PHY392T NOTES: TOPOLOGICAL PHASES OF MATTER

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Today we'll describe second quantization as a convenient way to describe many-particle quantum-mechanical systems.

In "first quantization" (only named because it came first) one considers a system of N identical particles, either bosons or fermions. The wavefunction $\psi(r_1, \dots, r_N)$ is redundant: if σ is a permutation of $\{1, \dots, N\}$, then

$$\psi(r_1, \dots, r_n) = (\pm 1)\psi(r_{\sigma(1)}, \dots, r_{\sigma(N)}), \tag{2.1}$$

where the sign depends on whether we have bosons or fermions, and on the parity of σ.

For fermionic systems specifically, $\psi(r_1, \dots, r_N)$ is the determinant of an $N \times N$ matrix, which leads to an exponential amount of information in N. It would be nice to have a more efficient way of understanding many-particle systems which takes advantage of the redundancy (2.1) somehow; this is what second quantization does.

Another advantage of second quantization is that it allows for systems in which the total particle number can change, as in some relativistic systems.

The idea of second quantization is to view every degree of freedom as a quantum harmonic oscillator

$$H := \frac{1}{2}\omega^2(p^2 + x^2). \tag{2.2}$$

We set the lowest eigenvalue to zero for convenience. If $a := (x + ip)/\sqrt{2}$ and $a^\dagger := (x - ip)/\sqrt{2}$, then $\hat{n} := a^\dagger a$ computes the eigenvalue of an eigenstate.

Now let's assume our particles are all identical bosons. Then we introduce these operators $a_\sigma(\mathbf{r}), a_\sigma^\dagger(\mathbf{r})$ which behave as annihilation, respectively creation operators, in that they satisfy the commutation relations

$$\begin{gathered}[a_\sigma^\dagger(\mathbf{r}), a_{\sigma'}(\mathbf{r}')] = -\delta_{\sigma\sigma'}\delta(\mathbf{r} - \mathbf{r}') \\ [a^\dagger, a^\dagger] = 0.\end{gathered} \tag{2.3}$$

The Hamiltonian is generally of the form

$$H := \sum_{\sigma,\sigma'} \int_{\mathbf{r},\mathbf{r}'} a_\sigma^\dagger(\mathbf{r}) h_{\sigma\sigma'}(\mathbf{r} - \mathbf{r}') a_{\sigma'}(\mathbf{r}) + V_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta, \tag{2.4}$$

where the first term is the free part and the second term determines a two-particle interaction.

Letting $n_\sigma(\mathbf{r}) \coloneqq a_\sigma^\dagger(\mathbf{r})a_\sigma(\mathbf{r})$, which is called the *number operator* (since it counts the number of particles in state σ), there is a state $|\varnothing\rangle$ called the *vacuum* which satisfies $n_\sigma(\mathbf{r})|\varnothing\rangle = 0$ and $a_\sigma(\mathbf{r})|\varnothing\rangle = 0$. Particle creation operators commute, in that

$$a^\dagger(\mathbf{r}_1)a^\dagger(\mathbf{r}_2)|\varnothing\rangle = a^\dagger(\mathbf{r}_2)a^\dagger(\mathbf{r}_1)|\varnothing\rangle. \tag{2.5}$$

This is encoding that the particles are bosons: we exchange them and nothing changes.

The fermionic story is similar, but things should anticommute rather than commute. Letting α be an index, let f_α, resp. $f_\alpha^\dagger$ be the annihilation, resp. creation operators for a fermion in state α. There's again a vacuum $|\varnothing\rangle$, with $f_\alpha|\varnothing\rangle = 0$ for all α. Now we impose the relation

$$f_\alpha^\dagger f_\beta^\dagger|\varnothing\rangle = -f_\beta^\dagger f_\alpha^\dagger|\varnothing\rangle. \tag{2.6}$$

That is, define the *anticommutator* by

$$\{f_\alpha^\dagger, f_\beta^\dagger\} \coloneqq f_\alpha^\dagger f_\beta^\dagger + f_\beta^\dagger f_\alpha^\dagger. \tag{2.7}$$

Then we ask that $\{f_\alpha^\dagger, f_\beta^\dagger\} = 0$, and $\{f_\alpha^\dagger, f_\beta\} = \delta_{\alpha\beta}$.

Again we have a number operator $n_\alpha \coloneqq f_\alpha^\dagger f_\alpha$; it satisfies $n_\alpha f_\alpha = f_\alpha(n_\alpha - 1)$, and measures the number of particles in the state α. Because

$$(f_\alpha^\dagger)^2 = f_\alpha^\dagger f_\alpha^\dagger = -f_\alpha^\dagger f_\alpha^\dagger = 0, \tag{2.8}$$

then n_α is a projector (i.e. $n_\alpha^2 = n_\alpha$), and therefore its eigenvalues can only be 0 or 1. This encodes the Pauli exclusion principle: there can be at most a single fermion in a given state.

We'd like to write our second-quantized systems with quadratic Hamiltonians, largely because these are tractable. Let $(h_{\alpha\beta})$ be a self-adjoint matrix and consider the Hamiltonian

$$H \coloneqq \sum_{\alpha,\beta} f_\alpha^+ h_{\alpha\beta} f_\beta. \tag{2.9}$$

The *number operator* $N \coloneqq \sum n_\alpha$ commutes with the Hamiltonian, which therefore defines a symmetry of the system. The associated conserved quantity is the particle number. Slightly more explicitly, we have a symmetry of the group U_1 (i.e. the unit complex numbers under multiplication): for $\theta \in [0, 2\pi)$, let

$$u_\theta \coloneqq \exp(i\theta N). \tag{2.10}$$

Then

$$u_\theta^\dagger H u_\theta = \sum_{\alpha,\beta} \underbrace{u_\theta^\dagger f_\alpha^\dagger u_\theta}_{=e^{-i\theta} f_\alpha^\dagger} h_{\alpha\beta} \underbrace{u_\theta^\dagger f_\beta u_\theta}_{=e^{i\theta} f_\beta} = H. \tag{2.11}$$

When you see a Hamiltonian, you should feel a deep-seated instinct to diagonalize it: we want to find $\lambda_n, v^{(n)}$ such that $h_{\alpha\beta}v_\beta^{(n)} = \lambda_n v_\alpha^{(n)}$ and $vv^\dagger = \mathrm{id}$. Let $v_{n\alpha} \coloneqq v_\alpha^{(n)}$ and

$$\psi_n \coloneqq \sum_\alpha v_{n\alpha} f_\alpha. \tag{2.12}$$

Then $\psi_n^\dagger$ and ψ_n satisfy the same creation and annihilation relations as $f_\alpha^\dagger$ and f_α:

$$\{\psi_n^\dagger, \psi_m\} = \{\sum_\alpha v_{n\alpha}^* f_\alpha^\dagger, \sum_\beta v_{m\beta} f_\beta\} \tag{2.13}$$

$$= \sum_{\alpha,\beta} v_{n\alpha}^* v_{m\beta} \underbrace{\{f_\alpha^\dagger, f_\beta\}}_{=\delta_{\alpha\beta}} \tag{2.14}$$

$$= \sum_\alpha v_{m\alpha}(v^\dagger)_{n\alpha} = \delta_{m,n}. \tag{2.15}$$

Let $\hat{n}_n \coloneqq \psi_n^\dagger \psi_n$. Now the Hamiltonian has the nice diagonal form

$$H = \sum_n \lambda_n \psi_n^\dagger \psi_n, \tag{2.16}$$

and we can explicitly calculate its action on a state:

$$H\psi_{n_1}^\dagger\psi_{n_2}^\dagger\cdots\psi_{n_N}^\dagger|\varnothing\rangle = \underbrace{\left(\sum_m \lambda_m\psi_m^\dagger\psi_m\psi_{n_1}^\dagger\right)}_{(*)}\psi_{n_2}^\dagger\cdots\psi_{n_N}^\dagger|\varnothing\rangle. \tag{2.17}$$

The term $(*)$ is equal to

$$\psi_m^\dagger(\delta_{mn} - \psi_{n_1}^\dagger\psi_m) = \delta_{mn_1}\psi_{n_1}^\dagger + \psi_{n_1}^\dagger\psi_m^\dagger\psi_m. \tag{2.18}$$

Then (2.17) is equal to

$$(2.17) = \lambda_{n_1}\psi_{n_1}^\dagger(\psi_{n_2}^\dagger\cdots\psi_{n_N}^\dagger)|\varnothing\rangle, \tag{2.19}$$

so we've split off a term and can induct. The final answer is

$$= \left(\sum_{i=1}^N \lambda_i\right)\psi_{n_1}^\dagger\cdots\psi_{n_N}^\dagger|\varnothing\rangle. \tag{2.20}$$

Example 2.21 (1d tight binding model)**.** Let's consider the system on a circle with L sites (you might also call this periodic boundary conditions). We have operators which create fermions at each state and also some sort of tunneling operators. The Hamiltonian is

$$H \coloneqq -t\sum_{j=1}^L (f_{j+1}^\dagger f_j + f_j^\dagger f_{j+1}) - \mu\sum_{j=1}^L f_j^\dagger f_j, \tag{2.22}$$

where $j+1$ is interpreted mod L as usual. One of t and N (TODO: which?) can be interpreted as the chemical potential. The eigenstates are the Fourier modes

$$\psi_k \coloneqq \frac{1}{\sqrt{L}}\sum_{j=1}^L e^{ikj}f_j, \tag{2.23}$$

where $k = 2\pi n/L$. Hence in particular $e^{ik(L+1)} = e^{ik}$. Now we can compute

$$\sum_{j=1}^L f_{j+1}^\dagger f_j = \frac{1}{L}\sum_{j,k,k'} e^{ik'(j+1)}e^{-ikj}\psi_{k'}^\dagger\psi_k \tag{2.24}$$

$$= \frac{1}{L}\sum_{k,k'} e^{ik'}\sum_j e^{ij(k-k')}\psi_{k'}^\dagger\psi_k \tag{2.25}$$

$$= \sum_k e^{ik}\psi_k^\dagger\psi_k. \tag{2.26}$$

That is, the diagonalized Hamiltonian is

$$H = \sum_{k=1}^L (-2t\cos k - \mu)\psi_k^\dagger\psi_k. \tag{2.27}$$

You can plot λ_k as a function of k, but really k is defined on the circle $\mathbb{R}/2\pi\mathbb{Z}$, which is referred to as the *Brillouin zone*. The ground state of the system is to fill all states with negative energy:

$$|\text{G.S.}\rangle = \left(\prod_{k:\lambda_k<0}\psi_k^\dagger\right)|\varnothing\rangle. \tag{2.28}$$

If L is fixed, k only takes on L different values, but implicitly we'd like to take some sort of thermodynamic limit $L\to\infty$, giving us the actually smooth function $\lambda_k = -2t\cos k - \mu$. ◀

We said that second quantization is useful when the particle number can change, so let's explore that now. This would involve a Hamiltonian that might look something like

$$H = f_\alpha^\dagger h_{\alpha\beta}f_\beta + \frac{1}{2}\Big(\Delta_{\alpha\beta}f_\alpha^\dagger f_\beta^\dagger + \Delta_{\alpha\beta}^\dagger f_\alpha f_\beta\Big). \tag{2.29}$$

These typically arise in mean-field descriptions of superconductors. This typically arises in situations where electrons are attracted to each other — this is a little bizarre, since electrons have the same charge, but you can imagine an electron moving in a crystalline solid with some positive ions. The electron attracts the ions, but they move more slowly, so the electron keeps moving and we get an accumulation of positive charge, and this can attract additional electrons.

This binds pairs of electrons together at a certain point, and this forms a *condensate*, i.e. a superposition of states with different particle numbers. (2.29) describes a superconducting condensate, in which $\Delta_{\alpha\beta}$ describes pairs of particles appearing or disappearing in the condensate. To learn more, take a solid-state physics class.

Remark 2.30. You have to have pairs of fermionic terms — if you try to include an odd number of fermions, or a single fermionic term, you'll get nonlocal interactions between the lone fermion and others. Thus, even though the particle number is not conserved, its value mod 2, which is called *fermion parity*, is conserved. ◀

If you try to directly diagonalize (2.29), some weird stuff happens, so we'll rewrite the Hamiltonian such that it looks like it's particle-conserving, and then apply our old trick. This approach is due to Nambu. Let

$$\Psi_{\alpha,\tau} \coloneqq \begin{pmatrix} f_\alpha \\ f_\alpha^\dagger \end{pmatrix}, \tag{2.31}$$

where τ denotes the vertical index. We can rewrite the Hamiltonian as

$$H = \frac{1}{2}\begin{pmatrix} f_\alpha^\dagger & f_\alpha \end{pmatrix}\begin{pmatrix} h_{\alpha\beta} & \Delta_{\alpha\beta} \\ \Delta_{\alpha\beta}^\dagger & -h_{\alpha\beta}^\dagger \end{pmatrix}\begin{pmatrix} f_\beta \\ f_\beta^\dagger \end{pmatrix} + (\text{constant}) = \frac{1}{2}\Psi_{\alpha\tau}^\dagger \mathcal{H}_{\alpha\beta\tau\tau'}\Psi_{\beta\tau'}. \tag{2.32}$$

However, Ψ and $\Psi^\dagger$ have some redundancy: if σ^x denotes the Pauli matrix $\left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$, then $\Psi_\tau^\dagger = \sigma_{\tau\tau'}^x \Psi_{\tau'}$.

This is telling us that Ψ and $\Psi^\dagger$ create particles with energies (say) e and $-e$, respectively. Now

$$\Psi^\dagger H \Psi = \Psi^{\mathrm{T}}\sigma^x H \sigma^x (\Psi^\dagger)^{\mathrm{T}} = -\Psi^\dagger \sigma^x H^{\mathrm{T}} \sigma^x \Psi, \tag{2.33}$$

and therefore $\mathcal{H} = -\sigma^x \mathcal{H}^* \sigma^x$. Using this, we can determine the eigenstates: $\mathcal{H}v = Ev$ iff $\mathcal{H}\sigma^x v^* = -E\sigma^x v^*$. Then

$$\mathcal{H}\sigma^x v^* = \sigma^x(\sigma^x \mathcal{H}\sigma^x)v^* = \sigma^x(\sigma^x\mathcal{H}^*\sigma^x v)^* = \sigma^x(-\mathcal{H}v)^* = -E\sigma^x v^* \tag{2.34}$$

and

$$\gamma_E \coloneqq \sum_{\alpha,\tau} v_{\alpha\tau}\Psi_{\alpha\tau} \tag{2.35}$$

satisfies $\gamma_{-E} = \gamma_E^\dagger$. TODO: what are we trying to show here?

This $E \leftrightarrow -E$ symmetry is an instance of what's traditionally called "particle-hole symmetry," but it's a little weird — we can't break this symmetry by introducing additional terms to the Hamiltonian. So it might be more accurate to call it *particle-hole structure*, which conveniently has the same acronym.

TODO: some other stuff I missed. I think $\{\Psi_{\alpha\tau}, \Psi_{\beta\tau'}^\dagger\} = \delta_{\alpha\beta}\delta_{\tau\tau'}$ and $\{\gamma_E, \gamma_{E'}^\dagger\} = \delta_{EE'}$, which tells us these (I think) behave like creation and annihilation operators.

At zero energy, $\gamma_0 = \gamma_0^\dagger$, so we have a fermion which is its own antiparticle. This is called a *Majorana fermion*. It will be helpful to have a slightly different normalization here, which we'll discuss more later.