Computational Methods for quantum many-body systems

Chapter 1: Quantum Field Theory (QFT) and Green functions

Why QFT in condensed matter?

classical FT → infinite degrees of freedom
(e.g., $\vec{E}(\vec{r},t)$)

QFT: no longer quantization of classical variables (such as $\vec{r}$ and $\vec{p}$)
Hilbert space

BUT quantization of fields (e.g.: electrical fields, particle fields, ...)
Fock space

QFT is de facto necessary in relativistic quantum mechanics, because of

·) "eigenstates" with unlimited negative energies, e.g. in the Dirac equation → hole theory, Fermi Sea of ∞ electrons with $E<0$
⇒ infinite degrees of freedom needed

·) number of "particles" not fixed
→ mass is not conserved, energy is ($E=mc^2$)

What about problems in condensed matter?

Typical Hamiltonian in condensed matter:

$$H = \sum_{\ell=1}^{N} \left[-\frac{\hbar^2 \vec{\nabla}_\ell^2}{2m} - \mu \hat{N} \right] + \frac{1}{2} \sum_{\ell \neq \ell'} V(|\vec{r}_\ell - \vec{r}_{\ell'}|)$$

kinetic energy of the ℓ-th electron

chemical potential

electronic interaction between electrons located at $\vec{r}_\ell$ and $\vec{r}_{\ell'}$ (e.g. Coulomb)

Our needs are not so different from those of the relativistic case

- not infinite, but $N = 10^{23}$ particles / degrees of freedom
- no particle conservation: grand-canonical ensemble, superconductivity, ...

Obviously, there are also significant differences, e.g.:

relativistic case		condensed matter
infrared divergences ($k \to 0$)	$\to$	only in thermodynamics (phase transitions)
ultraviolet divergences ($k \to \infty$)	$\to$	not present, because of the natural cut-off of the lattice ($k \lesssim \frac{1}{a}$)

lattice spacing

1.1 A Step towards QFT: Second quantization

Convenient "accounting" system for many particles

"First quantization" for many-particle systems

operators, wave functions and commutation relations

N identical particles: $\psi(\vec{r}) \to \psi(\vec{r}_1, \ldots, \vec{r}_N)$

$$|\psi(\vec{r}_1, \ldots, \vec{r}_N)|^2 \prod_{j=1}^{N} d^3 r_j = \left|\begin{array}{l}\text{probability of finding } N \\ \text{particles in volume } \prod d^3 r \text{ and } (\vec{r}_1, \ldots, \vec{r}_N)\end{array}\right|$$

quantum mechanics: indistinguishable particles

$$\psi(\vec{r}_1, \ldots, \vec{r}_j, \ldots, \vec{r}_k, \ldots, \vec{r}_N) = \lambda\, \psi(\vec{r}_1, \ldots, \vec{r}_k, \ldots, \vec{r}_j, \ldots, \vec{r}_N) =$$

$$= \lambda^2\, \psi(\vec{r}_1, \ldots, \vec{r}_j, \ldots, \vec{r}_k, \ldots, \vec{r}_N)$$

$$\Rightarrow \lambda = \begin{cases} +1 & \text{bosons} \\ -1 & \text{fermions (Pauli exclusion principle)} \end{cases}$$

single-particle basis: complete orthonormal $\{\psi_\nu(\vec{r})\}$ ← quantum number

$$\sum_\nu \psi_\nu^*(\vec{r})\psi_\nu(\vec{r}\,') = \delta(\vec{r}-\vec{r}\,'), \quad \int d^3 r\, \psi_\nu^*(\vec{r})\psi_{\nu'}(\vec{r}) = \delta_{\nu\nu'}$$

we project from $\psi(\vec{r}_1, \ldots, \vec{r}_N)$ on basis state $\psi_{\nu_1}(\vec{r}_1)$:

$$A_{\nu_1}(\vec{r}_2, \ldots, \vec{r}_N) \equiv \int d^3 r_1\, \psi_{\nu_1}^*(\vec{r}_1)\, \psi(\vec{r}_1, \ldots, \vec{r}_N)$$

and multiply by $\psi_{\nu_1}(\vec{r}_1)$, sum over ν_1, iterate

$$\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \sum_{\nu_1} \psi_{\nu_1}(\vec{r}_1)\, A_{\nu_1}(\vec{r}_2, \ldots, \vec{r}_N)$$

$$\Rightarrow \boxed{\Psi(\vec{r}_1,\dots,\vec{r}_N) = \sum_{\nu_1\dots\nu_N} \underbrace{A_{\nu_1\dots\nu_N}}_{\in\mathbb{C}} \psi_{\nu_1}(\vec{r}_1)\dots\psi_{\nu_N}(\vec{r}_N)}$$

symmetry of indistinguishable particles : symmetry of product

$$S_\pm \prod_{j=1}^{N} \psi_j(\vec{r}_j) = \begin{vmatrix} \psi_{\nu_1}(\vec{r}_1) & \psi_{\nu_1}(\vec{r}_2) & \dots \\ \psi_{\nu_2}(\vec{r}_1) & \ddots & \\ & & \psi_{\nu_N}(\vec{r}_N) \end{vmatrix}_\pm$$

$$\left.\begin{array}{l}\text{bosons: } + \ \dots \text{ permanent} \\ \text{fermions: } - \ \dots \text{ (Slater) determinant}\end{array}\right\} \text{physically valid bases}$$

$$\boxed{\Psi(\vec{r}_1,\dots,\vec{r}_N) = \sum_{\nu_1\dots\nu_N} B_{\nu_1\dots\nu_N} \hat{S}_\pm \psi_{\nu_1}(\vec{r}_1)\dots\psi_{\nu_N}(\vec{r}_N)}$$

Operators in 1st quantization

·) one-particle operators

$$T_{tot} = \sum_{j=1}^{N} T_j \ , \quad T_j = \sum_{\nu_a\nu_b} t_{\nu_a\nu_b} |\nu_b\rangle_j \langle\nu_a|_j$$

$$T_{\nu_a\nu_b} = \int d^3r\, \psi^*_{\nu_b}(\vec{r})\, T(\vec{r},\vec{\nabla}_r)\, \psi_{\nu_a}(\vec{r})$$

$$T_{tot} |\nu_1\rangle_1 |\nu_2\rangle_2 \dots |\nu_N\rangle_N = \sum_{j=1}^{N} \sum_{\nu_a\nu_b} T_{\nu_b\nu_a} \delta_{\nu_a\nu_j} |\nu_1\rangle_1 \dots |\nu_b\rangle_j \dots |\nu_N\rangle_N$$

·) two-particle operators

$$V_{tot} = \sum_{j<k}^{N} V_{jk} = \frac{1}{2}\sum_{j\neq k} V_{jk} \ , \quad V_{jk} = \sum_{\substack{\nu_a\nu_b \\ \nu_c\nu_d}} V_{\nu_c\nu_d\nu_a\nu_b} |\nu_c\rangle_j |\nu_d\rangle_k \langle\nu_a|_j \langle\nu_b|_k$$

$$V_{\nu_c\nu_d\nu_a\nu_b} = \int d^3r_j\, d^3r_k\, \psi^*_{\nu_c}(\vec{r}_j)\, \psi^*_{\nu_d}(\vec{r}_k)\, V(\vec{r}_j - \vec{r}_k)\, \psi_{\nu_a}(\vec{r}_j)\, \psi_{\nu_b}(\vec{r}_k)$$

$$V_{tot} |\nu_1\rangle_1 \dots |\nu_N\rangle_N = \frac{1}{2} \sum_{j\neq k} \sum_{\substack{\nu_a\nu_b \\ \nu_c\nu_d}} V_{\nu_c\nu_d\nu_a\nu_b}\, \delta_{\nu_a\nu_j}\, \delta_{\nu_b\nu_k}$$
$$|\nu_1\rangle_1 \dots |\nu_c\rangle_j \dots |\nu_d\rangle_k \dots |\nu_N\rangle_N$$

second quantization

idea: only occupied states play role in product

$\Rightarrow$ occupation number representation

We choose an ordered and complete single-particle basis

$$\{|\nu_1\rangle, \dots\}, \quad \hat{S}_\pm \, \psi_{\nu_{n_1}}(\vec{r}_1)\psi_{\nu_{n_2}}(\vec{r}_2)\dots\psi_{\nu_{n_N}}(\vec{r}_N)$$

and list the occupation number of each basis state

$$|n_{\nu_1}, n_{\nu_2}, \dots\rangle, \quad \sum_j n_{\nu_j} = N$$

$$n_{\nu_j} = \begin{cases} 0,1 & \text{for fermions (Pauli principle!)} \\ 0,1,2,\dots & \text{for bosons} \end{cases}$$

These are eigenstates of the occupation number operator:

$$\hat{n}_{\nu_j} |n_{\nu_j}\rangle = n_{\nu_j} |n_{\nu_j}\rangle$$

The spanned space is called a Fock space

$$F = F_0 \oplus F_1 \oplus F_2 \dots \quad F_N = \mathrm{Span}\{|n_{\nu_1} n_{\nu_2} \dots\rangle, \sum_j n_{\nu_j} = N\}$$

The empty state is called vacuum $|0\rangle = |0,0,\dots\rangle \neq 0$!

bosonic creation and annihilation operators

Creation operator: raises occupation of state $|\nu_j\rangle$ by 1 (cf. harmonic oscillator)

$$b^\dagger_{\nu_j} |\dots, n_{\nu_{j-1}}, n_{\nu_j}, n_{\nu_{j+1}}, \dots\rangle = B_+(n_{\nu_j}) |\dots, n_{\nu_{j-1}}, n_{\nu_j}+1, n_{\nu_{j+1}}, \dots\rangle$$

normalization (to be determined)

annihilation operator: lowers occupation of state $|v_j\rangle$ by 1

$$b_{v_j} |\dots, n_{v_{j-1}}, n_{v_j}-1, n_{v_{j+1}}, \dots\rangle = B_-(n_{v_j}) |\dots, n_{v_{j-1}}, n_{v_j}-1, n_{v_{j+1}}, \dots\rangle$$

bosons are symmetric in index v_j

$$\Rightarrow [b_{v_j}^+, b_{v_k}^+] = [b_{v_j}, b_{v_k}] = 0$$

care must be taken for $[b_{v_j}, b_{v_k}^+]$!

·) if $j \neq k$: different states, no problem

·) unoccupied state cannot be emptied further

$$b_{v_j} |\dots, 0, \dots\rangle = 0 \Rightarrow B_-(0) = 0$$

·) normalization (freedom)

$$b_{v_j}^+ |\dots, 0, \dots\rangle = |\dots, 1, \dots\rangle \Rightarrow B_+(0) = 1$$

·) since $\langle 1| b_{v_j}^+ |0\rangle^* = \langle 0| b_{v_j} |1\rangle$

$$\Rightarrow b_{v_j} |\dots, 1, \dots\rangle = |\dots 0 \dots\rangle \Rightarrow B_-(1) = 1$$

·) $b_{v_j} b_{v_j}^+ |0\rangle = |0\rangle$, $b_{v_j}^+ b_{v_j} |0\rangle = 0$

$$\Rightarrow [b_{v_j}, b_{v_j}^+]|0\rangle = (b_{v_j} b_{v_k}^+ - b_{v_j}^+ b_{v_j})|0\rangle = |0\rangle$$

$$\Rightarrow [b_{v_j}, b_{v_j}^+] = 1 \quad \text{for } |0\rangle, \quad \Rightarrow [b_{v_j}, b_{v_k}^+] = \delta_{jk}$$

We assume this commutation relation to be valid in general → What are the consequences?

What are remaining normalizations?

note that $[b_\nu^\dagger b_\nu, b_\nu] = -b_\nu$ and $[b_\nu^\dagger b_\nu, b_\nu^\dagger] = b_\nu^\dagger$

for any state $|\phi\rangle$ we note that $\langle\phi|b_\nu^\dagger b_\nu|\phi\rangle$ is the norm of state $b_\nu|\phi\rangle$ (positive, real number)

let $|\phi_\lambda\rangle$ be an eigenstate of $b_\nu^\dagger b_\nu \Rightarrow b_\nu^\dagger b_\nu|\phi_\nu\rangle = \lambda|\phi_\nu\rangle$
$\lambda > 0$

We choose a particular λ_0 and study $b_\nu|\phi_{\lambda_0}\rangle$:

$$(b_\nu^\dagger b_\nu) b_\nu |\phi_{\lambda_0}\rangle = (b_\nu b_\nu^\dagger - 1) b_\nu |\phi_{\lambda_0}\rangle = b_\nu (b_\nu^\dagger b_\nu - 1)|\phi_{\lambda_0}\rangle$$
$$= b_\nu (\lambda_0 - 1)|\phi_{\lambda_0}\rangle$$

$\Rightarrow$ also eigenstate, but with reduced occupation!

analogously: with $|\phi_\lambda\rangle = |n_\nu\rangle \Rightarrow b_\nu^\dagger b_\nu|n_\nu\rangle = n_\nu|n_\nu\rangle$
and $b_\nu|n_\nu\rangle \propto |n_\nu - 1\rangle$

$$(b_\nu^\dagger b_\nu) b_\nu^\dagger |n_\nu\rangle = (n+1) b_\nu^\dagger |n_\nu\rangle$$
$$\Rightarrow b_\nu^\dagger |n_\nu\rangle \propto |n_\nu + 1\rangle$$

normalizations: $\| b_\nu |n_\nu\rangle \|^2 = (b_\nu|n_\nu\rangle)^\dagger (b_\nu|n_\nu\rangle) =$
$$= \langle n_\nu | b_\nu^\dagger b_\nu | n_\nu\rangle = \underline{\underline{n_\nu}}$$
$$\| b_\nu^\dagger |n_\nu\rangle \|^2 = (b_\nu^\dagger|n_\nu\rangle)^\dagger (b_\nu^\dagger|n_\nu\rangle) =$$
$$= \langle n_\nu | b_\nu b_\nu^\dagger | n_\nu\rangle = \underline{\underline{n_\nu + 1}}$$

⇒ <u>for bosons:</u>

$$b_\nu^+ b_\nu = \hat{n}_\nu \,, \quad b_\nu^+ b_\nu |n_\nu\rangle = n_\nu |n_\nu\rangle \,, \quad n_\nu = 0,1,\ldots$$

$$b_\nu |n_\nu\rangle = \sqrt{n_\nu}\,|n_\nu - 1\rangle \,, \quad b_\nu^+ |n_\nu\rangle = \sqrt{n_\nu + 1}\,|n_\nu + 1\rangle$$

$$\hat{S}_+ |\nu_{n_1}\rangle_1 |\nu_{n_2}\rangle_2 \ldots |\nu_{n_N}\rangle_N \Leftrightarrow b^+_{\nu_{n_1}} b^+_{\nu_{n_2}} \ldots b^+_{\nu_{n_N}} |0\rangle$$

<u>for fermions:</u>

Anti-Commutators instead of commutators!

$$\{c^+_{\nu_j}, c^+_{\nu_k}\} = 0 \,, \quad \{c_{\nu_j}, c_{\nu_k}\} = 0 \,, \quad \{c_{\nu_j}, c^+_{\nu_k}\} = \delta_{\nu_j,\nu_k}$$

$$\Rightarrow (c^+_{\nu_j})^2 = 0 = (c_{\nu_j})^2 \quad \Rightarrow \text{Pauli principle!}$$

$$c_\nu^+ c_\nu = \hat{n}_\nu \,, \quad c_\nu^+ c_\nu |n_\nu\rangle = n_\nu |n_\nu\rangle \,, \quad n_\nu = 0,1$$

$$c_\nu|0\rangle = 0 \,, \quad c_\nu^+|0\rangle = |1\rangle \,, \quad c_\nu|1\rangle = |0\rangle \,, \quad c_\nu^+|1\rangle = 0$$

$$\hat{S}_- |\nu_{n_1}\rangle_1 |\nu_{n_2}\rangle_2 \ldots |\nu_{n_N}\rangle_N \Leftrightarrow c^+_{\nu_{n_1}} c^+_{\nu_{n_2}} \ldots c^+_{\nu_{n_N}} |0\rangle$$

⇒ We identified the bases!

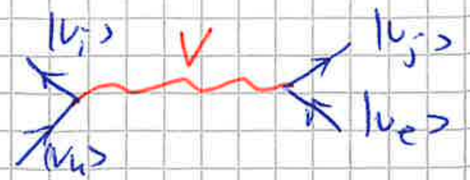
<u>Operators in second quantization</u>

<u>all operators</u> can be written with fundamental creation/annihilation operators

$$T_{tot} = \sum_{\nu_i \nu_j} T_{\nu_i \nu_j}\, a^+_{\nu_i} a_{\nu_j} \,, \quad T_{\nu_i \nu_j} = \int d^3r\, \psi^*_{\nu_i}(\vec{r})\, T(\vec{r}, \vec{\nabla}_r)\, \psi_{\nu_j}(\vec{r})$$

graphically (diagrammatically):

$$V_{tot} = \frac{1}{2} \sum_{\substack{\nu_i \nu_j \\ \nu_k \nu_l}} V_{\nu_i \nu_j \nu_k \nu_l} \, a_{\nu_i}^{\dagger} a_{\nu_j}^{\dagger} a_{l} a_{\nu_l}$$



⇒ linear combinations of products of creation / annihilation operators weighted by matrix elements of operators calculated in 1st quantization!

change of basis

$$\{|\nu_1\rangle, \ldots\} \to \{|\mu_1\rangle, \ldots\}$$

$$|\mu\rangle = \sum_{\nu} |\nu\rangle\langle\nu|\mu\rangle = \sum_{\nu} \langle\mu|\nu\rangle^{*} |\nu\rangle$$

$$a_{\mu}^{\dagger}|0\rangle = |\mu\rangle = \sum_{\nu} \langle\mu|\nu\rangle^{*} a_{\nu}^{\dagger}|0\rangle$$

$$\Rightarrow \boxed{a_{\mu}^{\dagger} = \sum_{\nu} \langle\mu|\nu\rangle^{*} a_{\nu}^{\dagger} \, , \; a_{\mu} = \sum_{\nu} \langle\mu|\nu\rangle a_{\nu}}$$

Special operators

particularly important: real-space basis

→ quantum field operators

$$\hat{\psi}^{\dagger}(\vec{r}) = \sum_{\nu} \langle\vec{r}|\nu\rangle^{*} a_{\nu}^{\dagger} = \sum_{\nu} \psi_{\nu}^{*}(\vec{r}) \, a_{\nu}^{\dagger}$$

↑ wave-function in real-space basis

$$\hat{\psi}(\vec{r}) = \sum_{\nu} \langle\vec{r}|\nu\rangle a_{\nu} = \sum_{\nu} \psi_{\nu}(\vec{r}) \, a_{\nu}$$

$\hat\psi^+$ ... "sum of all possible ways of adding a particle to the system at position $\vec r$ through any boson state $\psi_\nu(\vec r)$"

bosons: $[\hat\psi(\vec r_1), \hat\psi^+(\vec r_2)] = \delta(\vec r_1 - \vec r_2)$

fermions: $\{\hat\psi(\vec r_1), \psi^+(\vec r_2)\} = \delta(\vec r_1 - \vec r_2)$

Fourier transform: $$\hat\psi^+(\vec r) = \frac{1}{\sqrt V}\sum_{\vec k} e^{-i\vec k\vec r} a^+_{\vec k}$$

$$\hat\psi(\vec r) = \frac{1}{V}\sum_{\vec k} e^{i\vec k\vec r} a_{\vec k}$$

$$a_{\vec q}^+ = \frac{1}{\sqrt V}\int d^3r\, e^{i\vec q\vec r}\hat\psi^+(\vec r)$$

$$a_{\vec q} = \frac{1}{\sqrt V}\int d^3r\, e^{-i\vec q\vec r}\hat\psi(\vec r)$$

•) kinetic energy (tight binding)

$$T = -\sum_{ij\sigma} t_{ij}\, c^+_{i\sigma} c_{j\sigma}$$

•) kinetic energy (dispersion $\varepsilon_{\vec k}$)

$$T = \sum_{\vec k\sigma} \varepsilon_{\vec k}\, c^+_{\vec k\sigma} c_{\vec k\sigma} = \sum_{\vec k\sigma} \varepsilon_{\vec k}\, \hat n_{\vec k}$$

•) Coulomb interaction

$$V = \frac{1}{2V}\sum_{\sigma_1\sigma_2}\sum_{\vec k_1\vec k_2\vec q} V_{\vec q}\, a^+_{\vec k_1+\vec q,\sigma_1} a^+_{\vec k_2-\vec q,\sigma_2} a_{\vec k_2\sigma_2} a_{\vec k_1\sigma_1}$$

with $V_{\vec q} = \frac{e_0^2}{4\pi\varepsilon_0 q}$ unit charge