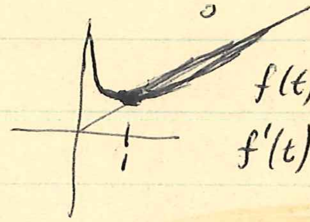
December 24, 1979

thermo formulas 500
spin waves 505 (fermion mistake)
fermion integration: 522-528

Correction terms to Stirling's formula by Feynman graphs.

$$n! = \int_0^\infty e^{-t} t^n \, dt = \int_0^\infty e^{-t + n\log t} \, dt = \int_0^\infty e^{-nt + n\log(nt)} \, n\,dt$$

$$= n e^{n\log n} \int_0^\infty e^{-n(t - \log t)} \, dt$$



$f(t) = t - \log t$

$f'(t) = 1 - \frac{1}{t} = 0$ at $t=1$

$$= n^{n+1} \int_{-1}^\infty e^{-n(1+x-\log(1+x))} \, dx$$

$$= n^{n+1} e^{-n} \int_{-1}^\infty e^{-n\left(+\frac{x^2}{2} - \frac{x^3}{3} + \cdots\right)} \, dx = \overbrace{n^{n+1} e^{-n} \frac{\sqrt{2\pi}}{\sqrt{n}}}^{n^n e^{-n}\sqrt{2\pi n}} \left(1 + O\left(\tfrac{1}{n}\right)\right)$$

The interaction is $+\frac{x^3}{3} - \frac{x^4}{4} + \cdots = 2\frac{x^3}{3!} - 3!\frac{x^4}{4!} + 4!\frac{x^5}{5!} - \cdots\cdots$

Loop formula:

$$l - 1 = \tfrac{1}{2}k_3 + k_4 + \tfrac{3}{2}k_5$$

No connected diagrams with $l=0$, $l=1$. For $l=2$ we have $k_4 = 1$

or $k_3 = 2$

The contribution is is

$$\frac{1}{8}(-6n)\frac{1}{n^2} + \frac{1}{12}(2n)^2\frac{1}{n^3} + \frac{1}{8}(2n)^2\frac{1}{n^3}$$

$$= \frac{1}{n}\left(-\frac{3}{4} + \frac{1}{3} + \frac{1}{2}\right) = \frac{1}{n}\left(-\frac{1}{4} + \frac{1}{3}\right) = \frac{1}{12n}$$

Thus

$$n! = n^n e^{-n}\sqrt{2\pi n} \; e^{\frac{1}{12n} + O\left(\frac{1}{n^2}\right)}$$

but computation of the next term leads to too many diagrams.

December 25, 1979

Summary: I am still trying to understand vertex functions, that is, to find a suitable way of thinking so they appear naturally. A good viewpoint does not seem to arise from the 0-dim case, so I consider a situation closer to the Schwinger-Feynman work, namely, 0+1 space-time dimensions. Thus I consider a generating function given by a path integral

$$\int \mathcal{D}q \; e^{-\int \left(\frac{1}{2}\dot{q}^2 + V(q) - J(t)q\right) dt}$$

The Green's functions which result by functional differentiation with respect to J can be interpreted in terms of the Hamiltonian

$$H = \frac{p^2}{2} + V$$

So let's begin with a review of the formulas. Let's consider first the case where the spectrum of H is discrete, say

$$H|n\rangle = E_n|n\rangle$$

with a non-degenerate ground state. Without needing this assumption, one has

$$\langle q=x \,|\, U_J(t,t') \,|\, q=x' \rangle = \int\limits_{\substack{q(t')=x' \\ q(t)=x}} \mathcal{D}q \; e^{-\int_{t'}^{t} \left(\frac{1}{2}\dot{q}^2 + V(q) - J(t)q\right) dt}$$

where $U_J(t,t')$ is the propagator for the imaginary time Schroed. equation

$$\frac{\partial \psi}{\partial t} = \left(-H + J(t) q\right)\psi .$$

Assuming discrete spectrum we have for $J=0$

$$U(t,t') = e^{-(t-t')H} = \sum_n |n\rangle e^{-(t-t')E_n} \langle n|$$

so that

$$\langle q=x|U(t,t')|q=x'\rangle = \sum_n \underbrace{\langle q=x|n\rangle}_{\varphi_n(x)} e^{-(t-t')E_n} \underbrace{\langle n|q=x'\rangle}_{\overline{\varphi_n(x')}}$$

$$\approx e^{-(t-t')E_0} \varphi_0(x)\overline{\varphi_0(x')} \qquad t-t' \to +\infty$$

$$= \langle 0|U(t,t')|0\rangle \varphi_0(x)\overline{\varphi_0(x')}$$

[redacted] Recall that the ground state eigenfn. doesn't vanish so that $\varphi_0(x) \neq 0$ for all x.

Feynman-Dyson expansion: Dyson's form:

$$U_J(t,t') = U(t,t') + \int_{t'}^{t} dt_1\, U(t,t_1) J(t_1) q\, U(t_1,t')$$

$$+ \int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2\, U(t,t_1) J(t_1) q\, U(t_1,t_2) J(t_2) q\, U(t_2,t')$$

$$+ \cdots\cdots$$

$$\langle x|U_J(t,t')|x'\rangle = \langle x|U(t,t')|x'\rangle + \int_{t'}^{t} dt_1\, J(t_1) \langle x|U(t,t_1) q\, U(t_1,t')|x'\rangle$$

$$+ \cdots$$

The same expansion can be obtained by expanding the J factor of the path integral

$$\int\limits_{\substack{q(t')=x' \\ q(t)=x}} \mathcal{D}q \; e^{-\int_{t'}^{t}\left(\frac{1}{2}\dot{q}^2 + V(q)\right)dt} \sum_{n\geq 0} \frac{1}{n!}\left(\int_{t'}^{t} J(t)q(t)\,dt\right)^n$$

$$= \int \mathcal{D}q \, e^{-\int \frac{1}{2}\dot{q}^2 + V} + \int_{t'}^{t} dt_1 \, J(t_1) \int \mathcal{D}q \, e^{-\int(\frac{1}{2}\dot{q}^2 + V(q))dt} q(t_1) + \cdots$$

If we put

$$\langle T[q(t_1)\cdots q(t_k)]\rangle = \frac{\int \mathcal{D}q \, e^{-\int(\frac{1}{2}\dot{q}^2+V)} q(t_1)\cdots q(t_k)}{\int \mathcal{D}q \, e^{-\int(\frac{1}{2}\dot{q}^2+V)}}$$

then we can write Dyson's expansion as

$$\frac{\langle x | U_J(t,t') | x' \rangle}{\langle x | U(t,t') | x' \rangle} = \sum_{k\geq 0} \frac{1}{k!} \int dt_1 \cdots dt_k \, J(t_1)\cdots J(t_k) \langle T[q(t_1)\cdots q(t_k)]\rangle$$

These formulas make sense without assuming the spectrum is discrete. Assume there is a non-degenerate discrete ground state $|0\rangle$ and take the limit as $t \to \infty$, $t' \to -\infty$. Then the Green's functions become in the limit

$$G(t_1, \ldots, t_k) = \frac{\langle 0 | U(T, t_1) q \, U(t_1, t_2) q \cdots U(t_k, -T) | 0 \rangle}{\langle 0 | U(T, -T) | 0 \rangle}$$

where $t_1 \geq \cdots \geq t_k$ and T is large

Digression: Let's think à la Feynman and concentrate on computing the Green's function

$$G(t_a, t_b) = \frac{\delta^2}{J(t_a) J(t_b)} \langle x | U_J(t,t') | x' \rangle \Big|_{J=0} \Big/ \langle x | U(t,t') | x' \rangle$$

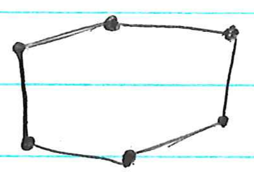
$$= \frac{\langle x \,|\, U(t,t_a)\, q\, U(t_a,t_b)\, q\, U(t_b,t') \,|\, x' \rangle}{\langle x \,|\, U(t,t') \,|\, x' \rangle}$$

when $H = \underbrace{\frac{p^2}{2}}_{H_0} + V$. For example, suppose $V = \frac{1}{2}\omega^2 x^2$.

This Green's function is a sum of terms indexed by diagrams. Look at the denominator first

$$\langle x | U(t,t') | x' \rangle = \int_{\substack{q(t')=x' \\ q(t)=x}} \mathcal{D}q \; e^{-\int \frac{1}{2}\dot{q}^2} \sum_{n \geq 0} \frac{(-1)^n}{n!} \left(\int \frac{1}{2!}\omega^2 q(t)^2 \right)^n$$

Suppose $x' = x = 0$. Then $\int \frac{1}{2}\dot{q}^2\, dt$ is a homogeneous quadratic function on the vector space of paths, so I can use Wick's thm. Let $G_0 = (-\Delta)^{-1}$ for fns. vanishing at t, t'. In this case the vertices have mult. 2, so the connected diagrams are loops



symmetry factor $\frac{1}{2n}$. So we get

$$\langle \underset{0}{\overset{}{x}} | U(t,t') | \underset{0}{x'} \rangle = \langle \underset{0}{x} | e^{-(t-t')\frac{p^2}{2}} | \underset{0}{x'} \rangle \, e^{\sum_{n \geq 1} \frac{1}{2n}(-\omega^2)^n \, \mathrm{tr}(G_0^n)}$$

January 27, 1979

Fermi gas: Consider a box of volume $V = L^3$ and a gas of scalar fermions in the box. The 1-particle eigenfunctions for $H = \frac{p^2}{2}$ are (assuming periodic bdry conditions)

$$u_{\mathbb{k}} = \frac{1}{\sqrt{V}} e^{-i\mathbb{k}\cdot x} \qquad \text{where } \mathbb{k} \in \left(\frac{2\pi}{L}\mathbb{Z}\right)^3$$

and $\quad H u_{\mathbb{k}} = \varepsilon_{\mathbb{k}} u_{\mathbb{k}} \qquad \varepsilon_{\mathbb{k}} = \frac{\mathbb{k}^2}{2}$. The N-particle Hilbert space is $\Lambda^N \mathcal{H}_1$ where $\mathcal{H}_1 = L^2(\text{box}) =$ 1-particle space. The N-particle eigenfunctions for H are

$$V^{-N/2}\, u_{\mathbb{k}_1} \wedge \cdots \wedge u_{\mathbb{k}_N} \qquad \mathbb{k}_1 < \cdots < \mathbb{k}_N$$

where we linearly order the $\mathbb{k}$ so that $\varepsilon_{\mathbb{k}}$ increases. The ground energy is

$$\varepsilon_{\mathbb{k}_1} + \cdots + \varepsilon_{\mathbb{k}_N}$$

Now we want to take the limit as $N, V \to \infty$. In order to obtain the ground state we fill up the energy levels in order, and since $\varepsilon_{\mathbb{k}} = \frac{k^2}{2}$ we get roughly a sphere in $\mathbb{k}$ spaces. A better parameter to describe what's happening is the radius k_F rather than N. Then

$$N = \sum_{|k|<k_F} 1 \approx \frac{V}{(2\pi)^3} \,\text{vol sphere radius } k_F = \frac{V}{(2\pi)^3} \frac{4}{3}\pi k_F^3$$

so requiring $\frac{N}{V}$ ~~to~~ have a limit as $N, V \to \infty$ is the same as fixing k_F. Also

$$E = \sum_{|k|<k_F} \varepsilon_k \approx \frac{V}{(2\pi)^3} \int_0^{k_F} \frac{k^2}{2} 4\pi k^2\, dk$$

so we have

$$\lim \frac{N}{V} = \frac{1}{(2\pi)^3} \frac{4}{3}\pi k_F^3$$

$$\lim \frac{E}{V} = \frac{1}{(2\pi)^3} 2\pi \frac{k_F^5}{5}$$

and the energy per particle is

$$\lim \frac{E}{N} = \frac{3}{10} k_F^2 = \frac{3}{5} \cdot \frac{k_F^2}{2}$$

which is $\frac{3}{5}$ the Fermi energy.

The preceding describes the ground state or 0-temperature situation. Next consider positive temperature. The partition function for N-particles is

$$Z_N = \sum_{k_1 < \cdots < k_N} e^{-\beta \sum \varepsilon_{k_i}}$$

but it is more convenient to work with the grand partition function which has a product expansion

$$Z_{gr} = \sum_{N \geq 0} z^N Z_N = \prod_{k} (1 + z e^{-\beta \varepsilon_k})$$

Then
$$Z_N = \frac{1}{2\pi i} \oint Z_{gr} \, z^{-N-1} \, dz.$$

Instead of the grand energy we want the internal energy

$$U = -\frac{\partial}{\partial \beta} \log Z_N = -\frac{\frac{\partial}{\partial \beta} \oint Z_{gr} \, z^{-N} \frac{dz}{z}}{\oint Z_{gr} \, z^{-N} \frac{dz}{z}}$$

Now recall that we want to take the limit as $N, V \to \infty$ with N/V const.

[redacted] Notice also that

$$\frac{1}{V} \log Z_{gr} = \frac{1}{V} \sum_{k} \log\left(1 + z e^{-\beta k^2/2}\right)$$

$$\longrightarrow \frac{1}{(2\pi)^3} \int_0^\infty \log\left(1 + z e^{-\beta k^2/2}\right) 4\pi k^2 \, dk$$

Consequently the integral

$$\oint Z_{gr} \, z^{-N} \frac{dz}{z} = \oint e^{N\left(\frac{1}{N} \log Z_{gr} - \log z\right)} \frac{dz}{z}$$

ought to be able to be evaluated by the saddle point method. The peak occurs at that z for which

$$\frac{d}{dz}\left(\lim \frac{V}{N} \frac{\log Z_{gr}}{V}\right) = \frac{1}{z}$$

or

$$\frac{N}{V} \; [redacted] = \int_0^\infty \frac{z e^{-\beta k^2/2}}{1 + z e^{-\beta k^2/2}} \, 4\pi k^2 \frac{dk}{(2\pi)^3}$$

This z should be the same as the one you get using Z_{gr} as the partition fn. and adjusting z so that

$$N \; [redacted] = \frac{\sum N z^N Z_N}{\sum z^N Z_N} = z \frac{d}{dz} \log Z_{gr}$$

which [redacted]. Formula recorded for latter use:

$$\boxed{\frac{N}{V} = z \frac{d}{dz}\left(\frac{1}{V} \log Z_{gr}\right)}$$

should put lims on both sides

Let's return to the internal energy

$$U = -\frac{\partial}{\partial \beta} \log Z_N = \frac{-\int \frac{\partial Z_{gr}}{\partial \beta} \frac{1}{Z_{gr}} \, Z_{gr} z^{-N} \frac{dz}{z}}{\int Z_{gr} \, z^{-N} \frac{dz}{z}}$$

As $N, V \to \infty$ the measure $Z_{gr}\, z^{-N} \frac{dz}{z}$ peaks around the point z we've determined so we get

$$\boxed{\left(\frac{U}{V}\right) = -\frac{\partial}{\partial\beta}\left(\frac{1}{V}\log Z_{gr}\right)}$$

For the Fermi gas

$$\frac{U}{V} = \int_0^\infty \frac{z e^{-\beta k^2/2}}{1 + z e^{-\beta k^2/2}}\, 2\pi k^4 \frac{dk}{(2\pi)^3}.$$

What is the pressure? Normally

$$Z = \sum e^{-\beta E_j(V)}$$

$$p = \sum \left(-\frac{\partial E_j}{\partial V}\right) e^{-\beta E_j(V)} \frac{1}{Z} = +\frac{1}{\beta}\frac{\partial}{\partial V}\log Z$$

so in our case

$$p = \frac{1}{\beta}\frac{\partial}{\partial V}\log Z_N = \frac{1}{\beta}\frac{\oint \frac{\partial Z_{gr}}{\partial V} z^{-N}\frac{dz}{z}}{\oint Z_{gr}\, z^{-N}\frac{dz}{z}}$$

$$\approx \frac{1}{\beta}\frac{\partial}{\partial V}\log Z_{gr}$$

$$\approx \frac{1}{\beta}\frac{\log Z_{gr}}{V} \qquad \text{because } \lim \frac{\log Z_{gr}}{V} \text{ exists}$$

So

$$\boxed{p = \frac{1}{\beta V}\log Z_{gr}}$$

for grand canonical ensemble

December 28, 1979:

Fermi's version of the thermodynamic formulas:

$$Z \overset{def}{=} \sum e^{-\beta E_n}$$

$$U \overset{def}{=} \sum E_n \frac{e^{-\beta E_n}}{Z} = -\frac{d}{d\beta} \log Z$$

$$S \overset{defn.}{=} \int \frac{dU}{T} = k\int \beta dU = k\left(\beta U - \int U d\beta\right)$$

$$\therefore \quad \frac{S}{k} = \beta U + \log Z$$

is the Legendre transform of $-\log Z$ wrt β

Also

$$F \overset{defn}{=} U - TS$$

$$= U - T(k\beta U + k \log Z) = -\frac{1}{\beta} \log Z$$

so that $Z = e^{-\beta F}$. The only other result is that

$$[redacted] \; -\sum p_n \log p_n = -\sum(-\beta E_n - \log Z) p_n = \beta U + \log Z.$$

or

$$\frac{S}{k} = -\sum p_n \log p_n$$

statistical interpretation of entropy

December 29, 1979

Goal: To find a good model of interacting fermions where one can see things happening. It should start with a Fock space or exterior algebra constructed from a 1-particle space having a basis of momentum eigenfunctions. The interaction should be understandable in terms of scattering between 1-particle states. We should also be able to take a infinite limit as $N, V \to \infty$. But before one takes the limit one ought to notice the features of the fixed but large N situation. The point is that even though the one and 2 particle situation is fairly simple, at high N things become complicated. One is interested in the ground state and fluctuations around it, i.e. "quasi-particles".

Question: Can you work with the Ising model at zero temperature? For each magnetization $\sum s_i = M$ one has a minimum energy. The question is whether I can handle this constraint "thermo-dynamically" i.e. by a Lagrange multiplier business. Thus instead of

$$\min \{ E_s \mid \sum s_i = M \}$$

I would like

$$\lim_{\beta \to \infty} -\frac{1}{\beta} \log \overbrace{\left(\sum_s e^{-\beta E_s + \beta H \sum s_i} \right)}^{Z(\beta, H)}$$

where H is adjusted so that $\frac{1}{\beta}\frac{\partial}{\partial H} \log Z = M$

December 30, 1979

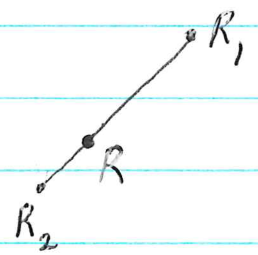
Suppose we have particles m_1 at R_1, m_2 at R_2 with aqual and opposite forces. Then

$$m_1 \ddot{R}_1 = - m_2 \ddot{R}_2 \qquad \text{or} \qquad (m_1 R_1 + m_2 R_2)^{\cdot\cdot} = 0$$

which means that the center of mass

$$R = \frac{m_1 R_1 + m_2 R_2}{m_1 + m_2}$$

has constant velocity. Set $\vec{r} = R_1 - R_2$ and think of $m_2 > m_1$. Let's compute the KE in terms of R, r.



$$R = \frac{m_1 R_1 + m_2 (R_1 - r)}{m_1 + m_2} = R_1 - \frac{m_2}{m_1 + m_2} r$$

$$R_1 = R + \frac{m_2}{m_1 + m_2} r$$

$$R_2 = R - \frac{m_1}{m_1 + m_2} r$$

Set $M = m_1 + m_2$

$$KE = \frac{1}{2} m_1 \left(\dot{R} + \frac{m_2}{M} \dot{r} \right)^2 + \frac{1}{2} m_2 \left(\dot{R} - \frac{m_1}{M} \dot{r} \right)^2$$

$$= \frac{1}{2} M \dot{R}^2 + \frac{1}{2} \underbrace{\frac{m_1 m_2}{m_1 + m_2}}_{\text{reduced mass}} \dot{r}^2$$

reduced mass $= \dfrac{m_1}{1 + \frac{m_1}{m_2}}$ ← reducing factor

If the ~~potential~~ forces on the particle is derived from a potential energy function of the form $V(R_1 - R_2)$, the Lagrangian in the R, r coord system is

$$L = \frac{1}{2} M \dot{R}^2 + \frac{1}{2} m_{red} \dot{r}^2 - V(r)$$

so
$$P = \frac{\partial L}{\partial \dot{R}} = M\dot{R} \qquad p = \frac{\partial L}{\partial \dot{r}} = m_{red}\dot{r}$$

and
$$H = \frac{P^2}{2M} + \frac{p^2}{2m_{red}} + V(r)$$

Let's consider next 2 particles of mass 1 with position coordinates x_1, x_2 with motion governed by the Hamiltonian

$$H = \frac{p_1^2}{2} + \frac{p_2^2}{2} + V(x_1 - x_2)$$

$$= \left(\frac{p_1+p_2}{2}\right)^2 + \left(\frac{p_1-p_2}{2}\right)^2 + V(x_1 - x_2)$$

Set $P = p_1 + p_2$. Then $[P, H] = 0$ so P, H can be simultaneously diagonalized. Let $\psi(x_1, x_2)$ be a wave function which is an eigenfunction for P with eigenvalue k:

$$P\psi = \left(\frac{1}{i}\frac{\partial}{\partial x_1} + \frac{1}{i}\frac{\partial}{\partial x_2}\right)\psi = k\psi$$

Then clearly
$$\psi(x_1, x_2) = e^{ik\left(\frac{x_1+x_2}{2}\right)} \tilde{\psi}(x_1, x_2)$$

where
$$P\tilde{\psi} = 0$$

The last condition is equivalent to $\tilde{\psi}$ being a function of $x_1 - x_2$. So

$$\psi(x_1, x_2) = e^{ik\left(\frac{x_1+x_2}{2}\right)} \tilde{\psi}(x_1 - x_2)$$

and

$$\frac{p_1-p_2}{2}\psi = e^{ik\left(\frac{x_1+x_2}{2}\right)} \frac{1}{2}\frac{1}{i}(\partial_{x_1}-\partial_{x_2})\tilde{\varphi}(x_1-x_2)$$

$$= e^{ik\left(\frac{x_1+x_2}{2}\right)} \frac{1}{i}(\nabla\tilde{\varphi})(x_1-x_2)$$

If we put $r = x_1 - x_2$ and $p = \frac{p_1-p_2}{2}$, then

$$H\psi = \left(\frac{k^2}{4} + p^2 + V(r)\right) e^{ik\left(\frac{x_1+x_2}{2}\right)}\tilde{\varphi}(r)$$

$$= e^{ik\left(\frac{x_1+x_2}{2}\right)}\left(\frac{k^2}{4} + -\nabla_r^2 + V(r)\right)\tilde{\varphi}(r).$$

Hence one is effectively reduced to understanding the operator $-\nabla_r^2 + V(r)$ on functions of r.

Notice that $\psi(x_2,x_1) = -\psi(x_1,x_2)$ means that $\tilde{\varphi}$ is odd:

$$\tilde{\varphi}(-r) = \tilde{\varphi}(r)$$

Of course we want $V(r) = V(-r)$ in order that H operate on anti-symmetric wave functions.

Next check that if one is working in a box [redacted] with periodic boundary conditions, then [redacted] things are OK. So suppose $\psi(x_1,x_2)$ is periodic in both x_1, x_2. Then adding the same period to x_1, x_2 doesn't change $\tilde{\varphi}$, and so we see k belongs to the dual lattice for the box. [redacted] Adding a period γ to x_1 and $-\gamma$ to x_2 shows that $\tilde{\varphi}$ is periodic for 2γ. Adding γ to x_1 and 0 to x_2 shows $\psi(r+\gamma) = \pm\psi(r)$ where the sign is $e^{ik\frac{\gamma}{2}}$.

In the situation I want to concentrate on, V will be a function of $|x|$ supported in an interval about 0 which is sufficiently small relative to the periods.

December 31, 1979

Look at Heisenberg chain. There is a site for each $n \in \mathbb{Z}/N\mathbb{Z}$ and a 2-dimensional spin space belonging to each site. The Hilbert space $\mathcal{H}$ is the tensor product of these spin spaces. It is therefore the exterior algebra on a vector space with orth basis e_n, $n \in \mathbb{Z}/N\mathbb{Z}$. $\mathcal{H}$ has an orthonormal basis given by spin assignments $s : (\mathbb{Z}/N\mathbb{Z}) \longrightarrow \pm 1$, and e_n corresponds to the s with one $-$ at the site n.

It might be convenient to eventually allow the lattice spacing to go to zero, so let the set of sites be $a\mathbb{Z}/Na\mathbb{Z}$.

The Hamiltonian on $\mathcal{H}$ is essentially given by $\sum_n P^{ex}_{n,n+a}$ where $P^{ex}_{n,n+a}$ exchanges the spins at the $n, n+a$ sites. The good choice for H seems to be

$$H = \sum_n \underbrace{\frac{1}{2}\left(1 - P^{ex}_{n,n+a}\right)}$$

this gives 0 when "support" of s doesn't meet $\{n, n+a\}$.

Then

$$He_n = \left\{\frac{1}{2}\left(1 - P^{ex}_{n,n+a}\right) + \frac{1}{2}\left(1 - P^{ex}_{n-a,n}\right)\right\} e_n$$

$$= e_n - \frac{1}{2}e_{n+a} - \frac{1}{2}e_{n-a}$$

so we get our familiar J-matrix. If we use the basis for the "1-particle" space $\mathcal{H}^1$ (spanned by the e_n) given by

$$u_k = \frac{1}{\sqrt{N}} \sum_n{}' e^{ikn} e_n \qquad k \in \frac{2\pi}{aN}\mathbb{Z} \Big/ \frac{2\pi}{a}\mathbb{Z}$$

Then

$$H u_k = \underbrace{\left(1 - \tfrac{1}{2} e^{-ika} - \tfrac{1}{2} e^{ika}\right)}_{\varepsilon_k \,=\, 1-\cos(ka) \;\approx\; \frac{1}{2}a^2k^2} u_k$$

Hence we want to divide by a^2 in order to have a good limit as the lattice spacing goes to 0.

The next thing I want to do is to understand H on the "2-particle" space $\mathcal{H}^2$ spanned by the $e_m \wedge e_n$. Let's compute $H(e_m \wedge e_n)$. First suppose $m+a<n$, so that

$$e_m \wedge e_n : \quad \cdots + + \overset{m}{-} \overset{m+a}{+} \overset{n}{-} + \cdots$$

Then in the sum $H = \sum_k{}' \frac{1}{2}(1 - P^{ex}_{k,k+a})$ we have contributions from $k = m-a, m, n-a, n$ and we get

$$H(e_m \wedge e_n) = \tfrac{1}{2} e_m \wedge e_n - \tfrac{1}{2} e_{m-a,n} + \tfrac{1}{2} e_m \wedge e_n - \tfrac{1}{2} e_{m+a} \wedge e_n$$
$$+ \tfrac{1}{2} e_m \wedge e_n - \tfrac{1}{2} e_m \wedge e_{n-a} + \tfrac{1}{2} e_m \wedge e_n - \tfrac{1}{2} e_m \wedge e_{n+a}$$
$$= (He_m) \wedge e_n + e_m \wedge (He_n)$$

Next suppose $m+a=n$

$$e_m \wedge e_{m+a} : \quad \cdots + + \overset{m}{-} \overset{m+a}{-} + + \cdots$$

Then in the sum for H we get contributions for $k = m-a, m+a$

and we have

$$H(e_m \wedge e_{m+a}) = \tfrac{1}{2} e_m \wedge e_{m+a} - \tfrac{1}{2} e_{m-a} \wedge e_{m+a}$$
$$+ \tfrac{1}{2} e_m \wedge e_{m+a} - \tfrac{1}{2} e_m \wedge e_{m+2a}$$

$$= He_m \wedge e_{m+a} + e_m \wedge He_{m+a} - e_m \wedge e_{m+a}$$

Thus we have on $\mathcal{H}^2 = \Lambda^2 \mathcal{H}^1$ that

$$H = H_0 - H'$$

where H_0 is the derivation extending H on $\mathcal{H}^1$ and where H' projects onto the subspace spanned by the $e_m \wedge e_{m+a}$.

Consider now an element of $\mathcal{H}^2$:

$$\psi = \tfrac{1}{2} \sum_{m,n} \psi(m,n)\, e_m \wedge e_n \qquad \psi(m,n) = -\psi(n,m)$$

Let's assume ψ is an eigenfunction for translation $e_m \mapsto e_{m+1}$ so that

$$\psi(m+1, n+1) = e^{-i\alpha} \psi(m,n)$$

Then we have $\psi(m,n) = e^{i\left(\frac{m+n}{2}\right)\alpha}\, \tilde{\psi}(m-n)$ where $\tilde{\psi}(-n) = -\tilde{\psi}(n)$. Then

$$H_0 \psi = \tfrac{1}{2} \sum_{m,n} \psi(m,n) \Big(-\tfrac{1}{2} e_{m-1} \wedge e_n + e_m \wedge e_n - \tfrac{1}{2} e_{m+1} \wedge e_n$$
$$- \tfrac{1}{2} e_m \wedge e_{n-1} + e_m \wedge e_n - \tfrac{1}{2} e_m \wedge e_{n+1} \Big)$$

$$= \tfrac{1}{2} \sum_{m,n} \begin{pmatrix} -\tfrac{1}{2}\psi(m+1,n) + \psi(m,n) - \tfrac{1}{2}\psi(m,n-1) \\ -\tfrac{1}{2}\psi(m,n+1) + \psi(m,n) - \tfrac{1}{2}\psi(m,n+1) \end{pmatrix} e_m \wedge e_n$$

$$= \tfrac{1}{2} \sum_{m,n} \begin{pmatrix} -\tfrac{1}{2} e^{i\alpha} \tilde{\psi}(m-n+1) + \tilde{\psi}(m-n) - \tfrac{1}{2} e^{-i\alpha} \tilde{\psi}(m-n+1) \\ -\tfrac{1}{2} e^{i\alpha} \tilde{\psi}(m-n-1) + \tilde{\psi}(m-n) - \tfrac{1}{2} e^{-i\alpha} \tilde{\psi}(m-n-1) \end{pmatrix} e^{i\frac{m+n}{2}\alpha} e_m \wedge e_n$$

$$= \frac{1}{2} \sum_{m,n} e^{i\left(\frac{m+n}{2}\right)\alpha} \left(-\cos\alpha\, \tilde{\psi}(m-n+1) + 2\tilde{\psi}(m-n) - \cos\alpha\, \tilde{\psi}(m-n-1)\right) e_m \wedge e_n$$

$$= (2-2\cos\alpha)\psi + 2\cos\alpha \; \frac{1}{2} \sum_{m,n} e^{i\left(\frac{m+n}{2}\right)\alpha} \left(-\tfrac{1}{2}\tilde{\psi}(m-n+1) + \tilde{\psi}(m-n) - \tfrac{1}{2}\tilde{\psi}(m-n-1)\right) e_m \wedge e_n$$

<u>Check</u>: If $\tilde{\psi}$ is an eigenfunction for ↑ with eigenvalue $1-\cos\beta$, then H_0 has the eigenvalue

$$2 - 2\cos\alpha + 2\cos\alpha(1-\cos\beta)$$

$$= 2 - 2\cos\alpha\cos\beta = 2 - \left(\cos\frac{\alpha+\beta}{2} + \cos\frac{\alpha-\beta}{2}\right)$$

$$= \left(1 - \cos\left(\frac{\alpha+\beta}{2}\right)\right) + \left(1 - \cos\left(\frac{\alpha-\beta}{2}\right)\right)$$

which is the sum of two 1-particle energies.

Let's now suppose $H\psi = \lambda\psi$

$$[\lambda-(2-2\cos\alpha)] \frac{1}{2} \sum e^{i\left(\frac{m+n}{2}\right)\alpha} \tilde{\psi}(m-n) e_m \wedge e_n = 2\cos\alpha \; \frac{1}{2} \sum e^{i\left(\frac{m+n}{2}\right)\alpha} (J\tilde{\psi}(m-n)) e_m \wedge e_n$$

$$- \underbrace{H'\psi}$$

$$\sum_m e^{i\left(\frac{2m+1}{m}\right)\alpha} \tilde{\psi}(+1) e_{m+1} \wedge e_m$$

This gives

$$(2\cos\alpha)\left[-\tfrac{1}{2}\tilde{\psi}(m+1) + \tilde{\psi}(m) - \tfrac{1}{2}\tilde{\psi}(m-1)\right] = [\lambda - (2-2\cos\alpha)]\tilde{\psi}(m)$$

for $m \neq 1, -1$

and it equals $[\lambda - (2-2\cos\alpha)]\tilde{\psi}(1) + \tilde{\psi}(1)$

for $m = 1$.