Quantum systems of many identical particles

Two approaches:

- Second quantization: 1-particle QM with multiple occupancies of eigenstates $\rightarrow$ Quantum Field
- Field quantization: Classical field with normal modes turned QM oscillators $\rightarrow$ Quantum Field

Comparison:

- different viewpoints: particles (1) vs. fields (2)
- Equivalent results
- Bosons & Fermions
- "2nd quantization" vs. "1st quantization": historic, the notation of QFT

The canonical field quantization approach

Recipe for quantizing fields:

- Determine the classical normal modes. If the equations are nonlinear, this may be difficult. Linearize the equations if necessary. The nonlinear terms can be included later as perturbations.
- Quantize the normal modes as simple harmonic oscillators.
- Classical fields become field-operators obeying free-field commutation relations
- From the distribution of the quantum states, predict thermodynamic quantities, correlation functions, etc.

Many-body QM. Basic structure

Hilbert space for N identical particles (B or F)

Fock space: $F_N = V_0 \oplus V_1 \oplus V_2 \oplus ... = \oplus_{n=0}^{\infty} SV^{\otimes n}$

V_0 vacuum, V_1 one-particle states, V_2 two-particle states (symmetric for B, antisymmetric for F), etc
Hamiltonian in F_N

$$H = -\sum_{i=1...N} -\frac{\hbar^2}{2m}\nabla_i^2 + V(\boldsymbol{r}_1...\boldsymbol{r}_N)$$

Eigenfunctions $H\psi_n(\boldsymbol{r}_1...\boldsymbol{r}_N) = E_n\psi_n(\boldsymbol{r}_1...\boldsymbol{r}_N)$
symmetric for B, antisymmetric for F

An equivalent quantum field picture (justify later)

Introduce field operators:

$$\psi(\mathrm{r}) = \sum_i \varphi_i(\mathrm{r}) c_i, \quad \psi^\dagger(\mathrm{r}) = \sum_i \varphi_i^*(\mathrm{r}) c_i^\dagger.$$

$\langle \varphi_i | \varphi_j \rangle = \delta_{ij}$, $[c_i, c_j^\dagger]_\pm = \delta_{ij}$.
The operator $\psi(\boldsymbol{r})$ annihilates particle at $\boldsymbol{r}$, $\psi^\dagger(\boldsymbol{r})$ creates particle at $\boldsymbol{r}$

$$[\psi(\boldsymbol{r}), \psi^\dagger(\boldsymbol{r}')]_\pm = \delta^{(3)}(\boldsymbol{r} - \boldsymbol{r}'), \quad [\psi(\boldsymbol{r}), \psi(\boldsymbol{r}')]_\pm = 0$$

notation: $[A, B]_\pm = AB \pm BA$

One-particle operators:

$$A = \sum_{i=1}^{N} A(\mathrm{r}_i) \;\rightarrow A = \sum_{\mathrm{pq}} A_{\mathrm{pq}} c_{\mathrm{p}}^{\dagger} c_{\mathrm{q}}$$

with $A_{\mathrm{pq}} = \int d^3 r \varphi_{\mathrm{p}}^{*}(\mathrm{r}) A \varphi_{\mathrm{q}}(\mathrm{r})$. Here $A(\boldsymbol{r})$, say, a 1-particle kinetic or potential energy operator:

$$A(\boldsymbol{r}) = -\frac{\hbar^2}{2m}\nabla^2, \quad A(\boldsymbol{r}) = U(\mathrm{r}), \text{ etc}$$

Two(three)-particle operators are constructed in a similar manner. The field operators appear to be basis-dependent. We'll show later that they are not.

An equivalent quantum field picture (justify later)

1-particle/many-particle correspondence:

$$\sum_i f(\boldsymbol{r}_i) \to \int d^3 r \psi^\dagger(\boldsymbol{r}) f(\boldsymbol{r}) \psi(\boldsymbol{r})$$

2-particle/many-particle correspondence:

$$\sum_{ij} g(\boldsymbol{r}_i, \boldsymbol{r}_j) \to \frac{1}{2} \int d^3 r_1 d^3 r_2 \psi^\dagger(\boldsymbol{r}_1) \psi^\dagger(\boldsymbol{r}_2) g(\boldsymbol{r}_1, \boldsymbol{r}_2) \psi(\boldsymbol{r}_2) \psi(\boldsymbol{r}_1)$$

and so on. For $V(\boldsymbol{r}_1 \ldots \boldsymbol{r}_N) = \sum_{ij} V(\boldsymbol{r}_i, \boldsymbol{r}_j)$ arrive at

$$H = \int d^3 r \psi^\dagger(\boldsymbol{r}) \frac{p^2}{2m} \psi(\boldsymbol{r}) + \frac{1}{2} \int d^3 r d^3 r' \psi^\dagger(\boldsymbol{r}) \psi^\dagger(\boldsymbol{r}') V(\boldsymbol{r}, \boldsymbol{r}') \psi(\boldsymbol{r}') \psi(\boldsymbol{r})$$

Properties:

- Define particle # operator $N = \int d^3\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r})$;
  N obeys:

  $$[N, H] = 0, \ [\psi(\boldsymbol{r}), N] = \psi(\boldsymbol{r})], \ [\psi^\dagger(\boldsymbol{r}), N] = -\psi^\dagger(\boldsymbol{r})$$

  same for B and F!
  Interpretation: action of ψ ($\psi^\dagger$) on eigenstate of N is to decrease (increase) eigenvalue by 1
- The vacuum state $\psi(\boldsymbol{r})|0\rangle = 0$ (for any $\boldsymbol{r}$) where $|0\rangle$ is a nonzero vector and 0 is the null vector
- Eigenstates of N: $\psi^\dagger(\boldsymbol{r}_1)\psi^\dagger(\boldsymbol{r}_2)...\psi^\dagger(\boldsymbol{r}_m)|0\rangle$ with the eigenvalue $N = m$

Second quantization (with justification)

Occupation number representation:
symmetrized products of complete ONB states (position eigenstates, momentum eigenstates, noninteracting H eigenstates, etc)

$$\psi_B(x_1, x_2 ... x_N) = c \sum_P \varphi_1(Px_1)\varphi_2(Px_2)...\varphi_N(Px_N)$$

φ_q occurs n_q times (n_q particles in state φ_q),
$q = 1...Q$
$N!$ permutations, $c = (N!/(n_1!...n_Q!))^{-1/2}$
Occupation $\#$ representation:

$$\psi_B = |n_1, n_2 ... n_Q ...\rangle, \quad n_q = 0, \; q > Q$$

Creation and annihilation operators

$$b_q^\dagger|n_1, n_2 ... n_q ... n_Q ...\rangle = \sqrt{n_q + 1}|n_1, n_2 ... n_q{+}1 ... n_Q ...\rangle$$

$$b_q|n_1, n_2 ... n_q ... n_Q ...\rangle = \sqrt{n_q}|n_1, n_2 ... n_q - 1 ... n_Q ...\rangle$$

prefactors $\sqrt{n_q + 1}$ and $\sqrt{n_q}$ motivated by the ladder operator results for simple harmonic oscillator
These operators obey

$$[b_r, b_s^\dagger] = \delta_{rs}, \quad [b_r, b_s] = [b_r^\dagger, b_s^\dagger] = 0$$

Consistent with the field normal modes quantized as independent oscillators

Fermions

Antisymmetrized states, the Slater determinant

$$\psi_F(\mathbf{x}_1, \mathbf{x}_2 ... \mathbf{x}_N) = c \sum_P (-1)^P \varphi_1(P\mathbf{x}_1)\varphi_2(P\mathbf{x}_2)...\varphi_N(P\mathbf{x}$$

all φ_i different (equiv Pauli exclusion)
$N!$ permutations, $c = (N!)^{-1/2}$
Occupation number representation:

$$\psi_F = |n_1, n_2, n_3 ...\rangle, \quad n_i = \begin{cases} 1 \text{ for } \varphi_1 ... \varphi_N \\ 0 \text{ else} \end{cases}$$

NB: order matters, affects the $(-1)^P$ sign

Fermion creation & annihilation operators

One particle: $|1\rangle$ a 1-particle state, $|0\rangle$ vacuum, or no-particle state

$a^\dagger|0\rangle = |1\rangle$, $a^\dagger|1\rangle = 0$, $a|1\rangle = |0\rangle$, $a|0\rangle = 0$

NB: $|0\rangle$ and 0 not the same!

Algebra: $[a, a^\dagger]_+ = 1$, $[a, a]_+ = [a^\dagger, a^\dagger]_+ = 0$

Many particles:

$$a_q|n_1, n_2 \ldots n_q \ldots\rangle = \begin{cases} (-1)^S |n_1, n_2 \ldots 0 \ldots\rangle, & n_q = 1 \\ 0, & n_q = 0 \end{cases}$$

$$a_q^\dagger|n_1, n_2 \ldots n_q \ldots\rangle = \begin{cases} 0, & n_q = 1 \\ (-1)^S |n_1, n_2 \ldots 1 \ldots\rangle, & n_q = 0 \end{cases}$$

with $S = n_1 + n_2 + \ldots + n_{q-1}$ to keep track of ordering condition

Full algebra:

$$[a_r, a_s^\dagger]_+ = \delta_{rs}, \quad [a_r, a_s]_+ = [a_r^\dagger, a_s^\dagger]_+ = 0$$

NB: $a_1^\dagger a_2^\dagger |0, 0, ...\rangle = -a_2^\dagger a_1^\dagger |0, 0, ...\rangle$ consistent with the Slater determinant definition

Particle number operators:

$$n_q = \begin{cases} b_q^\dagger b_q, & Bosons, \quad n_q = 0, 1, 2... \\ a_q^\dagger a_q, & Fermions, \quad n_q = 0, 1 \end{cases}$$

- $[n_s, n_r]_- = 0$ simultaneously diagonalizable
- For a general state $\langle\psi|n_q|\psi\rangle$ may be nonintegral

Summing up:

- Complicated many-particle wavefunction
- A more simple occupation $\#$ repres
- Algebra for a, $a^\dagger$ operators, states $a_1^\dagger \ldots a_s^\dagger |0\rangle$
- Few-body operators $T = \sum_i -\frac{1}{2m}\nabla_i^2$, $V = \sum_{i<j} u(x_i - x_j)$. Second-quantized?
- Basis dependent? Actually, basis independent (discuss later)

Physical operators

- One-body operators $O_1 = \sum_i f_i$.
  Second-quantized form $O_1 = \sum_{rs} \langle \varphi_r | \varphi_s \rangle c_r^\dagger c_s$
  with matrix elements
  $\langle \varphi_r | f | \varphi_s \rangle = \int d^3x \varphi_r^*(x) f(x) \varphi_s(x)$
  c_r repres a_r (fermions) or b_r (bosons)
- Two-body operators $O_2 = \sum_{i<j} f(x_i, x_j)$.
  Second quantized form $O_2 = \sum_{pqrs} f_{pqrs} c_p^\dagger c_q^\dagger c_r c_s$
  with matrix elements
  $f_{pqrs} = \int d^3x d^3x' \varphi_p^*(x) \varphi_q^*(x') f(x, x') \varphi_r(x) \varphi_s(x')$
  NB: the ordering matters for fermions, does not matter for bosons

Prove it for Fermions (more difficult)

$$R = \left(\sum_s f_s \right) A \left[\varphi_1(x_1)...\varphi_N(x_N) \right]$$

- move $\sum_s f_s$ inside A
- Use completeness
  $f(x)\varphi_s(x) = \sum_r \langle \varphi_r | f | \varphi_s \rangle \varphi_r(x)$
- Obtain a sum, with weights $\langle \varphi_r | f | \varphi_s \rangle$, of antisymmetric products in which $\varphi_s \to \varphi_r$
- But this is the content of 2nd quantization, $c_r^\dagger c_s$ gives just that. QED

Two-particle operators, analogously

- move $\sum_{r,s} f_{r,s}$ inside A
- Use completeness to replace $\varphi_r \varphi_s$ with $\sum_{p,q} f_{pqrs} \varphi_p \varphi_q$
- The correct ordering of the operators arises because

$$\left(c_p^\dagger c_q^\dagger c_s c_r\right) c_r^\dagger c_s^\dagger |0\rangle = c_p^\dagger c_q^\dagger |0\rangle$$

agrees with (anti)commutation rules

QED

Bogoliubov transformation

Diagonalizing quadratic Hamiltonians

$H = \sum_{ij} H_{ij} c_i^\dagger c_j$, where H_{ij} - hermitian, hence, can be diagonalized by a unitary transformation. Then

$$\alpha_l^\dagger = \sum_i c_i^\dagger \overset{\substack{\text{unitary}\\ \downarrow}}{U_{il}} \xrightarrow{\text{inversion}} \sum_l \alpha_l^\dagger \left(U^\dagger\right)_{lj} = c_j^\dagger \quad \Rightarrow \quad c_j = \sum_l U_{jl} \alpha_l .$$

Use transformed c, $c^\dagger$ operators to transform H:

$$H = \sum_{lm} \alpha_l^\dagger (U^\dagger H U)_{lm} \alpha_m = \sum_m \varepsilon_m \alpha_m^\dagger \alpha_m = \sum_m \varepsilon_m n_m .$$

NB: Operator algebra is basis independent:

$[c_i, c_j^\dagger]_\pm = \delta_{ij}$, $[c_i, c_j]_\pm = [c_i^\dagger, c_j^\dagger]_\pm = 0$

$UB = B$, $UF = F$ (statistics unchanged!)

Physically important systems (superconductors, superfluids, ferromagnets, antiferromagnets) all can be described by a quadratic H (approximately)

As an example take a boson Hamiltonian

$$H = \varepsilon(c_1^\dagger c_1 + c_2^\dagger c_2) + \lambda(c_1 c_2 + c_2^\dagger c_1^\dagger)$$

Try a linear transformation (with real u, v):

$$c_1 = ud_1 + vd_2^\dagger, \qquad c_1^\dagger = ud_1^\dagger + vd_2,$$
$$c_2 = ud_2 + vd_1^\dagger, \qquad c_2^\dagger = ud_2^\dagger + vd_1.$$

Bosonic algebra? 1) $[c_1^\dagger, c_2^\dagger] = 0$ for any u and v.
2) $[c_1, c_1^\dagger] = u^2[d_1, d_2] - v^2[d_2, d_2^\dagger] = 1$, giving

$$u^2 - v^2 = 1$$

Hence we make a *Minkowski* (special relativity) parameterization

$$u^2 - v^2 = 1: \qquad \begin{aligned} u &= \cosh\theta, \\ v &= \sinh\theta. \end{aligned}$$

The matrix form of our transformation reads

$$\begin{pmatrix} c_1 \\ c_2^\dagger \end{pmatrix} = \begin{pmatrix} u & v \\ v & u \end{pmatrix} \begin{pmatrix} d_1 \\ d_2^\dagger \end{pmatrix}$$

Diagonalize H? **The key idea: mix c_1 with $c_2^\dagger$ and c_2 with $c_1^\dagger$.** Change order, $c_2^\dagger c_2 = c_2 c_2^\dagger - \hat{1}$,

$$H = (c_1^\dagger \; c_2) \begin{pmatrix} \varepsilon & \lambda \\ \lambda & \varepsilon \end{pmatrix} \begin{pmatrix} c_1 \\ c_2^\dagger \end{pmatrix} - \overset{\substack{\text{const (ignore)} \\ \downarrow}}{\varepsilon}$$

Write in terms of d, $d^\dagger$:

$$H = (d_1^\dagger \; d_2) \begin{pmatrix} u & v \\ v & u \end{pmatrix} \begin{pmatrix} \varepsilon & \lambda \\ \lambda & \varepsilon \end{pmatrix} \begin{pmatrix} u & v \\ v & u \end{pmatrix} \begin{pmatrix} d_1 \\ d_2^\dagger \end{pmatrix}$$

Can use 2×2 Pauli matrices notation $H = d_i^\dagger H'_{ij} d_j$
$\tilde{H} = (u\hat{1} + v\sigma_1)(\varepsilon\hat{1} + \lambda\sigma_1)(u\hat{1} + v\sigma_1)$

$$\tilde{H} = \hat{1}(\varepsilon(u^2 + v^2) + \lambda uv) + \sigma_1(2\varepsilon uv + \lambda[u^2 + v^2]).$$

Setting $\tanh 2\theta = -\lambda/\varepsilon$ obtain

$$\tilde{H} = \tilde{\varepsilon}\hat{1} + \tilde{\lambda}\sigma_1, \quad \tilde{\varepsilon} = \sqrt{\varepsilon^2 - \lambda^2}, \quad \tilde{\lambda} = 0.$$

This gives **two decoupled bosons:**

$$H = \tilde{\varepsilon}(d_1^\dagger d_1 + d_2^\dagger d_2) - \varepsilon + \tilde{\varepsilon}$$

The condition $\varepsilon > |\lambda|$ is required for stability.

A toy model that illustrates how a system of interacting particles is represented as a system of noninteracting quasiparticles

Particle nonconserving transformations? Meaning?

Recall a, $a^\dagger$ for a harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right),$$

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(q + \frac{i}{m\omega}p\right), \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(q - \frac{i}{m\omega}p\right)$$

Take a', $a'^\dagger$ with a ‘wrong’ value ω' instead of ω.
These operators describe squeezed states, representing H as a hermitian and yet particle-nonconserving operator!

$$H_\omega = H_{\omega'} + \left(\frac{m\omega^2}{2} - \frac{m\omega'^2}{2}\right)q^2 = \hbar\omega'\left(a^\dagger a + \frac{1}{2}\right) + \frac{m\Delta(\omega^2)}{2}\frac{\hbar}{2m\omega'}\left(a' + a'^\dagger\right)^2$$

$$= \hbar\frac{\omega^2 + \omega'^2}{2\omega'}a'^\dagger a' + \frac{m\Delta(\omega^2)}{4\omega'}\left(a'a' + a'^\dagger a'^\dagger\right).$$

1. Affords a natural generalization to many modes
2. Works for both B & F (will discuss later).

Squeezing as a unitary transformation?

Wanted: $UH_{\omega'}U^{-1} \sim H_\omega$
This is achieved by a norm-preserving scaling transformation $U_g: \ \psi(q) \to \sqrt{g}\psi(gq)$. A dilation for parameter values $0 < g < 1$ and squeezing for $g > 1$, respectively.
Since $U_g q U_g^{-1} = gq$, $U_g p U_g^{-1} = g^{-1}p$ and $U_g \left(\frac{p^2}{2m} + \frac{m\omega'^2}{2} q^2 \right) U_g^{-1} = \frac{p^2}{2mg^2} + g^2 \frac{m\omega'^2}{2} q^2$, for the value $g = (m/m')^{1/2}$ we have $UH_{\omega'}U^{-1} \sim H_\omega$ and
$Ua'U^{-1} = ua + va^\dagger$, $Ua'^\dagger U^{-1} = ua^\dagger + va$,
with the values $u = \frac{1}{2}(g + g^{-1})$, $v = \frac{1}{2}(g - g^{-1})$.
On the side: $U_g = e^{\lambda q \frac{d}{dq}} = 1 + \lambda q \frac{d}{dq} + \frac{\lambda^2}{2} \left(q \frac{d}{dq} \right)^2 + \ldots$ with $\lambda = \ln(g)$