Quantum Field Theory

Edition: 1

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1 Making second quantization work

Why there is a minus in

$$\hat{H} = \sum_{ij} (-t_{ij}) \hat{c}_i^{\dagger} \hat{c}_j$$

I think I am still not very accustomed to the second quantization. And I can't tell the relation between writing an operator in terms of second quantization and in terms of field operators, and what is their separate lien with momentum and position?

A calculation work: The Hamiltonian for the Hubbard model is

$$\hat{H} = \sum_{ij\sigma} (-t_{ij}) \hat{c_{i\sigma}}^{\dagger} \hat{c_{j\sigma}} + U \sum_{i} \hat{n_{i\uparrow}} \hat{n_{i\downarrow}}$$

and we write a general state as $|\psi\rangle = a\,|\uparrow\downarrow, 0\rangle + b\,|\uparrow, \downarrow\rangle + c\,|\downarrow, \uparrow\rangle + d\,|0, \uparrow\downarrow\rangle$ and prove that in this basis the Hubbard Hamiltonian is

$$\hat{H} = \begin{pmatrix} U & -t & -t & 0 \\ -t & 0 & 0 & -t \\ -t & 0 & 0 & -t \\ 0 & -t & -t & U \end{pmatrix}$$

We calculate $\hat{H}\,|\uparrow\downarrow, 0\rangle$

$$\begin{aligned} \hat{H}\,|\uparrow\downarrow, 0\rangle &= (-t_{11}) \hat{c_{1\sigma}}^{\dagger} \hat{c_{1\sigma}}\,|\uparrow\downarrow, 0\rangle + (-t_{21}) \hat{c_{2\sigma}}^{\dagger} \hat{c_{1\sigma}}\,|\uparrow\downarrow, 0\rangle + U \hat{n_{1\uparrow}} \hat{n_{1\downarrow}}\,|\uparrow\downarrow, 0\rangle\,|\uparrow\downarrow, 0\rangle \\ &= {\color{red}?} + U.1.1\,|\uparrow\downarrow, 0\rangle \end{aligned}$$

$$\begin{aligned} (-t_{21}) \hat{c_{2\uparrow}}^{\dagger} \hat{c_{1\uparrow}}\,|\uparrow\downarrow, 0\rangle &= (-t_{21})((-1)^{n_0=0}\sqrt{1}) \hat{c_{2\uparrow}}^{\dagger}\,|\downarrow, 0\rangle \\ &= (-t_{21})((-1)^0\sqrt{1})((-1)^0\sqrt{1-0})\,|\downarrow, \uparrow\rangle \\ &= (-t_{21})\,|\downarrow, \uparrow\rangle \end{aligned}$$

$$\begin{aligned} (-t_{11}) \hat{c_{1\uparrow}}^{\dagger} \hat{c_{1\uparrow}}\,|\uparrow\downarrow, 0\rangle &= (-t_{11})((-1)^0\sqrt{1}) \hat{c_{1\uparrow}}^{\dagger}\,|\downarrow, 0\rangle \\ &= (-t_{11})((-1)^0\sqrt{1})((-1)^0\sqrt{1-0})\,|\uparrow\downarrow, 0\rangle \\ &= (-t_{11})\,|\uparrow\downarrow, 0\rangle \end{aligned}$$

$$\begin{aligned} (-t_{11}) \hat{c_{1\downarrow}}^{\dagger} \hat{c_{1\downarrow}}\,|\uparrow\downarrow, 0\rangle &= (-t_{11})((-1)^{n_{2-1}=n_1=1}\sqrt{1}) \hat{c_{1\downarrow}}^{\dagger}\,|\uparrow, 0\rangle \\ &= (-t_{11})((-1)^{n_{2-1}=n_1=1}\sqrt{1})((-1)^{n_{2-1}=n_1=1}\sqrt{1-0})\,|\uparrow\downarrow, 0\rangle \\ &= (-t_{11})\,|\uparrow\downarrow, 0\rangle \end{aligned}$$

But $t_{11} = 0$, so we don't keep these terms in our final result.

References