_\varepsilon = e^{\varepsilon t} V \psi_\varepsilon$$

and construct the solution by iteration starting from $\psi_\varepsilon^{(0)} = e^{-iE_a t}\varphi_a$. The DE has constant coefficients, so by undetermined coefficients we get

$$\psi_\varepsilon^{(1)} = e^{-iE_a t}\varphi_a + e^{-iE_a t + \varepsilon t}\frac{1}{E_a - H_0 + i\varepsilon} V\varphi_a$$

and continuing we get the series

$$\psi_\varepsilon(t) = e^{-iE_a t}\varphi_a + e^{-iE_a t + \varepsilon t}\frac{1}{E_a - H_0 + i\varepsilon} V\varphi_a$$
$$+ e^{-iE_a t + 2\varepsilon t}\frac{1}{E_a - H_0 + 2i\varepsilon} V \frac{1}{E_a - H_0 + i\varepsilon} V\varphi_a + \cdots$$

which one can assume converges (no problem in the fin. diml case because one has a factorial-like denominator). Now the idea is to renormalize ψ_ε so that it converges as $\varepsilon \to 0$. The Gell-Mann-Low renormalization is

$$\frac{\psi_\varepsilon}{\langle \varphi_a | \psi_\varepsilon(0)\rangle}.$$

This ought to approach as $\varepsilon \to 0$ a solution of $i\frac{\partial}{\partial t}\psi = H\psi$.

Actually one can be clearer. Replace V by λV so

$$\psi_\varepsilon(0) = \varphi_a + \frac{1}{E_a - H_0 + i\varepsilon}\lambda V\varphi_a + \frac{1}{E_a - H_0 + 2i\varepsilon}\lambda V \frac{1}{E_a - H_0 + i\varepsilon}\lambda V\varphi_a + \cdots$$

Then $i\varepsilon\lambda\frac{\partial}{\partial\lambda}$ multiplies the nth term by $ni\varepsilon$ so that

$$\left(E_a - H_0 + i\varepsilon\lambda\frac{\partial}{\partial\lambda}\right)\psi_\varepsilon(0) = \lambda V \psi_\varepsilon(0)$$

and hence provided $\psi_\varepsilon(0)$ can be normalized so as to converge as $\varepsilon \to 0$, then it approaches an eigenvector for [redacted] $H_0 + \lambda V$ with eigenvalue E_a? Something is screwy!

Let us assume whatever limits needed to exist do so that

$$\psi_a = \lim_{\varepsilon \to 0} \frac{\psi_\varepsilon}{\langle \varphi_a | \psi_\varepsilon \rangle}$$

exists and is the eigenvector of H which φ_a evolves into. Then the new eigenvalue is

$$\tilde{E}_a = \frac{\langle \varphi_a | \overset{H_0+V}{H} | \psi_a \rangle}{\underbrace{\langle \varphi_a | \psi_a \rangle}_{1}} = E_a + \lim \frac{\langle \varphi_a | V | \psi_\varepsilon \rangle}{\langle \varphi_a | \psi_\varepsilon \rangle}$$

Thus

$$\Delta E_a = \lim \frac{\langle \varphi_a | V | \psi_\varepsilon \rangle}{\langle \varphi_a | \psi_\varepsilon \rangle} = \lim \frac{\langle \varphi_a | V | \varphi_a \rangle + \langle \varphi_a | V \frac{1}{E_a - H_0 + i\varepsilon} V | \varphi_a \rangle + \cdots}{1 + \langle \varphi_a | \frac{1}{E_a - H_0 + i\varepsilon} V | \varphi_a \rangle + \cdots}$$

February 1, 1980

The principle behind adiabatic switching seems to be that if you turn on the interaction slowly the free eigenstate φ_0 should change into the corresponding eigenstate for H. Feynman's idea is that the H-eigenstate is the free eigenstate φ_0 modified by the influence of the perturbation: This gives the formula

$$(1)\qquad \begin{aligned}\psi(t) = {} & e^{-iE_0 t}\varphi_0 + \int_{-\infty}^{t} e^{-iH_0(t-t_1)}\tfrac{1}{i}V e^{-iE_0 t_1}\varphi_0\, dt_1 \\ & + \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2\, e^{-iH_0(t-t_1)}\tfrac{1}{i}V e^{-iH(t_1-t_2)}\tfrac{1}{i}V e^{-iE_0 t_2}\varphi_0 + \cdots\end{aligned}$$

which is the iteration solution of

$$\psi(t) = e^{-iE_0 t}\varphi_0 + \int_{-\infty}^{t} dt'\, e^{-iH_0(t-t')}\tfrac{1}{i}V\psi(t')$$

or

$$\begin{cases} i\dfrac{\partial}{\partial t}\psi = (H_0+V)\psi \\ \psi \sim e^{-iE_0 t}\varphi_0 \qquad \text{at } t\to-\infty \end{cases}$$

However if one does the integrations in (1) one gets

$$\psi(t) = e^{-iE_0 t}\left(\varphi_0 + \frac{1}{E_0-H_0}V\varphi_0 + \cdots\cdots\right)$$

which has problems because since E_0 is an eigenvalue of H_0, $E_0 - H_0$ isn't invertible. This formula does make sense in the scattering situation, and it gives us the $(+)$ eigenstate of H corresponding to φ_0.

So the game is to make sense out of the Feynman prescription (1). The adiabatic method replaces V by $e^{\varepsilon t}V$. In some sense this is like turning on the interaction for the time $\sim \frac{1}{\varepsilon}$, so let's consider having the interaction on for a time T and letting $T \to \infty$.

Thus what you want is to look at $e^{-iHT}\varphi_0$ as $T \to \infty$. Let $H = \sum' |\psi_n\rangle \tilde{E}_n \langle\psi_n|$, whence

$$e^{-iHT}\varphi_0 = \sum_n{}' |\psi_n\rangle e^{-i\tilde{E}_n T}\langle\psi_n|\varphi_0\rangle$$

If one gives T an increasing negative imaginary part: $T = (1-i\varepsilon)R$ with $R \to +\infty$, then

$$e^{-iHT}\varphi_0 \sim |\psi_0\rangle e^{-i\tilde{E}_0 T}\langle\psi_0|\varphi_0\rangle$$

so therefore one does get the H-ground state (assuming $\langle\psi_0|\varphi_0\rangle \neq 0$ which is a standard operating assumption.)

A simpler way to obtain ψ_0 from φ_0 is to use imaginary time:

$$e^{-\beta H}\varphi_0 = \sum_n{}' \psi_n e^{-\beta\tilde{E}_n}\langle\psi_n|\varphi_0\rangle \sim \psi_0 e^{-\beta\tilde{E}_0}\langle\psi_0|\varphi_0\rangle$$

Therefore $\cancel{\frac{\psi_0}{\langle\varphi_0|\psi_0\rangle} = \lim \frac{e^{-\beta H}\varphi_0}{\langle\varphi_0|e^{-\beta H}|\varphi_0\rangle}}$ one has the formula

$$\boxed{\frac{\psi_0}{\langle\varphi_0|\psi_0\rangle} = \lim_{\beta\to\infty} \frac{e^{-\beta H}\varphi_0}{\langle\varphi_0|e^{-\beta H}\varphi_0\rangle}}$$

to replace the adiabatic switching formula.

February 2, 1980.

Goldstone diagrams and why they are inefficient: According to RD Mattuck's book the RS series for the ground energy shift can be obtained as a sum over Goldstone diagrams. I now understand what this means.

Let's begin with $H_0 = \sum |n\rangle \mu_n \langle n|$ where $\mu_0 < 0$ and $\mu_n > 0$ for $n \neq 0$, and let $H = H_0 + V$ be a small perturbation. I need a time-dependent formula for the shift $\Delta E = \tilde{\mu}_0 - \mu_0$ in the ground energy. Let us extend H to a derivation $\hat{H}$ on the exterior algebra $\Lambda \mathcal{H}_1$. Because we have adjusted energy levels so that $\mu_0 < 0$ and the others are > 0, we know the ground energy for $\hat{H}$ is the same as for H. Now we use the formula

$$\frac{\operatorname{Tr}\left(e^{-\beta \hat{H}}\right)}{\operatorname{Tr}\left(e^{-\beta \hat{H}_0}\right)} \sim e^{-\beta(\Delta E)} \qquad \text{as } \beta \to \infty$$

and the basic theory (Dyson, Wick) which allow us to compute the former as exp of connected diagrams. Doing this computation gives

$$\log \frac{\operatorname{Tr}(e^{-\beta \hat{H}})}{\operatorname{Tr}(e^{-\beta \hat{H}_0})} = \operatorname{tr}(G_0 V) - \frac{1}{2} \operatorname{tr}\left((G_0 V)^2\right) + \frac{1}{3}\left(\operatorname{tr}(G_0 V)^3\right) - \cdots$$

where $G_0 = \left(\frac{d}{dt} + H_0\right)^{-1}$ on functions from $[0, \beta]$ to $\mathcal{H}$, with anti-periodic boundary conditions. So now we want to divide by β and let $\beta \to \infty$. Now

$$G_0^\beta(t,t') = \frac{1}{\beta}\sum_k \frac{e^{ik(t-t')}}{ik+H_0} \qquad k \in \frac{2\pi}{\beta}\left(\tfrac{1}{2}+\mathbb{Z}\right)$$

$$\longrightarrow \int \frac{dk}{2\pi}\frac{e^{ik(t-t')}}{ik+H_0} = G_0^\infty(t,t') = \begin{cases}\text{inverse of } \frac{d}{dt}+H_0 \\ \text{in } L^2(\mathbb{R})\end{cases}$$

$$tr(G_0V) = \int_0^\beta tr_{\mathcal{H}_1}\left(G_0^\beta(t^-,t)\,V\right)dt = \sum_k tr_{\mathcal{H}_1}\left(\frac{e^{-ik\varepsilon}}{ik+H_0}V\right)$$

$$\sim \beta \underbrace{\int \frac{dk}{2\pi}\, tr_{\mathcal{H}_1}\left(\frac{e^{-ik\varepsilon}}{ik+H_0}V\right)}_{tr_{\mathcal{H}_1}\left(G_0^\infty(0^-,0)V\right)}$$

similarly

$$tr\,(G_0^\beta V)^p = \sum_k tr_{\mathcal{H}_1}\left(\frac{1}{ik+H_0}V\right)^p \sim \beta\int\frac{dk}{2\pi}\,tr\left(\frac{1}{ik+H_0}V\right)^p$$

$$= \beta \int_{t_1=0} dt_2\cdots dt_p\; tr_{\mathcal{H}_1}\left(G_0^\infty(t_1,t_2)V\,G_0^\infty(t_2,t_3)V\cdots G_0^\infty(t_p,t_1)V\right)$$

as one sees by substituting in $G_0^\infty(t_1,t_2) = \int \frac{dk}{2\pi}\frac{e^{ik(t_1-t_2)}}{ik+H_0}$.
So basic time-dependent expression is

$$\Delta E = -tr_{\mathcal{H}_1}\left(G_0^\infty(0^-,0)V\right) + \frac{1}{2}\int_{t_1=0} dt_2\; tr_{\mathcal{H}_1}\left(G_0^\infty(t_1,t_2)V\,G_0^\infty(t_2,t_1)V\right) - \frac{1}{3}\cdots$$

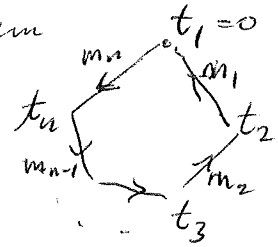
This is the Feynman diagram expression for the energy shift in the coordinate repn.

The next step is to insert matrix elements

$$V_{mn} = \langle m|V|n\rangle$$

$$G_0^\infty(t,t')_{mm} = \begin{cases} e^{-\mu_m(t-t')}\,\theta(t-t') & \mu_m>0 \\ -e^{\mu_0(t-t')}\,\theta(t'-t) & \mu_0<0\end{cases}$$

One takes the nth order term for ΔE which belongs to the n diagram

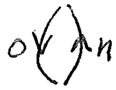


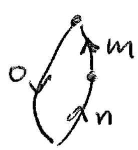
and breaks up the integral into $n!$ integrals indexed by the different time orderings. A lots of these integrals are zero because $|m\rangle$ propagates forward in time for $m \neq 0$ and $|0\rangle$ goes backward in time. These time-ordered diagrams with "particles" going forward and "holes" going backwards are the <u>Goldstone</u> diagrams.

Calculate:

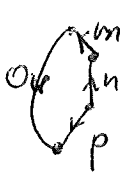
The Rayleigh-Schroed. series for the ground energy shift is the sum of following terms

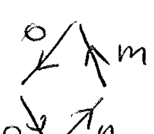
$p=1$  V_{00}

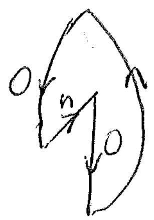
$p=2$  $$\sum_{n \neq 0} - \frac{V_{0n} V_{n0}}{\mu_n - \mu_0}$$

$p=3$  $$\sum_{m,n \neq 0} \frac{V_{0m} V_{mn} V_{n0}}{(\mu_m - \mu_0)(\mu_n - \mu_0)}$$

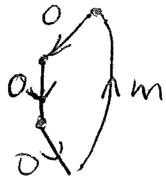
 $$\sum_{m \neq 0} - \frac{V_{0m} V_{m0} V_{00}}{(\mu_m - \mu_0)^2}$$

$p=4$  $$\sum_{m,n,p \neq 0} - \frac{V_{0m} V_{mn} V_{np} V_{p0}}{(\mu_m - \mu_0)(\mu_n - \mu_0)(\mu_p - \mu_0)}$$

 $$\sum_{m,n \neq 0} \frac{V_{0m} V_{mn} V_{n0} V_{00}}{(\mu_m - \mu_0)(\mu_n - \mu_0)} \left(\frac{1}{\mu_m - \mu_0} + \frac{1}{\mu_n - \mu_0} \right)$$



$$\frac{1}{2}\sum_{m,n\neq 0} \frac{V_{om}V_{mo}V_{on}V_{no}}{(\mu_m-\mu_o)(\mu_n-\mu_o)}\left(\frac{1}{\mu_m-\mu_o}+\frac{1}{\mu_n-\mu_o}\right)$$



$$\sum_{m\neq 1} -\frac{V_{om}V_{mo}V_{oo}^2}{(\mu_m-\mu_o)^3}$$

$p=5$ assuming V_{oo} you have 2 terms

 and 

In the above one uses the formula

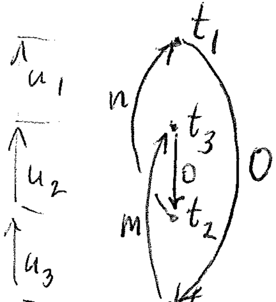
$$\Delta E = \sum_{p\geq 1}\frac{1}{p}\sum_{m_1\cdots m_p} V_{m_1m_2}V_{m_2m_3}\cdots V_{m_pm_1}\frac{1}{2\pi i}\oint\frac{ds}{\prod_{i=1}(s-\mu_{m_i})}$$

where the contour gets the residue at μ_o. Since

$$\frac{1}{s-\mu_m} = -\frac{1}{\mu_m-\mu_o}\frac{1}{1-\frac{s-\mu_o}{\mu_m-\mu_o}} = -\frac{1}{\mu_m-\mu_o}\left(1+\frac{s-\mu_o}{\mu_m-\mu_o}+\frac{(s-\mu_o)^2}{(\mu_m-\mu_o)^2}+\cdots\right)$$

it's clear that the residue gives denominators which are products of $(\mu_m-\mu_o)$ for $m\neq 0$.

But consider the Goldstone diagram:

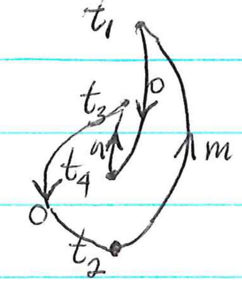


The contribution is

$$\int_{u_1,u_2,u_3\geq 0} du_1du_2du_3\; e^{-\mu_n(u_1+u_2)}V_{no}(-)e^{\mu_o u_2}V_{om}\,e^{-\mu_m(u_2+u_3)}V_{mo}(-)e^{\mu_o(u_1+u_2+u_3)}V_{on}$$

$$= \frac{V_{no}V_{om}V_{mo}V_{on}}{(\mu_n-\mu_o)(\mu_n-\mu_o+\mu_m-\mu_o)(\mu_m-\mu_o)}$$

which has the strange denominator factor $(\mu_m+\mu_n-2\mu_0)$.
However one also has the Goldstone diagrams:



which contributes

$$\frac{V_{om}V_{mo}V_{on}V_{no}}{(\mu_m-\mu_0)^2(\mu_m+\mu_n-2\mu_0)}$$

and the point is that

$$\frac{1}{\mu_m+\mu_n-2\mu_0}\left[\frac{1}{(\mu_m-\mu_0)^2}+\frac{1}{(\mu_n-\mu_0)^2}+\frac{2}{(\mu_m-\mu_0)(\mu_n-\mu_0)}\right]$$

$$=\frac{1}{\mu_m+\mu_n-2\mu_0}\left(\frac{1}{\mu_m-\mu_0}+\frac{1}{\mu_n-\mu_0}\right)^2=\frac{1}{(\mu_m-\mu_0)(\mu_n-\mu_0)}\left(\frac{1}{\mu_m-\mu_0}+\frac{1}{\mu_n-\mu_0}\right)$$

so these strange denominators disappear under summation.

Let's consider the boson analogue of the path integral

$$\int e^{-\int \tilde{\psi}\left(\frac{d}{dt}+\mu\right)\psi}$$

encountered above (p. 582). Start with finite-dim'l formula

$$(1) \qquad \int e^{-\sum \bar{z}_i a_{ij} z_j} \underset{\substack{\text{Lebesgue} \\ \text{measures} \\ \text{on } \mathbb{C}^n}}{dV} = \frac{\text{const}}{\det(a_{ij})}$$

valid for a complex matrix whose hermitian part is positive-definite. Notice that $z \longmapsto z^* a z$ is a quadratic function on $\mathbb{C}^n$ regarded as a real vector space whose real part is

$$\operatorname{Re}(z^* a z) = \frac{1}{2}\left(z^* a z + z^* a^* z\right) = z^* \underbrace{\left(\frac{a+a^*}{2}\right)}_{\text{hermitian part of } a.} z$$

and hence (1) makes sense when $\frac{a+a^*}{2}$ is positive-definite. Also the integral should be a real analytic function of the matrix a_{ij}, so that by analytic continuation it suffices to check the formula when a is pos-definite. In this case we can diagonalize a by a unitary transformation, so one is reduced to computing

$$\int e^{-\bar{z} a z}\, dx\,dy = \int e^{-\frac{2a}{2}(x^2+y^2)}\, dx\,dy = \left(\frac{\sqrt{2\pi}}{\sqrt{2a}}\right)^2 = \frac{\pi}{a}$$

for $a>0$. So a better form of (1) is

$$(2) \qquad \int e^{-\sum \bar{z}_i a_{ij} z_j} \prod_{j=1}^{n} dx_j\, dy_j = \frac{\pi^n}{\det(a_{ij})} .$$

Then
$$\frac{\int e^{-\sum \bar{z}_i a_{ij} z_j} z_k \bar{z}_\ell}{\int e^{-\sum \bar{z}_i a_{ij} z_j}} = -\frac{\partial}{\partial a_{\ell k}} \log\left(\int e^{-\sum \bar{z}_i a_{ij} z_j}\right)$$

$$= \frac{\partial}{\partial a_{\ell k}} \log\det(a_{ij}) = \frac{\ell k\text{-th cofactor}}{\det(a_{ij})} = b_{k\ell} \quad \text{where } (b_{k\ell}) = (a_{ij})^{-1}.$$

We want to determine a so that

$$\frac{\int e^{-\int \bar{\psi} a \psi} \psi(t)\bar{\psi}(t')}{\int e^{-\int \bar{\psi} a \psi}} = \langle T[a(t)a^*(t')]\rangle$$

Since $\left(\frac{d}{dt}+\mu\right) a(t) = 0$ and $aa^* - a^*a = 1$, the latter is the kernel of $\left(\frac{d}{dt}+\mu\right)^{-1}$, so $a = \frac{d}{dt}+\mu$, so

$$\boxed{\frac{\int e^{-\int \bar{\psi}\left(\frac{d}{dt}+\mu\right)\psi} \psi(t)\bar{\psi}(t')}{\int e^{-\int \bar{\psi}\left(\frac{d}{dt}+\mu\right)\psi}} = \langle T[a(t)a^*(t')]\rangle}$$

In the above integrals ψ is a complex-valued function of t and $\bar{\psi}$ is its conjugate. I have forgotten to check that $\frac{d}{dt}+\mu$ has pos. definite hermitian part, but the boundary conditions implicit in the above formula make $\frac{d}{dt}$ skew-hermitian, so the hermitian part is μ which is >0.

The question is how the above path integral compares with the path integral one constructs by the Feynman method for the operator $H_0 = \mu a^* a$. Let's do this in two ways. First we use paths $p(t), q(t)$, and then let's try to [redacted] work out the analogue in the holomorphic functions repn.

Let's recall that the ground state for $\frac{p^2}{2}+\mu^2\frac{q^2}{2}$ is $e^{-\frac{1}{2}\mu x^2}$ which is killed by $\frac{d}{dx}+\mu x = \mu q + ip$. So

$$a = \frac{1}{\sqrt{2\mu}}(\mu q + ip)$$

$$a^* = \frac{1}{\sqrt{2\mu}}(\mu q - ip)$$

$$[a, a^*] = \frac{1}{2\mu}\left([\mu q, -ip] + [ip, \mu q]\right) = 1$$

$$\mu a^* a = \frac{1}{2}\left(\mu^2 q^2 + p^2 + \mu[q, ip]\right) = \frac{p^2+\mu^2 q^2}{2} - \frac{\mu}{2}$$

so $$\langle x | e^{-\varepsilon \frac{p^2}{2}} | x' \rangle = \int \frac{dp}{2\pi}\, e^{-\underbrace{\varepsilon}_{dt} \frac{p^2}{2}} e^{ip\underbrace{(x-x')}_{dx}}$$

hence the Feynman method gives

$$\mathrm{Tr}\, e^{-\beta\left(\frac{p^2}{2}+\frac{1}{2}\mu^2 q^2\right)} = \int \mathcal{D}p\,\mathcal{D}q\; e^{-\int_0^\beta \left[\left(\frac{p^2}{2}+\frac{1}{2}\mu^2 q^2\right) - ip\dot{q}\right] dt}$$

Now if we relate paths $p(t), q(t)$ to path $\psi(t)$ by

$$\psi = \frac{1}{\sqrt{2\mu}}(\mu q + ip)$$

$$\bar{\psi} = \frac{1}{\sqrt{2\mu}}(\mu q - ip)$$

then $$\int \bar{\psi}\left(\frac{d}{dt}+\mu\right)\psi = \int \frac{1}{2\mu}(\mu q - ip)(\mu \dot{q} + i\dot{p}) + \int \mu \frac{1}{2\mu}(\mu^2 q^2 + p^2).$$

[redacted] since $\int q\dot{q} = \int p\dot{p} = \int p\dot{q} + \dot{p}q = 0$ by periodicity, we have

$$\int \bar{\psi}\left(\frac{d}{dt}+\mu\right)\psi = \int \frac{1}{2}\left(p^2+\mu^2 q^2\right) - p\dot{q}$$

hence the agreement is perfect.

2nd method is to compute $e^{-\beta a^* a}$ in the holomorphic representation.