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Quantum field theory and Green's function approach

8.1. Background

8.1.1. Why QFT?

Same as second quantization. As long as one uses second quantization c and $c^\dagger$, QFT will emerge naturally.

Why second quantization? We want to handle large numbers of indistinguishable particles.

n indistinguishable particles:

$$\Psi(r_1, r_2, r_{3,} ..., r_n) = \sum_{\mathcal{P}} (\pm 1)^{\mathcal{P}} \, \psi_{i_1}(r_1) \, \psi_{i_2}(r_2) \, ... \psi_{i_n}(r_n) \tag{8.1}$$

where $\mathcal{P}$ represents all permutations and there are n! terms here. For large n, this is an extremely complicated wavefunction. For even ten particles, n=10, there are 2.6 million terms.

Same is true for high energy. Although the colliders focus on the collisions between two particles, there are many "virtue particles".

8.1.2. Expectation value at finite T (quantum statistical physics)

For classical statistical physics, we know that the expectation value of some quantity is (grand canonical ensemble)

$$\langle X \rangle = \frac{\sum_n X_n \exp[-\beta(E_n - \mu N)]}{\sum_n \exp[-\beta(E_n - \mu N)]} \tag{8.2}$$

For a quantum system, the expectation value is

$$\langle X \rangle = \frac{\sum_n \langle n \mid \hat{X} \exp[-\beta(\hat{H} - \mu \hat{N})] \mid n \rangle}{\sum_n \langle n \mid \exp[-\beta(\hat{H} - \mu \hat{N})] \mid n \rangle} = \frac{\mathrm{Tr}\{\hat{X} \exp[-\beta(\hat{H} - \mu \hat{N})]\}}{\mathrm{Tr}\{\exp[-\beta(\hat{H} - \mu \hat{N})]\}} \tag{8.3}$$

Here the $\sum_n$ is summing over a complete basis of the Hilbert space.

8.1.3. Second quantization

Operators: Every operator is written in terms of creation and annihilation operators c s and $c^\dagger$s: $\hat{X} = c_{k1} \, c_{k2} \, ... \, c_{kn} \, c_{q1}{}^\dagger \, c_{q2}{}^\dagger \, ... c_{qm}{}^\dagger$

Physical observables: Every observables are the expectation values of operators, which are products of cs and $c^\dagger$s: $\langle \hat{X} \rangle = \langle c_{k1} \, c_{k2} \, ... \, c_{kn} \, c_{q1}{}^\dagger \, c_{q2}{}^\dagger \, ... c_{qm}{}^\dagger \rangle$.

Tasks: compute these type of things: $\langle c_{k1} \, c_{k2} \, ... \, c_{kn} \, c_{q1}{}^\dagger \, c_{q2}{}^\dagger \, ... c_{qm}{}^\dagger \rangle$, which are known as correlation functions.

Consider a system with particle number conservation law (no superfluid, no superconductivity), it is easy to notice that $\langle c \rangle = \langle c^\dagger \rangle = 0$. This is because $\langle n|c|n \rangle = 0$.

In other words, the simplest correlation function one can imagine is $\langle c_k \, c_k{}^\dagger \rangle$

8.1.4. Normal order

Let's consider a system with Hamiltonian:

$$H = \int dr \, \frac{\nabla \psi^\dagger(r) \, \nabla \psi(r)}{2\,m} + \frac{1}{2} \int dr \, dr' \, V(\,|\,r-r'\,|\,) \, \psi^\dagger(r) \, \psi(r) \, \psi^\dagger(r') \, \psi(r') =$$

$$\int dr \, \frac{\nabla \psi^\dagger(r) \, \nabla \psi(r)}{2\,m} + \frac{1}{2} \int dr \, dr' \, V(\,|\,r-r'\,|\,) \, \psi^\dagger(r) \, \psi^\dagger(r') \, \psi(r') \, \psi(r) + \frac{1}{2} \int dr \, dr' \, V(\,|\,r-r'\,|\,) \, \delta(r-r') \, \psi^\dagger(r) \, \psi(r')$$

$$= \int dr \, \frac{\nabla \psi^\dagger(r) \, \nabla \psi(r)}{2\,m} + \frac{1}{2} \int dr \, dr' \, V(\,|\,r-r'\,|\,) \, \psi^\dagger(r) \, \psi^\dagger(r') \, \psi(r') \, \psi(r) + \frac{1}{2} \int dr \, V(0) \, \psi^\dagger(r) \, \psi(r')$$

$$= \int dr \, \frac{\nabla \psi^\dagger(r) \, \nabla \psi(r)}{2\,m} + \frac{1}{2} \int dr \, dr' \, V(\,|\,r-r'\,|\,) \, \psi^\dagger(r) \, \psi^\dagger(r') \, \psi(r') \, \psi(r) + \frac{V(0)\,N}{2}$$

(8.4)

We can drop the last term, which is a constant. (It is canceled by the potential energy from the nucleons). This procedure is known as "normal order", i.e. putting creation operators on the left and annihilation operators on the right.

$$H = \int dr \, \frac{\nabla \psi^\dagger(r) \, \nabla \psi(r)}{2\,m} + \frac{1}{2} \int dr \, dr' \, V(\,|\,r-r'\,|\,) \, \psi^\dagger(r) \, \psi^\dagger(r') \, \psi(r') \, \psi(r)$$

(8.5)

8.1.5. Equation of motion for operators

In general, for an operator X

$$i \, \frac{\partial X(t)}{\partial t} = [X(t), \, H(t)]$$

(8.6)

For operator ψ, we have

$$i \, \frac{\partial \psi(r_0, t)}{\partial t} = [\psi(r_0), \, H] = \int dr \, \frac{\nabla \delta(r-r_0) \, \nabla \psi(r)}{2\,m} +$$

$$\frac{1}{2} \int dr \, dr' \, \delta(r-r_0) \, V(\,|\,r-r'\,|\,) \, \psi^\dagger(r') \, \psi(r') \, \psi(r) + \frac{1}{2} \int dr \, dr' \, V(\,|\,r-r'\,|\,) \, \delta(r'-r_0) \, \psi^\dagger(r) \, \psi(r') \, \psi(r)$$

$$= -\frac{\nabla^2 \psi(r_0, t)}{2\,m} + \int dr \, V(\,|\,r_0-r\,|\,) \, \psi^\dagger(r) \, \psi(r) \, \psi(r_0)$$

(8.7)

Similarly, for the conjugate operator $\psi^\dagger$, we have

$$-i \, \frac{\partial \psi^\dagger(r_0, t)}{\partial t} = -\frac{\nabla^2 \psi^\dagger(r_0, t)}{2\,m} + \psi^\dagger(r_0) \int dr \, V(\,|\,r_0-r\,|\,) \, \psi^\dagger(r) \, \psi(r)$$

(8.8)

8.1.6. Equation of motion for correlation functions

Define

$$\tilde{G}(r_1, t_1; r_2 \, t_2) = \frac{1}{i} \left\langle \psi(r_1, t_1) \, \psi^\dagger(r_2, t_2) \right\rangle$$

(8.9)

For systems with translational symmetry in space and time, $\tilde{G}(r_1, t_1; r_2 \, t_2) = \tilde{G}(r_1 - r_2, t_1 - t_2) = \tilde{G}(r, t)$.

Q: What is the equations of motion for $G(r, \, t)$?

$$\partial_t \tilde{G}(r.t) = \partial_{t_1} \frac{1}{i} \left\langle \psi(r_1, t_1) \, \psi^\dagger(r_2, t_2) \right\rangle = \left\langle -i \, \partial_{t_1} \psi(r_1, t_1) \, \psi^\dagger(r_2, t_2) \right\rangle$$

$$= -\left\langle \left[-\frac{\nabla^2 \psi(r_1, t_1)}{2\,m} + \int dr \, V(\,|\,r_0-r\,|\,) \, \psi^\dagger(r) \, \psi(r) \, \psi(r_1, t_1) \right] \psi^\dagger(r_2, t_2) \right\rangle$$

(8.10)

$$= \frac{1}{2\,m}\,\partial_{r_1}{}^2 \left\langle \psi(r_1,\, t_1)\, \psi^\dagger(r_2,\, t_2) \right\rangle - V \left\langle \psi^\dagger\, \psi^\dagger\, \psi\, \psi \right\rangle = \frac{i}{2\,m}\,\nabla^2\,\tilde{G}(r,\, t) - V < \psi^\dagger\, \psi^\dagger\, \psi\, \psi >$$

If $V = 0$ (free systems), we have a closed partial differential equation for two fermion correlation functions.

$$i\,\partial_t\,\tilde{G}_0(r.t) + \frac{\nabla^2}{2\,m}\,\tilde{G}_0(r,\, t) = 0 \tag{8.11}$$

We can just solve this partial differential equation (with proper initial conditions and boundary conditions), and we get the correlation function.

However, for $V \neq 0$, the story is not as simple. We need to solve a more complicate equation.

$$i\,\partial_t\,\tilde{G}(r.t) + \frac{\nabla^2}{2\,m}\,\tilde{G}(r,\, t) = -i\,V < \psi^\dagger\, \psi^\dagger\, \psi\, \psi > \tag{8.12}$$

So we are having an Inhomogeneous partial differential equation.

$$i\,\partial_t\,\tilde{G}(r.t) + \frac{\nabla^2}{2\,m}\,\tilde{G}(r,\, t) = f(r,\, t) \tag{8.13}$$

Q: How do we solve Inhomogeneous partial differential equation?

A: Let's look at E&M

8.1.7. E&M: electric potential ϕ(r) for charge distribution ρ(r)

Gauss's law

$$\nabla \cdot \vec{E}(r) = \rho(r) \tag{8.14}$$

We know that

$$\vec{E}(r) = -\nabla\,\phi(r) \tag{8.15}$$

so

$$\nabla^2\,\phi(r) = \rho(r) \tag{8.16}$$

This is an Inhomogeneous equation. How do we solve it?

We first solve a different equation:

$$\nabla^2\,G(r,\, r_0) = \delta(r_0) \tag{8.17}$$

$G(r,\, r_0)$ is the electric potential for a point charge at position r_0. We know the solution of this equation, which is just the Coulomb's law

$$G(r,\, r_0) = \frac{1}{4\,\pi}\,\frac{1}{|r - r_0|} \tag{8.18}$$

Then, we know that

$$\phi(r) = \int d\,r_0\; G(r,\, r_0)\, \rho(r_0) = \int d\,r_0\; \frac{1}{4\,\pi}\,\frac{1}{|r - r_0|}\,\rho(r_0) \tag{8.19}$$

Mathematicians calls $G(r,\, r_0)$ Green's function. And this methods of solving inhomogeneous PDEs are known as the Green's function approach.

In general, one first change the inhomogeneous part with a delta function. Then, one solve this PDE first and the solution is known as the Green's function. Then one use this Integral to find the solution for the original inhomogeneous PDE.

8.1.8. A trick to get delta function: time ordering

Define time-ordered correlation functions (Green's functions)

$$G(r_1,\, t_1;\, r_2\, t_2) = \frac{1}{i}\,\left\langle \mathcal{T}\psi(r_1,\, t_1)\, \psi^\dagger(r_2,\, t_2) \right\rangle \tag{8.20}$$

Here $\mathcal{T}\psi^\dagger(r_1, t_1)\,\psi(r_2, t_2)$ is known as the time − ordered product.

$$
\begin{aligned}
\mathcal{T}\,\psi(r_1, t_1)\,\psi^\dagger(r_2, t_2) &= \psi(r_1, t_1)\,\psi^\dagger(r_2, t_2) \quad \text{if } t_1 > t_2 \\
&= \pm\,\psi^\dagger(r_2, t_2)\,\psi(r_1, t_1) \ \text{ if } t_1 < t_2
\end{aligned}
\tag{8.21}
$$

For bosons, we use the + sign and for fermions we use the - sign

In other words,

$$
\mathcal{T}\,\psi(r_1, t_1)\,\psi^\dagger(r_2, t_2) = \psi(r_1, t_1)\,\psi^\dagger(r_2, t_2)\,\eta(t_1 - t_2) \pm \psi^\dagger(r_2, t_2)\,\psi(r_1, t_1)\,\eta(t_2 - t_1)
\tag{8.22}
$$

where $\eta(x)$ is the step function $\eta(x)=1$ for x>0 and $\eta(x)=0$ for x<0

Now, let's consider the EOM for $G(r, t)$

$$
\begin{aligned}
\partial_t \tilde{G}(r.t) &= \partial_{t_1} \frac{1}{i}\left\langle \mathcal{T}\,\psi(r_1, t_1)\,\psi^\dagger(r_2, t_2)\right\rangle = -i\,\partial_{t_1}\left\langle \psi(r_1, t_1)\,\psi^\dagger(r_2, t_2)\,\eta(t_1 - t_2) \pm \psi^\dagger(r_2, t_2)\,\psi(r_1, t_1)\,\eta(t_2 - t_1)\right\rangle \\
&= \left\langle -i\,\partial_{t_1}\psi(r_1, t_1)\,\psi^\dagger(r_2, t_2)\,\eta(t_1 - t_2)\right\rangle \pm \left\langle \psi^\dagger(r_2, t_2)\,(-i\,\partial_{t_1})\,\psi(r_1, t_1)\,\eta(t_2 - t_1)\right\rangle - \\
&\quad\ i\left\langle \psi(r_1, t_1)\,\psi^\dagger(r_2, t_2) \mp \psi^\dagger(r_2, t_2)\,\psi(r_1, t_1)\right\rangle \delta(t_1 - t_2) \\
&= \frac{1}{2m}\,\partial_{r_1}^{\,2}\left\langle \mathcal{T}\psi(r_1, t_1)\,\psi^\dagger(r_2, t_2)\right\rangle - V\left\langle \mathcal{T}\,\psi^\dagger\,\psi^\dagger\,\psi\,\psi\right\rangle - i\,\delta(r_1 - r_2)\,\delta(t_1 - t_2) \\
&= \frac{i}{2m}\,\nabla^2 G(r, t) - V\left\langle \mathcal{T}\,\psi^\dagger\,\psi^\dagger\,\psi\,\psi\right\rangle - i\,\delta(r_1 - r_2)\,\delta(t_1 - t_2)
\end{aligned}
\tag{8.23}
$$

If $V = 0$

$$
i\,\partial_t G_0(r.t) + \frac{1}{2m}\,\nabla^2 G_0(r, t) = \delta(r)\,\delta(t)
\tag{8.24}
$$

Bottom line, by time-ordering, we automatically got the Green's function.

$$
\left(i\,\partial_t + \frac{\nabla^2}{2m}\right) G_0(r, t) = \delta(r)\,\delta(t)
\tag{8.25}
$$

$$
\int dr\,dt\,\exp[-i\,k\,r + i\,\omega\,t]\left(i\,\partial_t + \frac{\nabla^2}{2m}\right) G_0(r, t) = \int dr\,dt\,\exp[-i\,k\,r + i\,\omega\,t]\,\delta(r)\,\delta(t)
\tag{8.26}
$$

$$
\int dr\,dt\left(-i\,\partial_t + \frac{\nabla^2}{2m}\right) \exp[-i\,k\,r + i\,\omega\,t]\,G_0(r, t) = 1
\tag{8.27}
$$

$$
\left(\omega - \frac{k^2}{2m}\right)\int dr\,dt\,\exp[-i\,k\,r + i\,\omega\,t]\,G_0(r, t) = 1
\tag{8.28}
$$

$$
\left(\omega - \frac{k^2}{2m}\right) G_0(k, \omega) = 1
\tag{8.29}
$$

$$
G_0(k, \omega) = \frac{1}{\omega - \frac{k^2}{2m}}
\tag{8.30}
$$

More generally, for free particles (without interactions), $G_0 = \frac{1}{\omega - \epsilon_k}$

8.1.9. Note: there are many other reason to use $\mathcal{T}$.

(1) Path integral leads to $\mathcal{T}$ naturally.

(2) The evaluational operator $\mathcal{T}\exp[i\int dt\ \mathrm{H}(t)\,t]$

(3) With $\mathcal{T}$, bosons and fermions are unified together. Same theory with two different boundary conditions.