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PHYS 535 MANY-BODY QUANTUM-MECHANICS OF DEGENERATE GASES

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Literature:

No single textbook

- R. Shankar „Principles of Q.M.") too little
- J.J. Sakurai „Modern Q.M"
- Negele and Orland „Quantum many particle systems" (too much
- Fetter and Walecka „Quantum theory of many-particle systems"
- Pethick and Smith „Bose-Einstein Condensation in dilute gases"
- L. Schiff „Quantum Mechanics"
- ... ? Bruus, Flensberg „Introduction to Many-Body QM in cond. mat"

Assessment:

Online-Quiz	20%
Assignments	10% → See "Rules", speech
Mid-Sem	30%
End-Sem	40%

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Office Hours: Thursdays 14:00–17:00
(please confirm online)

Course Outline: (tentative)

1) Motivation and Review ~1 week

- fields that require Many-Body QM, why degenerate gases
- review of essential pieces from single-particle QM

2) Quantum-many-body formalism ~4 weeks

- Second quantisation, Bosons vs. Fermions, quantum field operators, coherent states

3) Bose-Einstein condensates ~4 weeks

- Symmetry breaking / mean field, critical temperature, Gross-Pitaevskii equation, Bogoliubov quasi-particles, Quantum-field theory of BEC

4) Degenerate Fermi Gases ~ 3 weeks

- Fermi surface, degeneracy pressure, Neutron stars, electron gas, pairing, superconductivity

5) Quantum Simulators ~2 weeks

Analog and digital quantum simulation, Bose-Hubbard model, BEC-BCS cross-over

1) MOTIVATION AND REVIEW

1.1) Quantum Many-Body theory and QFT

Single quantum particle $|\varphi(\vec{x})\rangle$

Many particles, symmetries

$$\psi(\vec{x}_1, \vec{x}_2) = \frac{1}{\sqrt{2}}\left(|\varphi_1(\vec{x}_1)\varphi_2(\vec{x}_2)\rangle \pm |\varphi_2(\vec{x}_1)\varphi_1(\vec{x}_2)\rangle\right)$$

Particle creation/destruction

$\psi(\vec{x}_1)$

$\psi(\vec{x}_1, \vec{x}_2)$ $\hat{=}$ Fock Space

$\psi(\vec{x}_1, \vec{x}_2, \vec{x}_3)$

Second quantization, creation and destruction operators

$\hat{a}$, $\hat{a}^+$ (same algebra as S.H.O. ladder operators)

Quantum field theory

$$\hat{\psi}(x) = \sum_n \underbrace{\varphi_n(\vec{x})}_{\text{waves}} \underbrace{\hat{a}_n^+}_{\text{particles}}$$

- $\hat{\psi}$ can be viewed as type of destruction operator
- classical field theory → now field itself quantized

not here $v \approx c$ → relativistic quantum mechanics & quantum field theory (Elementary Particle physics) ↓ only Spin-Statistics theorem

also not here → Advanced QFT techniques, Greens-functions, Path-Integrals, Keldysh Formalism, thermal field theory

1.2. Disciplines with many-body QM (ASK)

- Atomic Molecular Physics (many e^-)
- Chemistry (more e^-)
- Nuclear Physics (many n, p)
- Particle Physics (several elementary particles, but more concerned with creation / destruction / conversion / symmetries than with many)
- Condensed matter physics (10^{23} e^-. Or quasi particles (Spinon, Magnon, Plasmon, Sth.on))
- (Astro physics ?) (Even more e^-/ n)

Recently: Quantum Optics (many γ, usually non-interacting)
Information (many 0,1)

1.3. Review

also establish notation

1.3.1. Single-particle states

In this course, we will always assume the problem of a single particle to be solved. E.g. in

Time-independent Schrödinger equation (TISE)

$$\boxed{\mathcal{H}_0 |\varphi_n\rangle = E_n |\varphi_n\rangle \qquad (1.1)}$$

- $\mathcal{H}_0$ is the single-body Hamiltonian (depends on co-ordinates of just one particle)
- $|\varphi_n\rangle$ is the (typically) infinite single-particle basis
- E_n are single particle energies.

Examples:

(i) free particles in volume V

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

$$|\varphi_n\rangle \rightsquigarrow |\phi_{\vec{k}}\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\vec{x}}$$ wavenumber $\vec{k}$

sloppy on "ket" versus position-space rep. Explain

(ii) Spin-$\frac{1}{2}$ states

$$H_0 = \Delta E\, \sigma_3 \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad E_{\uparrow,\downarrow} = \pm \Delta E$$

$$|\varphi_{\uparrow,\downarrow}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \mathrel{\hat{=}} |\uparrow\rangle \quad \text{or} \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix} \mathrel{\hat{=}} |\downarrow\rangle$$

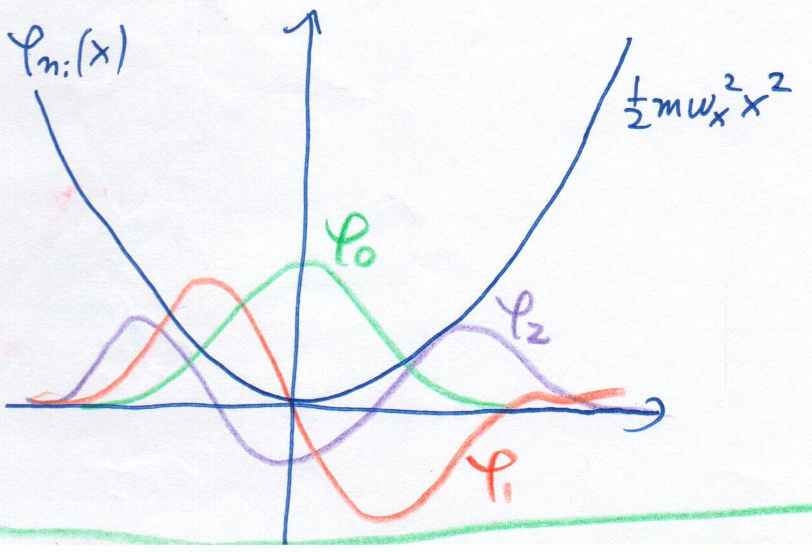
(iii) Simple harmonic oscillator states (3D)

$$H_0 = \frac{\vec{p}^2}{2m} + \frac{1}{2} m \left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right)$$

$$|\varphi_{\vec{n}}\rangle = |\varphi_{n_x n_y n_z}\rangle = \varphi_{n_x}(x)\, \varphi_{n_y}(y)\, \varphi_{n_z}(z) \quad \left(= |\varphi_{\vec{n}}(\vec{x})\rangle\right) \qquad (1.2)$$

$$\varphi_{n_i}(x_i) = \underbrace{\frac{1}{\sqrt{2^{n_i}(n_i)!\sqrt{\pi}\,\sigma_i}}}_{\equiv N} e^{-\frac{x^2}{2\sigma_i^2}} H_{n_i}\left(\frac{x_i}{\sigma_i}\right)$$

$x_i \in \{x, y, z\}$



$$\boxed{\begin{aligned} E_n &= \hbar\omega_x\left(n_x + \tfrac{1}{2}\right) \\ &+ \hbar\omega_y\left(n_y + \tfrac{1}{2}\right) \\ &+ \hbar\omega_z\left(n_z + \tfrac{1}{2}\right) \end{aligned}} \qquad (1.3)$$

We can show $[\hat{b}, \hat{b}^+] = 1$ (from $[\hat{x}, \hat{p}] = i\hbar$)

New Hamiltonian using ladder operators (from 1D version of (1.2))

$$\hat{H}_0 = \hbar\omega\left(\hat{b}^+\hat{b} + \frac{1}{2}\right) \quad (1.5)$$

We can now show (e.g Shankar ≈ pp. 204) the

~~that~~ function of lowering operator ($\hat{a}$) and raising operator

$$\hat{b}|\varphi_n\rangle = \sqrt{n}\,|\varphi_{n-1}\rangle \qquad \hat{b}|\varphi_0\rangle = 0$$

$$\hat{b}^+|\varphi_n\rangle = \sqrt{n+1}\,|\varphi_{n+1}\rangle \quad (1.6)$$

Number-operator: $\hat{N} = \hat{b}^+\hat{b}$ $\quad \hat{N}|\varphi_n\rangle = n|\varphi_n\rangle$

- these properties follow solely from the commutation relation $[\hat{b}, \hat{b}^+] = 1$, we would NOT need to know the position space representation (1.2).

1.3.2 Single particle density matrices

(maybe not review? See: Schiff p. 378 ff)

QM: superpositions: $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$

Classical: Probability distribution e.g. $P(\uparrow) = 50\%$, $P(\downarrow) = 50\%$
(let $\uparrow, \downarrow$ be "head"/"tail" for a coin here).

Want Mathematics to describe both simultaneously.

Density matrix / operator:

$$\hat{\rho} = \sum_{nm} \rho_{nm} |\varphi_n\rangle\langle\varphi_m| \quad (1.7)$$

where $|\varphi_n\rangle$ is a chosen single particle basis as in (1.5).

- Pure quantum: $\hat{\rho} = |\psi\rangle\langle\psi|$
- Pure classical $\rho_{nm} = 0$ for $n \neq m$

(see examples later)

Density Matrix properties:

$\hat{\rho}$ hermitian, $\hat{\rho}^2 = \hat{\rho}$ for pure state, $\mathrm{trace}(\hat{\rho}) = 1$

expectation value of observable $\hat{O}$: $\langle \hat{O} \rangle = \mathrm{trace}(\hat{\rho} \cdot \hat{O})$ (1.8)

~~Timeevolution for pure states~~

$\underbrace{\mathrm{trace}\,(\hat{\rho}^2)}_{=\text{Purity}} \leq 1 \Rightarrow =1$ for pure states

else is called mixed state

Time-evolution ~~for pure states~~

$$i\hbar \frac{\partial}{\partial t} \hat{\rho} = [\hat{H}, \hat{\rho}] \qquad \text{von-Neumann equation} \qquad (1.9)$$

Example: Single spin-$\frac{1}{2}$ (see (ii) earlier)

(i) Let $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$

$$\hat{\rho} = |\psi\rangle\langle\psi| = \frac{1}{2}\Big(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| + |\uparrow\rangle\langle\downarrow| + |\uparrow\rangle\langle\downarrow|\Big) \rightarrow$$

ρ_{nm} in matrix form:

$$\underline{\underline{\rho}} = \begin{array}{cc} & \begin{array}{cc} |\uparrow\rangle & |\downarrow\rangle \end{array} \\ & \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array} \end{array}$$

(ii)
If we had a classical mixture (50% $\uparrow$, 50% $\downarrow$)

$$\hat{\rho} = \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) \rightarrow \underline{\underline{\rho}} = \begin{array}{cc} & \begin{array}{cc} |\uparrow\rangle & |\downarrow\rangle \end{array} \\ & \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array} \end{array}$$

Diagonal elements: „populations" / „probabilities"

$\rho_{nn} \;\hat{=}\;$ Probability to find system in state n

Off-diagonal elements: „coherences"

$\rho_{12} \;\hat{=}\;$ coherence between state 1&2
(=0 classically)

Consequences:

$$\langle \hat{\sigma}_x \rangle = \begin{cases} \langle\psi|\hat{\sigma}_x|\psi\rangle = \hbar/2 & \text{(for case (i), pure)} \\ \text{versus} & \\ \mathrm{Tr}[\hat{\rho}\hat{\sigma}_x] = \mathrm{Tr}\begin{bmatrix} 0 & \frac{\hbar}{2\sqrt{2}} \\ \frac{\hbar}{2\sqrt{2}} & 0 \end{bmatrix} = 0 & \text{(for case (ii) mixed)} \end{cases}$$

1.3.3. Many-particle states

Generalisation of (1.1) to many-particles, is to add one co-ordinate per particle:

Many-Body TISE (general case) (1.10)

$$\hat{H}(\vec{x}_1, \dots, \vec{x}_n, \hat{p}_1, \dots \hat{p}_N) \, |\psi_K(\vec{x}_1, \dots, \vec{x}_N)\rangle = E_K \, |\psi_K(\vec{x}_1, \dots \vec{x}_N)\rangle$$

- Typically very (too) high dimensional PDE (e.g. 9D for 3 particles in 3D space)
- K may contain many indices
- Can write many body state in terms of single-body ones:

show vector analogy

$$|\psi_K(\vec{x}_1, \dots \vec{x}_N)\rangle \doteq \sum_{\boxed{n_1, \dots n_N}} C_{k; n_1, \dots n_N} \, |\varphi_{n_1}(\vec{x}_1)\rangle \otimes |\varphi_{n_2}(\vec{x}_2)\rangle \otimes \dots |\varphi_{n_N}(\vec{x}_N)\rangle \quad (1.11)$$

see φ for S.H.O (Eq. (1.2))

Insertion:

See 1.3.4 page 10

Orthogonality: $\langle \varphi_{n_1}(\vec{x}_1) | \langle \varphi_{n_2}(\vec{x}_2) | \varphi_{n_1'}(\vec{x}_1)\rangle | \varphi_{n_2'}(\vec{x}_2)\rangle = \delta_{n_1 n_1'} \delta_{n_2 n_2'}$

1.3.5. Indistinguishable particles

A statement like (11), "particle 1 in state n_1", "particle 2 in state n_2", etc., makes sense if the particles are distinguishable (say $1 = e^-$, $2 = p$, $3 = \gamma$)

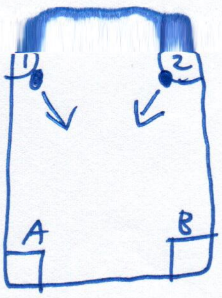
For <u>indistinguishable particles</u>, the uncertainty relation forces us to abandon the label "particle 1" (See Box on "trajectories" next page)

Mathematically the state $\psi(x_a, x_b)$ <u>must be</u> "equivalent" to $\psi(x_b, x_a)$

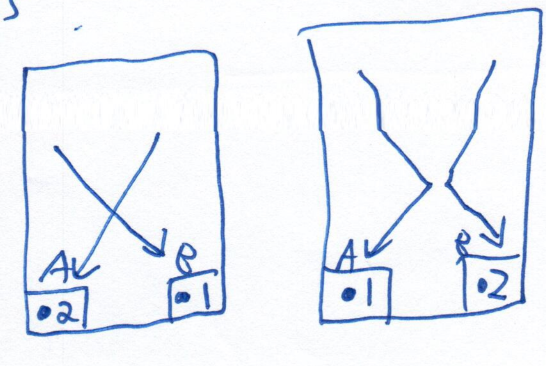
particle 1 particle 2

Trajectories of indistinguishable particles (see Shankar p. 260)

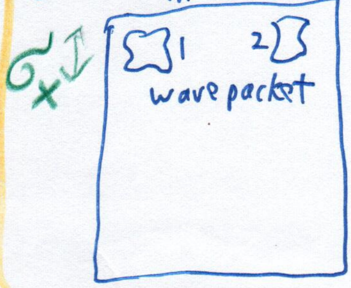
Classical identical billiard balls



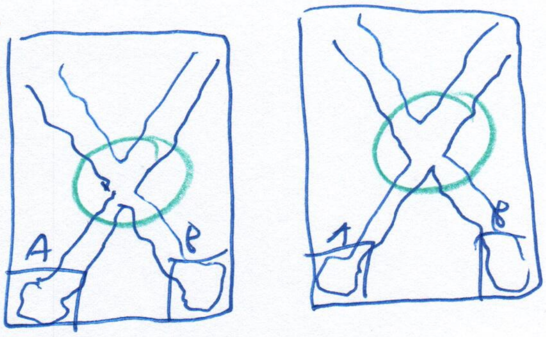
distinguish final states via history/trajectory



Quantum Mechanical



cannot distinguish via history



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equivalent still allows

$$\psi(x_a, x_b) = \pm\, \psi(x_b, x_a) \qquad \begin{array}{l} \oplus \text{ Bosons} \\ \ominus \text{ Fermions} \end{array} \qquad (1.12)$$

Bosons = symmetric under exchange of any two indistinguishable particles

Fermions = Anti-symmetric

Comment: the need for special treatment of indistinguishable particles comes from region ◯, i.e. when the matter waves overlapp.

If this never happens, particles can be tracked and (anti-) symmetrization is irrelevant (we can still do it, but it makes no difference to the math).

Examples: One e^- inside you and another on the moon.

(See also Shankar p. 273)

1.3.4 Entanglement

A many-body state is called <u>seperable</u>, if it can be writen as a <u>product</u> of states for each particle

$$\Psi_{sep}(\vec{x}_1 \dots \vec{x}_n) = \prod_{i=1}^{N} \varphi_{n_i}(x_i) \qquad (1.13)$$

All states that are not seperable are called <u>entangled</u>.

<u>Examples:</u>

Seperable: $|\psi\rangle = |\uparrow\uparrow\rangle = |\uparrow\rangle \otimes |\uparrow\rangle$

$|\psi\rangle = \frac{1}{2}(|\uparrow\rangle + |\downarrow\rangle) \otimes (|\uparrow\rangle + |\downarrow\rangle) = \frac{1}{2}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$

$\psi(x_1 x_2) = \frac{1}{\sqrt{V}} e^{i(k_1 x_1)} \cdot N \exp\left(-\frac{x_2}{2\sigma^2}\right)$

Entangled: $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$

$\psi(x_1 x_2) = N \exp\left(-\frac{(x_1 - x_2)^2}{2\sigma_\perp^2} - \frac{(x_1 + x_2)^2}{2\sigma_\parallel^2}\right)$

- In an entangled state (for two systems A, B), if I measure system A I typically know also about system B.
- Entanglement implies classical <u>correlations</u>, but is much more than that (Keywords: EPR paradox, Bell-theorem)
- The definition gets a bit more complicated for mixed states ($\hat{\rho}$).