Physics 307

Mathematical Physics

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Partial Differential Equations II

4.1 Taxonomy ✓

4.2 Wave Equation ✓

4.3 Diffusion Equation

4.4 Laplace Equation

Answering Ivan's Question

Diffusion Equation

The diffusion equation is a partial differential equation
which describes density dynamics in a material undergoing diffusion

Heat flow is a particular case of diffusive behavior
in which the collective diffusion coefficient is constant

4.3.1. Heat flow

Heat equation is a parabolic partial differential equation
which describes distribution of heat in a given region over time
(or variation in temperature)

Consider a long thin bar of heat conducting material

Length coordinate may be taken to be x

Let σ be the specific heat per unit length
(i.e. the capacity of a unit length of the material to hold heat)
and κ the heat conductivity

Let us assume that temperature in the subinterval $I_k = [x_{k-1}, x_k]$
at a given time t
can be adequately approximated by scalar function $u_k(t)$

Heat contained in I_k is then $\Delta x \, \sigma \, u_k(t)$ ☛ $\Delta x = x_k - x_{k-1}$

The heat conductivity coefficient expresses relationship between rate of flow of heat & temperature differential per unit length u_x

Since our model is spatially discrete so far

we approximate $u_x(x_k)$ by $[u_k(t) - u_{k-1}(t)]/\Delta x$

Rate of heat flow emanating from I_k is ☛ $\Delta x\,\sigma\, du_k/dt$

while flow of heat into I_k $\begin{cases} \text{from } I_{k+1} \text{ is ☛ } \kappa\,[u_{k+1}(t) - u_k(t)]\,/\Delta x \\ \text{from } I_{k-1} \text{ is ☛ } \kappa\,[u_{k-1}(t) - u_k(t)]\,/\Delta x \end{cases}$

Assuming heat is conserved we obtain

$$\Delta x\,\sigma\,\frac{du_k}{dt} = \frac{\kappa}{\Delta x}\,[u_{k+1}(t) - 2u_k(t) + u_{k-1}(t)] \qquad (4.3.112.)$$

Dividing by Δx we have

$$\sigma\,\frac{du_k}{dt} = \kappa\,\frac{u_{k+1}(t) - 2u_k(t) + u_{k-1}(t)}{(\Delta x)^2} \qquad (4.3.113.)$$

If we assume actual heat distribution is a function $u(x,t)$

fraction on right ☛ a second difference divided by $(\Delta x)^2$

may be regarded as an approximation to u_{xx}

In limit $\Delta x \to 0$ ☛ we obtain the partial differential equation

$$u_t(x,t) - \alpha\, u_{xx}(x,t) = 0 \qquad (4.3.114.)$$

with $\alpha = \kappa/\sigma > 0$

If there are external heat sources or losses which can be represented by a function $f_\sigma(x,t)$

equation is augmented to more general form

$$u_t(x,t) - \alpha u_{xx}(x,t) = \overline{f}_\sigma(x,t) \qquad (4.3.115.)$$

Both (4.3.114.) and (4.3.115.)

are valid for arbitrary number of space dimensions

4.3.2. Diffusion in an infinitely long metal bar

Let us first study initial value problem of heat flow on an infinite bar $-\infty < x < \infty$

The system is described by (4.3.114.)
and we assume initial heat distribution $u(x,0) = f(x)$ (4.3.116.)
is at least piecewise continuous as a function of x

Fourier transform of solution is

$$\hat{u}(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x,t)\, e^{-ikx}\, dx \qquad (4.3.117.)$$

and so

$$u(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{u}(k,t)\, e^{ikx}\, dx \qquad (4.3.118.)$$

Substituting (4.3.117.) and (4.3.118.) into (4.3.114.) we obtain

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{u}_t(k,t) e^{ikx} dk + \frac{\alpha}{\sqrt{2\pi}} \int_{-\infty}^{\infty} k^2 \hat{u}(k,t) e^{ikx} dk = 0$$

(4.3.119.)

regrouping terms (4.3.119.) becomes

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \left[\hat{u}_t(k,t) + \alpha\ k^2 \hat{u}(k,t)\right] e^{ikx} dk = 0$$

(4.3.120.)

Given that Fourier transform of bracket is zero

bracket must cancel ☛ $\hat{u}_t(k,t) + \alpha k^2 \hat{u}(k,t) = 0$ (4.3.121.)

Solution of (4.3.121.) is found to be

$$\hat{u}(k,t) = \hat{f}(k) e^{-\alpha k^2 t}$$

(4.3.122.)

Let us now reconstruct full solution by inverse Fourier transform

$$u(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}(k)\ e^{-\alpha k^2 t} e^{ikx} dk \qquad (4.3.123.)$$

Function $\hat{f}(k)$ so far undetermined

is specified by imposing initial condition

$$u(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}(k)\ e^{ikx} dk = f(x) \qquad (4.3.124.)$$

$\hat{f}(k)$ is Fourier transform of initial temperature distribution

Thus ☛

$$\begin{aligned} u(x,t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{-a^2 k^2 t} e^{ikx} \int_{-\infty}^{\infty} dx' f(x') e^{-ikx'} \\ &= \int_{-\infty}^{\infty} dx'\ K(x-x',t) f(x') \qquad (4.3.125.) \end{aligned}$$

with $$K(x-x',t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ik(x-x')-\alpha k^2 t} \qquad (4.3.126.)$$

This is one integral that we can solve explicitly

so we turned out our problem completely

Before calculating the explicit expression of K

we verify that $K(x,t)$ is the fundamental solution

in sense that it satisfies

$$K_t(x,t) = \alpha K_{xx}(x,t), \quad \text{with} \quad K(x,0) = \delta(x) \qquad (4.3.127.)$$

Note that if $f(x) = \delta(x)$ then

$$\begin{aligned} u(x,t) &= \int_{-\infty}^{\infty} K(x-x',t)\ f(x')dx' \\ &= \int_{-\infty}^{\infty} K(x-x',t)\ \delta(x')dx' \\ &= K(x,t) \qquad (4.3.128.) \end{aligned}$$

Therefore ☛ K is response at any point and any time

to an initial distribution of unitary temperature

concentrated on a single point

To determine explicit form of K we complete square in exponent

$$\begin{aligned}\exp[ikx-\alpha k^2 t] &= \exp\left[-\left(\alpha k^2 t - ikx - \frac{x^2}{4\alpha t}\right)\right]\,\exp\left[-\frac{x^2}{4\alpha t}\right] \\ &= \exp\left[-\left(\frac{ix}{\sqrt{4\alpha t}} - k\sqrt{\alpha t}\right)^2\right]\,\exp\left[-\frac{x^2}{4\alpha t}\right]\end{aligned}$$

yielding

$$\begin{aligned}K(x,t) &= \frac{e^{-x^2/(4\alpha t)}}{2\pi}\int_{-\infty}^{\infty} e^{-\left(ix/\sqrt{4\alpha t}-k\sqrt{\alpha t}\right)^2}\,dk \\ &= \frac{e^{-x^2/(4\alpha t)}}{\sqrt{\alpha\, t}\;\;2\pi}\int_{-\infty}^{\infty} e^{-z^2}dz \qquad (4.3.129.)\end{aligned}$$

with $z=\sqrt{\alpha t}-ix/\sqrt{4\alpha t}$ and $dz=\sqrt{\alpha t}\,dk$

We then have to compute integral $\quad I=\int_{-\infty}^{\infty} e^{-z^2}dz$

not over real axis ☛ but displaced on imaginary axis to $-x/\sqrt{4\alpha t}$

However ☛ given that e^{-z^2} is analytical in entire plane

$I = \int_{-\infty}^{\infty} e^{-z^2} dz$ gives the same integrate along real axis

$$\int_{-\infty}^{\infty} e^{-z^2}\, dz = \int_{-\infty}^{\infty} e^{-\zeta^2}\, d\zeta, \quad \zeta \in \mathbb{R} \qquad (4.3.130.)$$

This integral is easily solved in polar coordinates

$$\begin{aligned} I^2 &= \int_{-\infty}^{\infty} d\zeta\, e^{-\zeta^2} \int_{-\infty}^{\infty} d\eta\, e^{-\eta^2} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d\zeta\, d\eta\, e^{-(\zeta^2+\eta^2)} \\ &= \int_0^{\infty}\int_0^{2\pi} r\, dr\, d\phi\, e^{-r^2} = 2\pi \int_0^{\infty} r\, dr\, e^{-r^2} = \pi \int_0^{\infty} du\, e^{-u} = \pi \end{aligned}$$

Finally ☛ $I = \sqrt{\pi}$ and (4.3.129.) becomes

$$K(x,t) = \frac{1}{\sqrt{4\alpha\pi t}}\, e^{-x^2/(4\alpha t)}, \quad t > 0 \qquad (4.3.131.)$$

$K(x-x',t)$ is response function of heat equation
for an infinite bar

It describes temperature $u(x,t)$ at position x and time $t>0$
for an initial temperature distribution $u(x,0)=\delta(x-x')$
located at x'

As a consequence of this description $K(x-x',t)$
is referred to as heat kernel

It follows a Gaussian distribution centered at $x=x'$
that spreads over time with standard deviation $\sigma(t)=\sqrt{2\alpha t}$

Since total heat is conserved
using normalization of initial condition $\int_{-\infty}^{+\infty}\delta(x-x')dx=1$

we obtain $\forall t$ ☛ $\int_{-\infty}^{\infty}K(x,t)\,dx=1$ (4.3.132.)

With increasing t ☛ heat kernel flattens and spreads preserving its area

For a fix $x \neq 0, K(x,t)$ has a maximum at $t_0 = x^2/(2\alpha)$

with $K(x,t_0) = 1/(\sqrt{2\pi}x)$

decreasing then as $t^{-1/2}$ for $t \to \infty$

Note also that if $t > 0, K(x,t) \neq 0 \; \forall x \neq 0$

which indicates an infinite speed of heat transmission

(4.2.114.) is clearly not invariant under Lorentz transformations

(as opposed to wave equation)

However ☛ $K(x,t)$ is very small for $x \gg \sigma(t)$

Example 4.3.1.

For $u(x,0) = A\ \cos(kx) = A\ \Re\mathrm{e}\ [e^{ikx}]$

it follows that

$$u(x,t) = A\ \Re\mathrm{e}\ [e^{ikx-\alpha k^2 t}] = A\ \cos(kx)\ e^{-\alpha k^2 t} \qquad (4.3.133.)$$

General solution (4.3.125.) is therefore
"sum" of elementary solutions for initial conditions $u(x,0) = \hat{u}(k,0)$

Note that initial spatial fluctuations of temperature
decay much more rapidly for higher frequency k

If $k = 0, u(x,t) = A$

Example 4.3.2.

For $u(x,0) = A\ e^{-x^2/r}/\sqrt{\pi r}$, with $r > 0$

(Gaussian initial distribution of temperatures)

it follows that

$$u(x,t) = A\frac{e^{-x^2/(r+4\alpha t)}}{\sqrt{\pi(r+4\alpha t)}} = AK(x,t+t_0), \quad t_0 = \frac{r}{4\alpha}$$

Temperature distribution remains Gaussian $\forall t > 0$

If $r \to 0^+$ then $u(x,t) \to AK(x,t)$

4.3.3. Diffusion in a finite metal bar

(i) Homogeneous equation

Consider evolution of temperature $u(x,t)$ in a bar of finite length L

with boundary conditions $u(0,t) = u(L,t) = 0$

and initial condition $u(x,0) = f(x)$

The temperature is assumed separable in x and t

and we write $u(x,t) = X(x)T(t)$ so that (4.3.114.) becomes

$$\frac{1}{\alpha}\frac{T'(t)}{T(t)} = \frac{X''(x)}{X(x)} = -k^2 \quad \text{(4.3.135.)}$$

where k^2 is separation constant and $X(0) = X(L) = 0$

The spatial equation is then $X'' + k^2 X = 0$

which is simple harmonic motion equation

with trigonometric solutions

$$X(x) = A\cos\ (kx) + B\sin\ (kx) \qquad \text{(4.3.136.)}$$

Now ☛ applying boundary conditions we find

$$X(x) = \sin(n\pi x/L) \quad (4.3.137.)$$

For such values of k we have

$$T_n(t) = b_n e^{-(n\pi/L)^2 \alpha t} \quad (4.3.138.)$$

We take most general solution

by adding together all possible solutions

satisfying boundary conditions

$$u(x,t) = \sum_{n=1}^{\infty} b_n e^{-(n\pi/L)^2 \alpha t} \sin(n\pi x/L) \quad (4.3.139.)$$

Final step is to apply initial conditions

$$u(x,0) = \sum_{n=1}^{\infty} b_n \sin(n\pi x/L) = f(x) \quad (4.3.140.)$$

and invert Fourier series to determine coefficients b_n

We do this by multiplying equation by $\sin\ (m\pi x/L)$

and integrating over interval $[0, L]$

$$b_n = \frac{2}{L}\int_0^L f(s)\ \sin\ (n\pi s/L)\ ds \quad (4.3.141.)$$

Solution is then

$$u(x,t) = \sum_{n=1}^{\infty} \frac{2}{L}\int_0^L f(s)\sin(n\pi s/L)\sin(n\pi x/L)e^{-(n\pi/L)^2\alpha t} ds$$

(4.3.142.)

Note that due to rapid decrease in exponential when n grows

series is strongly convergent

Moreover ☛ given that $|u_n(x,t)| < |c_n|\ \forall t, 0 \leq x \leq L$

and that series of absolute value of Fourier coefficients converges

if f is continuous with continuous derivative to pieces

(with $f(0) = f(L) = 0$)

series $\sum_{n=1}^{\infty} u_n$ converges uniformly

and determines a continuous function for $t \geq 0$

Due to uniform convergence

we can swap order of integral and sum to obtain

$$u(x,t) = \int_0^L f(s)\, K(x,s,t)\, ds \quad (4.3.143.)$$

where

$$K(x,s,t) = \frac{2}{L}\sum_{n=1}^{\infty} \sin(n\pi s/L)\sin(n\pi x/L)e^{-(n\pi/L)^2\alpha t} \quad (4.3.144.)$$

is fundamental solution that satisfies boundary conditions

$$K(0,s,t) = K(L,s,t) = 0$$

Fundamental solution decays exponentially in time

and hence describes a transient process

i.e. if we wait long enough then $K(x,s,t)$ decays away

Other boundary conditions

lead to different eigenvalues and eigenfunctions for spatial part

e.g. ☛ if edges are isolated $X'' + k^2 X = 0, \quad X'(0) = X'(L) = 0$

From these boundary conditions we obtain

$$X(x) = \cos(n\pi x/L), \quad n = 0, 1, \ldots \qquad (4.3.146.)$$

and so $$u(x,t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \, e^{-(nx/L)^2 \alpha t} \; \cos(n\pi x/L) \qquad (4.3.147.)$$

Initial condition yields $$f(s) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos(n\pi x/L) \qquad (4.3.148.)$$

and so $$\begin{aligned} a_n &= \frac{2}{L}\int_0^L f(s)\cos(n\pi s/L)\; ds\,, \\ a_0 &= \frac{2}{L}\int_0^L f(s)\; ds \end{aligned} \qquad (4.3.149.)$$

Note that terms with $n \geq 1$ are transient

Stationary term of solution $a_0/2$ is independent of x
and gives average of initial temperatures

Problem with fixed temperature at edges

$$u(0,t) = T_0, \quad \text{and} \quad u(L,t) = T_L \qquad (4.3.150.)$$

with T_0 and T_L independent of t

can be reduced to previous problem with substitution

$$u(x,t) = w(x,t) + T_0 + \frac{x}{L}(T_L - T_0) \qquad (4.3.151.)$$

Note that linear function on right is a stationary solution of diffusion equation that satisfies boundary conditions (4.3.150.)

whereas $w(x,t)$ also satisfies homogeneous diffusion equation but with homogeneous boundary conditions

$$w(x,0) = u(x,0) - T_0 - x(T_L - T_0)/L)$$

In this case $\displaystyle \lim_{t\to\infty} u(x,t) = T_0 + \frac{x}{L}(T_L - T_0) \qquad (4.3.152.)$

(ii) Inhomogeneous equation

Solution of inhomogeneous equation (4.3.115.)
with initial condition

$$u(x,0)=0, \quad \text{for} \quad 0 \le x \le L \qquad (4.3.153.)$$

and boundary conditions

$$u(0,t)=u(L,t)=0, \quad \text{for} \quad 0 \le x \le L \qquad (4.3.154.)$$

is given by

$$u(x,t)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G(x,x',t-t')\ \overline{f}_{\sigma}(x',t')dx'\ dt' \qquad (4.3.155.)$$

where $G(x,x',t-t')$ satisfies differential equation

$$G_t(x,x',t-t')-\alpha^2 G_{xx}(x,x',t-t')=\delta(x-x')\delta(t-t') \qquad (4.3.156.)$$

with $G(0,x',t-t')=G(L,x',t-t')=0$

We have seen that solution of homogeneous equation (4.3.114.) can be expanded in a Fourier sine series ☛

$$G(x, x', t-t') = \sum_{n=1}^{\infty} g_n(x', t-t') \ \sin\left(\frac{n\pi x}{L}\right) \qquad (4.3.157.)$$

We have also seen that a Fourier series expansion of $\delta(x-x')$ gives

$$\delta(x-x') = \frac{2}{L}\sum_{n=1}^{\infty} \sin\left(\frac{n\pi x'}{L}\right) \ \sin\left(\frac{n\pi x}{L}\right) \qquad (4.3.158.)$$

Substituting (4.3.157.) and (4.3.158.) into (4.3.156.) we obtain

$$\begin{aligned}\frac{2}{L}\sum_{n=1}^{\infty} \sin\left(\frac{n\pi x'}{L}\right) \delta(t-t') \ \sin\left(\frac{n\pi x}{L}\right) &= \sum_{n=1}^{\infty} \sin\left(\frac{n\pi x}{L}\right) \left[\frac{\partial g_n}{\partial t}(x', t-t') \right. \\ &\quad + \left. \alpha\left(\frac{n\pi}{L}\right)^2 g_n(x', t-t')\right]\end{aligned}$$

and so Fourier coefficients of G satisfy

$$\frac{\partial g_n}{\partial t}(x', t-t') + \alpha\left(\frac{n\pi}{L}\right)^2 g_n(x', t-t') = \frac{2}{L} \sin\left(\frac{n\pi x'}{L}\right) \ \delta(t-t') \qquad (4.3.159.)$$

To determine $g_n(x', t-t')$

we write it in terms of its Fourier transform

$$g_n(x, t-t') = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{g}_n(x', \omega) e^{i\omega(t-t')} d\omega \quad (4.3.160.)$$

Substituting Fourier-integral expression for delta function

$$\delta(t-t') = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega(t-t')} d\omega \quad (4.3.161.)$$

and (4.3.160.) into (4.3.159.) we obtain

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \left[i\omega + \alpha \left(\frac{n\pi}{L} \right)^2 \right] \hat{g}_n(x', \omega) e^{i\omega(t-t')} d\omega = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega e^{i\omega(t-t')} \frac{2}{L} \sin\left(\frac{n\pi x'}{L} \right)$$

which leads to

$$\left[i\omega + \alpha \left(\frac{n\pi}{L} \right)^2 \right] \hat{g}_n(x', \omega) = \frac{1}{\sqrt{2\pi}} \frac{2}{L} \sin\left(\frac{n\pi x'}{L} \right) \quad (4.3.162.)$$

and so $$\hat{g}_n(x', \omega) = \frac{1}{L} \sqrt{\frac{2}{\pi}} \frac{\sin(n\pi x'/L)}{i\omega + \alpha(n\pi/L)^2} \quad (4.3.163.)$$

Now ☛ we must solve anti-Fourier transformation

$$g_n(x', t-t') = \frac{1}{L}\sqrt{\frac{2}{\pi}}\frac{\sin(n\pi x'/L)}{\sqrt{2\pi}}\int_{-\infty}^{\infty} d\omega \frac{e^{i\omega(t-t')}}{i\omega + \alpha(n\pi/L)^2}$$

This integral can be performed in complex plane ω

closing contour on upper half-plane

(where exponential function decreases at infinity)

$$\int_{-\infty}^{\infty} d\omega \frac{e^{i\omega(t-t')}}{i\omega + \alpha(n\pi/L)^2} = 2\pi e^{\alpha(n\pi/L)^2(t-t')}$$

Therefore

$$g_n(x, t-t') = \frac{2}{L} e^{-\alpha(n\pi/L)^2(t-t')} \sin\left(\frac{n\pi x'}{L}\right)$$

and

$$G(x, x', t-t') = \frac{2}{L}\sum_{n=1}^{\infty} e^{-\alpha(n\pi/L)^2(t-t')} \sin\left(\frac{n\pi x'}{L}\right) \sin\left(\frac{n\pi x}{L}\right)$$

4.2.5 Schrödinger & Klein-Gordon equation

A quantum mechanical description of a relativistic free particle results from applying correspondence principle

which allows one to replace classical observables

by quantum mechanical operators acting on wave functions

In position representation the correspondence principle states

$$E \to -\frac{\hbar}{i}\frac{\partial}{\partial t} \equiv -\frac{\hbar}{i}\partial_t, \qquad \mathbf{p} \to \frac{\hbar}{i}\nabla \qquad (4.2.58.)$$

which in four-vector notation reads

$$p_\mu \to i\hbar(\partial_t, \nabla) = i\hbar\partial_\mu\,; \qquad p^\mu \to i\hbar(\partial_t, -\nabla) = i\hbar\partial^\mu$$

$$\mu = 0, 1, 2, 3 \equiv t, x, y.z$$

General prescription for obtaining Schrödinger equation

for a free particle of mass m is to substitute differential operators into classical energy momentum relation

$$E = \frac{\mathbf{p}^2}{2m} \qquad (4.2.59.)$$

Resulting operator equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi = i\,\hbar\,\partial_t\psi \qquad (4.2.60.)$$

is understood to act on a (complex) wavefunction $\psi(\mathbf{x}, t)$

Schrödinger equation can be viewed as a diffusion equation

with imaginary diffusion constant $i\hbar/(2m)$

or mathematically as diffusion equation in imaginary time it

with a real diffusion constant $\hbar/(2m)$

Wavefunction does not have any physical interpretation

but we interpret $\rho = |\psi|^2$ as probability density ☛ that is

$|\psi|^2 d^3x$ ➡ probability of finding particle in volume element d^3x

Because of its parabolic anatomy (4.2.60) violates Lorentz invariance

and is not suitable for a particle that moves relativistically

Applying correspondence principle

to relativistic energy-momentum relation $E^2 = \mathbf{p}^2 + m^2$ (4.2.61.)

one obtains wave equation $$(\hbar^2\partial^\mu\partial_\mu + m^2)\psi = 0 \qquad (4.2.62.)$$

where $\psi(\mathbf{x}, t)$ is a scalar complex-valued wavefunction

Hereafter we work with natural units $\hbar = c = 1$

In natural units quantities:

energy, momentum, mass, $(\text{length})^{-1}$ and $(\text{time})^{-1}$

☛ all have the same dimension

In these units (4.2.60.) reads $(\Box^2 + m^2)\psi = 0$ (4.2.61.)

$\Box^2 \equiv \partial_\mu \partial^\mu$ is invariant d'Alembertian operator

Partial differential equation (4.2.61) is called Klein-Gordon equation

Multiplying Klein-Gordon equation by $-i\psi^*$

and complex conjugate equation by $-i\psi$

and subtracting ☛ leads continuity equation

$$\partial_t \underbrace{[i(\psi^* \partial_t \psi - \psi \partial_t \psi^*)]}_{\text{probability density}} + \nabla . \underbrace{[-i(\psi^* \nabla \psi - \psi \nabla \psi^*)]}_{\text{density flux of a beam of particles}} = \mathbf{0} \quad (4.2.62.)$$

Hints for the calculation

$$\partial_\mu(\phi^*\partial^\mu\phi) = \partial_\mu\phi^*\partial^\mu\phi + \phi^*\partial_\mu\partial^\mu\phi$$

$$\begin{aligned} -i\phi^*\partial_\mu\partial^\mu\phi - i\phi^*m^2\phi + i\phi\partial_\mu\partial^\mu\phi^* + i\phi m^2\phi^* &= -i\phi^*\partial_\mu\partial^\mu\phi + i\phi\partial_\mu\partial^\mu\phi^* \\ &= 0 \end{aligned}$$

Considering motion a free particle of energy E and momentum $\mathbf{p}$

described by Klein-Gordon solution $\psi = N\, e^{i(\mathbf{p}\,.\mathbf{x} - Et)}$ (4.2.63.)

from (4.2.62.) we find

$\rho = -i(2\,i\,E)|N|^2 = 2\,E\,|N|^2$ and $\mathbf{j} = -i(2\,i\,\mathbf{p})|N|^2 = 2\,\mathbf{p}\,|N|^2$

We note that probability density ρ

is timelike component of a four-vector

$$\rho \propto E = \pm(\mathbf{p}^{\,2} + m^2)^{1/2} \qquad (4.2.64.)$$

In addition to acceptable $E > 0$ solutions

we have negative energy solutions

which have associated a negative probability density

We cannot simply discard negative energy solutions

as we have to work with a complete set of states

and this set inevitably includes unwanted states

Prescription for handling negative energy configurations
was put forward by Stückelberg and by Feynman

Expressed most simply ☛ idea is that a negative energy solution describes a particle which propagates backwards in time

or equivalently

a positive energy antiparticle propagating forward in time

To master this idea ☛ consider a spin-zero particle of:

energy E

three-momentum $\mathbf{p}$

and charge $-e$

generally referred to as spinless electron

Substituting (4.2.63.) into the charge current density of electron

$$j^\mu = -i\,e\,(\psi^*\ \partial^\mu \psi - \psi\ \partial^\mu \psi^*) \qquad (4.2.65.)$$

we obtain the electromagnetic four-vector current

$$j^\mu(e^-) = -2e|N|^2(E,\ \mathbf{p}) \qquad (4.2.66.)$$

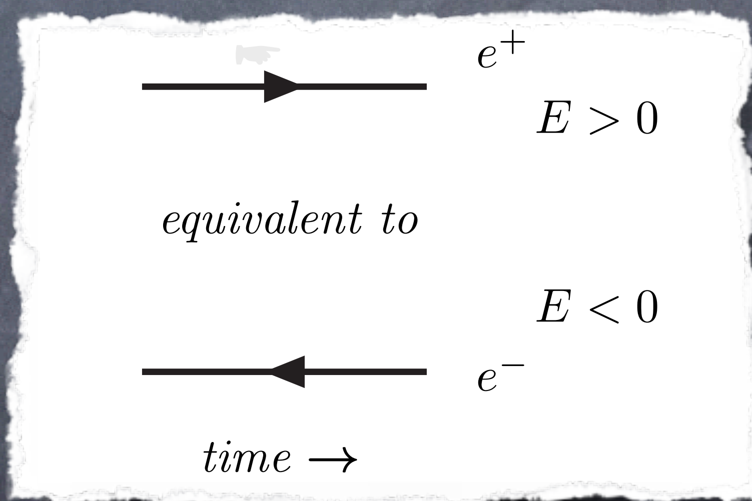
Now ☛ taking its antiparticle e^+ of same $(E, \mathbf{p})$
because its charge is $+e$ we obtain

$$\begin{aligned} j^\mu(e^+) &= 2e|N|^2(E, \mathbf{p}) \\ &= -2e|N|^2(-E, -\mathbf{p}) \end{aligned} \qquad (4.2.67.)$$

which is exactly same as current of original particle with $-E, -\mathbf{p}$

Hence ☛ as far as a system is concerned
emission of an antiparticle with energy E
is the same as absorption of a particle of energy $-E$

Pictorially



$-E$ particle solutions going backward in time
describe E antiparticle solutions going forward in time

this identification can be made because $e^{-i(-E)(-t)} = e^{-iEt}$

Green function (or propagator) of spinless electron satisfies

$$(\Box^2 + m^2)\, G_F(x - x') = \delta^{(4)}(x - x') \qquad (4.2.68.)$$

To define Green function entirely

one also needs to fix boundary condition

Retarded (advanced) Green function is defined to be

non-vanishing for positive (negative) values of time $t - t'$

Boundary conditions for Feynman propagator are causal:

positive (negative) solutions propagate forward (backward) in time

To solve (4.2.68.) ☛ we first Fourier transform to momentum space

$$G_F(x - x') = \frac{1}{(2\pi)^4} \int S_F(p)\, e^{-ip\cdot(x - x')}\, d^4p \qquad (4.2.69.)$$

Then ☛ on substituting into (4.2.68.) we obtain

$$\frac{1}{(2\pi)^4}\int (p^2 - m^2)\; S_F(p)\; e^{-ip\cdot(x-x')} d^4p = \frac{1}{(2\pi)^4}\int e^{-ip\cdot(x-x')}\; d^4p$$

right-hand side is Fourier representation of delta function

In momentum space ☛ (4.2.68.) therefore becomes simply

$$(p^2 - m^2)\; S_F(p) = 1 \qquad (4.2.71.)$$

that is ☛ $$S_F(p) = \frac{1}{p^2 - m^2} \qquad (4.2.72.)$$

To complete determination of $S_F(p)$

we need to know how to treat singularities at

$$p^2 - \mu^2 = p_0{}^2 - (\mathbf{p}^2 + m^2) = (p_0 - E)\;(p_0 + E) = 0$$

To obtain correct prescription for integration over poles at $p_0 = \pm E$

we need to impose appropriate boundary conditions on $G_F(x - x')$

From (4.2.101.) and (4.2.104.)

$$G_F(x-x') = \frac{1}{(2\pi)^4}\int \frac{1}{(p_0-E)(p_0+E)} e^{-ip\cdot(x-x')} d^4p \qquad \text{(4.2.105.)}$$

$$= \frac{1}{(2\pi)^4}\int d^3p\; e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')} \int_{-\infty}^{\infty} \frac{e^{-ip_0(t-t')}}{(p_0-E)(p_0+E)}\, dp_0$$

$G_F(x-x')$ represents wave produced at x by a unit source at x'

That is ☛ propagation is from x' to x

We will see that $S_F(p)$ which is associated with propagation of positive-energy spinless electrons forward in time $(t > t')$ and with negative energy spinless electrons backwards in time $(t < t')$

This can be accomplished by performing p_0 integration in complex plane using Cauchy residue theorem

To do this ☛ we rewrite propagator as

$$S_F(p) = \frac{1}{p^2 - m^2 - \epsilon^2} \qquad (4.2.106.)$$

introduction of $+i\epsilon$ (with ϵ infinitesimal and positive) has the effect of displacing $p_0 = \pm E$ poles slightly off axis

There are two poles one just above real axis and one just below

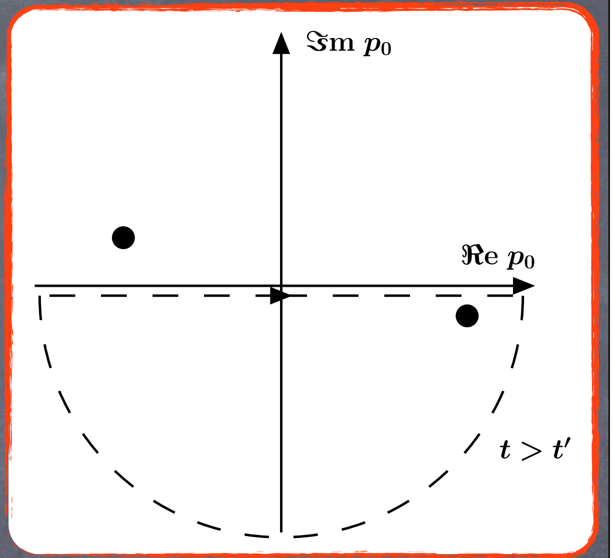
First pole has

$$\text{location} \to \quad +\left(E - \frac{i\epsilon}{2E}\right) \quad \text{residue} \to \quad \frac{\exp\{+i(E - i\epsilon/2E)(t-t')\}}{2(E - i\epsilon/2E)}$$

while second has

$$\text{location} \to \quad -\left(E - \frac{i\epsilon}{2E}\right) \quad \text{residue} \to \quad -\frac{\exp\{-i(E - i\epsilon/2E)(t-t')\}}{2(E - i\epsilon/2E)}$$

If $t > t'$ from (4.2.105) we see that to ensure that contribution from semicircle vanishes we must close contour in lower half-plane



We therefore enclose pole at $p_0 = +E$ to obtain (in limit $\epsilon \to 0$)

$$\int_{-\infty}^{\infty} \frac{e^{-ip_0(t-t')}}{(p_0 - E)(p_0 + E)}\, dp_0 = -2\pi i \left(+ \frac{e^{-iE(t-t')}}{2E} \right) \qquad (4.2.107.)$$

Substituting this result into (4.2.105.)

$$\begin{aligned} G_F(x - x') &= \frac{-2\pi i}{(2\pi)^4} \int \frac{d^3p}{(2E)}\, e^{-ip\cdot(x-x')} \\ &= \frac{-i}{(2\pi)^3} \int \frac{d^3p}{2E}\, e^{-ip\cdot(x-x')} \qquad (4.2.108.) \end{aligned}$$

$S_F(p)$ represents propagation of $+E$ spinless electrons forward in time

For $t < t'$ semicircle contribution will vanish
provided we close contour in upper half-plane

We now enclose pole at $p_0 = -E$ and so

$$\int_{-\infty}^{\infty} \frac{e^{-ip_0(t-t')}}{(p_0 - E)(p_0 + E)}\, dp_0 = +2\pi i \left(-\frac{e^{-i(-E)(t-t')}}{2E} \right) \quad (4.2.109.)$$

yielding $G_F(x - x') \ = \ \frac{2\pi i}{(2\pi)^4} \int \frac{d^3 p}{(-2E)} e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')}\, e^{-i(-E)(t-t')}$

Since we are integrating over all of three-momentum space

G_F is unchanged by substitution $\mathbf{p} \to -\mathbf{p}$

we obtain $G_F(x - x') = \frac{-i}{(2\pi)^3} \int \frac{d^3 p}{2E}\, e^{ip\cdot(x-x')}$ (4.2.111.)

$S_F(p)$ represents propagation of $-E, -\mathbf{p}$
spinless electrons backward in time

which is equivalent to propagation of $+E, +\mathbf{p}$
spinless positrons forward in time

We see that origin of antiparticle states is pole at $p_0 = -E$
which is not present in a nonrelativistic theory


TO BE
CONTINUED....