Quantum Many-Body Problem

- Quantum liquids
- cold atoms
- Atomic nuclei
- Neutron stars

Physical System
Energy and length scales of the probes

$\Longrightarrow$ Constituents

$\Downarrow$

Masses
Interactions

$\Downarrow$

Hamiltonian
non-relativistic
Indistinguisibility

$\Longrightarrow$ Schrödinger Equation

$\Downarrow$

Methods to solve the Schrödinger equation
- Perturbation theory
- Variational method
- Propagators. Green's function
- QMC

$\Downarrow$

Predictions

Experimental information
- Binding energy
- Scattering $\Rightarrow$ elastic & inelastic

The characteristic length and energy scales of the systems under consideration run over many orders of magnitude. However, in many cases the physics and the methods are very similar

Bibliography

* "Quantum theory of many-particle systems"
Alexander Fetter & John Dirk Walecka

* "A guide to Feynman diagrams in the many-body problem"
Richard Mattuck, Dover

* "Many-Body theory Exposed!"
Willem Dickhoff & Dimitri Van Neck
World Scientific 2005. Now 2º edition.

Propagators in one-particle quantum mechanics

- Time evolution is determined by the Hamiltonian of the physical system.

- In quantum mechanics, the state of a particle with quantum numbers α at time t_0 is denoted by

$$|\alpha; t_0\rangle$$

at a time later one has $|\alpha, t_0; t\rangle$ (which can have other quantum numbers).

- For a time independent Hamiltonian:

$$\boxed{|\alpha, t_0; t\rangle = \underbrace{e^{-\frac{i}{\hbar} H (t-t_0)}}_{\text{time evolution operator}} |\alpha, t_0\rangle}$$

which is consistent with the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\alpha, t_0; t\rangle = H |\alpha, t_0; t\rangle$$

$$\Downarrow$$

$$i\hbar \frac{\partial}{\partial t} \left\{ e^{-\frac{i}{\hbar} H(t-t_0)} |\alpha, t_0\rangle \right\} = i\hbar \left(-\frac{i}{\hbar}\right) H \, e^{-\frac{i}{\hbar} H(t-t_0)} |\alpha, t_0\rangle$$

$$= H \, |\alpha, t_0; t\rangle$$

Projecting these equations in $\vec{r}$- representati[on]

$$\Psi(\vec{r},t) = \langle \vec{r} \,|\alpha, t_0; t\rangle = \langle \vec{r} \,|\, e^{-\frac{i}{\hbar} H(t-t_0)} |\alpha, t_0\rangle$$

$$= \int d^3r' \langle \vec{r} \,|\, e^{-\frac{i}{\hbar} H(t-t_0)} |\vec{r}\,'\rangle\langle \vec{r}\,'|\alpha, t_0\rangle$$

$$I = \int d^3r' |\vec{r}\,'\rangle\langle\vec{r}\,'|$$

$$= i\hbar \int d^3r' \; G(\vec{r},\vec{r}\,'; t-t_0)\; \Psi(\vec{r}\,', t_0)$$

$$\boxed{G(\vec{r},\vec{r}\,'; t-t_0) \equiv -\frac{i}{\hbar} \langle \vec{r} \,|\, e^{-\frac{i}{\hbar} H(t-t_0)} |\vec{r}\,'\rangle}$$

* The propagator is the expectation value of the time evolution operator in coordinate representation.

* The knowledge of the wave function at the time t_0, together with the propagator allows for the calculation of the wave function at any $t > t_0$.

Several ways to write the propagator

taking into account the eigenvectors of H.

$$H\,|n\rangle = \varepsilon_n\,|n\rangle$$

assuming a discrete spectrum:

$$G(\vec{r},\vec{r}\,';t-t_0) = -\frac{i}{\hbar}\langle \vec{r}\,|\,e^{-\frac{i}{\hbar}H(t-t_0)}\,|\vec{r}\,'\rangle =$$

$$= -\frac{i}{\hbar}\langle 0|\,\hat{\Psi}(r)\;e^{-\frac{i}{\hbar}H(t-t_0)}\,\hat{\Psi}^{+}(\vec{r}\,')\,|0\rangle =$$

$$= -\frac{i}{\hbar}\sum_n \langle 0|\,\hat{\Psi}(r)\,|n\rangle\langle n|\,\hat{\Psi}^{+}(\vec{r}\,')\,|0\rangle\;e^{-\frac{i}{\hbar}\varepsilon_n(t-t_0)}$$

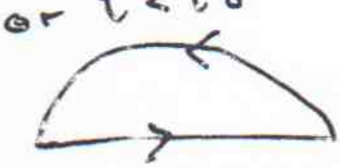
$$= -\frac{i}{\hbar}\sum_n u_n(\vec{r})\,u_n^{*}(\vec{r}\,')\;e^{-\frac{i}{\hbar}\varepsilon_n(t-t_0)}$$

- To incorporate causality explicitly, $t>t_0$, we introduce the step function $\theta(t-t_0)$.
- We are interested in the Fourier transform of the propagator and to this end it will be useful the integral representation of $\theta(t-t_0)$

$$\theta(t-t_0) = -\int_{-\infty}^{\infty}\frac{dE'}{2\pi i}\;\frac{e^{-iE'(t-t_0)/\hbar}}{E'+i\eta} \qquad \eta\to 0^{+}$$

For $t>t_0$

for $t<t_0$



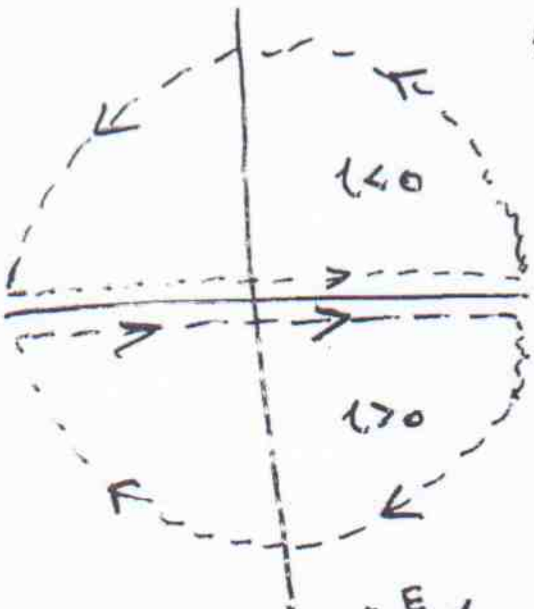
At $t=t_0$ $\theta(t-t_0)$ jumps from 0 to 1

$$\frac{d}{dt}\,\theta(t-t_0) = \delta(t-t_0)$$

Integral representation of the step function

$$\Theta(t) = -\frac{1}{2\pi i} \lim_{\varepsilon \to 0^+} \int_{-\infty}^{\infty} dE \, \frac{e^{-i\frac{Et}{\hbar}}}{E + i\varepsilon}$$

this integral is performed in the complex plane!



* The integrand has a pole in the complex plane E, located at $E = -i\varepsilon$

* For $t<0$, the circuit is closed by the upper part ⇒ the contribution in the semicircle is zero!

$$f(\rho,\phi) = \frac{e^{-i\frac{E}{\hbar}t}}{E} = \frac{e^{-i\frac{1}{\hbar}\rho t(\cos\phi + i\sin\phi)}}{\rho e^{i\phi}}$$

$$= e^{-i\frac{1}{\hbar}\rho t\cos\phi} \, \frac{e^{\rho/\hbar \, t \sin\phi}}{\rho e^{i\phi}}$$

$$|f(\rho,\phi)| = \frac{e^{\frac{\rho t}{\hbar}\sin\phi}}{\rho}$$ for $t<0 \to 0$ when $\rho \to \infty$

⇒ The contribution of the semicircle is smaller than

$$\pi\rho \, |f(\rho,\phi)| = \pi\cancel{\rho} \, \frac{e^{-\frac{\rho}{\hbar}|t|\sin\phi}}{\cancel{\rho}} \Rightarrow 0 \;(\rho \to \infty)$$

As there are no poles inside the circuit

$$\oint = \int + \underbrace{\int_{\frown}}_{=0} = 0 \Rightarrow \int = 0 \Rightarrow \Theta(t) = 0 \quad t<0$$

$$\boxed{\Theta(t) = 0 \quad t<0}$$

for $t>0$, the circle should be closed below!

$$t>0 \qquad \pi\rho\,|f(\rho,\phi)| = \frac{\pi\cancel{\rho}\, e^{-\frac{\rho}{\hbar}t|\sin\phi|}}{\cancel{\rho}} \longrightarrow 0 \quad (\rho\to\infty) \qquad \sin\phi<0$$

$$f(\rho,\phi) = e^{-i\frac{\rho}{\hbar}t\cos\phi}\,\frac{e^{\frac{\rho}{\hbar}t\sin\phi}}{\rho\, e^{i\phi}}$$

we have a pole of order 1 at $E=-i\varepsilon$

$$\text{Res} = \lim_{E\to -i\varepsilon^+} \frac{e^{-i\frac{E}{\hbar}t}}{\cancel{E+i\varepsilon}}\,\cancel{(E+i\varepsilon)} = \lim_{\substack{E\to -i\varepsilon^+\\ \varepsilon\to 0^+}} e^{-i\frac{1}{\hbar}(-i\varepsilon)t} = 1$$

- For $t>0$,

$$\lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty} dE\,\frac{e^{-i\frac{E}{\hbar}t}}{E+i\varepsilon} = \underset{\substack{\text{clock}\\ \text{wise}}}{\underset{\downarrow}{(-1)}}\ \underset{\substack{\text{Cauchy}\\ \text{theorem}}}{\underset{\downarrow}{2\pi i}}\cdot 1$$

- Therefore:

$$\Theta(t<0) = 0$$

$$\Theta(t>0) = -\frac{1}{2\pi i}\lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty} dE\,\frac{e^{-i\frac{E}{\hbar}t}}{E+i\varepsilon} = -\frac{1}{2\pi i}(-1)\,2\pi i = 1$$

- Besides:

$$\frac{d\Theta(t)}{dt} = -\frac{1}{2\pi i}\lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty}\frac{d}{dt}\,\frac{e^{-i\frac{E}{\hbar}t}}{E+i\varepsilon}\,dE =$$

$$= -\frac{1}{2\pi i}\lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty}\frac{-iE}{E+i\varepsilon}\,e^{-i\frac{E}{\hbar}t}\,d\!\left(\frac{E}{\hbar}\right) =$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\frac{E}{\hbar}t}\,d\!\left(\frac{E}{\hbar}\right) = \delta(t)$$

$$\boxed{\frac{d\Theta(t)}{dt} = \delta(t)}$$

Fourier transform

$$\boxed{G(\vec{r},\vec{r}\,';E) = \int_{-\infty}^{\infty} d(t-t_0)\, e^{\frac{i E (t-t_0)}{\hbar}}\, G(\vec{r},\vec{r}\,'; t-t_0)}$$

depends on the time difference

$$= -\frac{i}{\hbar}\int_{-\infty}^{\infty} d(t-t_0)\, e^{\frac{i}{\hbar}E(t-t_0)} \left\{\theta(t-t_0) \sum_n{}' u_n(\vec{r})\, u_n^*(\vec{r}\,')\, e^{-\frac{i}{\hbar}\varepsilon_n(t-t_0)}\right\}$$

$$= -\frac{i}{\hbar}\int_{-\infty}^{\infty} d(t-t_0)\, e^{\frac{i}{\hbar}E(t-t_0)} \left\{-\int \frac{dE'}{2\pi i}\, \frac{e^{-\frac{i}{\hbar}E'(t-t_0)}}{E'+i\eta}\right\}\left(\sum_n{}' u_n(\vec{r})\, u_n^*(\vec{r}\,')\, e^{-\frac{i}{\hbar}\varepsilon_n(t-t_0)}\right)$$

$$= \int_{-\infty}^{\infty} dE'\, \frac{1}{E'+i\eta} \sum_n{}' u_n(\vec{r})\, u_n^*(\vec{r}\,')\, \underbrace{\frac{1}{2\pi}\int_{-\infty}^{\infty} d\left(\frac{t-t_0}{\hbar}\right) e^{\frac{i}{\hbar}(t-t_0)(E-E'-\varepsilon_n)}}_{\delta(E-E'-\varepsilon_n)}$$

$$= \sum_n{}' \frac{u_n(\vec{r})\, u_n^*(\vec{r}\,')}{E-\varepsilon_n+i\eta} = \sum_n{}' \frac{\langle 0|\hat{\psi}(\vec{r})|n\rangle\langle n|\hat{\psi}^\dagger(\vec{r}\,')|0\rangle}{E-\varepsilon_n+i\eta}$$

$$= \langle 0|\hat{\psi}(\vec{r})\, \frac{1}{E-H+i\eta}\, \hat{\psi}^\dagger(\vec{r}\,')|0\rangle = \langle \vec{r}|\frac{1}{E-H+i\eta}|\vec{r}\,'\rangle$$

$$\boxed{G(\vec{r},\vec{r}\,';E) = \langle \vec{r}|\frac{1}{E-H+i\eta}|\vec{r}\,'\rangle}$$

* Notice that the presence of the $i\eta$ term in the denominator originates from the inclusion of the condition $t>t_0$ (forward propagation)

* One can study the propagator in any basis!
→ The Hamiltonian could be diagonal or not in this basis!

$$\boxed{G(\alpha,\beta;E) = \langle 0|a_\alpha \frac{1}{E-H+i\eta} a_\beta^\dagger|0\rangle}$$

Expansion of the propagator

The exact propagator can be related to an approximate one by using a decomposition of the Hamiltonian:

$$H = H_0 + V$$

H_0 is the unperturbed Hamiltonian
the associated $G^{(0)}$ is readily available!
Could be the kinetic energy!

Use the operatorial identity!

$$\frac{1}{A-B} = \frac{1}{A} + \frac{1}{A} B \frac{1}{A-B}$$

$$\frac{1}{A}\left(1 + B\frac{1}{A-B}\right) = \frac{1}{A}\left((A-B)\cancel{\frac{1}{A-B}} + B\cancel{\frac{1}{A-B}}\right) = \frac{1}{A} A \frac{1}{A-B} = \frac{1}{A-B}$$

$$\left.\begin{array}{l} A = E - H_0 + i\eta \\ B = V \end{array}\right\}$$ we can relate G and $G^{(0)}$

$$G = \frac{1}{E - H + i\eta} \qquad G^{(0)} = \frac{1}{E - H_0 + i\eta}$$

$$\boxed{G = G^{(0)} + G^{(0)} V G}$$

this equation can be solved iteratively
$\Downarrow$
expansion in terms of $G^{(0)}$ and V

$$G^{(1)} = G^{(0)} + G^{(0)} V G^{(0)}$$

$$G^{(2)} = G^{(0)} + G^{(0)} V \left[G^{(0)} + G^{(0)} V G^{(0)}\right] =$$

$$= G^{(0)} + G^{(0)} V G^{(0)} + G^{(0)} V G^{(0)} V G^{(0)}$$

$$G = G^{(0)} + G^{(0)} V G^{(0)} + G^{(0)} V G^{(0)} V G^{(0)} + \dots$$

using a particular basis →

$$G^{(0)}(\alpha, \beta; E) = \langle \alpha | \frac{1}{E - H_0 + i\eta} | \beta \rangle$$

and the equation is written as:

$$\langle \alpha | \frac{1}{E - H + i\eta} | \beta \rangle = \langle \alpha | \frac{1}{E - H_0 + i\eta} | \beta \rangle +$$

$$+ \sum_{\gamma\delta} \langle \alpha | \frac{1}{E - H_0 + i\eta} | \gamma \rangle \langle \gamma | V | \delta \rangle \langle \delta | \frac{1}{E - H + i\eta} | \beta \rangle$$

$$\Downarrow$$

$$\boxed{G(\alpha, \beta; E) = G^{(0)}(\alpha, \beta; E) + \sum_{\gamma\delta} G^{(0)}(\alpha, \gamma; E) \langle \gamma | V | \delta \rangle G(\delta, \beta; E)}$$

* In general, it is useful to use a diagonal basis for $G^{(0)}$.

* The operatorial equation $G = G^{(0)} + G^{(0)} V G$ and its series expansion can be rearrange in several ways.

$$\begin{aligned} G &= G^{(0)} + G^{(0)} V G^{(0)} + G^{(0)} V G^{(0)} V G^{(0)} + \dots \\ &= G^{(0)} + G^{(0)} V \{ G^{(0)} + G^{(0)} V G^{(0)} + \dots \} = G^{(0)} + G^{(0)} V G \\ &= G^{(0)} + \{ G^{(0)} + G^{(0)} V G^{(0)} + \dots \} V G^{(0)} = G^{(0)} + G V G^{(0)} \\ &= G^{(0)} + G^{(0)} \{ V + V G^{(0)} V + \dots \} G^{(0)} = G^{(0)} + G^{(0)} T G^{(0)} \end{aligned}$$

we have introduced a new operator: T-matrix

..

T-matrix also fulfils an integral equation:
the Lippman - Schwinger equation

$$T = V + V G^{(0)} V + V G^{(0)} V G^{(0)} V + \dots$$
$$= V + V G^{(0)} \{ V + V G^{(0)} V + \dots \}$$
$$= V + V G^{(0)} T = V + T G^{(0)} V = V + V G V$$

$$\boxed{\begin{array}{l} T = V + V G^{(0)} T = V + V G V \\ T \simeq V \quad \text{Born approximation} \end{array}}$$

FREE PARTICLE STATES

$$H_0 = \frac{\vec{p}^2}{2m} = - \frac{\hbar^2 \vec{\nabla}^2}{2m}$$

eigenstates: $\frac{p^2}{2m} |\vec{p}'\rangle = \frac{(p')^2}{2m} |\vec{p}'\rangle$

wave function: $\langle \vec{r} | \vec{p} \rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{i \frac{\vec{p}\vec{r}}{\hbar}}$

normalization:

$$\langle \vec{p}' | \vec{p} \rangle = \frac{1}{(2\pi\hbar)^3} \int d^3 r \; e^{\frac{i}{\hbar}(\vec{p} - \vec{p}')\vec{r}} = \delta(\vec{p}' - \vec{p})$$

$$I = \int d^3 p \; |\vec{p}\rangle\langle\vec{p}|$$

wave number notation

$\vec{p} = \hbar \vec{k}$

$$\langle \vec{r} | \vec{k} \rangle = \frac{1}{(2\pi)^{3/2}} e^{i \vec{k} \vec{r}}$$
$$\langle \vec{k} | \vec{k}' \rangle = \delta(\vec{k} - \vec{k}')$$
$$I = \int d^3 k \; |\vec{k}\rangle\langle\vec{k}|$$

Also useful box normalization

The particle is confined to a cubic box with sides L and volume $\Omega = L^3$

$$\langle \vec{r} \,|\, \vec{k} \rangle = \frac{1}{\Omega^{1/2}} e^{i\bar{k}\bar{r}}$$

$$\langle \bar{k}' \,|\, \bar{k} \rangle = \delta_{\bar{k}',\bar{k}} = \frac{1}{\Omega} \int_{\Omega} d^3 r \, e^{i(\bar{k}-\bar{k}')\bar{r}} = \underbrace{\delta_{\bar{k}',\bar{k}}}_{\text{delta Kronecker}}$$

$$I = \int_{\Omega} d^3 r \, |\vec{r}\rangle\langle\vec{r}| = \sum_{\vec{k}} |\bar{k}\rangle\langle\bar{k}|$$

Diagrammatic notation

* Physicists like diagrammatic notation. They prefere to draw diagrams instead of writing integrals or long expre sions.

* You need a dictionary to interpret diagrams. Once you are used, they are more transparent and easy to interpret in physical terms.

* Convenient to use a basis $\{|\alpha\rangle\}$ to be eigenstates of H_0, whose eigenvalues are ε_α.

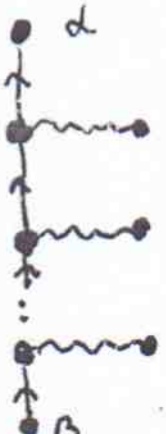
$$G^{(0)}(\alpha,\beta;E) = \frac{\delta_{\alpha,\beta}}{E-\varepsilon_\alpha+i\eta} \qquad H = H_0 + V$$

$$G(\alpha,\beta;E) = G^{(0)}(\alpha,\beta;E) + \sum_{\gamma,\delta} G^{(0)}(\alpha,\gamma;E)\langle\gamma|V|\delta\rangle G(\delta,\beta;E)$$

* It is possible to generate a series of diagrams that represent the contributions to the single-particle propagator in a perturbation expansion in the potential. The terms of the expansion can be derived algebraically by iterating the equation for G.

Diagram rules : For the K^{th} order in V

(1) Draw a directed line with a K wavy horizontal interaction lines V and $K+1$ directed unperturbed propagators $G^{(0)}$



(2) Label external points (α and β)
Label each V

$\langle\gamma|V|\delta\rangle$

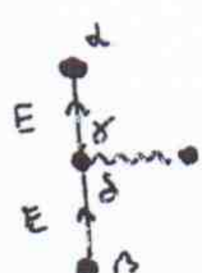
For each full line with arrow write

$G^{(0)}(\mu,\nu;E)$

(3) Sum (integrate) over all internal quantum numbers

Examples

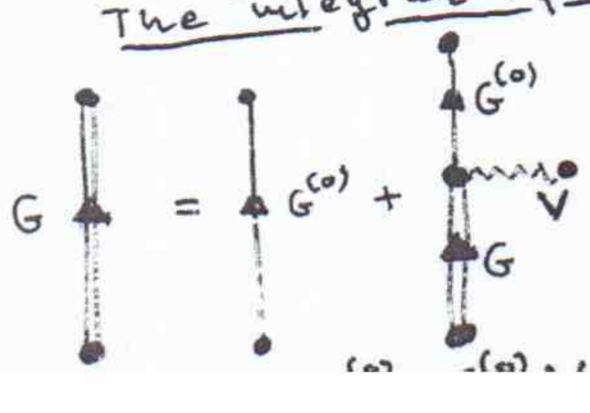
$G^{(0)}(\alpha,\beta;E)$

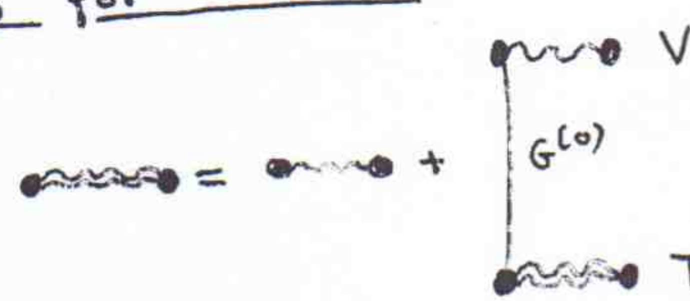


$\sum_{\gamma\delta} G^{(0)}(\alpha,\gamma;E)\langle\gamma|V|\delta\rangle G^{(0)}(\delta,\beta;E)$

first order

The integral equations for G and T





$T = V + V G^{(0)} T$