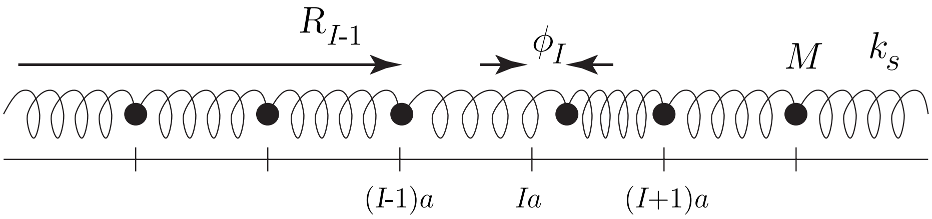
# Lecture I: Collective Excitations: From Particles to Fields

## Free Scalar Field Theory: Phonons

*The aim of this course is to develop the machinery to explore the properties of quantum systems with very large or infinite numbers of degrees of freedom. To represent such systems it is convenient to abandon the language of individual elementary particles and speak about quantum fields. In this lecture, we will consider the simplest physical example of a free or non-interacting many-particle theory which will exemplify the language of classical and quantum fields. Our starting point is a toy model of a mechanical system describing a classical chain of atoms coupled by springs.*

▷ Discrete elastic chain




Equilibrium position $\bar{x}_n \equiv na$; natural length $a$; spring constant $k_s$

Goal: to construct and quantise a classical field theory
for the collective (longitundinal) vibrational modes of the chain

▷ Discrete Classical Lagrangian:

$$L = T - V = \sum_{n=1}^{N} \Big( \overbrace{\frac{m}{2}\dot{x}_n^2}^{\text{k.e.}} - \overbrace{\frac{k_s}{2}(x_{n+1} - x_n - a)^2}^{\text{p.e. in spring}} \Big)$$

assume periodic boundary conditions (p.b.c.) $x_{N+1} = Na + x_1$ (and set $\dot{x}_n \equiv \partial_t x_n$)

Using displacement from equilibrium $\phi_n = x_n - \bar{x}_n$

$$L = \sum_{n=1}^{N} \left( \frac{m}{2}\dot{\phi}_n^2 - \frac{k_s}{2}\left(\phi_{n+1} - \phi_n\right)^2 \right), \qquad \text{p.b.c}: \quad \phi_{N+1} \equiv \phi_1$$

In principle, one can obtain exact solution of discrete equation of motion — see PS I

However, typically, one is not concerned with behaviour on 'atomic' scales:

1. for such purposes, modelling is too primitive! *viz. anharmonic contributions*
2. such properties are in any case 'non-universal'

Aim here is to describe low-energy collective behaviour — generic, i.e. <u>universal</u>

*In this case, it is often permissible to neglect the discreteness of the microscopic entities of the system and to describe it in terms of effective continuum degrees of freedom.*

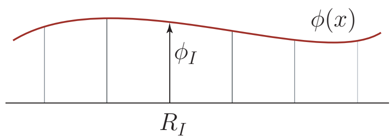
▷ Continuum Lagrangian

Describe $\phi_n$ as a smooth function $\phi(x)$ of a continuous variable $x$;

makes sense if $\phi_{n+1} - \phi_n \ll a$ (i.e. gradients small)

$$\phi_n \to a^{1/2}\phi(x)\Big|_{x=na}, \qquad \phi_{n+1}-\phi_n \to a^{3/2}\partial_x\phi(x)\Big|_{x=na}, \qquad \sum_n \longrightarrow \frac{1}{a}\int_0^{L=Na} dx$$

N.B. $[\phi(x)] = L^{1/2}$




$$\overbrace{L[\phi] = \int_0^L dx\ \mathcal{L}(\phi, \partial_x\phi, \dot\phi)}^{\text{Lagrangian functional}}, \qquad \overbrace{\mathcal{L}(\phi, \partial_x\phi, \dot\phi) = \frac{m}{2}\dot\phi^2 - \frac{k_s a^2}{2}(\partial_x\phi)^2}^{\text{Lagrangian density}}$$

▷ Classical action

$$\boxed{S[\phi] = \int dt\ L[\phi] = \int dt \int_0^L dx\ \mathcal{L}(\phi, \partial_x\phi, \dot\phi)}$$

- $N$-point particle degrees of freedom $\mapsto$ continuous classical field $\phi(x)$
- Dynamics of $\phi(x)$ specified by functionals $L[\phi]$ and $S[\phi]$

What are the corresponding equations of motion...?

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▷ Hamilton's Extremal Principle: (Revision)

Suppose classical point particle $x(t)$ described by action $S[x] = \int dt\ L(x, \dot x)$

Configurations $x(t)$ that are realised are those that extremise the action

i.e. for any smooth function $\eta(t)$, the "variation",

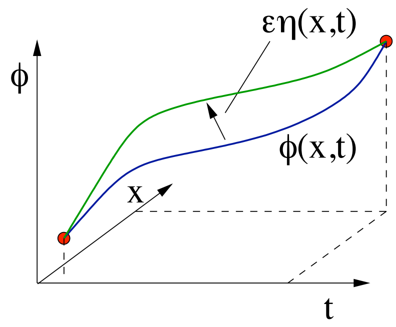
$\delta S[x] \equiv \lim_{\epsilon\to 0}\frac{1}{\epsilon}(S[x+\epsilon\eta] - S[x]) = 0$ is stationary

$\rightsquigarrow$ Euler-Lagrange equations of motion

$$S[x+\epsilon\eta] = \int_0^t dt\, L(x+\epsilon\eta, \dot x + \epsilon\dot\eta) = \int_0^t dt\,(L(x,\dot x) + \epsilon\eta\partial_x L + \epsilon\dot\eta\partial_{\dot x}L) + O(\epsilon^2)$$

$$\delta S[x] = \int dt\,(\eta\partial_x L + \dot\eta\partial_{\dot x}L) \overset{\text{by parts}}{=} \int dt\ \overbrace{\left(\partial_x L - \frac{d}{dt}(\partial_{\dot x}L)\right)}^{=0}\ \eta = 0$$

Note: boundary term, $\eta\partial_{\dot x}L|_0^t$ vanishes by construction




▷ Generalisation to continuum field $x \mapsto \phi(x)$?

Apply same extremal principle: $\phi(x,t) \mapsto \phi(x,t) + \epsilon\eta(x,t)$
with both $\phi$ and $\eta$ periodic in $x$, i.e. $\phi(x+L) = \phi(x)$

$$S[\phi + \epsilon\eta] = S[\phi] + \epsilon \int_0^t dt \int_0^L dx \left( m\dot{\phi}\dot{\eta} - k_s a^2 \partial_x\phi\partial_x\eta \right) + O(\epsilon^2).$$

Integrating by parts *boundary terms vanish by construction:* $\eta\dot{\phi}|_0^t = 0 = \eta\partial_x\phi|_0^L$

$$\delta S = -\int_0^t dt \int_0^L dx \left( m\ddot{\phi} - k_s a^2 \partial_x^2 \phi \right) \eta = 0$$

Since $\eta(x,t)$ is an arbitrary smooth function, $\left(m\partial_t^2 - k_s a^2\partial_x^2\right)\phi = 0$,
i.e. $\phi(x,t)$ obeys classical wave equation

General solutions of the form: $\phi_+(x+vt) + \phi_-(x-vt)$
where $v = a\sqrt{k_s/m}$ is sound wave velocity and $\phi_\pm$ are arbitrary smooth functions


▷ <u>COMMENTS</u>

- Low-energy <u>collective</u> excitations – phonons – are lattice vibrations
propagating as sound waves at constant velocity $v$

- Trivial behaviour of model is consequence of simplistic definition:
  Lagrangian is quadratic in fields $\mapsto$ linear equation of motion
  Higher order gradients in expansion (i.e. $(\partial^2\phi)^2$) $\mapsto$ dispersion
  Higher order terms in potential (i.e. interactions) $\mapsto$ dissipation

- $L$ is said to be a 'free (i.e. non-interacting) scalar (i.e. one-component) field theory'

- In higher dimensions, field has vector components $\mapsto$ transverse and longintudinal modes

Variational principle is example of <u>FUNCTIONAL ANALYSIS</u>
– useful (but not essential method for this course) – see lecture notes

# Lecture II: Collective Excitations: From Particles to Fields

## Quantising the Classical Field

*Having established that the low energy properties of the atomic chain are represented by a free scalar classical field theory, we now turn to the formulation of the quantum system.*

▷ CANONICAL QUANTISATION PROCEDURE

Recall point particle mechanics:

1. Define canonical momentum, $p = \partial_{\dot{x}} L$
2. Construct Hamiltonian, $H = p\dot{x} - L(p, x)$
3. Promote position and momentum to operators with canonical commutation relations

$$x \mapsto \hat{x}, \qquad p \mapsto \hat{p}, \qquad [\hat{p}, \hat{x}] = -i\hbar, \qquad H \mapsto \hat{H}$$

Natural generalisation to continuous field:

1. Canonical momentum, $\pi(x) \equiv \dfrac{\partial \mathcal{L}}{\partial \dot{\phi}(x)}$, i.e. applied to chain, $\pi = \partial_{\dot{\phi}}(m\dot{\phi}^2/2) = m\dot{\phi}$
2. Classical Hamiltonian

$$H[\phi, \pi] \equiv \int dx \; \overbrace{\left[\pi\dot{\phi} - \mathcal{L}(\partial_x \phi, \dot{\phi})\right]}^{\text{Hamiltonian density } \mathcal{H}(\phi,\pi)}, \qquad \text{i.e.} \qquad \mathcal{H}(\phi, \pi) = \frac{1}{2m}\pi^2 + \frac{k_s a^2}{2}(\partial_x \phi)^2$$

3. Canonical Quantisation
   (a) promote $\phi(x)$ and $\pi(x)$ to operators: $\phi \mapsto \hat{\phi}$, $\pi \mapsto \hat{\pi}$
   (b) generalise commutation relations, $[\hat{\pi}(x), \hat{\phi}(x')] = -i\hbar\delta(x - x')$
   N.B. $[\delta(x - x')] = [\text{Length}]^{-1}$ (Ex.)

Operator-valued functions $\hat{\phi}$ and $\hat{\pi}$ referred to as quantum fields

*$\hat{H}$ represents a quantum field theoretical formulation of elastic chain, but not yet a solution.*

As with any function, $\hat{\phi}(x)$ and $\hat{\pi}(x)$ can be expressed as Fourier expansion:

$$\left\{\begin{array}{l}\hat{\phi}(x)\\ \hat{\pi}(x)\end{array}\right. = \frac{1}{L^{1/2}}\sum_k e^{\pm ikx}\left\{\begin{array}{l}\hat{\phi}_k\\ \hat{\pi}_k\end{array}\right., \qquad \left\{\begin{array}{l}\hat{\phi}_k\\ \hat{\pi}_k\end{array}\right. \equiv \frac{1}{L^{1/2}}\int_0^{L=Na} dx\, e^{\mp ikx}\left\{\begin{array}{l}\hat{\phi}(x)\\ \hat{\pi}(x)\end{array}\right.$$

$\sum_k$ runs over all discrete wavevectors $k = 2\pi m/L$, $m \in \mathcal{Z}$, Ex: confirm $[\hat{\pi}_k, \hat{\phi}_{k'}] = -i\hbar\delta_{kk'}$

ADVICE: *Maintain strict conventions(!) — we will pass freely between real and Fourier space.*

Hermiticity: $\hat{\phi}^\dagger(x) = \hat{\phi}(x)$, implies $\hat{\phi}_k^\dagger = \hat{\phi}_{-k}$ (similarly $\hat{\pi}$). Using

$$\int_0^L dx\ (\partial\hat{\phi})^2 = \sum_{k,k'} (ik\hat{\phi}_k)(ik'\hat{\phi}_{k'})\ \overbrace{\frac{1}{L}\int_0^L dx\, e^{i(k+k')x}}^{\delta_{k+k',0}} = \sum_k k^2\hat{\phi}_k\hat{\phi}_{-k}$$

$$\hat{H} = \sum_k \left[\frac{1}{2m}\hat{\pi}_k\hat{\pi}_{-k} + \overbrace{\frac{k_s a^2}{2}k^2}^{m\omega_k^2/2}\ \hat{\phi}_k\hat{\phi}_{-k}\right], \qquad \omega_k = v|k|, \qquad v = a(k_s/m)^{1/2}$$

i.e. 'modes $k$' decoupled

COMMENTS:

- $\hat{H}$ describes low-energy excitations of system (waves) in terms of microscopic constituents (atoms)
- However, it would be more desirable to develop picture where relevant excitations appear as fundamental units:

▷ QUANTUM HARMONIC OSCILLATOR (REVISITED)

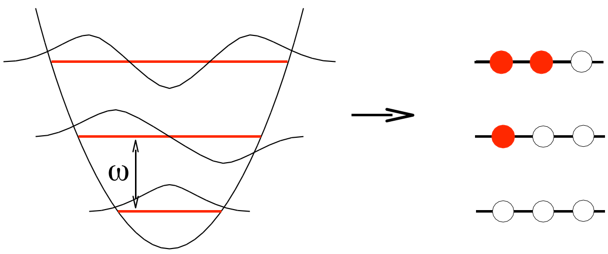
$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2$$

Defining ladder operators

$$\hat{a} \equiv \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right), \qquad \hat{a}^\dagger \equiv \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right) \quad \rightsquigarrow \quad \hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$$

If we find state $|0\rangle$ s.t. $\hat{a}|0\rangle = 0 \rightsquigarrow \hat{H}|0\rangle = \frac{\hbar\omega}{2}|0\rangle$, i.e. $|0\rangle$ is g.s.

Using commutation relations $[\hat{a}, \hat{a}^\dagger] = 1$, one may then show $|n\rangle \equiv \hat{a}^{\dagger n}|0\rangle$ is eigenstate with eigenvalue $\hbar\omega(n + \frac{1}{2})$




<u>COMMENTS</u>: Although single-particle, $a$-representation suggests many-particle interpretation

- $|0\rangle$ represents 'vacuum', i.e. state with no particles
- $\hat{a}^\dagger|0\rangle$ represents state with single particle of energy $\hbar\omega$
- $\hat{a}^{\dagger n}|0\rangle$ is $n$-body state, i.e. operator $\hat{a}^\dagger$ <u>creates</u> particles

- In 'diagonal' form $\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2})$ simply counts particles (viz. $\hat{a}^\dagger\hat{a}|n\rangle = n|n\rangle$)
  and assigns an energy $\hbar\omega$ to each

▷ Returning to harmonic chain, consider

$$a_k \equiv \sqrt{\frac{m\omega_k}{2\hbar}}\left(\hat{\phi}_k + \frac{i}{m\omega_k}\hat{\pi}_{-k}\right), \qquad a_k^\dagger \equiv \sqrt{\frac{m\omega_k}{2\hbar}}\left(\hat{\phi}_{-k} - \frac{i}{m\omega_k}\hat{\pi}_k\right)$$

*N.B. By convention, drop hat from operators a*

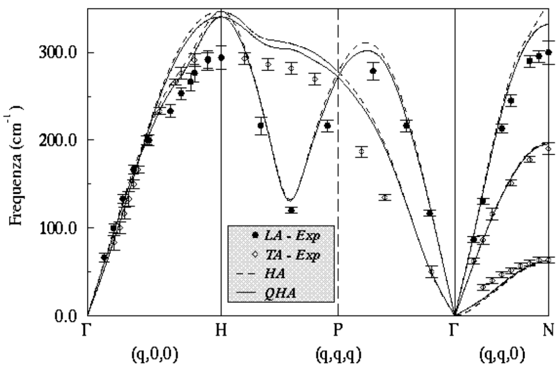
with $[a_k, a_{k'}^\dagger] = \frac{i}{2\hbar}\Big(\overbrace{[\hat{\pi}_{-k}, \hat{\phi}_{-k'}]}^{-i\hbar\delta_{kk'}} - [\hat{\phi}_k, \hat{\pi}_{k'}]\Big) = \delta_{kk'}$

▷ And obtain (Ex. - PS I)

$$\boxed{\hat{H} = \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2}\right)}$$

Elementary collective excitations of quantum chain (phonons)
created/annihilated by operators $a_k^\dagger$ and $a_k$

Spectrum of excitations is linear $\omega_k = v|k|$ (cf. relativistic)




COMMENTS:

- Low-energy excitations of discrete model involve slowly varying <u>collective</u> modes;
  i.e. each mode involves many atoms;
- Low-energy ($k \to 0$) $\mapsto$ long-wavelength excitations,
  i.e. <u>universal</u>, insensitive to microscopic detail;
- Allows many different systems to be mapped onto a few classical field theories;
- Canonical quantisation procedure for point mechanics generalises to quantum field theory;
- Simplest model actions (such as the one considered here) are quadratic in fields
  – known as <u>free field theory</u>;
- More generally, interactions $\rightsquigarrow$ non-linear equations of motion viz. interacting QFTs.

▷ Other examples? †<u>Quantum Electrodynamics</u>

EM field — specified by 4-vector potential $A(x) = (\phi(x), \mathbf{A}(x))$ $(c = 1)$

$$\text{Classical action}: \quad \boxed{S[A] = \int d^4x \; \mathcal{L}(A), \qquad \mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu}}$$

$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ — EM field tensor

Classical equation of motion:

$$\overbrace{\partial_{A^\alpha} \mathcal{L} - \partial^\beta \frac{\partial \mathcal{L}}{\partial(\partial^\beta A^\alpha)} = 0}^{\text{Euler} - \text{Lagrange eqns.}} \qquad \mapsto \qquad \overbrace{\partial_\alpha F^{\alpha\beta} = 0}^{\text{Maxwell's eqns.}}$$

Quantisation of classical field theory identifies elementary excitations: photons

*for more details, see handout, or go to QFT!*

## Lecture III: Second Quantisation

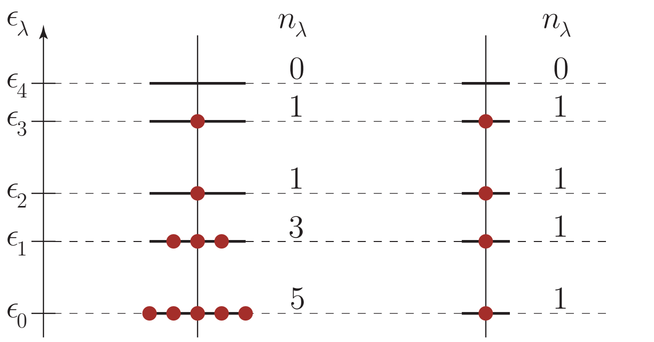
*We have seen how the elementary excitations of the quantum chain can be presented in terms of new elementary quasi-particles by the ladder operator formalism. Can this approach be generalised to accommodate other many-body systems? The answer is provided by the method of second quantisation — an essential tool for the development of interacting many-body field theories. The first part of this section is devoted largely to formalism – the second part to applications aimed at developing fluency. Reference: see, e.g., Feynman's book on "Statistical Mechanics"*

▷ Notations and Definitions

Starting with single-particle Schrodinger equation,

$$\boxed{\hat{H}|\psi_\lambda\rangle = \epsilon_\lambda|\psi_\lambda\rangle}$$

how can one construct many-body wavefunction?




Particle indistinguishability demands symmetrisation:
e.g. two-particle wavefunction for fermions *i.e. particle 1 in state 1, particle 2...*

$$\psi_F(x_1,x_2) \equiv \frac{1}{\sqrt{2}}(\overbrace{\psi_1(x_1)}^{\text{state 1, particle 1}}\psi_2(x_2) - \psi_2(x_1)\psi_1(x_2))$$

In Dirac notation: $|1,2\rangle_F \equiv \frac{1}{\sqrt{2}}\left(|\psi_1\rangle \otimes |\psi_2\rangle - |\psi_2\rangle \otimes |\psi_1\rangle\right)$

*N.B.* $\otimes$ *denotes outer product of state vectors*

▷ General normalised, symmetrised, $N$-particle wavefunction of bosons ($\zeta = +1$) or fermions ($\zeta = -1$)

$$\boxed{|\lambda_1,\lambda_2,\ldots\lambda_N\rangle \equiv \frac{1}{\sqrt{N!\prod_{\lambda=0}^{\infty} n_\lambda!}}\sum_{\mathcal{P}} \zeta^{\mathcal{P}}|\psi_{\lambda_{\mathcal{P}1}}\rangle \otimes |\psi_{\lambda_{\mathcal{P}2}}\rangle \ldots \otimes |\psi_{\lambda_{\mathcal{P}N}}\rangle}$$

- $n_\lambda$ — no. of particles in state $\lambda$; (for fermions, Pauli exclusion: $n_\lambda = 0, 1$)

- $\sum_{\mathcal{P}}$: Summation over $N!$ permutations of $\{\lambda_1, \ldots \lambda_N\}$
  required by particle indistinguishability
- Parity $\mathcal{P}$ — no. of transpositions of two elements which brings permutation
  $(\mathcal{P}_1, \mathcal{P}_2, \cdots \mathcal{P}_N)$ back to ordered sequence $(1, 2, \cdots N)$

In particular, for fermions, $\langle x_1, \ldots x_N|\lambda_1, \ldots \lambda_N\rangle$ is Slater determinant, $\det \psi_i(x_j)$

Evidently, "first quantised" representation looks clumsy!
motivates alternative representation...

▷ <u>Second quantisation</u>

Define vacuum state: $|\Omega\rangle$, and set of <u>field operators</u> $a_\lambda$ and adjoints $a^\dagger_\lambda$ — no hats!

$$a_\lambda|\Omega\rangle = 0, \qquad \frac{1}{\sqrt{\prod_{\lambda=0}^\infty n_\lambda!}} \prod_{i=1}^N a^\dagger_{\lambda_i}|\Omega\rangle = |\lambda_1, \lambda_2, \ldots \lambda_N\rangle$$

cf. ladder operators for phonons *N.B. ambiguity of ordering?*

Field operators fulfil commutation relations for bosons (fermions)

$$[a_\lambda, a^\dagger_\mu]_{-\zeta} = \delta_{\lambda\mu}, \qquad [a_\lambda, a_\mu]_{-\zeta} = [a^\dagger_\lambda, a^\dagger_\mu]_{-\zeta} = 0$$

where $[\hat{A}, \hat{B}]_{-\zeta} \equiv \hat{A}\hat{B} - \zeta\hat{B}\hat{A}$ is the commutator (anti-commutator)

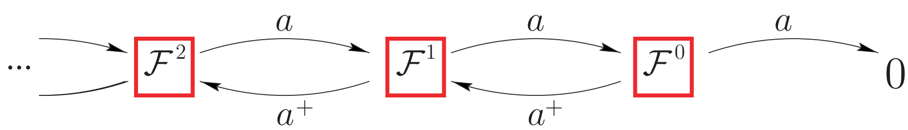
- Operator $a^\dagger_\lambda$ creates particle in state $\lambda$, and $a_\lambda$ annihilates it
- Commutation relations imply Pauli exclusion for fermions: $a^\dagger_\lambda a^\dagger_\lambda = 0$
- <u>Any</u> $N$-particle wavefunction can be generated by application of set of
  $N$ operators to a unique vacuum state

$$\text{e.g.} \qquad |1, 2\rangle = a^\dagger_2 a^\dagger_1|\Omega\rangle$$

- Symmetry of wavefunction under particle interchange maintained by
  commutation relations of field operators

$$\text{e.g.} \qquad |1, 2\rangle = a^\dagger_2 a^\dagger_1|\Omega\rangle = \zeta a^\dagger_1 a^\dagger_2|\Omega\rangle = \zeta|2, 1\rangle$$

(Providing one maintains a consistent ordering convention,
the nature of that convention doesn't matter)




▷ <u>Fock space</u>: Defining $\mathcal{F}_N$ to be linear span of all $N$-particle states $|\lambda_1, \ldots \lambda_N\rangle$,
Fock space $\mathcal{F}$ is defined as 'direct sum' $\oplus_{N=0}^\infty \mathcal{F}_N$

operators $a$ and $a^\dagger$ connect different subspaces $\mathcal{F}_N$

- General state $|\phi\rangle$ of the Fock space is linear combination of states with any no. of particles
- Note that vacuum $|\Omega\rangle$ (sometimes written as $|0\rangle$) is distinct from zero!

▷ Change of basis:

Using resolution of identity $\mathbf{1} \equiv \sum_\lambda |\lambda\rangle\langle\lambda|$, we have $\overbrace{|\tilde{\lambda}\rangle}^{a^\dagger_{\tilde{\lambda}}|\Omega\rangle} = \sum_\lambda \overbrace{|\lambda\rangle}^{a^\dagger_\lambda|\Omega\rangle} \langle\lambda|\tilde{\lambda}\rangle$

$$\text{i.e.} \quad a^\dagger_{\tilde{\lambda}} = \sum_\lambda \langle\lambda|\tilde{\lambda}\rangle a^\dagger_\lambda, \qquad \text{and} \quad a_{\tilde{\lambda}} = \sum_\lambda \langle\tilde{\lambda}|\lambda\rangle a_\lambda$$

e.g. Fourier representation: $a_\lambda \equiv a_k$, $a_{\tilde{\lambda}} \equiv a(x)$

$$a(x) = \sum_k \overbrace{\langle x|k\rangle}^{e^{ikx}/\sqrt{L}} a_k, \qquad a_k = \frac{1}{\sqrt{L}}\int_0^L dx\; e^{-ikx} a(x)$$

▷ Occupation number operator: $\hat{n}_\lambda = a^\dagger_\lambda a_\lambda$ measures no. of particles in state $\lambda$

e.g. (bosons)

$$a^\dagger_\lambda a_\lambda (a^\dagger_\lambda)^n|\Omega\rangle = a^\dagger_\lambda \overbrace{a_\lambda a^\dagger_\lambda}^{1+a^\dagger_\lambda a_\lambda} (a^\dagger_\lambda)^{n-1}|\Omega\rangle = (a^\dagger_\lambda)^n|\Omega\rangle + (a^\dagger_\lambda)^2 a_\lambda (a^\dagger_\lambda)^{n-1}|\Omega\rangle = \cdots = n(a^\dagger_\lambda)^n|\Omega\rangle$$

Ex: check for fermions

*So far we have developed an operator-based formulation of many-body states. However, for this representation to be useful, we have to understand how the action of first quantised operators on many-particle states can be formulated within the framework of the second quantisation. To do so, it is natural to look for a formulation in the diagonal basis and recall the action of the particle number operator. To begin, let us consider...*

## Second Quantised Representation of Operators

▷ One-body operators: *i.e. operators which address only one particle at a time*

$$\hat{\mathcal{O}}_1 = \sum_{n=1}^N \hat{o}_n, \qquad \text{e.g. k.e.} \;\; \hat{T} = \sum_{n=1}^N \frac{\hat{p}_n^2}{2m}$$

Suppose $\hat{o}$ diagonal in orthonormal basis $|\lambda\rangle$, i.e. $\hat{o} = \sum_{\lambda=0}^\infty |\lambda\rangle o_\lambda \langle\lambda|$, $\quad o_\lambda = \langle\lambda|\hat{o}|\lambda\rangle$

e.g. k.e., $|\lambda\rangle \equiv |p\rangle$ and $o_p = p^2/2m$

$$\begin{aligned} \langle\lambda'_1, \cdots \lambda'_N|\hat{\mathcal{O}}_1|\lambda_1, \cdots \lambda_N\rangle &= \left(\sum_{i=1}^N o_{\lambda_i}\right) \langle\lambda'_1, \cdots \lambda'_N|\lambda_1, \cdots \lambda_N\rangle \\ &= \langle\lambda'_1, \cdots \lambda'_N| \sum_{\lambda=0}^\infty o_\lambda \hat{n}_\lambda |\lambda_1, \cdots \lambda_N\rangle, \end{aligned}$$

Since this holds for any basis state, $\hat{\mathcal{O}}_1 = \sum_{\lambda=0}^{\infty} o_\lambda \hat{n}_\lambda = \sum_{\lambda=0}^{\infty} o_\lambda a_\lambda^\dagger a_\lambda$

*i.e. in diagonal representation, simply count number of particles in state* $\lambda$ *and multipy by corresponding eigenvalue of one-body operator*

Transforming to general basis (recall $a_\lambda = \sum_\nu \langle\lambda|\nu\rangle a_\nu$)

$$\boxed{\hat{\mathcal{O}}_1 = \sum_{\lambda\mu\nu} \langle\mu|\lambda\rangle o_\lambda \langle\lambda|\nu\rangle a_\mu^\dagger a_\nu = \sum_{\mu\nu} \langle\mu|\hat{o}|\nu\rangle a_\mu^\dagger a_\nu}$$

i.e. $\hat{\mathcal{O}}_1$ scatters particle from state $\nu$ to $\mu$ with probability amplitude $\langle\mu|\hat{o}|\nu\rangle$

▷ Examples of one-body operators:

1. Total number operator: $\hat{N} = \int dx\ a^\dagger(x)a(x) = \sum_k a_k^\dagger a_k$
2. Electron spin operator: $\hat{\mathbf{S}} = \sum_{\alpha\beta} \mathbf{S}_{\alpha\beta} a_\alpha^\dagger a_\beta$, $\quad \mathbf{S}_{\alpha\beta} = \langle\alpha|\hat{\mathbf{S}}|\beta\rangle = \frac{1}{2}\sigma_{\alpha\beta}$
   where $\alpha = \uparrow, \downarrow$, and $\sigma$ are Pauli spin matrices

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mapsto \hat{S}^z = \frac{1}{2}(\hat{n}_\uparrow - \hat{n}_\downarrow), \qquad \sigma_+ = \sigma_x + i\sigma_y = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \mapsto \hat{S}^+ = a_\uparrow^\dagger a_\downarrow$$

3. Free particle Hamiltonian

$$\sum_p \frac{p^2}{2m} a_p^\dagger a_p \overset{\text{Ex.}}{=} \int_0^L dx\ a^\dagger(x) \frac{(-\hbar^2\partial_x^2)}{2m} a(x)$$

i.e. $$\boxed{\hat{H} = \hat{T} + \hat{V} = \int_0^L dx\ a^\dagger(x) \left[\frac{\hat{p}^2}{2m} + V(x)\right] a(x)}$$ where $\hat{p} = -i\hbar\partial_x$

▷ Two-body operators: *i.e. operators which address two-particles*

E.g. symmetric pairwise interaction: $V(x,x') \equiv V(x',x)$ (such as Coulomb) acting between two-particle states *N.B.* 1/2 *for double counting*

$$\hat{V} = \frac{1}{2}\int dx \int dx'\ |x,x'\rangle V(x,x') \langle x,x'|$$

When acting on $N$-body states,

$$\hat{V}|x_1, x_2, \cdots x_N\rangle = \frac{1}{2}\sum_{n\neq m}^{N} V(x_n, x_m)|x_1, x_2, \cdots x_N\rangle$$

In second quantised form, it is straightforward to show that (Ex.)

$$\hat{V} = \frac{1}{2}\int dx \int dx'\ a^\dagger(x) a^\dagger(x') V(x,x') a(x') a(x)$$

*i.e. annihilation operators check for presence of particles at x and x' – if they exist, asign the potential energy and then recreate particles in correct order (viz. statistics)*

N.B. $\frac{1}{2}\int dx \int dx'\ V(x,x')\hat{n}(x)\hat{n}(x')$ does *not* reproduce the two-body operator

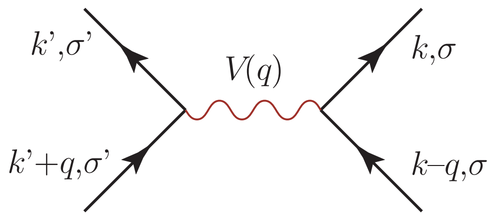
▷ In non-diagonal basis

$$\boxed{\hat{\mathcal{O}}_2 = \sum_{\lambda\lambda'\mu\mu'} \mathcal{O}_{\mu,\mu',\lambda,\lambda'} a^\dagger_{\mu'} a^\dagger_{\mu} a_\lambda a_{\lambda'}, \qquad \mathcal{O}_{\mu,\mu',\lambda,\lambda'} \equiv \langle \mu,\mu'|\hat{\mathcal{O}}_2|\lambda,\lambda'\rangle}$$

e.g. in Fourier basis: $a^\dagger(x) = \frac{1}{L^{1/2}}\sum_k e^{ikx} a^\dagger_k$ can show that (Ex.)

$$\frac{1}{2}\int dxdx'\ a^\dagger(x)a^\dagger(x')V(x-x')a(x')a(x) = \sum_{k_1,k_2,q} V(q)a^\dagger_{k_1}a^\dagger_{k_2}a_{k_2+q}a_{k_1-q}$$

Feynman diagram:



## Lecture IV: Applications of Second Quantisation

1. Phonons: oscillator states $|k\rangle$ form a Fock space:
   for each mode $k$, arbitrary state of excitation can be created from vacuum

$$|k\rangle = a_k^\dagger|\Omega\rangle, \qquad a_k|\Omega\rangle = 0, \qquad [a_k, a_{k'}^\dagger] = \delta_{kk'}$$

   Hamiltonian, $\hat{H} = \sum_k \hbar\omega_k(a_k^\dagger a_k + 1/2)$ is diagonal:
   $|k_1, k_2, ...\rangle = a_{k_1}^\dagger a_{k_2}^\dagger \cdots |\Omega\rangle$ is eigenstate of $\hat{H}$ with energy $\hbar\omega_{k_1} + \hbar\omega_{k_2} + \cdots$

2. Interacting Electron Gas

   (i) Free-electron Hamiltonian

$$\hat{H}^{(0)} = \sum_{\sigma=\uparrow,\downarrow} \int dx\, c_\sigma^\dagger(x) \left[\frac{\hat{p}^2}{2m} + V(x)\right] c_\sigma(x), \qquad [c_\sigma(x), c_{\sigma'}^\dagger(x')] = \delta(x-x')\delta_{\sigma,\sigma'}$$

   (ii) Interacting electron gas:

$$\hat{H} = \hat{H}^{(0)} + \frac{1}{2}\int dx \int dx' \sum_{\sigma\sigma'} c_\sigma^\dagger(x) c_{\sigma'}^\dagger(x') \frac{e^2}{|x-x'|} c_{\sigma'}(x') c_\sigma(x)$$

▷ COMMENTS:

- ▷ Phonon Hamiltonian is example of 'free field theory':
  involves field operators at only quadratic order...
- ▷ (whereas) electron Hamiltonian is typical of an interacting field theory
  and is infinitely harder to analyze...

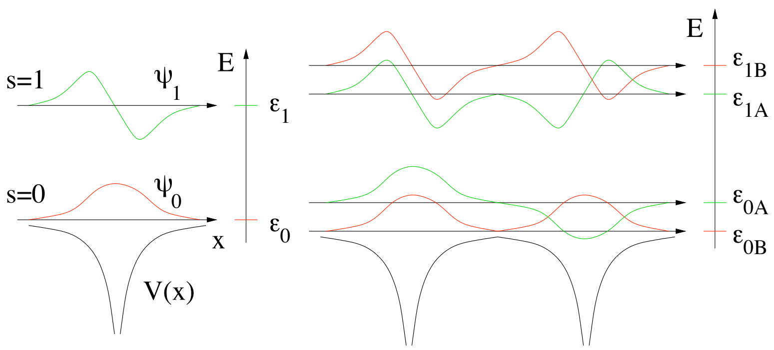
*To familiarise ourselves with second quantisation, in the remainder of this and the next lecture, we will explore several case studies: 'Atomic limit' of strongly interacting electron gas: electron crystallisation and Mott transition; Quantum magnetism; and weakly interacting Bose gas*

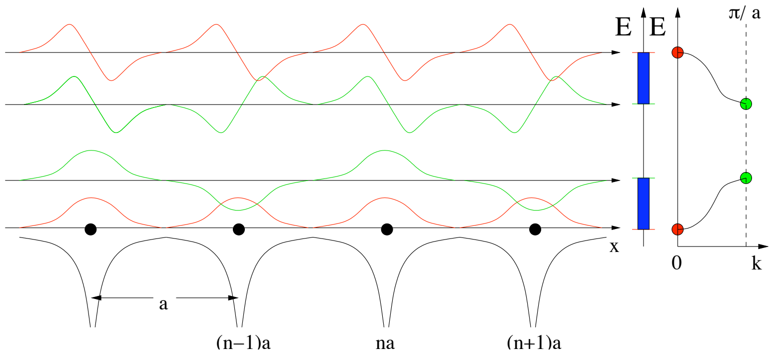
## Tight-binding and the Mott transition

*According to band picture of non-interacting electrons, a 1/2-filled band of states is metallic. But strong Coulomb interaction of electrons can effect a transition to a crystalline phase in which electrons condense into an insulating magnetic state – Mott transition. We will employ the second quantisation to explore the basis of this phenomenon.*

▷ 'Atomic Limit' of crystal

How do atomic orbitals broaden into band states? `Show transparencies`

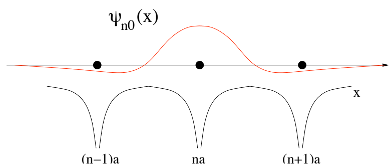



Weak overlap of tightly bound orbital states $\mapsto$ narrow band of Bloch states $|\psi_{ks}\rangle$,
specified by band index $s$, $k \in [-\pi/a, \pi/a]$ in first Brillouin zone.

Bloch states can be used to define <u>'Wannier basis'</u>, cf. discrete Fourier decomposition

$$|\psi_{ns}\rangle \equiv \frac{1}{\sqrt{N}} \sum_{k\in[-\pi/a,\pi/a]}^{\text{B.Z.}} e^{-ikna}|\psi_{ks}\rangle, \qquad |\psi_{ks}\rangle \equiv \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ikna}|\psi_{ns}\rangle, \qquad k = \frac{2\pi}{Na}m$$




In 'atomic limit', Wannier states $|\psi_{ns}\rangle$ mirror atomic orbital $|s\rangle$ on site $n$

Field operators associated with Wannier basis: $\overbrace{|\psi_{ns}\rangle}^{c^\dagger_{ns}|\Omega\rangle} = \int dx \overbrace{|x\rangle}^{c^\dagger(x)|\Omega\rangle} \overbrace{\langle x|\psi_{ns}\rangle}^{\psi_{ns}(x)}$

$$c^\dagger_{ns} \equiv \int dx\ \psi_{ns}(x) c^\dagger(x)$$

and using completeness $\sum_{ns} \psi^*_{ns}(x')\psi_{ns}(x) = \delta(x - x')$

$$c^\dagger(x) = \sum_{ns} \psi^*_{ns}(x) c^\dagger_{ns}, \qquad [c_{ns}, c^\dagger_{n's'}]_+ = \delta_{nn'}\delta_{ss'}$$

i.e. (if we include spin index $\sigma$) operators $c^\dagger_{ns\sigma}/c_{ns\sigma}$ create/annihilate electrons at site $n$ in band $s$ with spin $\sigma$

▷ In atomic limit, bands are well-separated in energy.
If electron densities are low, we may focus on lowest band $s = 0$.

Transforming to Wannier basis,

$$\hat{H} = \sum_{\sigma=\uparrow,\downarrow} \int dx\, c^\dagger_\sigma(x) \left[\frac{\hat{p}^2}{2m} + V(x)\right] c_\sigma(x) + \frac{1}{2}\int dx \int dx' \sum_{\sigma\sigma'} c^\dagger_\sigma(x) c^\dagger_{\sigma'}(x') V(x-x') c_{\sigma'}(x') c_\sigma(x)$$
$$= \sum_{mn,\sigma} t_{mn} c^\dagger_{m\sigma} c_{n\sigma} + \sum_{mnrs,\sigma\sigma'} U_{mnrs} c^\dagger_{m\sigma} c^\dagger_{n\sigma'} c_{r\sigma'} c_{s\sigma'}$$

where "hopping" matrix elements $t_{mn} = \langle\psi_m|[\frac{\hat{p}^2}{2m} + V(x)]|\psi_n\rangle = t^*_{nm}$ and "interaction parameters"

$$U_{mnrs} = \frac{1}{2}\int dx \int dx' \psi^*_m(x)\psi^*_n(x') \frac{e^2}{|x-x'|}\psi_r(x')\psi_s(x)$$

(For lowest band) representation is exact:
but, in atomic limit, matrix elements decay exponentially with lattice separation

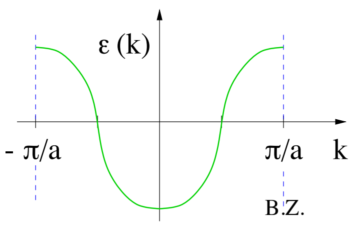
(i) "Tight-binding" approximation:

$$t_{mn} = \begin{cases} \epsilon & m=n \\ -t & mn \text{ neighbours} \\ 0 & \text{otherwise} \end{cases}, \qquad \hat{H}^{(0)} \simeq \sum_{n\sigma} \epsilon\, c^\dagger_{n\sigma} c_{n\sigma} - t\sum_{n\sigma}\left(c^\dagger_{n+1\sigma} c_{n\sigma} + \text{h.c.}\right)$$

In discrete Fourier basis: $c^\dagger_{n\sigma} = \frac{1}{\sqrt{N}} \sum_{k\in[-\pi/a,\pi/a]}^{\text{B.Z.}} e^{-ikna} c^\dagger_{k\sigma}$

$$-t\sum_{n\sigma}^{N}\left(c^\dagger_{n+1\sigma}c_{n\sigma} + \text{h.c.}\right) = -t\sum_{kk'\sigma} \overbrace{\frac{1}{N}\sum_n e^{-i(k-k')na}}^{\delta_{kk'}} e^{-ika} c^\dagger_{k\sigma} c_{k'\sigma} + \text{h.c.} = -2t\sum_{k\sigma}\cos(ka)\, c^\dagger_{k\sigma} c_{k\sigma}$$

$$\boxed{\hat{H}^{(0)} = \sum_{k\sigma}(\epsilon - 2t\cos ka) c^\dagger_{k\sigma} c_{k\sigma}}$$




As expected, as $k \to 0$, spectrum becomes free electron-like:
$\epsilon_k \to \epsilon - 2t + t(ka)^2 + \cdots$ (with $m^* = \hbar^2/2a^2t$)

(ii) Interaction

- Focusing on lattice sites $m \neq n$:
  1. Direct terms $U_{mnnm} \equiv V_{mn}$ — couple to density fluctuations: $\sum_{m\neq n} V_{mn}\hat{n}_m\hat{n}_n$
     $\rightsquigarrow$ potential for charge density wave instabilities
  2. Exchange coupling $J^F_{mn} \equiv U_{mnmn}$ (Ex. – see handout)

$$\sum_{m\neq n,\sigma\sigma'} U_{mnmn} c^\dagger_{m\sigma} c^\dagger_{n\sigma'} c_{m\sigma'} c_{n\sigma} = -2 \sum_{m\neq n} J^F_{mn} \left(\hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_n + \frac{1}{4}\hat{n}_m\hat{n}_n\right), \qquad \hat{\mathbf{S}}_m = \frac{1}{2} c^\dagger_{m\alpha}\sigma_{\alpha\beta}c_{m\beta}$$

i.e. weak ferromagnetic coupling ($J_F > 0$) cf. Hund's rule in atoms

*spin alignment $\mapsto$ symmetric spin state and asymmetric spatial state lowers p.e.*

But, in atomic limit, both $V_{mn}$ and $J^F_{mn}$ exponentially small in separation $|m-n|a$

- 'On-site' Coulomb or 'Hubbard' interaction

$$\sum_{n\sigma\sigma'} U_{nnnn} c^\dagger_{n\sigma} c^\dagger_{n\sigma'} c_{n\sigma'} c_{n\sigma} = U \sum_n \hat{n}_{n\uparrow}\hat{n}_{n\downarrow}, \qquad U \equiv 2U_{nnnn}$$

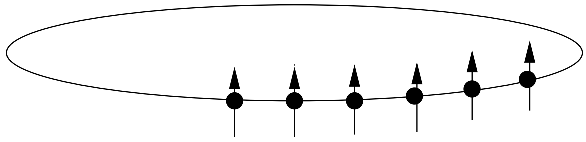
▷ Minimal model for strong interaction: Mott-Hubbard Hamiltonian

$$\boxed{\hat{H} = -t\sum_{n\sigma}(c^\dagger_{n+1\sigma}c_{n\sigma} + \text{h.c.}) + U\sum_n \hat{n}_{n\uparrow}\hat{n}_{n\downarrow}}$$

*...could have been guessed on phenomenological grounds*

`Transparencies on Mott-Insulators and the Magnetic State`

# Lecture V: Quantum Magnetism and the Ferromagnetic Chain




▷ Spin $S$ Quantum Heisenberg Magnet *spin analogue of discrete harmonic chain*

$$\boxed{\hat{H} = -J\sum_{m=1}^{N}\hat{\mathbf{S}}_m\cdot\hat{\mathbf{S}}_{m+1}} \qquad \text{p.b.c. } \hat{\mathbf{S}}_{n+N} = \hat{\mathbf{S}}_n$$

Sign of exchange constant $J$ depends on material parameters *c.f. previous lecture.*

*Our aim is to uncover ground states and nature of low-energy (collective) excitations.*

▷ Classical ground states

- Ferromagnet: all spins aligned along a given (arbitrary) direction
  ⇒ manifold of continuous degeneracy (cf. crystal)
- Antiferromagnet: Néel state – (where possible) all neighbouring spins antiparallel

▷ Quantum ground states:

$$\hat{H} = -J\sum_m\Big[\hat{S}^z_m\hat{S}^z_{m+1} + \overbrace{\hat{S}^x_m\hat{S}^x_{m+1} + \hat{S}^y_m\hat{S}^y_{m+1}}^{\frac{1}{2}(\hat{S}^+_m\hat{S}^-_{m+1} + \hat{S}^-_m\hat{S}^+_{m+1})}\Big]$$

where $\hat{S}^\pm = \hat{S}^x \pm i\hat{S}^y$ denotes spin raising/lowering operator

- Ferromagnet: as classical, e.g. $|\text{g.s.}\rangle = \otimes_{m=1}^N|S^z_m = S\rangle$

  No spin dynamics in $|\text{g.s.}\rangle$, i.e. no zero-point energy! (cf. phonons)

  Manifold of degeneracy explored by action of total spin lowering operator $\sum_m \hat{S}^-_m$

- Antiferromagnet: spin exchange interaction (viz. $\hat{S}^+_m\hat{S}^-_{m+1}$) ⇝ zero point fluctuations which, depending on dimensionality, may or may not destroy ordered ground state

▷Elementary excitations

Development of ordered state breaks continuous spin rotation symmetry ⇝ low-energy collective excitations (spin waves or magnons) – cf. phonons in a crystal

Example of general principle known as Goldstone's theorem: Breaking of a continuous symmetry accompanied by appearance of gapless excitations

However, as with lattice vibrations, 'general theory' is nonlinear.
Fortunately, low-energy excitations described by free theory

To see this, for large spin $S$, it is helpful to switch to representation in which spin deviations are parameterised as bosons:

$$\begin{array}{ll} |S^z = S\rangle & |n=0\rangle \\ |S^z = S-1\rangle & |n=1\rangle \\ \vdots & \vdots \\ |S^z = -S\rangle & |n=2S\rangle \end{array}$$

i.e. a maximum of $n$ bosons per lattice site ("softcore" constraint)

For ferromagnet with spins oriented along $z$-axis,
the g.s. coincides with vacuum $|\text{g.s.}\rangle \equiv |\Omega\rangle$, i.e. $a_m|\Omega\rangle = 0$

Mapping useful when spin wave excitation involves $n \ll 2S$

▷ Mapping of operators:

(Setting $\hbar = 1$) operators obey quantum spin algebra

$$[\hat{S}^\alpha, \hat{S}^\beta] = i\epsilon^{\alpha\beta\gamma}\hat{S}^\gamma \qquad \rightsquigarrow \qquad [\hat{S}^+, \hat{S}^-] = 2\hat{S}^z, \qquad [\hat{S}^z, \hat{S}^\pm] = \pm\hat{S}^\pm$$

cf. bosons: $[a, a^\dagger] = 1$

According to mapping, $\hat{S}^z = S - a^\dagger a$;
therefore, to leading order in $S \gg 1$ (spin-wave approximation),

$$\hat{S}^- \simeq (2S)^{1/2} a^\dagger, \qquad \hat{S}^+ \simeq (2S)^{1/2} a$$

In fact, exact mapping provided by Holstein-Primakoff transformation (Ex.)

$$\hat{S}^- = a^\dagger \left(2S - a^\dagger a\right)^{1/2}, \qquad \hat{S}^+ = (\hat{S}^-)^\dagger, \qquad \hat{S}^z = S - a^\dagger a$$

▷ Applied to ferromagnetic Heisenberg spin $S$ chain, 'spin-wave' approximation:

$$\begin{aligned} \hat{H} &= -J\sum_{m=1}^{N}\left\{\hat{S}^z_m\hat{S}^z_{m+1} + \frac{1}{2}(\hat{S}^+_m\hat{S}^-_{m+1} + \hat{S}^-_m\hat{S}^+_{m+1})\right\} \\ &= -J\sum_m\left\{S^2 - S(a^\dagger_m a_m - a^\dagger_{m+1}a_{m+1}) + S(a_m a^\dagger_{m+1} + a^\dagger_m a_{m+1}) + O(S^0)\right\} \\ &= -J\sum_m\left\{S^2 - 2Sa^\dagger_m a_m + S\left(a^\dagger_m a_{m+1} + \text{h.c.}\right) + O(S^0)\right\} \end{aligned}$$

with p.b.c. $\hat{S}_{m+N} = \hat{S}_m$ and $a_{m+N} = a_m$

To leading order in $S$, Hamiltionian is bilinear in Bose operators;
diagonalised by discrete Fourier transform (Ex.)

$$a_k^\dagger = \sum_n \overbrace{\langle n|k\rangle}^{e^{ikn}/\sqrt{N}} a_n^\dagger, \qquad a_n^\dagger = \frac{1}{\sqrt{N}} \sum_k^{\text{B.Z.}} e^{-ikn} a_k^\dagger, \qquad [a_k, a_{k'}^\dagger] = \delta_{kk'}$$

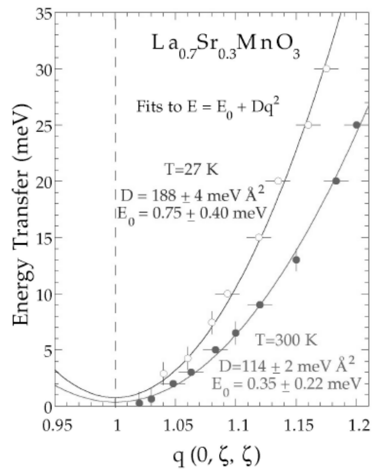
Noting

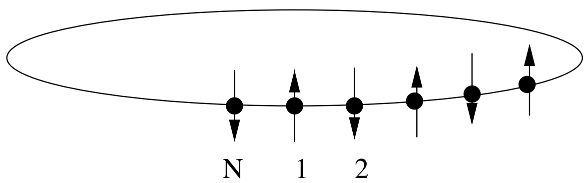
$$\sum_m (a_m^\dagger a_{m+1} + \text{h.c.}) = \sum_{kk'} \overbrace{\frac{1}{N}\sum_m e^{-i(k-k')m}}^{\delta_{kk'}} e^{-ika} a_k^\dagger a_{k'} + \text{h.c.} = \sum_k \cos k \; a_k^\dagger a_k$$

$$\hat{H} = -JNS^2 + \sum_k^{\text{B.Z.}} \omega_k a_k^\dagger a_k + O(S^0), \quad \text{where } \omega_k = 2JS(1-\cos k) = 4JS\sin^2(k/2)$$

At low energy ($k \to 0$), spin waves have free particle-like spectrum

Terms of higher order in $S \rightsquigarrow$ spin-wave interactions




▷ <u>Spin $S$ Quantum Heisenberg Antiferromagnet</u>

$$\hat{H} = J\sum_{m=1}^{N} \hat{\mathbf{S}}_m \cdot \hat{\mathbf{S}}_{m+1}, \qquad J > 0, \qquad \text{p.b.c. } \hat{\mathbf{S}}_{m+N} = \hat{\mathbf{S}}_m$$

Classical (Néel) ground state no longer an eigenstate;
nevertheless, it serves as useful reference for spin-wave expansion

In this case, useful to rotate spins on one sublattice, say $B$, through $180^o$ about $x$,
i.e. $\hat{S}^x_B \longmapsto \hat{S}^x_B, \qquad \hat{S}^y_B \longmapsto -\hat{S}^y_B, \qquad \hat{S}^z_B \longmapsto -\hat{S}^z_B$

Transformation is said to be canonical in that it respects spin commutation relations

Under mapping $\hat{S}^{\pm}_{\rm B} \longmapsto \hat{S}^{\mp}_{\rm B}$

$$\hat{H} = -J\sum_m \left[\hat{S}^z_m \hat{S}^z_{m+1} - \frac{1}{2}(\hat{S}^+_m \hat{S}^+_{m+1} + \hat{S}^-_m \hat{S}^-_{m+1})\right]$$

In rotated frame, classical ground state is ferromagnetic
but $\hat{S}^-_m \hat{S}^-_{m+1} \rightsquigarrow$ zero-point fluctuations (ZPF)

Applying spin wave approximation: $\hat{S}^z_m = S - a^\dagger_m a_m$, $\hat{S}^-_m \simeq (2S)^{1/2} a^\dagger_m$, etc.

$$\hat{H} = -NJS^2 + JS\sum_m \left[a^\dagger_m a_m + a^\dagger_{m+1} a_{m+1} + a_m a_{m+1} + a^\dagger_m a^\dagger_{m+1}\right] + O(S^0)$$

$\rightsquigarrow$ processes that do not conserve particle number! (ZPF)

Turning to Fourier representation: $a_m = \frac{1}{N^{1/2}}\sum_k e^{ikm} a_k$, etc., and using

$$\sum_{m=1}^N a_m a_{m+1} = \sum_{kk'} \overbrace{\frac{1}{N}\sum_{m=1}^N e^{i(k+k')m}}^{\delta_{k+k',0}} e^{ik} a_{k'} a_k = \sum_k a_{-k} a_k e^{ik} \equiv \sum_k a_{-k} a_k \overbrace{\frac{1}{2}(e^{ik} + e^{-ik})}^{\gamma_k = \cos k}$$

$$\begin{aligned}\hat{H} &= -NJS^2 + JS\sum_k [a^\dagger_k a_k + \overbrace{a^\dagger_k a_k}^{a_k a^\dagger_k - 1} + \gamma_k (a_{-k} a_k + a^\dagger_k a^\dagger_{-k})] \\ &= -NJS(S+1) + JS\sum_k \begin{pmatrix} a^\dagger_k & a_{-k}\end{pmatrix} \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1\end{pmatrix} \begin{pmatrix} a_k \\ a^\dagger_{-k}\end{pmatrix} + O(S^0)\end{aligned}$$

To diagonalise $\hat{H}$, we must implement only operator transformations that preserve
canonical commutation relations:

i.e. setting $\mathbf{A} = \begin{pmatrix} a_k \\ a^\dagger_{-k}\end{pmatrix}$ ($k$ index suppressed), we must implement transformations

$$\mathbf{A} \mapsto \widetilde{\mathbf{A}} = \mathbf{L}\mathbf{A} \text{ such that } [\widetilde{A}_i, \widetilde{A}^\dagger_j] = [A_i, A^\dagger_j] = g_{ij}, \text{ with } \mathbf{g} = \begin{pmatrix} 1 & 0 \\ 0 & -1\end{pmatrix}$$

Consider operator transformation $\mathbf{A} \mapsto \widetilde{\mathbf{A}} = \mathbf{L}\mathbf{A}$; we require

$$[\widetilde{A}_i, \widetilde{A}^\dagger_j] \stackrel{!}{=} g_{ij} = L_{im} L^*_{nj} [A_m, A^\dagger_n] = (\mathbf{L}\,\mathbf{g}\,\mathbf{L}^\dagger)_{ij}$$

i.e. $\mathbf{L}$ belongs to the group of Lorentz transformations. For real elements,

$$\mathbf{L} = \begin{pmatrix} \cosh\theta_k & \sinh\theta_k \\ \sinh\theta_k & \cosh\theta_k\end{pmatrix} \qquad \text{Bogoliubov transformations}$$

## Lecture VI: Bogoliubov Theory

Inverse transformation

$$\mathbf{A} = \mathbf{L}^{-1}\widetilde{\mathbf{A}}, \qquad \begin{pmatrix} a_k \\ a^\dagger_{-k} \end{pmatrix} = \begin{pmatrix} \cosh\theta_k & -\sinh\theta_k \\ -\sinh\theta_k & \cosh\theta_k \end{pmatrix} \begin{pmatrix} \alpha_k \\ \alpha^\dagger_{-k} \end{pmatrix}$$

Applied to Hamiltonian,

$$\begin{aligned} \mathbf{A}^\dagger \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \mathbf{A} &= \widetilde{\mathbf{A}}^\dagger \mathbf{L}^{-1} \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \mathbf{L}^{-1} \widetilde{\mathbf{A}} \\ &= \widetilde{\mathbf{A}}^\dagger \begin{pmatrix} \cosh(2\theta_k) - \gamma_k \sinh(2\theta_k) & \gamma_k \cosh(2\theta_k) - \sinh(2\theta_k) \\ \text{as “12”} & \text{as “11”} \end{pmatrix} \widetilde{\mathbf{A}} \end{aligned}$$

if $\tanh(2\theta_k) = \gamma_k$, off-diagonal elements vanish.

With $\cosh(2\theta_k) = \dfrac{1}{(1-\tanh^2(2\theta_k))^{1/2}} = \dfrac{1}{(1-\gamma_k^2)^{1/2}}$

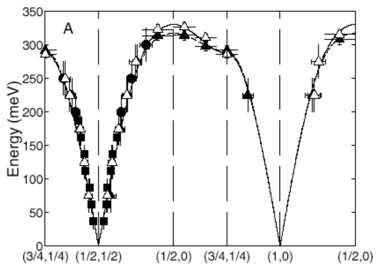
diagonal elements given by $(1-\gamma_k^2)^{1/2} = |\sin k|$, i.e.

$$\begin{aligned} \hat{H} &= -NJS(S+1) + JS\sum_k |\sin k| \left(\alpha^\dagger_k \alpha_k + \alpha_{-k}\alpha^\dagger_{-k}\right) + O(S^0) \\ &= -NJS(S+1) + 2JS\sum_k |\sin k| \left[\alpha^\dagger_k \alpha_k + \frac{1}{2}\right] + O(S^0) \end{aligned}$$

Ground state defined by $\alpha_k|\text{g.s}\rangle$

and spectrum of excitations are linear (i.e. relativistic), (cf. phonons, photons, etc.)

*Experiment?*




▷ Do ZPF destroy long-range order?

Referring to sublattice magnetisation

$$\begin{aligned} \langle \text{g.s.}|\frac{1}{N}\sum_n (-1)^n \hat{S}^z_n|\text{g.s.}\rangle &= S - \langle \text{g.s.}|\frac{1}{N}\sum_k a^\dagger_k a_k|\text{g.s.}\rangle \\ &= S - \frac{1}{N}\sum_k \langle \text{g.s.}|(-\sinh\theta_k \alpha_{-k} + \cosh\theta_k \alpha^\dagger_k)(\cosh\theta_k \alpha_k - \sinh\theta_k \alpha^\dagger_{-k})|\text{g.s.}\rangle \\ &= S - \frac{1}{N}\sum_k \sinh^2\theta_k = S - \int \frac{d^dk}{(2\pi)^d}\frac{1}{2}\left[(1-\gamma_k^2)^{-1/2} - 1\right] \sim \int_0^{1/a} k^{d-1} dk \frac{1}{k} \end{aligned}$$

i.e. quantum fluctuations destroy long range AFM order in 1d – spin liquid

▷ FRUSTRATION

On "bipartite" lattice, AF LRO survives ZPF in $d > 1$

For non-bipartite lattice (e.g. triangular), system is said to be frustrated
$\rightsquigarrow$ spin liquid phase in higher dimension

## Bogoliubov Theory of weakly interacting Bose gas

*Although strong interactions can lead to the formation of unusual ground states of electron system, the properties of the weakly interacting system mirror closely the trivial behaviour of the non-interacting Fermi gas. By contrast, even in the weakly interacting system, the Bose gas has the capacity to form a correlated phase known as a Bose-Einstein condensate. The aim of this lecture is to explore the nature of the ground state and the character of the elementary excitation spectrum in the condensed phase.*

Consider $N$ bosons confined to volume $L^d$. If non-interacting, at $T = 0$ all bosons condensed in lowest energy state of single-particle system, viz. $|\text{g.s.}\rangle_0 = \frac{1}{\sqrt{N!}}(a_0^\dagger)^N|\Omega\rangle$

How is g.s. and excitation spectrum influenced by weak (repulsive) interaction?

$$\hat{H} = \sum_{\mathbf{k}} \overbrace{\frac{\hbar^2\mathbf{k}^2}{2m}}^{\epsilon_k^{(0)}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \overbrace{\frac{1}{2}\int d^dx\, d^dx'\, a^\dagger(\mathbf{x})a^\dagger(\mathbf{x}')V(\mathbf{x}-\mathbf{x}')a(\mathbf{x}')a(\mathbf{x})}^{\hat{H}_I}$$

$$\hat{H}_I = \frac{1}{2L^d}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V(\mathbf{q})\, a_{\mathbf{k}'}^\dagger a_{\mathbf{k}}^\dagger a_{\mathbf{k}-\mathbf{q}} a_{\mathbf{k}'+\mathbf{q}}$$

If interaction is sufficiently weak, g.s. still condensed
with lowest single-particle state macroscopically occupied, i.e. $\frac{N_{k=0}}{N} = \mathcal{O}(1)$

Therefore, since $\hat{N}_0 = a_{k=0}^\dagger a_{k=0} = O(N) \gg 1$ and $a_0 a_0^\dagger - a_0^\dagger a_0 = 1$,
$a_0$ and $a_0^\dagger$ can be approximated by $C$-number $\sqrt{N_0}$

Taking (for simplicity) $V(\mathbf{q}) = V$ const.,
i.e. a contact interaction $V(\mathbf{x}-\mathbf{x}') = V\delta^d(\mathbf{x}-\mathbf{x}')$, expansion in $N_0$ obtains

$$\hat{H}_I = \frac{V}{2L^d}N_0^2 + \frac{V}{L^d}N_0\sum_{\mathbf{k}\neq 0}\left[2a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{1}{2}\left(a_{-\mathbf{k}}a_{\mathbf{k}} + a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger\right)\right] + O(N_0^{1/2})$$

cf. quantum AF in spin-wave approximation

*N.B. Momentum conservation eliminates terms at* $O(N_0^{3/2})$

▷ Physical interpretation of components:

- $Va^\dagger_{\mathbf{k}}a_{\mathbf{k}}$ represents the 'Hartree-Fock energy' of excited particles interacting with condensate
  N.B. Contact interaction disguises presence of direct and exchange contributions
- $V(a_{-\mathbf{k}}a_{\mathbf{k}} + a^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}})$ represents creation or annihilation of particle pairs from condensate
  *Note that, in this approximation, total no. of particles is not conserved*

Finally, using $N = N_0 + \sum_{\mathbf{k}\neq 0} a^\dagger_{\mathbf{k}}a_{\mathbf{k}}$ to trade $N_0$ for $N$, and defining density, $n = \frac{N}{L^d}$

$$\hat{H} = \frac{VnN}{2} + \sum_{\mathbf{k}\neq 0}\left[\left(\epsilon^{(0)}_{\mathbf{k}} + Vn\right) a^\dagger_{\mathbf{k}}a_{\mathbf{k}} + \frac{Vn}{2}\left(a_{-\mathbf{k}}a_{\mathbf{k}} + a^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}}\right)\right]$$

As with quantum AF, $\hat{H}$ diagonalised by Bogoluibov transformation:

$$\begin{pmatrix} a_{\mathbf{k}} \\ a^\dagger_{-\mathbf{k}} \end{pmatrix} = \begin{pmatrix} \cosh\theta_{\mathbf{k}} & -\sinh\theta_{\mathbf{k}} \\ -\sinh\theta_{\mathbf{k}} & \cosh\theta_{\mathbf{k}} \end{pmatrix}\begin{pmatrix} \alpha_{\mathbf{k}} \\ \alpha^\dagger_{-\mathbf{k}} \end{pmatrix}, \quad \text{with } \tanh(2\theta_k) = \frac{Vn}{\epsilon^{(0)}_{\mathbf{k}} + Vn}$$

$$\hat{H} = \frac{VnN}{2} - \frac{1}{2}\sum_{\mathbf{k}\neq 0}(\epsilon^{(0)}_{\mathbf{k}} + nV) + \sum_{\mathbf{k}\neq 0} \overbrace{\left[\left(\epsilon^{(0)}_{\mathbf{k}} + Vn\right)^2 - (Vn)^2\right]^{1/2}}^{\epsilon_{\mathbf{k}}} \left(\alpha^\dagger_{\mathbf{k}}\alpha_{\mathbf{k}} + \frac{1}{2}\right)$$

In particular, for $|\mathbf{k}| \to 0$, low-energy excitations have linear (relativistic)
dispersion, $\epsilon_{\mathbf{k}} = [\epsilon^{(0)}_{\mathbf{k}}(2Vn + \epsilon^{(0)}_{\mathbf{k}})]^{1/2} \simeq \hbar c|\mathbf{k}|$ with 'sound' speed $c = \left(\frac{Vn}{m}\right)^{1/2}$.

At high energies ($|\mathbf{k}| > k_0 = mc/\hbar$), spectrum becomes free particle-like.

▷ $^\dagger$<u>Ground state wavefunction</u>: defined by condition $\alpha_{\mathbf{k}}|\text{g.s.}\rangle = 0$

Since Bogoluibov transformation can be written as $\alpha_{\mathbf{k}} = \hat{U}a_{\mathbf{k}}\hat{U}^{-1}$ where (exercise)

$$\hat{U} = \exp\left[\sum_{\mathbf{k}\neq 0}\frac{\theta_{\mathbf{k}}}{2}(a^\dagger_{\mathbf{k}}a^\dagger_{-\mathbf{k}} - a_{\mathbf{k}}a_{-\mathbf{k}})\right]$$

may infer true g.s. from non-interacting g.s. as $|\text{g.s.}\rangle = \hat{U}|\text{g.s.}\rangle_0$

▷ <u>Experiment?</u> `transparencies`

*When cooled to $T \sim 2K$, liquid $^4He$ undergoes transition to Bose-Einstein condensed state*

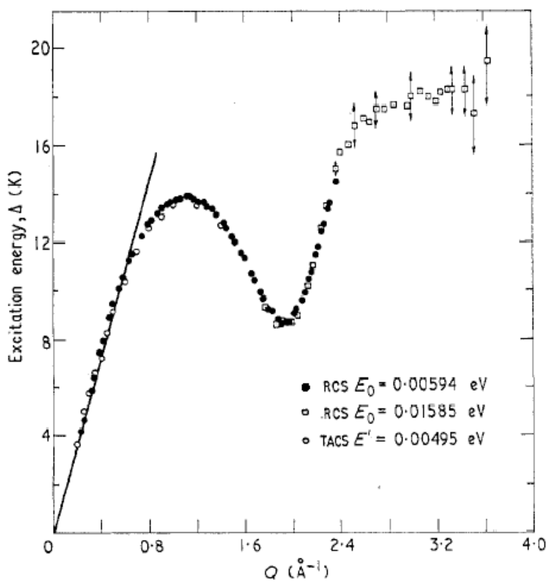
*Neutron scattering can be used to infer spectrum of collective excitations*

*In Helium, steric interactions are strong and at higher energy scales an important second branch of excitations known as rotons appear*

*A second example of BEC is presented by ultracold atomic gases:*

*By confining atoms to a magnetic trap, time of flight measurements can be used to monitor momentum distribution of condensate*

*Moreover, the perturbation imposed by a laser due to the optical dipole interaction provides a means to measure the sound wave velocity*


Excitation energy, Δ (K)
20
16
12
8
4
0
0·8
1·6
2·4
3·2
4·0
Q (Å⁻¹)
RCS $E_0$ = 0·00594 eV
RCS $E_0$ = 0·01585 eV
TACS $E'$ = 0·00495 eV

# Lecture VII: Feynman Path Integral

▷ Motivation:

- Alternative formulation of QM (cf. canonical quantisation)
- Close to classical construction — i.e. semi-classics easily accessed
- Effective formulation of non-perturbative approaches
- Prototype of higher-dimensional field theories

▷ Time-dependent Schrödinger equation

$$\boxed{i\hbar\partial_t|\Psi\rangle = \hat{H}|\Psi\rangle}$$

Formal solution: $|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle = \sum_n e^{-iE_nt/\hbar}|n\rangle\langle n|\psi(0)\rangle$

▷ Time-evolution operator

$$|\Psi(t')\rangle = \hat{U}(t',t)|\Psi(t)\rangle, \qquad \hat{U}(t',t) = e^{-\frac{i}{\hbar}\hat{H}(t'-t)}\theta(t'-t) \qquad \text{N.B. Causal}$$

- Real-space representation:

$$\Psi(q',t') \equiv \langle q'|\Psi(t')\rangle = \langle q'|\hat{U}(t',t)\underset{\wedge}{\int dq|q\rangle\langle q|}|\Psi(t)\rangle = \int dq\, U(q',t';q,t)\Psi(q,t),$$

where $U(q',t';q,t) = \langle q'|e^{-\frac{i}{\hbar}\hat{H}(t'-t)}|q\rangle\theta(t'-t)$ — propagator or Green function:

$$\left(i\hbar\partial_{t'} - \hat{H}\right)\hat{U}(t'-t) = i\hbar\delta(t'-t) \qquad \text{N.B. } \partial_{t'}\theta(t'-t) = \delta(t'-t)$$

Physically: $U(q',t';q,t)$ describes probability amplitude for particle to propagate from $q$ at time $t$ to $q'$ at time $t'$

▷ Construction of Path Integral

Feynman's idea: divide time evolution into $N \to \infty$ discrete time steps $\Delta t = t/N$

$$e^{-i\hat{H}t/\hbar} = [e^{-i\hat{H}\Delta t/\hbar}]^N$$

*Then separate the operator content so that momentum operators stand to the left and position operators to the right:*

$$e^{-i\hat{H}\Delta t/\hbar} = e^{-i\hat{T}\Delta t/\hbar}e^{-i\hat{V}\Delta t/\hbar} + O(\Delta t^2)$$

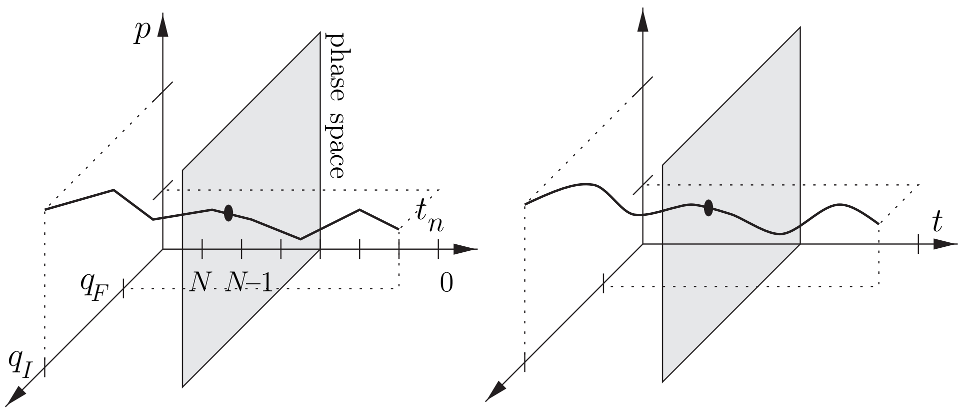
$$\langle q_F|[e^{-i\hat{H}\Delta t/\hbar}]^N|q_I\rangle \simeq \langle q_F|_{\wedge} e^{-i\hat{T}\Delta t/\hbar}e^{-i\hat{V}\Delta t/\hbar}{}_{\wedge}\cdots{}_{\wedge} e^{-i\hat{T}\Delta t/\hbar}e^{-i\hat{V}\Delta t/\hbar}|q_I\rangle$$

Inserting at $\wedge$ resol. of id. $= \int dq_n \int dp_n |q_n\rangle\langle q_n|p_n\rangle\langle p_n|$, and using $\langle q|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{iqp/\hbar}$,

$$e^{-i\hat{V}\Delta t/\hbar}|q_n\rangle\langle q_n|p_n\rangle\langle p_n|e^{-i\hat{T}\Delta t/\hbar} = |q_n\rangle e^{-iV(q_n)\Delta t/\hbar}\langle q_n|p_n\rangle e^{-iT(p_n)\Delta t/\hbar}\langle p_n|,$$

$$\text{and} \quad \langle p_{n+1}|q_n\rangle\langle q_n|p_n\rangle = \frac{1}{2\pi\hbar} e^{iq_n(p_n - p_{n+1})}$$

$$\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle = \int_{q_N=q_F, q_0=q_I} \prod_{n=1}^{N-1} dq_n \prod_{n=1}^{N} \frac{dp_n}{2\pi\hbar} \exp\left[-\frac{i}{\hbar}\Delta t \sum_{n=0}^{N-1}\left(V(q_n) + T(p_{n+1}) - p_{n+1}\frac{q_{n+1}-q_n}{\Delta t}\right)\right]$$




i.e. at each time step, integration over the classical phase space coords. $x_n \equiv (q_n, p_n)$

Contributions from trajectories where $(q_{n+1} - q_n)p_{n+1} > \hbar$ are negligible
— motivates continuum limit

$$\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle = \overbrace{\int_{q_N=q_F, q_0=q_I} \prod_{n=1}^{N-1} dq_n \prod_{n=1}^{N} \frac{dp_n}{2\pi\hbar}}^{\int_{q(t)=q_F, q(0)=q_I} D(q,p)} \exp\Big[-\frac{i}{\hbar} \overbrace{\Delta t \sum_{n=0}^{N-1}}^{\int_0^t dt'} (\overbrace{V(q_n) + T(p_{n+1})}^{H(q,p|_{t'=t_n})} - \overbrace{p_{n+1}\frac{q_{n+1}-q_n}{\Delta t}}^{p\dot{q}|_{t'=t_n}})\Big]$$

Propagator expressed as FUNCTIONAL INTEGRAL:
<u>Hamiltonian formulation of Feynman Path Integral</u>

$$\boxed{\langle q_F|e^{-i\hat{H}t/\hbar}|q_I\rangle = \int_{q(t)=q_F, q(0)=q_I} D(q,p) \exp\Big[\frac{i}{\hbar} \overbrace{\int_0^t dt' \overbrace{(p\dot{q} - H(p,q))}^{\text{Lagrangian}}}^{\text{Action}}\Big]}$$

*Quantum transition amplitude expressed as sum over all possible phase space trajectories (subject to appropriate b.c.) and weighted by classical action*

▷ Lagrangian formulation: for "free-particle" Hamiltonian $H(p,q) = \frac{p^2}{2m} + V(q)$

$$\langle q_F | e^{-i\hat{H}t/\hbar} | q_I \rangle = \int_{q(t)=q_F, q(0)=q_I} Dq \; e^{-(i/\hbar)\int_0^t dt' V(q)} \int Dp \overbrace{\exp\left[-\frac{i}{\hbar}\int_0^t dt' \left(\frac{p^2}{2m} - p\dot{q}\right)\right]}^{\text{Gaussian integral on p}}$$

$$\frac{p^2}{2m} - p\dot{q} \mapsto \frac{1}{2m}\overbrace{(p - m\dot{q})^2}^{p'^2} - \frac{1}{2}m\dot{q}^2$$

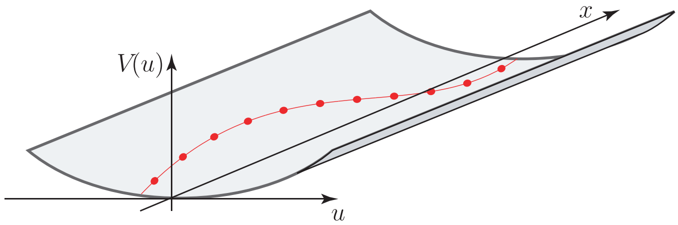
*Functional integral justified by discretisation*

$$\boxed{\langle q_F | e^{-i\hat{H}t/\hbar} | q_I \rangle = \int_{q(t)=q_F, q(0)=q_I} Dq \exp\left[\frac{i}{\hbar}\int_0^t dt' \left(\frac{m\dot{q}^2}{2} - V(q)\right)\right]}$$

$$Dq \to \widetilde{D}q = \lim_{N\to\infty} \left(\frac{Nm}{it2\pi\hbar}\right)^{N/2} \prod_{n=1}^{N-1} dq_n$$

▷ Connection of path integral to classical statistical mechanics

Consider flexible string held under constant tension, $T$,
and confined to 'gutter-like' potential, $V(u)$




i.e. $u(x)$ is displacement from potential minimum

Potential energy stored in spring due to line tension:

$$\text{from } x \text{ to } x + dx,\; dV_T = T\,\overbrace{\left[(dx^2 + du^2)^{1/2} - dx\right]}^{\text{extension}} \simeq \frac{T}{2}\,dx\,(\partial_x u)^2$$

$$V_T[\partial_x u] \equiv \int dV_T = \frac{1}{2}\int_0^L dx\; T\,(\partial_x u(x))^2$$

and from external (gutter) potential: $V_{\text{ext}}[u] \equiv \int_0^L dx\; V[u(x)]$

According to Boltzmann principle,
equilibrium partition function of periodic system ($\beta = 1/k_B T$)

$$\boxed{\mathcal{Z} = \text{tr}\left(e^{-\beta F}\right) = \int_{u(L)=u(0)} Du(x)\; \exp\left[-\beta\int_0^L dx \left(\frac{T}{2}(\partial_x u)^2 + V(u)\right)\right]}$$

"tr" denotes sum over configurations, cf. quantum transmission amplitude

▷ Mapping:

$$\langle q'|e^{-i\hat{H}t/\hbar}|q\rangle = \int Dq(t)\ \exp\left[\frac{i}{\hbar}\int_0^t dt'\left(\frac{m\dot{q}^2}{2} - V(q)\right)\right]$$

Wick rotation $t \to -i\tau \mapsto$ imaginary (Euclidean) time path integral

$$\int_0^t idt'\ (\partial_{t'}q)^2 \longrightarrow -\int_0^\tau d\tau'(\partial_{\tau'}q)^2, \qquad -\int_0^t idt' V(q) \longrightarrow -\int_0^\tau d\tau' V(q)$$

$$\langle q'|e^{-i\hat{H}t/\hbar}|q\rangle = \int Dq \exp\left[-\frac{1}{\hbar}\int_0^\tau d\tau'\left(\frac{m}{2}(\partial_{\tau'}q)^2 + V(q)\right)\right] \qquad \text{N.B. change of relative sign!}$$

(a) Classical partition function of 1d system coincides with QM amplitude

$$\mathcal{Z} = \int dq\ \langle q|e^{-i\hat{H}t/\hbar}|q\rangle\Big|_{t=-i\tau}$$

where time is imaginary, and $\hbar$ play role of temperature, $1/\beta$

Generally, path integral for quantum field $\phi(\mathbf{q}, t)$ in $d$ space dimensions
corresponds to classical statistical mechanics of $d+1$-dim. system

(b) Quantum partition function

$$\mathcal{Z} = \mathrm{tr}(e^{-\beta\hat{H}}) = \int dq\,\langle q|e^{-\beta\hat{H}}|q\rangle$$

i.e. $\mathcal{Z}$ is transition amplitude $\langle q|e^{-i\hat{H}t/\hbar}|q\rangle$ evaluated at imaginary time $t = -i\hbar\beta$.

(c) Semi-classics

As $\hbar \to 0$, PI dominated by stationary config. of action $S[p,q] = \int dt(p\dot{q} - H(p,q))$

$$\delta S = S[p+\delta p, q+\delta q] - S[p,q] = \int dt\,[\delta p\,\dot{q} + p\,\delta\dot{q} - \delta p\,\partial_p H - \delta q\,\partial_q H] + O(\delta p^2, \delta q^2, \delta p\delta q)$$
$$= \int dt\,[\delta p\,(\dot{q} - \partial_p H) + \delta q\,(-\dot{p} - \partial_q H)] + O(\delta p^2, \delta q^2, \delta p\delta q)$$

i.e. Hamilton's classical e.o.m.: $\dot{q} = \partial_p H$, $\dot{p} = -\partial_q H$ with b.c. $q(0) = q_I$, $q(t) = q_F$

Similarly, with Lagrangian formulation: $\delta S = 0 \Rightarrow \partial_t(\partial_{\dot{q}}L) - \partial_q L = 0$

What about contributions from fluctuations around classical paths?

Usually, exact evaluation of PI impossible — must resort to approximation schemes...

▷ SADDLE-POINT AND STATIONARY PHASE ANALYSIS

Principle: consider integral over single variable,

$$I = \int_{-\infty}^{\infty} dz\, e^{-f(z)}$$

Expect integral to be dominated by minima of $f(z)$; suppose unique i.e. $f'(z_0) = 0$

$$f(z) = f(z_0) + (z - z_0)\overbrace{f'(z_0)}^{\mapsto 0} + \frac{1}{2}(z - z_0)^2 f''(z_0) + \cdots$$

$$I \simeq e^{-f(z_0)} \int_{-\infty}^{\infty} dz\, e^{-(z-z_0)^2 f''(z_0)/2} = \sqrt{\frac{2\pi}{f''(z_0)}} e^{-f(z_0)}$$

$$\text{Example :} \quad \overbrace{\Gamma(s+1)}^{= s! \text{ if } s \in Z} = \int_0^{\infty} dz\, z^s e^{-z} = \int_0^{\infty} dz\, e^{-f(z)}, \qquad f(z) = z - s \ln z$$

$f'(z) = 1 - \frac{s}{z}$ i.e. $z_0 = s$, $f''(z_0) = \frac{s}{z_0^2} = \frac{1}{s}$
i.e. $\Gamma(s+1) \simeq \sqrt{2\pi s} e^{-(s - s\ln s)}$ — Stirling's formula

If minima not on integration contour – deform contour through saddle-point
e.g. $\Gamma(s+1)$, $s$ complex

What if exponent pure imaginary? Fast phase fluctuations $\rightsquigarrow$ cancellation
i.e. expand around region of slowest (i.e. stationary) phase and use identity

$$\int_{-\infty}^{\infty} dz\, e^{iaz^2/2} = \sqrt{\frac{2\pi}{a}} e^{i\pi/4}$$

▷ Can we apply same approach to analyse PI? Yes
but we must develop basic tool of QFT – Gaussian functional integral!

## Lecture VIII: Quantum Harmonic Oscillator

▷ Free particle propagator: Difficult to obtain from PI, but useful for normalization,

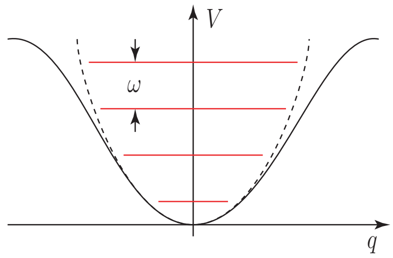
and easily obtained from equation for Green function, $(i\hbar\partial_t - \hat{H})\hat{G}_{\rm free}(t) = i\hbar\delta(t)$, which in Euclidean time $t = -i\tau$ becomes a diffusion equation,

$$\left(\hbar\partial_\tau - \frac{\hbar^2\nabla^2}{2m}\right) G_{\rm free}(q_{\rm F}, q_{\rm I}, t) = \hbar\delta(q_{\rm F} - q_{\rm I})\delta(\tau)$$

Solution: (PS3)

$$G_{\rm free}(q_F, q_I; t) \equiv \langle q_F|e^{-i\hat{p}^2 t/2m\hbar}|q_I\rangle\theta(t) = \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} \exp\left[\frac{i}{\hbar}\frac{m(q_F - q_I)^2}{2t}\right]\theta(t)$$

▷ Quantum particle in single (symmetric) well: $V(q) = V(-q)$




e.g. QM amplitude

$$G(0,0;t) \equiv \langle 0|e^{-i\hat{H}t/\hbar}|0\rangle\,\theta(t) = \int_{q(t)=q(0)=0} Dq \exp\left[\frac{i}{\hbar}\int_0^t dt'\left(\frac{m\dot{q}^2}{2} - V(q)\right)\right]$$

▷ Evaluate PI by stationary phase approx: *general recipe*

(i) Parameterise path as $q(t) = q_{\rm cl}(t) + r(t)$ and expand action in $r(t)$

$$S[\bar{q}+r] = \int_0^t dt'\Big[\frac{m}{2}\overbrace{(\dot{q}_{\rm cl}+\dot{r})^2}^{\dot{q}_{\rm cl}{}^2 + 2\dot{q}_{\rm cl}\dot{r} + \dot{r}^2} - \overbrace{V(q_{\rm cl}+r)}^{V(q_{\rm cl}) + rV'(q_{\rm cl}) + \frac{r^2}{2}V''(q_{\rm cl}) + \cdots}\Big]$$

$$= S[q_{\rm cl}] + \int_0^t dt' r(t')\overbrace{\left[-m\ddot{q}_{\rm cl} - V'(q_{\rm cl})\right]}^{\frac{\delta S}{\delta q(t')}=0} + \frac{1}{2}\int_0^t dt' r(t')\overbrace{\left[-m\partial_{t'}^2 - V''(q_{\rm cl})\right]}^{\frac{\delta^2 S}{\delta q(t')\delta q(t'')}} r(t') + \cdots$$

(ii) Classical trajectory: $m\ddot{q}_{\rm cl} = -V'(q_{\rm cl})$

Many solutions – choose non-singular $q_{\rm cl} = 0$, i.e. $S[q_{\rm cl}] = 0$ and $V''(q_{\rm cl}) = m\omega^2$ const.

$$G(0,0;t) \simeq \int_{r(0)=r(t)=0} Dr \exp\left[\frac{i}{\hbar}\int_0^t dt' r(t')\frac{m}{2}\left(-\partial_{t'}^2 - \omega^2\right)r(t')\right]$$

*N.B. if $V$ was quadratic, expression trivially exact*

More generally, $q_{\rm cl}(t)$ non-trivial $\mapsto$ non-vanishing $S[q_{\rm cl}]$ — see PS3

Fluctuations? — example of a...

▷ <u>Gaussian functional integration:</u> *mathematical interlude*

- One variable Gaussian integral: $(\int_{-\infty}^{\infty} dv\, e^{-av^2/2})^2 = 2\pi \int_0^\infty r\, dr\, e^{-ar^2/2} = \frac{2\pi}{a}$

$$\int_{-\infty}^{\infty} dv\, e^{-\frac{a}{2}v^2} = \sqrt{\frac{2\pi}{a}}, \qquad \text{Re}\, a > 0$$

- Many variables:

$$\int d\mathbf{v}\, e^{-\frac{1}{2}\mathbf{v}^T\mathbf{A}\mathbf{v}} = (2\pi)^{N/2} \det \mathbf{A}^{-1/2}$$

$\mathbf{A}$ is +ve definite real symmetric $N \times N$ matrix

Proof: $\mathbf{A}$ diagonalised by orthogonal trans: $\mathbf{D} = \mathbf{O}\mathbf{A}\mathbf{O}^T$

Change of variables: $\mathbf{v} = \mathbf{O}^T\mathbf{w}$ (Jacobian $\det(\mathbf{O}) = 1$) $\rightsquigarrow$ $N$ decoupled Gaussian integrations: $\mathbf{v}^T\mathbf{A}\mathbf{v} = \mathbf{w}^T\mathbf{D}\mathbf{w} = \sum_i^N d_i w_i^2$ and $\prod_{i=1}^N d_i = \det \mathbf{D} = \det \mathbf{A}$

- Infinite number of variables; interpret $\{v_i\} \mapsto v(t)$ as continuous field and $A_{ij} \mapsto A(t,t') = \langle t|\hat{A}|t'\rangle$ as operator kernel

$$\int Dv(t)\, \exp\left[-\frac{1}{2}\int dt \int dt'\, v(t)A(t,t')v(t')\right] \propto (\det \hat{A})^{-1/2}$$

(iii) Applied to QW, $A(t,t') = -\frac{i}{\hbar}m\delta(t-t')(-\partial_{t'}^2 - \omega^2)$ and

$$G(0,0;t) \simeq J \det\left(-\partial_{t'}^2 - \omega^2\right)^{-1/2}$$

where $J$ absorbs constant prefactors ($im, \hbar$, etc.)

What does 'det' mean? Effectively, we can expand trajectories $r(t')$ in eigenbasis of $\hat{A}$ subject to b.c. $r(t) = r(0) = 0$

$$\left(-\partial_t^2 - \omega^2\right) r_n(t) = \epsilon_n r_n(t), \qquad \text{cf. PIB}$$

i.e. Fourier series expansion: $r_n(t') = \sin(\frac{n\pi t'}{t})$, $\quad n = 1, 2, \ldots, \quad \epsilon_n = (\frac{n\pi}{t})^2 - \omega^2$

$$\det\left(-\partial_t^2 - \omega^2\right)^{-1/2} = \prod_{n=1}^{\infty} \epsilon_n^{-1/2} = \prod_{n=1}^{\infty}\left(\left(\frac{n\pi}{t}\right)^2 - \omega^2\right)^{-1/2}$$

▷ For $V = 0$, $G = G_{\rm free}$ known — use to eliminate constant prefactor $J$

$$G(0,0;t) = \frac{G(0,0;t)}{G_{\rm free}(0,0;t)} G_{\rm free}(0,0;t) = \prod_{n=1}^{\infty}\left[1 - \left(\frac{\omega t}{n\pi}\right)^2\right]^{-1/2} \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} \Theta(t)$$

Applying identity $\prod_{n=1}^{\infty}[1-(\frac{x}{n\pi})^2]^{-1} = \frac{x}{\sin x}$

$$G(0,0;t) \simeq \sqrt{\frac{m\omega}{2\pi i\hbar \sin(\omega t)}}\Theta(t)$$

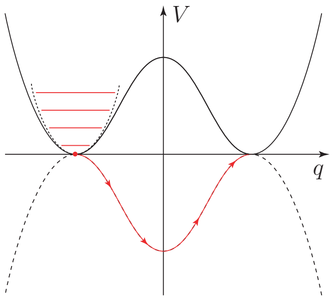
(exact for harmonic oscillator)

*Singular behaviour is a feature of ladder-like states of harmonic oscillator leading to periodic coherent superposition and dynamical echo (see PS3).*

## Double Well: Tunneling and Instantons

How can QM tunneling be described by path integral? No semi-classical expansion!

▷ E.g transition amplitude in double well: $G(a,-a;t) \equiv \langle a|e^{-i\hat{H}t/\hbar}|-a\rangle$




▷ Feynman PI:

$$G(a,-a;t) = \int_{q(0)=-a}^{q(t)=a} Dq \exp\left[\frac{i}{\hbar}\int_0^t dt' \left(\frac{m}{2}\dot{q}^2 - V(q)\right)\right]$$

Stationary phase analysis: classical e.o.m. $m\ddot{q} = -\partial_q V$

$\mapsto$ only singular (high energy) solutions *Switch to alternative formulation...*

▷ Imaginary (Euclidean) time PI: Wick rotation $t = -i\tau$

N.B. (relative) sign change! "$V \to -V$"

$$G(a,-a;\tau) = \int_{q(0)=-a}^{q(\tau)=a} Dq \exp\left[-\frac{1}{\hbar}\int_0^\tau d\tau' \left(\frac{m}{2}\dot{q}^2 + V(q)\right)\right]$$

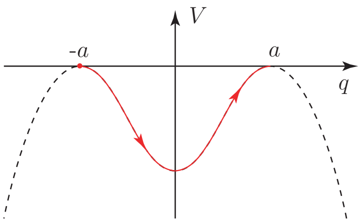
Saddle-point analysis: classical e.o.m. $m\ddot{q} = +V'(q)$ in inverted potential!

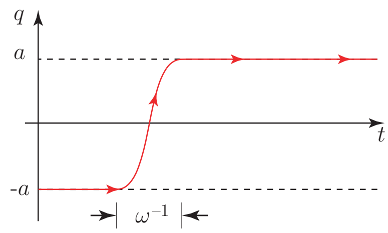
solutions depend on b.c.

(1) $G(a,a;\tau) \rightsquigarrow q_{\rm cl}(\tau) = a$
(2) $G(-a,-a;\tau) \rightsquigarrow q_{\rm cl}(\tau) = -a$
(3) $G(a,-a;\tau) \rightsquigarrow q_{\rm cl}$ : rolls from $-a$ to $a$

*Combined with small fluctuations,* (1) and (2) recover propagator for single well

(3) accounts for tunneling – known as "instanton" (or "kink")




▷ Instanton: classically forbidden trajectory connecting two degenerate minima

— i.e. topological, and therefore particle-like

For $\tau$ large, $\dot{q_{\rm cl}} \simeq 0$ (*evident*), i.e. "first integral" $m\dot{q_{\rm cl}}^2/2 - V(q_{\rm cl}) = \epsilon \overset{\tau\to\infty}{\to} 0$

*precise value of $\epsilon$ fixed by b.c. (i.e. $\tau$)*

Saddle-point action *(cf. WKB $\int dq p(q)$)*

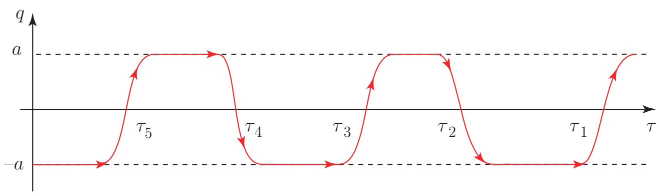
$$S_{\rm inst.} = \int_0^\tau d\tau' \left(\frac{m}{2}\dot{q}_{\rm cl}^2 + V(q_{\rm cl})\right) \simeq \int_0^\tau d\tau' m\dot{q}_{\rm cl}^2 = \int_{-a}^a dq_{\rm cl} m\dot{q}_{\rm cl} = \int_{-a}^a dq_{\rm cl}(2mV(q_{\rm cl}))^{1/2}$$

Structure of instanton: For $q \simeq a$, $V(q) = \frac{1}{2}m\omega^2(q-a)^2 + \cdots$, i.e. $\dot{q}_{\rm cl} \overset{\tau\to\infty}{\simeq} \omega(q_{\rm cl} - a)$

$$q_{\rm cl}(\tau) \overset{\tau\to\infty}{=} a - e^{-\tau\omega}, \text{ i.e. temporal extension set by } \omega^{-1} \ll \tau$$

Imples existence of approximate saddle-point solutions

involving many instantons (and anti-instantons): instanton gas




▷ Accounting for fluctuations around n-instanton configuration

$$G(a, \pm a; \tau) \simeq \sum_{n \text{ even}/\text{odd}} K^n \int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n \overbrace{A_n(\tau_1, \ldots, \tau_n)}^{A_{n,\rm cl.}A_{n,\rm qu.}},$$

constant $K$ set by normalisation

$A_{n,\rm cl.} = e^{-nS_{\rm inst.}/\hbar}$ — 'classical' contribution

$A_{n,\rm qu.}$ — quantum fluctuations (cf. single well): $G_{\rm s.w.}(0,0;t) \sim \frac{1}{\sqrt{\sin\omega t}}$

$$A_{n,\rm qu.} \sim \prod_i^n \frac{1}{\sqrt{\sin(-i\omega(\tau_{i+1} - \tau_i))}} \sim \prod_i^n e^{-\omega(\tau_{i+1}-\tau_i)/2} \sim e^{-\omega\tau/2}$$

$$G(a, \pm a; \tau) \simeq \sum_{n \text{ even}/\text{odd}} K^n e^{-nS_{\rm inst.}/\hbar} e^{-\omega\tau/2} \overbrace{\int_0^\tau d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n}^{\tau^n/n!}$$

$$= \sum_{n \text{ even / odd}} e^{-\omega\tau/2} \frac{1}{n!} \left(\tau K e^{-S_{\text{inst.}}/\hbar}\right)^n$$

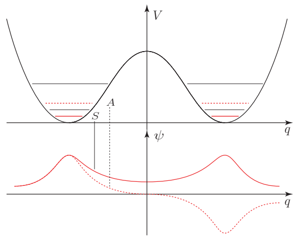
Using $e^x = \sum_{n=0}^{\infty} x^n/n!$, N.B. non-perturbative in $\hbar$!

$$G(a, a; \tau) \simeq Ce^{-\omega\tau/2} \cosh\left(\tau K e^{-S_{\text{inst.}}/\hbar}\right), \qquad G(a, -a; \tau) \simeq Ce^{-\omega\tau/2} \sinh\left(\tau K e^{-S_{\text{inst.}}/\hbar}\right)$$

Consistency check: main contribution from

$$\bar{n} = \langle n \rangle \equiv \frac{\sum_n nX^n/n!}{\sum_n X^n/n!} = X = \tau K e^{-S_{\text{inst.}}/\hbar}$$

no. per unit time, $\bar{n}/\tau$ exponentially small, and indep. of $\tau$, i.e. dilute gas




▷ Physical interpretation: For infinite barrier, oscillators independent, coupling splits degeneracy – symmetric/antisymmetric

$$G(a, \pm a; \tau) \simeq \langle a|S\rangle e^{-\epsilon_S\tau/\hbar}\langle S| \pm a\rangle + \langle a|A\rangle e^{-\epsilon_A\tau/\hbar}\langle A| \pm a\rangle$$

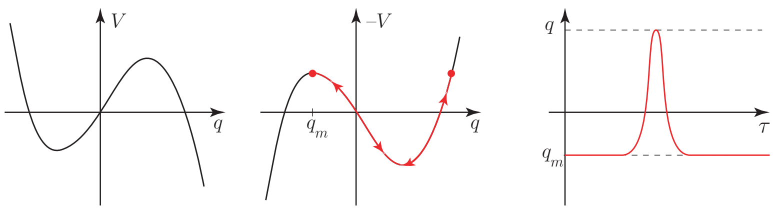
Setting $\epsilon_{A/S} = \hbar\omega/2 \pm \frac{\Delta\epsilon}{2}$, and noting $|\langle a|S\rangle|^2 = \langle a|S\rangle\langle S| - a\rangle = \frac{C}{2} = |\langle a|A\rangle|^2 = -\langle a|A\rangle\langle A| - a\rangle$

$$G(a, \pm a; \tau) \simeq \frac{C}{2}\left(e^{-(\hbar\omega - \Delta\epsilon)\tau/2\hbar} \pm e^{-(\hbar\omega+\Delta\epsilon)\tau/2\hbar}\right) = Ce^{-\omega\tau/2}\left\{\begin{array}{l}\cosh(\Delta\epsilon\tau/\hbar)\\ \sinh(\Delta\epsilon\tau/\hbar)\end{array}\right. .$$

▷ Remarks:

(i) Legitimacy? How do (neglected) terms $O(\hbar^2)$ compare to $\Delta\epsilon$?

In fact, such corrections are bigger but act equally on $|S\rangle$ and $|A\rangle$ i.e. $\Delta\epsilon = \hbar K e^{-S_{\text{inst.}}/\hbar}$ is dominant contribution to splitting




(ii) Unstable States and Bounces: survival probability: $G(0, 0; t)$? No even/odd effect:

$$G(0, 0; \tau) = Ce^{-\omega\tau/2} \exp\left[\tau K e^{-S_{\text{inst}}/\hbar}\right] \overset{\tau=it}{\equiv} Ce^{-i\omega t/2} \exp\left[-\frac{\Gamma}{2}t\right]$$

True decay rate has additional factor of 2: $\Gamma \sim |K|e^{-S_{\text{inst}}/\hbar}$ (i.e. $K$ imaginary) *see Coleman for details*

## Lecture IX: Coherent States

Generalisation of PI to many-body systems problematic due to particle indistinguishability. Can second quantisation help? *automatically respects particle statistics*

Require complete basis on Fock space to construct PI

i.e. analogue of $\int dq\, dp\, |q\rangle\langle q|p\rangle\langle p| = \text{id}$.

Such eigenstates exist and are known as... *reference: Negele and Orland*

▷ Coherent States (Bosons)

What are eigenstates of Fock space operators: $a_i$ and $a_i^\dagger$ with $[a_i, a_j^\dagger] = \delta_{ij}$?

As a state of the Fock space, an eigenstate $|\phi\rangle$ can be expanded as

$$|\phi\rangle = \sum_{n_1,n_2,\cdots} C_{n_1,n_2,\cdots} \frac{(a_1^\dagger)^{n_1}}{\sqrt{n_1}} \frac{(a_2^\dagger)^{n_2}}{\sqrt{n_2}} \cdots |0\rangle$$

*N.B. notation $|0\rangle$ for vacuum state!*

(i) $a_i^\dagger|\phi\rangle = \phi_i|\phi\rangle$? — clearly, eigenstate of $a_i^\dagger$ can not exist:

if minimum occupation of $|\phi\rangle$ is $n_0$, minimum of $a_i^\dagger|\phi\rangle$ is $n_0+1$

(ii) $a_i|\phi\rangle = \phi_i|\phi\rangle$? — can exist and given by: $\boxed{|\phi\rangle \equiv \exp[\sum_i \phi_i a_i^\dagger]|0\rangle}$ i.e. $\phi \equiv \{\phi_i\}$

Proof: *since $a_i$ commutes with all $a_j^\dagger$ for $j \neq i$ — focus on one element $i$*

$$ae^{\phi a^\dagger}|0\rangle = [a, e^{\phi a^\dagger}]|0\rangle = \sum_{n=0}^\infty \frac{\phi^n}{n!}[a, (a^\dagger)^n]|0\rangle = \sum_{n=1}^\infty \frac{n\phi^n}{n!}(a^\dagger)^{n-1}|0\rangle = \phi \exp(\phi a^\dagger)|0\rangle$$

$$a(a^\dagger)^n = aa^\dagger(a^\dagger)^{n-1} = (1 + a^\dagger a)(a^\dagger)^{n-1} = (a^\dagger)^{n-1} + a^\dagger a(a^\dagger)^{n-1} = n(a^\dagger)^{n-1} + (a^\dagger)^n a$$

i.e. $|\phi\rangle$ is eigenstate of all $a_i$ with eigenvalue $\phi_i$

▷ Properties of coherent state $|\phi\rangle$

- Hermitian conjugation:

$$\forall i: \quad \langle\phi|a_i^\dagger = \langle\phi|\bar{\phi}_i$$

$\bar{\phi}_i$ is complex conjugate of $\phi_i$

- By direct application of $\partial_{\phi_i}$ (and operator commutativity):

$$\forall i: \quad a_i^\dagger|\phi\rangle = \partial_{\phi_i}|\phi\rangle$$

- Overlap: with $\langle\theta| = |\theta\rangle^\dagger = \langle 0|e^{\sum_i \bar\theta_i a_i}$

$$\langle\theta|\phi\rangle = \langle 0|e^{\sum_i \bar\theta_i a_i}|\phi\rangle = e^{\sum_i \bar\theta_i \phi_i}\langle 0|\phi\rangle = \exp\left[\sum_i \bar\theta_i\phi_i\right]$$

i.e. states are not orthogonal! *operators not Hermitian*

- Norm: $\langle\phi|\phi\rangle = \exp\left[\sum_i \bar\phi_i\phi_i\right]$

- Completeness — resolution of id. (for proof see notes)

$$\boxed{\int \prod_i \frac{d\bar\phi_i d\phi_i}{\pi} e^{-\sum_i \bar\phi_i\phi_i}|\phi\rangle\langle\phi| = \mathbf{1}_{\mathcal{F}}}$$

where $d\bar\phi_i d\phi_i = d\mathrm{Re}\,\phi_i d\mathrm{Im}\,\phi_i$

▷ Coherent States (Fermions)

Following bosonic case, seek state $|\eta\rangle$ s.t.

$$a_i|\eta\rangle = \eta_i|\eta\rangle, \qquad \eta = \{\eta_i\}$$

But anticommutativity $[a_i, a_j]_+ = 0$ $(i \neq j)$ demands that $a_i a_j|\eta\rangle = -a_j a_i|\eta\rangle$
i.e. eigenvalues $\eta_i$ must anticommute!!

$$\eta_i\eta_j = -\eta_j\eta_i$$

$\eta_i$ can not be ordinary numbers — in fact, they obey...

▷ Grassmann Algebra

In addition to anticommutativity, defining properties:

(i) $\eta_i^2 = 0$ (cf. fermions) but note: these are not operators, i.e. $[\eta_i, \bar\eta_i]_+ \neq 1$

(ii) Elements $\eta_i$ can be added to, and multiplied, by ordinary complex numbers

$$c + c_i\eta_i + c_j\eta_j, \qquad c_i, c_j \in \mathcal{C}$$

(iii) Grassmann numbers anticommute with fermionic creation/annihilation operators
$[\eta_i, a_j]_+ = 0$

▷ Calculus of Grassmann variables:

(iv) Differentiation: $\partial_{\eta_i}\eta_j = \delta_{ij}$
N.B. ordering matters $\partial_{\eta_i}\eta_j\eta_i = -\eta_j\partial_{\eta_i}\eta_i = -\eta_j$ for $i \neq j$

(v) Integration: $\int d\eta_i = 0, \quad \int d\eta_i\eta_i = 1$
i.e. differentiation and integration have the same effect!!

▷ Gaussian integration:

$$\int d\bar{\eta}d\eta\, e^{-\bar{\eta}a\eta} = \int d\bar{\eta}d\eta\,(1-\bar{\eta}a\eta) = a\int d\bar{\eta}\bar{\eta}\int d\eta\eta = a$$

$$\int \prod_i d\bar{\eta}_i d\eta_i\, e^{-\bar{\eta}^T\mathbf{A}\eta} = \det\mathbf{A} \qquad \text{(exercise)}$$

cf. ordinary complex variables

▷ Functions of Grassmann variables:

Taylor expansion terminates at low order since $\eta^2 = 0$, e.g.

$$F(\eta) = F(0) + \eta F'(0)$$

Using rules

$$\int d\eta F(\eta) = \int d\eta\,[F(0)+\eta F'(0)] = F'(0) \equiv \partial_\eta F[\eta]$$

i.e. differentiation and integration have same effect on $F[\eta]$!

Usually, one has a function of many variables $F[\eta]$, say $\eta = \{\eta_1, \cdots \eta_N\}$

$$F(\eta) = \sum_{n=0}^{\infty} \frac{1}{n!}\frac{\partial^n F(0)}{\partial\eta_i\cdots\partial\eta_j}\eta_j\cdots\eta_i$$

but series must terminate at $n = N$

*with these preliminaries we are in a position to introduce the*

▷ Fermionic coherent state: $\boxed{|\eta\rangle = \exp[-\sum_i \eta_i a_i^\dagger]|0\rangle}$ i.e. $\eta = \{\eta_i\}$

Proof (cf. bosonic case)

$$a\exp(-\eta a^\dagger)|0\rangle = a(1-\eta a^\dagger)|0\rangle = \eta a a^\dagger|0\rangle = \eta|0\rangle = \eta\exp(-\eta a^\dagger)|0\rangle$$

Other defining properties mirror bosonic CS — *problem set*

▷ Differences:

(i) Adjoint: $\langle\eta| = \langle 0|e^{-\sum_i a_i\bar{\eta}_i} \equiv \langle 0|e^{\sum_i \bar{\eta}_i a_i}$ but N.B. $\bar{\eta}_i$ not related to $\eta_i$!

(ii) Gaussian integration: $\int d\bar{\eta}d\eta\, e^{-\bar{\eta}\eta} = 1$ N.B. no $\pi$'s

Completeness relation

$$\boxed{\int \prod_i d\bar{\eta}_i d\eta_i e^{-\sum_i \bar{\eta}_i\eta_i}|\eta\rangle\langle\eta| = \mathbf{1}_F}$$

## Lecture X: Many-body (Coherent State) Path Integral

*Having obtained a complete coherent state basis for the creation and annihilation operators, we could proceed by constructing path integral for the quantum time evolution operator. However, since we will be interested in application involving a phase transition, it is more convenient to begin with the quantum partition function.*

▷ Quantum partition function

$$\mathcal{Z} = \sum_{\{n\}\in\text{Fock Space}} \langle n|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle, \qquad F = -k_{\rm B}T\ln\mathcal{Z}$$

$\beta = \frac{1}{k_{\rm B}T}$, $\mu$ — chemical potential

In coherent state basis

$$\mathcal{Z} = \int d[\bar{\psi},\psi]e^{-\sum_i \bar{\psi}_i\psi_i}\sum_n \langle n|\psi\rangle\langle\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle$$

Elimination of $|n\rangle$ requires identity: $\langle n|\psi\rangle\langle\psi|n\rangle = \langle\zeta\psi|n\rangle\langle n|\psi\rangle$

Proof: for, e.g., $|n\rangle = a_1^\dagger a_2^\dagger\cdots a_n^\dagger|0\rangle$

$$\begin{aligned}\langle n|\psi\rangle &= \langle 0|a_n\cdots a_2a_1|\psi\rangle = \psi_n\cdots\psi_2\psi_1\langle 0|\psi\rangle = \psi_n\cdots\psi_2\psi_1\\ \langle\psi|n\rangle &= \bar{\psi}_1\bar{\psi}_2\cdots\bar{\psi}_n\\ \langle n|\psi\rangle\langle\psi|n\rangle &= \psi_n\cdots\psi_2\psi_1\bar{\psi}_1\bar{\psi}_2\cdots\bar{\psi}_n = \psi_1\bar{\psi}_1\psi_2\bar{\psi}_2\cdots\psi_n\bar{\psi}_n\\ &= (\zeta\bar{\psi}_1\psi_1)(\zeta\bar{\psi}_2\psi_2)\cdots(\zeta\bar{\psi}_n\psi_n) = \langle\zeta\psi|n\rangle\langle n|\psi\rangle\end{aligned}$$

*Note that $\hat{H}$ and $\hat{N}$ even in operators allowing matrix element to be commuted through*

$$\boxed{\mathcal{Z} = \int d[\bar{\psi},\psi]e^{-\sum_i\bar{\psi}_i\psi_i}\langle\zeta\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|\psi\rangle}$$

▷ Coherent State Path Integral

Applied to many-body Hamiltonian of fermions or bosons

$$\hat{H}-\mu\hat{N} = \sum_{ij}(h_{ij}-\mu\delta_{ij})a_i^\dagger a_j + \sum_{ij}V_{ij}\ a_i^\dagger a_j^\dagger a_j a_i$$

N.B. operators are normal ordered

Follow general strategy of Feynman:

(i) Divide 'time' interval, $\beta$, into $N$ segments of length $\Delta\beta = \beta/N$

$$\langle\zeta\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|\psi\rangle = \langle\zeta\psi|e^{-\Delta\beta(\hat{H}-\mu\hat{N})}{}_{\wedge}e^{-\Delta\beta(\hat{H}-\mu\hat{N})}{}_{\wedge}\cdots e^{-\Delta\beta(\hat{H}-\mu\hat{N})}|\psi\rangle$$

(ii) At each position '$_\wedge$' insert resolution of id.

$$\mathbf{1}_{\mathcal{F}} = \int d[\bar{\psi}_n, \psi_n] e^{-\bar{\psi}_n \cdot \psi_n} |\psi_n\rangle\langle\psi_n|$$

*i.e. N-independent sets* N.B. each $\psi_n$ is a vector with elements $\{\psi_i\}_n$

(iii) Expand exponent in $\Delta\beta$

$$\begin{aligned}
\langle\psi'|e^{-\Delta\beta(\hat{H}-\mu\hat{N})}|\psi\rangle &= \langle\psi'|\left[1-\Delta\beta(\hat{H}-\mu\hat{N})\right]|\psi\rangle + O(\Delta\beta)^2 \\
&= \langle\psi'|\psi\rangle - \Delta\beta\langle\psi'|(\hat{H}-\mu\hat{N})|\psi\rangle + O(\Delta\beta)^2 \\
&= \langle\psi'|\psi\rangle\left[1-\Delta\beta\left(H(\psi',\psi)-\mu N(\psi',\psi)\right)\right] + O(\Delta\beta)^2 \\
&\simeq e^{\psi'\cdot\psi} e^{-\Delta\beta(H(\psi',\psi)-\mu N(\psi',\psi))}
\end{aligned}$$

$$\text{with} \qquad H(\psi',\psi) = \frac{\langle\psi'|\hat{H}|\psi\rangle}{\langle\psi'|\psi\rangle} = \sum_{ij} h_{ij}\bar{\psi}'_i\psi_j + \sum_{ij} V_{ij}\bar{\psi}'_i\bar{\psi}'_j\psi_j\psi_i$$

similarly $N(\psi',\psi)$ *N.B.* $\langle\psi'|\psi\rangle$ *bilinear in* $\psi$*, i.e. commutes with everything*

$$\mathcal{Z} = \int_{\bar{\psi}_N=\zeta\bar{\psi}_0,\psi_N=\zeta\psi_0} \prod_{n=0}^{N} d[\bar{\psi}_n,\psi_n] e^{-\sum_{n=1}^{N}\left[\bar{\psi}_n\cdot(\psi_n-\psi_{n-1})+\Delta\beta(H(\bar{\psi}_n,\psi_{n-1})-\mu N(\bar{\psi}_n,\psi_{n-1}))\right]}$$

Continuum limit $N\to\infty$

$$\Delta\beta\sum_{n=0}^{N} \to \int_0^\beta d\tau, \qquad \frac{\psi_n-\psi_{n-1}}{\Delta\beta} \to \partial_\tau\psi\Big|_{\tau=n\Delta\beta}, \qquad \prod_{n=0}^{N} d[\bar{\psi}_n,\psi_n] \to D(\bar{\psi},\psi)$$

*comment on "small" Grassmann nos.*

$$\boxed{\mathcal{Z} = \int_{\substack{\bar{\psi}(\beta)=\zeta\bar{\psi}(0)\\ \psi(\beta)=\zeta\psi(0)}} D(\bar{\psi},\psi)e^{-S[\bar{\psi},\psi]}, \qquad S[\bar{\psi},\psi] = \int_0^\beta d\tau\left(\bar{\psi}\cdot\partial_\tau\psi + H(\bar{\psi},\psi) - \mu N(\bar{\psi},\psi)\right)}$$

With particular example:

$$S[\bar{\psi},\psi] = \int_0^\beta d\tau\left[\sum_{ij}\bar{\psi}_i(\tau)\left[(\partial_\tau-\mu)\delta_{ij}+h_{ij}\right]\psi_j(\tau) + \sum_{ij} V_{ij}\,\bar{\psi}_i(\tau)\bar{\psi}_j(\tau)\psi_j(\tau)\psi_i(\tau)\right]$$

quantum partition function expressed as path integral over fields $\psi_i(\tau)$

▷ Matsubara frequency representation

Often convenient to express path integral in frequency domain

$$\psi(\tau) = \frac{1}{\sqrt{\beta}}\sum_{\omega_n}\psi_n e^{-i\omega_n\tau}, \qquad \psi_{\omega_n} = \frac{1}{\sqrt{\beta}}\int_0^\beta d\tau\,\psi(\tau)e^{i\omega_n\tau}$$

where, since $\psi(\tau) = \zeta\psi(\tau+\beta)$

$$\omega_n = \begin{cases} 2n\pi/\beta, & \text{bosons,} \\ (2n+1)\pi/\beta, & \text{fermions} \end{cases}, \quad n \in \mathcal{Z}$$

$\omega_n$ are known as Matsubara frequencies

Using $\displaystyle\frac{1}{\beta}\int_0^\beta d\tau\; e^{i(\omega_n-\omega_m)\tau} = \delta_{\omega_n\omega_m}$

$$S[\bar\psi,\psi] = \sum_{ij\omega_n} \bar\psi_{i\omega_n}\left[(-i\omega_n-\mu)\,\delta_{ij}+h_{ij}\right]\psi_{j\omega_n} + \\ +\frac{1}{\beta}\sum_{ij}\sum_{\omega_{n_1}\omega_{n_2}\omega_{n_3}\omega_{n_4}} V_{ij}\bar\psi_{i\omega_{n_1}}\bar\psi_{j\omega_{n_2}}\psi_{j\omega_{n_3}}\psi_{i\omega_{n_4}}\delta_{\omega_{n_1}+\omega_{n_2},\omega_{n_3}+\omega_{n_4}}$$

e.g. Harmonic chain: $\hat H = \sum_k \hbar\omega_k(a_k^\dagger a_k + 1/2)$

$$S = \int_0^\beta d\tau \sum_k \bar\psi_k(\partial_\tau + \hbar\omega_k - \mu)\psi_k$$

e.g. Electron gas: $\hat H = \sum_\sigma \int dr\; c_\sigma^\dagger(\mathbf{r})\frac{\hat p^2}{2m}c_\sigma(\mathbf{r}) - \sum_{\sigma\sigma'}\int dr\,dr'\; c_\sigma^\dagger(\mathbf{r})c_{\sigma'}^\dagger(\mathbf{r}')\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}c_{\sigma'}(\mathbf{r}')c_\sigma(\mathbf{r})$

$$S = \int_0^\beta d\tau \sum_\sigma \int dr \bar\psi_\sigma(\mathbf{r},\tau)(\partial_\tau + \frac{\hat p^2}{2m} - \mu)\psi_\sigma(\mathbf{r},\tau) \\ -\int_0^\beta d\tau \sum_{\sigma,\sigma'}\int dr\,dr'\bar\psi_\sigma(\mathbf{r},\tau)\bar\psi_{\sigma'}(\mathbf{r}',\tau)\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\psi_{\sigma'}(\mathbf{r}',\tau)\psi_\sigma(\mathbf{r},\tau)$$

▷ Connection between coherent state and Feynman Path integral

e.g. QHO: $\hat H = \hbar\omega(a^\dagger a + 1/2)$, $\quad [a, a^\dagger] = 1$, i.e. bosons! $\qquad e^{-\beta\hbar\omega/2}$ *in* $D(\bar\psi,\psi)$

$$\mathcal{Z} = \mathrm{tr}\, e^{-\beta\hat H} = \int_{\psi(\beta)=\psi(0)} D(\bar\psi,\psi)\exp\left[-\int_0^\beta d\tau\,\bar\psi(\partial_\tau+\hbar\omega)\psi\right]$$

Setting $\psi(\tau) = \left(\frac{m\omega}{2\hbar}\right)^{1/2}[q(\tau) + \frac{i}{m\omega}p(\tau)]$, with $p, q$ real, and noting $\displaystyle\int_0^\beta d\tau\, q\dot p = -\int_0^\beta d\tau\, p\dot q$

$$\mathcal{Z} = \int_{\text{p.b.c}} D(p,q)\exp\left[-\int_0^\beta d\tau\left(\frac{p^2}{2m}+\frac{1}{2}m\omega^2q^2 - \frac{ip\dot q}{\hbar}\right)\right]$$

cf. (Euclidean time) FPI; $\beta = \dfrac{i}{\hbar}t, \quad \tau = \dfrac{i}{\hbar}t', \quad \dfrac{i}{\hbar}\dfrac{\partial q}{\partial\tau} = \dfrac{\partial q}{\partial t'}$

$$\mathcal{Z} = \int D(p,q)\exp\left[\frac{i}{\hbar}\int_0^t dt'\,(p\dot q - H(p,q))\right]$$

▷ Evaluation of $\mathcal{Z}$ from field integral

(i) 'Bosonic' oscillator: $\hat{H} = \hbar\omega(a^\dagger a + 1/2)$

$$\mathcal{Z}_{\rm B} = \overbrace{\int D(\bar\psi,\psi)\exp\left[-\int_0^\beta d\tau\,\bar\psi\,(\partial_\tau+\hbar\omega)\,\psi\right]}^{J\det(\partial_\tau+\hbar\omega)^{-1}} = \int (\prod_n d\bar\psi_{\omega_n} d\psi_{\omega_n})\, e^{-\sum_n \bar\psi_{\omega_n}(-i\omega_n+\hbar\omega)\psi_{\omega_n}}$$

$$= J\prod_{\omega_n}[\beta(-i\omega_n+\hbar\omega)]^{-1} = \frac{J}{\hbar\omega\beta}\prod_{n=1}^{\infty}\left[(\hbar\omega\beta)^2+(2n\pi)^2\right]^{-1} = \frac{J'}{\hbar\omega\beta}\prod_{n=1}^{\infty}\left[1+\left(\frac{\hbar\omega\beta}{2\pi n}\right)^2\right]^{-1}$$

$$= \frac{J'}{2\sinh(\hbar\omega\beta/2)} \qquad \text{where} \quad \prod_{n=1}^{\infty}\left[1+\left(\frac{x}{\pi n}\right)^2\right]^{-1} = \frac{x}{\sinh x}$$

Normalisation: as $T\to 0$, $\mathcal{Z}_{\rm B}$ dominated by g.s., i.e. $\lim_{\beta\to\infty}\mathcal{Z}_{\rm B} = e^{-\beta\hbar\omega/2}$

$$\text{i.e. } J' = 1, \qquad \mathcal{Z}_{\rm B} = \frac{1}{2\sinh(\hbar\beta\omega/2)}$$

(ii) 'Fermionic' oscillator: $\hat{H} = \hbar\omega(a^\dagger a + 1/2)$, $[a,a^\dagger]_+ = 1$

Gaussian Grassmann integration

$$\mathcal{Z}_{\rm F} = J\det(\partial_\tau+\hbar\omega) = J\prod_{\omega_n}[\beta(-i\omega_n+\hbar\omega)] = J\prod_{n=0}^{\infty}\left[(\hbar\omega\beta)^2+((2n+1)\pi)^2\right]$$

$$= J'\prod_{n=1}^{\infty}\left[1+\left(\frac{\hbar\omega\beta}{(2n+1)\pi}\right)^2\right] = J'\cosh(\hbar\omega\beta/2), \qquad \prod_{n=1}^{\infty}\left[1+\left(\frac{x}{\pi(2n+1)}\right)^2\right] = \cosh(x/2)$$

Using normalisation: $\lim_{\beta\to\infty}\mathcal{Z}_{\rm F} = e^{-\beta\hbar\omega/2}$

$$J' = 2e^{-\beta\hbar\omega} \qquad \mathcal{Z}_F = 2e^{-\beta\hbar\omega}\cosh(\hbar\beta\omega/2).$$

cf. direct computation: $\mathcal{Z}_B = e^{-\beta\hbar\omega/2}\sum_{n=0}^{\infty}e^{-n\beta\hbar\omega}$, $\mathcal{Z}_F = e^{-\beta\hbar\omega/2}\sum_{n=0}^{1}e^{-n\beta\hbar\omega}$.

*Note that normalising prefactor $J'$ involves only a constant offset of free energy,*
$F = -\frac{1}{\beta}\ln\mathcal{Z}$ *statistical correlations encoded in content of functional integral*

## Lecture XI: Matsubara frequency summations

▷ Quantum partition function of ideal (i.e. non-interacting) gas (from coherent states)

*Useful for "normalisation" of interacting theories*

e.g. (1) Fermions: $\hat{H} = \sum_\alpha \epsilon_\alpha a_\alpha^\dagger a_\alpha$

As a warm-up, in coherent state representation:

$$\mathcal{Z}_0 = \mathrm{tr}\; e^{-\beta(\hat{H}-\mu\hat{N})} = \sum_n \langle n|e^{-\beta(\hat{H}-\mu\hat{N})}|n\rangle = \int d(\bar{\psi},\psi) e^{-\sum_\alpha \bar{\psi}_\alpha \psi_\alpha} \langle -\psi|e^{-\beta(\hat{H}-\mu\hat{N})}|\psi\rangle$$

Using identity

$$e^{-\beta(\hat{H}-\mu\hat{N})} = e^{-\beta\sum_\alpha(\epsilon_\alpha-\mu)a_\alpha^\dagger a_\alpha} = \prod_\alpha e^{-\beta(\epsilon_\alpha-\mu)\hat{n}_\alpha} = \prod_\alpha \left[1 + \left(e^{-\beta(\epsilon_\alpha-\mu)} - 1\right)\hat{n}_\alpha\right]$$

$$\mathcal{Z}_0 = \int d(\bar{\psi},\psi) e^{-\sum_\alpha \bar{\psi}_\alpha\psi_\alpha} \prod_\alpha \Big\{ \overbrace{e^{-\bar{\psi}_\alpha\psi_\alpha}}^{\langle -\psi|\psi\rangle} \left[1 + \left(e^{-\beta(\epsilon_\alpha-\mu)} - 1\right)(-\bar{\psi}_\alpha\psi_\alpha)\right] \Big\}$$

$$= \prod_\alpha \int d\bar{\psi}_\alpha d\psi_\alpha \quad \overbrace{e^{-2\bar{\psi}_\alpha\psi_\alpha}}^{1-2\bar{\psi}_\alpha\psi_\alpha} \left[1 + \left(e^{-\beta(\epsilon_\alpha-\mu)} - 1\right)(-\bar{\psi}_\alpha\psi_\alpha)\right]$$

$$= \prod_\alpha \int d\bar{\psi}_\alpha d\psi_\alpha \left[1 - 2\bar{\psi}_\alpha\psi_\alpha - \left(e^{-\beta(\epsilon_\alpha-\mu)} - 1\right)\bar{\psi}_\alpha\psi_\alpha\right]$$

$$= \prod_\alpha \int d\bar{\psi}_\alpha d\psi_\alpha \left[-\bar{\psi}_\alpha\psi_\alpha(1 + e^{-\beta(\epsilon_\alpha-\mu)})\right]$$

$$= \prod_\alpha \left[1 + e^{-\beta(\epsilon_\alpha-\mu)}\right] \qquad \text{i.e. Fermi} - \text{Dirac distribution}$$

Exercise: show (using CS) that in Bosonic case

$$\mathcal{Z}_0 = \prod_\alpha \sum_{n=0}^\infty e^{-n\beta(\epsilon_\alpha-\mu)} = \prod_\alpha \left[1 - e^{-\beta(\epsilon_\alpha-\mu)}\right]^{-1} \qquad \text{i.e. Bose} - \text{Einstein distribution}$$

What about field integral...?

▷ Quantum partition function of ideal gas:

$$\mathcal{Z}_0 = \int_{\text{b.c.}} D(\bar{\psi},\psi) \exp\left[-\int_0^\beta d\tau \sum_\alpha \bar{\psi}_\alpha(\partial_\tau + \epsilon_\alpha - \mu)\psi_\alpha\right]$$

$$= \int D(\bar{\psi},\psi) \exp\left[-\sum_{\alpha,\omega_n} \bar{\psi}_{\alpha,\omega_n}(-i\omega_n + \epsilon_\alpha - \mu)\psi_{\alpha,\omega_n}\right] = J \prod_{\alpha,\omega_n} [\beta(-i\omega_n + \epsilon_\alpha - \mu)]^{-\zeta}$$

where $J$ absorbs constant prefactors

From $\mathcal{Z}_0 = \mathrm{tr}\, e^{-\beta(\hat{H}-\mu\hat{N})}$ we can obtain thermal occupation number:

$$n(T) \equiv \frac{1}{\mathcal{Z}_0}\mathrm{tr}[\hat{N}\, e^{-\beta(\hat{H}-\mu\hat{N})}] = \frac{1}{\beta\mathcal{Z}_0}\partial_\mu \mathcal{Z}_0 = \frac{1}{\beta}\partial_\mu \ln \mathcal{Z}_0 \equiv -\partial_\mu F = -\frac{\zeta}{\beta}\sum_{\alpha,\omega_n}\frac{1}{i\omega_n - \epsilon_\alpha + \mu}$$

▷ To perform summations of the form, $I = \sum_{\omega_n} h(\omega_n)$, helpful to introduce complex auxiliary function $g(z)$ with simple poles at $z = i\omega_n$

$$\text{e.g.} \quad g(z) = \begin{cases} \dfrac{\beta}{\exp(\beta z) - 1}, & \text{bosons} \\ \dfrac{\beta}{\exp(\beta z) + 1}, & \text{fermions} \end{cases}$$

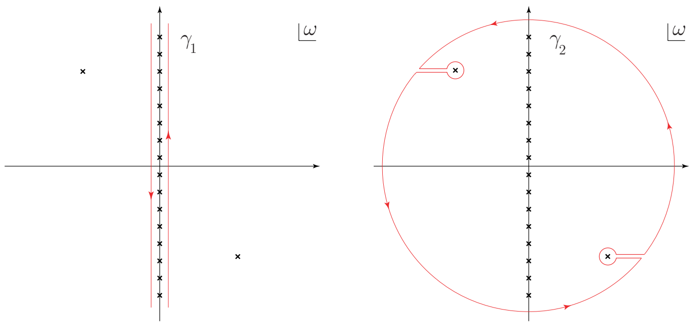
In bosonic case: poles when $\beta z = 2\pi i n$, i.e. $z = i\omega_n$; close to pole,

$$\frac{\beta}{e^{\beta(i\omega_n + \delta z)} - 1} = \frac{\beta}{e^{\beta\,\delta z} - 1} \simeq \frac{1}{\delta z}$$

noting that $g(z)$ has simple poles with residue $\zeta$,

$$I = \frac{\zeta}{2\pi i}\oint_{\gamma_1} dz\, g(z) h(-iz) = \zeta \sum_{\omega_n} \mathrm{Res}\,[g(z)h(-iz)]|_{z=i\omega_n}$$

where contour encircles poles




As long as we don't to cross singularities of $g(z)h(-iz)$, we are free to distort contour

If $g(z)h(-iz)$ decays sufficiently fast at $|z| \to \infty$ (i.e. faster than $z^{-1}$), useful to 'inflate' contour to infinite circle when integral along outer perimeter vanishes and

$$I = \frac{\zeta}{2\pi i}\oint_{\gamma_2} h(-iz)g(z) \overbrace{=}^{\text{N.B.}} - \zeta\sum_k \mathrm{Res}\,[h(-iz)g(z)]|_{z=z_k}$$

For problem at hand,

$$h(\omega_n) = -\frac{\zeta}{\beta}\sum_\alpha \frac{1}{i\omega_n - \epsilon_\alpha + \mu}, \qquad h(-iz) = -\frac{\zeta}{\beta}\sum_\alpha \frac{1}{z - \epsilon_\alpha + \mu}$$

Although $h(-iz)$ seems to scale as $1/z$ at infinity,

this reflects failure of continuum limit of the action: $\bar{\psi}_m \frac{(\psi_{m+1} - \psi_m)}{\Delta\beta} \mapsto \bar{\psi}\partial_\tau\psi$

Integral made convergent by including infinitesimal

$$(i\omega_n - \epsilon_\alpha + \mu) \mapsto (i\omega_n e^{-i\omega_n 0^+} - \epsilon_\alpha + \mu)$$

Since $h(-iz)$ involves simple poles at $z = \epsilon_\alpha - \mu$,

$$n(T) = -\zeta \sum_\alpha \text{Res}\left[g(z)h(-iz)\right]\Big|_{z=\epsilon_\alpha-\mu} = \sum_\alpha \frac{1}{e^{\beta(\epsilon_\alpha-\mu)} - \zeta} = \sum_\alpha \begin{cases} n_{\rm B}(\epsilon_\alpha), & \text{bosons,} \\ n_{\rm F}(\epsilon_\alpha), & \text{fermions} \end{cases}$$

where $n_{\rm F/B}$ are Fermi/Bose distribution functions

▷ Applications of Field Integral:

In remaining lectures we will address two case studies which exhibit phase transition to non-trivial ground state at low temperatures

- Bose-Einstein condensation and superfluidity
- Superconductivity

BOSE-EINSTEIN CONDENSATION FROM FIELD INTEGRAL

*Although we could start our analysis of application of the field integral with the weakly interacting electron gas, we would find that correlation effects could be considered perturbatively. Our analysis of the field integral would not engage any non-trivial field configurations of the action: the platform of the non-interacting electron system remains adiabatically connected to that of the weakly interacting system. In the following we will explore a problem in which the development of a non-trivial ground state — the Bose-Einstein condensate — is accompanied by the appearance of collective modes absent in the non-interacting system.*

▷ Consider Bose gas subject to weak short-ranged repulsive contact interaction:

$$\hat{H} = \int d^d r\, a^\dagger(\mathbf{r}) \hat{H}_0\, a(\mathbf{r}) + \frac{g}{2} \int d^d r\, a^\dagger(\mathbf{r}) a^\dagger(\mathbf{r}) a(\mathbf{r}) a(\mathbf{r})$$

▷ Expressed as field integral: $\mathcal{Z} = \mathrm{tr}\, e^{-\beta(\hat{H}-\mu\hat{N})} = \int_{\psi(\beta)=\psi(0)} D(\bar{\psi},\psi)\, e^{-S[\bar{\psi},\psi]}$, where

$$S = \int_0^\beta d\tau \int d^d r \left[ \bar{\psi}(\partial_\tau + \hat{H}_0 - \mu)\psi + \frac{g}{2}(\bar{\psi}\psi)^2 \right]$$

As a warm-up exercise, consider first the...

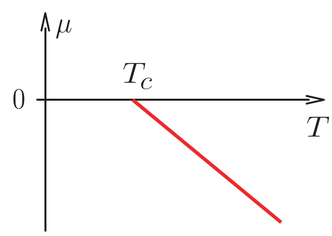
▷ NON-INTERACTING BOSE GAS ($g = 0$)

$$\mathcal{Z}_0 \equiv \mathcal{Z}\Big|_{g=0} = \int_{\psi(\beta)=\psi(0)} D(\bar{\psi},\psi)\, e^{-\sum_{a,\omega_n} \bar{\psi}_{a,\omega_n}(-i\omega_n + \epsilon_a - \mu)\psi_{a,\omega_n}} = J \prod_{a,\omega_n} \frac{1}{\beta(-i\omega_n + \epsilon_a - \mu)}$$

where eigenvalues of $\hat{H}_0$, $\epsilon_a \geq 0$ and $\epsilon_0 = 0$

While stability requires $\mu \leq 0$, precise value fixed by condition $N = \sum_a n_{\mathrm{B}}(\epsilon_a)$

▷ Bose-Einstein condensation (BEC)




- As $T$ reduced, $\mu$ increases until, at $T = T_{\mathrm{c}}$, $\mu = 0$
- For $T < T_{\mathrm{c}}$, $\mu$ remains zero and a macroscopic number of particles, $N_0 = N - N_1$, condense into ground state: BEC

$$\text{i.e. for } T < T_{\mathrm{c}}, \qquad \sum_a n_{\mathrm{B}}(\epsilon_a)\Big|_{\mu=0} \equiv N_1 < N$$

▷ How can this phenomenon be incorporated into path integral?

Although condensate characterised by g.s. component $\psi_0 \equiv \psi_{a=0,\omega_n=0}$, for $T < T_c$, fluctuations seemingly unbound (i.e. $\mu = \epsilon_0 = 0$ and action for $\psi_0$ vanishes!)

In this case, we must treat $\psi_0$ as a Lagrange multiplier which fixes particle number below $T_c$:

$$S_0|_{\mu=0^-} = -\beta\,\bar\psi_0\mu\psi_0 + {\sum_{a,\omega_n}}' \bar\psi_{a\omega_n}\left(-i\omega_n + \epsilon_a - \mu\right)\psi_{a\omega_n}$$

$$\mathcal{Z}_0 = e^{\beta\,\bar\psi_0\mu\psi_0} \times J {\prod_{a,\omega_n}}' \frac{1}{\beta(-i\omega_n + \epsilon_a - \mu)}$$

$$\text{i.e. } N = \frac{1}{\beta}\partial_\mu \ln \mathcal{Z}_0|_{\mu=0^-} = \bar\psi_0\psi_0 - \frac{1}{\beta}{\sum_{a,\omega_n}}' \frac{1}{i\omega_n - \epsilon_a} = \bar\psi_0\psi_0 + N_1$$

i.e. $\bar\psi_0\psi_0 = N_0$ translates to no. of particles in condensate

▷ <u>Weakly Interacting Bose Gas</u>

Bosons confined to box of size $L$ with p.b.c. and $\hat H_0 = \hat{\mathbf{p}}^2/2m$ described by action

$$S = \int_0^\beta d\tau \int d^d r \left[\bar\psi(\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu)\psi + \frac{g}{2}(\bar\psi\psi)^2\right]$$

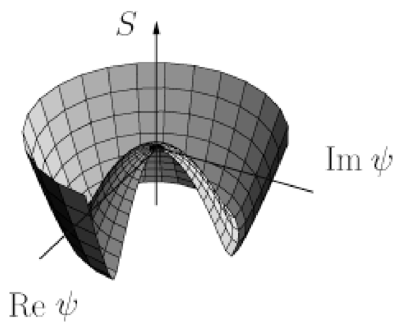
Since field integral intractable, turn to MEAN-FIELD THEORY (a.k.a. "saddle-point" approximation – Landau theory) valid for $T \ll T_c$

Variation of action w.r.t. $\bar\psi$ obtains the saddle-point equation:

$$\left(\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu + g\bar\psi\psi\right)\psi = 0$$

solved by constant $\psi(\mathbf{r},\tau) \equiv \frac{1}{L^{d/2}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}\psi_{\mathbf{k}}(\tau) = \frac{\psi_0}{L^{d/2}}$ where $\psi_0$ minimises saddle-point action

$$\frac{1}{\beta}S[\bar\psi_0,\psi_0] = -\mu\bar\psi_0\psi_0 + \frac{g}{2L^d}(\bar\psi_0\psi_0)^2, \qquad \text{i.e.} \quad \left(-\mu + \frac{g}{L^d}\bar\psi_0\psi_0\right)\psi_0 = 0$$



- For $\mu < 0$, only trivial solution $\psi_0 = 0$ – no condensate
- For $\mu \geq 0$, s.p.e. solved by any configuration with $|\psi_0| = \gamma \equiv \sqrt{\mu L^d/g}$

  N.B. interaction allows $\mu > 0$; $\bar{\psi}_0\psi_0 \propto L^d$ reflects macroscopic population of g.s.
- Condensation of Bose gas is example of a continuous phase transition, i.e. "order parameter" $\psi_0$ grows continuously from zero
- saddle-point solution is "continuously degenerate", $\psi_0 = \gamma \exp(i\phi), \phi \in [0, 2\pi]$
- One ground state chosen $\rightsquigarrow$ spontaneous symmetry breaking – Goldstone's theorem: expect branch of gapless excitations

Taking into account fluctuations, we may address the phenomenon of superfluidity...

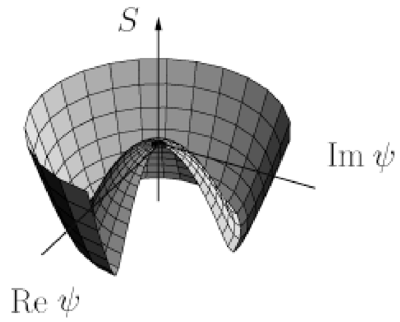
## Lecture XII: Superfluidity

*Previously, we have seen that, when treated in a mean-field or saddle-point approximation, the field theory of the weakly interacting Bose gas shows a transition to a Bose-Einstein condensed phase when $\mu = 0$ where the order parameter, the complex condensate wave-function $\psi_0$ acquires a non-zero expectation value, $|\psi_0| = \gamma \equiv \sqrt{\mu L^d/g}$. The spontaneous breaking of the continuous symmetry associated with the phase of the order parameter is accompanied by the appearance of massless collective phase fluctuations. In the following, we will explore the properties of these fluctuations and their role in the phenomenon of superfluidity.*

▷ Starting with the model action for a Bose system, ($\hbar = 1$)

$$S[\bar{\psi}, \psi] = \int_0^\beta d\tau \int d^d r \left[ \bar{\psi} \left( \partial_\tau - \frac{\partial^2}{2m} - \mu \right) \psi + \frac{g}{2} (\bar{\psi}\psi)^2 \right]$$

saddle-point analysis revealed that, for $\mu > 0$, $\psi$ acquires a non-zero expectation value: $|\psi_0| = (\mu L^d/g)^{1/2}$




Phase transition accompanied by spontaneous symmetry breaking (of $U(1)$ field associated with phase of global $\psi$)

To investigate consequence of transition, must explore role of fluctuations

To do so, it is convenient to parameterise $\psi(\mathbf{r}, \tau) = [\rho(\mathbf{r}, \tau)]^{1/2} e^{i\phi(\mathbf{r}, \tau)}$

Using

1. $$\int_0^\beta d\tau\, \bar{\psi}\partial_\tau \psi = \overbrace{\int_0^\beta d\tau \rho^{1/2}\partial_\tau \rho^{1/2}}^{\frac{1}{2}\int_0^\beta d\tau\, \partial_\tau(\rho^{1/2}\rho^{1/2}) = -\frac{\rho}{2}\Big|_0^\beta = 0} + \int_0^\beta d\tau\, i\rho\partial_\tau \phi$$
2. $$\partial(\rho^{1/2} e^{i\phi}) = e^{i\phi} \left( \frac{1}{2\rho^{1/2}} \partial\rho + i\rho^{1/2} \partial\phi \right)$$
3. $$\int_0^\beta d\tau\, \bar{\psi}\partial^2 \psi = -\int_0^\beta d\tau\, \partial\bar{\psi} \cdot \partial\psi = -\int_0^\beta d\tau \left( \frac{1}{4\rho} (\partial\rho)^2 + \rho(\partial\phi)^2 \right)$$

$$S[\rho, \phi] = \int_0^\beta d\tau \int d^d r \left\{ i\rho\partial_\tau \phi + \frac{1}{2m} \left[ \frac{1}{4\rho} (\partial\rho)^2 + \rho(\partial\phi)^2 \right] - \mu\rho + \frac{g\rho^2}{2} \right\}$$

Expansion of action around saddle-point: $\rho(\mathbf{r},\tau) = (\rho_0 + \delta\rho(\mathbf{r},\tau))\, e^{i\phi(\mathbf{r},\tau)}$,

$$S[\delta\rho,\phi] = \int_0^\beta d\tau \int d^d r \left\{ -\mu(\rho_0+\delta\rho) + \frac{g(\rho_0+\delta\rho)^2}{2} \right.$$
$$\left. + i(\rho_0+\delta\rho)\partial_\tau\phi + \frac{1}{2m}\left[\frac{1}{4(\rho_0+\delta\rho)}(\partial(\delta\rho))^2 + (\rho_0+\delta\rho)(\partial\phi)^2\right]\right\}$$
$$= S_0[\rho_0] + \int_0^\beta d\tau \int d^d r \Big\{ \overbrace{(-\mu + g\rho_0)}^{=0}\,\delta\rho + \frac{g\delta\rho^2}{2}$$
$$+ \overbrace{i\rho_0\partial_\tau\phi}^{\mapsto 0} + i\delta\rho\partial_\tau\phi + \frac{1}{2m}\left[\frac{1}{4\rho_0}(\partial(\delta\rho))^2 + \rho_0(\partial\phi)^2\right]\Big\} + O(\delta\rho^3, \delta\rho, \partial\phi)$$

Finally, discarding gradient terms involving massive fluctuations $\delta\rho$,

$$S[\delta\rho,\phi] \simeq S_0[\rho_0] + \int_0^\beta d\tau \int d^d r \left[ i\delta\rho\,\partial_\tau\phi + \frac{g}{2}\delta\rho^2 + \frac{\rho_0}{2m}(\partial\phi)^2\right]$$

- First term has canonical structure 'momentum $\times\, \partial_\tau$ (coordinate)', cf. "$p\dot{q}$"
- Second term describes "massive" fluctuations in "Mexican hat" potential
- Third term measures energy cost of spatially varying massless phase flucutations: i.e. $\phi$ is a Goldstone mode

Gaussian integration over $\delta\rho$:

$$\int D(\delta\rho)\exp\left[-\int_0^\beta d\tau\int d^d r\, \overbrace{\left(i\delta\rho\,\partial_\tau\phi + \frac{g\delta\rho^2}{2}\right)}^{\frac{g}{2}\left(\delta\rho + \frac{i}{g}\partial_\tau\phi\right)^2 + \frac{(\partial_\tau\phi)^2}{2g}}\right] = \text{const.}\times\exp\left[-\int_0^\beta d\tau\int d^d r \frac{(\partial_\tau\phi)^2}{2g}\right]$$

$\rightsquigarrow$ effective action for low-energy degrees of freedom, $\phi$,

$$S[\phi] \simeq S_0 + \frac{1}{2}\int_0^\beta d\tau \int d^d r\left[\frac{1}{g}(\partial_\tau\phi)^2 + \frac{\rho_0}{m}(\partial\phi)^2\right].$$

cf. Lagrangian formulation of harmonic chain (or massless Klein-Gordon field)

$$S = \int dt \int d^d r \left[\frac{m}{2}\dot{\phi}^2 - \frac{1}{2}k_s a^2(\partial\phi)^2\right] = \int dx\, \partial^\mu\phi\partial_\mu\phi$$

i.e. low-energy excitations involve collective phase fluctuations with a spectrum $\omega_{\mathbf{k}} = \frac{g\rho_0}{m}|\mathbf{k}|$

However, action differs from harmonic chain in that phase field $\phi$ is periodic on $2\pi$ – i.e. the space is not simply connected

This means that it can support topologically non-trivial field configurations involving windings – i.e. vortices

▷ PHYSICAL RAMIFICATIONS: current density

$$\hat{\mathbf{j}}(\mathbf{r},\tau) = \frac{1}{2}\left[a^\dagger(\mathbf{r},\tau)\frac{\hat{\mathbf{p}}}{m}a(\mathbf{r},\tau) - \left(\frac{\hat{\mathbf{p}}}{m}a^\dagger(\mathbf{r},\tau)\right)a(\mathbf{r},\tau)\right]$$

$$\stackrel{\text{fun. int}}{\longrightarrow} \frac{i}{2m}\left[(\partial\bar{\psi}(\mathbf{r},\tau))\psi(\mathbf{r},\tau) - \bar{\psi}(\mathbf{r},\tau)\partial\psi(\mathbf{r},\tau)\right] \simeq \frac{\rho_0}{m}\partial\phi(\mathbf{r},\tau)$$

i.e. $\partial\phi$ is measure of (super)current flow

Variation of action $S[\delta\rho, \phi] \rightsquigarrow$

$$i\partial_\tau\phi = -g\delta\rho, \qquad i\partial_\tau\delta\rho = \frac{\rho_0}{m}\partial^2\phi = \partial\cdot\mathbf{j}$$

- First equation: system adjusts to fluctuations of density by dynamical phase fluctuation
- Second equation $\rightsquigarrow$ continuity equation (conservation of mass)

Crucially, s.p.e. possess steady state solutions with non-vanishing current flow: if $\phi$ independent of $\tau$, $\delta\rho = 0$ and $\dfrac{\rho_0}{m}\partial^2\phi = \partial\cdot\mathbf{j} = 0$

For $T < T_c$, a configuration with a uniform density profile can support a steady state divergenceless (super)flow

Superflow imposed by boundary conditions, cf. Coulomb: $\partial^2\phi = -\dfrac{\rho(\mathbf{r})}{\epsilon}$

e.g. $\phi(\mathbf{r}) \simeq -\phi_0 \ln|x^2 + y^2|$ translates to a line vortex

Notice that a 'mass term' in the phase action (viz. $m_\phi\phi^2$) would spoil this property, i.e. the phenomenon of superflow is intimately linked to the Goldstone mode

▷ Steady state current flow in normal environments is prevented by the mechanism of energy dissipation, i.e. particles scatter off imperfections inside the system and thereby convert part of their energy into the creation of elementary excitations

How can dissipative loss of energy be avoided?

Trivially, no energy can be exchanged if there are no elementary excitations to create

In reality, this means that the excitations of the system should be energetically inaccessible (k.e. of carriers too small to create excitations)

But this is not the case here! there is no energy gap ($\omega_{\mathbf{k}} = v_s|\mathbf{k}|$)

However, there is an ingenuous argument due to Landau (see notes) showing that a linear excitation spectrum can stabilize dissipationless transport for $v < v_s$

## Cooper instability of electron gas

*In the final section of the course, we will explore a pairing instability of the electron gas which leads to condensate formation and the phenomenon of superconductivity.*

▷ History:

- 1911 discovery of superconductivity (Onnes)
- 1950 Development of (correct) phenomenology (Ginzburg-Landau)
- 1951 "isotope effect" — clue to (conventional) mechanism
- 1957 BCS theory of conventional superconductivity (Bardeen-Cooper-Schrieffer)
- 1976 Discovery of "unconventional" superconductivity (Steglich)
- 1986 Discovery of high temperature superconductivity in cuprates (Bednorz-Müller)
- ???? awaiting theory?

▷ (Conventional) mechanism: exchange of phonons induces non-local electron interaction

$$\hat{H}' = \hat{H}_0 + \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \frac{|M_{\mathbf{q}}|^2 \hbar\omega_{\mathbf{q}}}{(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}})^2 - (\hbar\omega_{\mathbf{q}})^2} c^\dagger_{\mathbf{k}-\mathbf{q}\sigma} c^\dagger_{\mathbf{k}'+\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma}$$

*Electrons can lower their energy by sharing lattice polarisation*

As a result electrons can condense as pairs into state with energy gap to excitations

▷ Cooper instability

Consider two electrons above filled Fermi sea:
Is weak pair interaction $V(\mathbf{r}_1 - \mathbf{r}_2)$ sufficient to create bound state?

Consider variational state

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \overbrace{\frac{1}{\sqrt{2}}(|\uparrow_1\rangle \otimes |\downarrow_2\rangle - |\uparrow_2\rangle \otimes |\downarrow_1\rangle)}^{\text{spin singlet}} \overbrace{\sum_{|\mathbf{k}|\geq k_{\mathrm{F}}} g_{\mathbf{k}}\, e^{i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}_2)}}^{\text{spatial symm. } g_{\mathbf{k}} = g_{-\mathbf{k}}}$$

Applied to (spin-independent) Schrödinger equation: $\hat{H}\psi = E\psi$

$$\sum_{\mathbf{k}} g_{\mathbf{k}} \left[2\,\epsilon_{\mathbf{k}} + V(\mathbf{r}_1 - \mathbf{r}_2)\right] e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)} = E \sum_{\mathbf{k}} g_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)}$$

Fourier transforming equation: $\times \frac{1}{L^d}\int_0^L d^d(\mathbf{r}_1 - \mathbf{r}_2) e^{-i\mathbf{k}'\cdot(\mathbf{r}_1-\mathbf{r}_2)}$

$$\sum_{\mathbf{k}'} V_{\mathbf{k}-\mathbf{k}'} g_{\mathbf{k}'} = (E - 2\epsilon_{\mathbf{k}}) g_{\mathbf{k}}, \qquad V_{\mathbf{k}-\mathbf{k}'} = \frac{1}{L^d}\int d^d r\, V(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}$$

If we assume $V_{\mathbf{k}-\mathbf{k}'} = \begin{cases} -\frac{V}{L^d} & \{|\epsilon_\mathbf{k} - \epsilon_F|, |\epsilon_{\mathbf{k}'} - \epsilon_F|\} < \omega_D \\ 0 & \text{otherwise} \end{cases}$

$$-\frac{V}{L^d}\sum_{\mathbf{k}'} g_{\mathbf{k}'} = (E - 2\epsilon_\mathbf{k})g_\mathbf{k} \mapsto -\frac{V}{L^d}\sum_\mathbf{k} \frac{1}{E - 2\epsilon_\mathbf{k}} \sum_{\mathbf{k}'} g_{\mathbf{k}'} = \sum_\mathbf{k} g_\mathbf{k} \mapsto -\frac{V}{L^d}\sum_\mathbf{k} \frac{1}{E - 2\epsilon_\mathbf{k}} = 1$$

Using $\frac{1}{L^d}\sum_\mathbf{k} = \int \frac{d^d k}{(2\pi)^d} = \int \nu(\epsilon)\, d\epsilon \sim \nu(\epsilon_F)\int d\epsilon$, where $\nu(\epsilon) = \frac{1}{|\partial_\mathbf{k}\epsilon_\mathbf{k}|}$ is DoS

$$-\frac{V}{L^d}\sum_\mathbf{k} \frac{1}{E - 2\epsilon_\mathbf{k}} \simeq -\nu(\epsilon_F)V \int_{\epsilon_F}^{\epsilon_F+\omega_D} \frac{d\epsilon}{E - 2\epsilon} = \frac{\nu(\epsilon_F)V}{2} \ln\left(\frac{E - 2\epsilon_F - 2\omega_D}{E - 2\epsilon_F}\right) = 1$$

In limit of "weak coupling", i.e. $\nu(\epsilon_F)V \ll 1$

$$E \simeq 2\epsilon_F - 2\omega_D e^{-\frac{2}{\nu(\epsilon_F)V}}$$

- i.e. pair forms a bound state (no matter how small interaction!)
- energy of bound state is non-perturbative in $\nu(\epsilon_F)V$

▷ Radius of pair wavefunction: $g(\mathbf{r}) = \sum_\mathbf{k} g_\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{r}}$,

Using $g_\mathbf{k} = \frac{1}{2\epsilon_\mathbf{k} - E} \times$ const., $\partial_\mathbf{k} = \frac{\partial\epsilon_\mathbf{k}}{\partial\mathbf{k}}\frac{\partial}{\partial\epsilon_\mathbf{k}} = \mathbf{v}\frac{\partial}{\partial\epsilon_\mathbf{k}}$, and

$$\frac{1}{L^d}\sum_\mathbf{k} |\partial_\mathbf{k} g_\mathbf{k}|^2 = \int d^d r\, d^d r'\, \mathbf{r}\cdot\mathbf{r}' \overbrace{\frac{1}{L^d}\sum_\mathbf{k} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}^{\delta(\mathbf{r}-\mathbf{r}')} g(\mathbf{r})g^*(\mathbf{r}') = \int d^d r\, \mathbf{r}^2 |g(\mathbf{r})|^2,$$

$$\langle \mathbf{r}^2 \rangle = \frac{\int d^d r\, \mathbf{r}^2 |g(\mathbf{r})|^2}{\int d^d r |g(\mathbf{r})|^2} = \frac{\sum_\mathbf{k} |\partial_\mathbf{k} g_\mathbf{k}|^2}{\sum_\mathbf{k} |g_\mathbf{k}|^2} = \frac{\int_{\epsilon_F}^{\epsilon_F+\omega_D} d\epsilon\, \nu(\epsilon)\, \mathbf{v}^2 \left(\frac{\partial}{\partial\epsilon}\frac{1}{2\epsilon - E}\right)^2}{\int_{\epsilon_F}^{\epsilon_F+\omega_D} d\epsilon\, \nu(\epsilon) \frac{1}{(2\epsilon - E)^2}}$$

$$\simeq \frac{v_F^2 \int_{\epsilon_F}^{\epsilon_F+\omega_D} \frac{4d\epsilon}{(2\epsilon - E)^4}}{\int_{\epsilon_F}^{\epsilon_F+\omega_D} \frac{d\epsilon}{(2\epsilon - E)^2}} = \frac{4}{3}\frac{v_F^2}{(2\epsilon_F - E)^2}$$

if binding energy $2\epsilon_F - E \sim k_\mathrm{B}T_c$, $T_c \sim 10\mathrm{K}$, $v_F \sim 10^8 \mathrm{cm/s}$, $\xi_0 = \langle \mathbf{r}^2 \rangle^{1/2} \sim 10^4 \mathring{A}$,
i.e. other electrons must be important

▷ BCS WAVEFUNCTION

Two electrons in a paired state has wavefunction

$$\phi(\mathbf{r}_1 - \mathbf{r}_2) = \frac{1}{\sqrt{2}}(|\uparrow_1\rangle \otimes |\downarrow_2\rangle - |\downarrow_1\rangle \otimes |\uparrow_2\rangle) g(\mathbf{r}_1 - \mathbf{r}_2)$$

Drawing analogy with Bose condensate, consider variational state

$$\psi(\mathbf{r}_1 \cdots \mathbf{r}_{2N}) = \mathcal{N} \prod_{n=1}^{N/2} \phi(\mathbf{r}_{2n-1} - \mathbf{r}_{2n})$$

Is $\psi$ compatible with Pauli principle? For a single pair,

$$|\phi\rangle = \frac{1}{L^d}\int_0^L d^d r_1 \int_0^L d^d r_2\, g(\mathbf{r}_1 - \mathbf{r}_2) c^\dagger_\uparrow(\mathbf{r}_1) c^\dagger_\downarrow(\mathbf{r}_2)|\Omega\rangle$$

$$= \sum_{\mathbf{k},\mathbf{k}'} \overbrace{\frac{1}{L^{2d}}\int_0^L d^d r_1 \int_0^L d^d r_2\, g(\mathbf{r}_1 - \mathbf{r}_2) e^{i\mathbf{k}\cdot\mathbf{r}_1} e^{i\mathbf{k}'\cdot\mathbf{r}_2}}^{\delta_{\mathbf{k}+\mathbf{k}',0}\, g_\mathbf{k}}\; c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{\mathbf{k}'\downarrow}|\Omega\rangle = \sum_\mathbf{k} g_\mathbf{k} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}|\Omega\rangle$$

where $g_\mathbf{k} = \frac{1}{L^d}\int d^d r\, g(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}$

Then, of the terms in the expansion of

$$|\psi\rangle = \prod_{n=1}^N \left[\sum_{\mathbf{k}_n} g_{\mathbf{k}_n} c^\dagger_{\mathbf{k}_n\uparrow} c^\dagger_{-\mathbf{k}_n\downarrow}\right]|\Omega\rangle$$

those with all $\mathbf{k}_n$s different survive

Generally, more convenient to work in grand canonical ensemble
where one allows for (small) fluctuations in the total particle number, viz.

$$|\psi\rangle = \prod_\mathbf{k}(u_\mathbf{k} + v_\mathbf{k} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})|\Omega\rangle \;\sim\; \overbrace{\exp\left[\sum_\mathbf{k} g_\mathbf{k} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}\right]|\Omega\rangle}^{\text{cf. coherent state of pairs}}$$

where normalisation demands $u^2_\mathbf{k} + v^2_\mathbf{k} = 1$ (exercise)

In non-interacting electron gas $v_\mathbf{k} = \begin{cases} 1 & |\mathbf{k}| < k_F \\ 0 & |\mathbf{k}| > k_F \end{cases}$

In interacting system, to determine the variational parameters, $(u_\mathbf{k}, v_\mathbf{k})$,
one can use a variational principle, i.e. to minimise $\langle\psi|\hat{H} - \epsilon_F \hat{N}|\psi\rangle$

▷ BCS Hamiltonian

However, since we are interested in both the g.s. energy and spectrum of excitations,
we will follow a different route and explore the model Hamiltonian

$$\hat{H} = \sum_\mathbf{k} \epsilon_\mathbf{k} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \frac{V}{L^d}\sum_{\mathbf{k}\mathbf{k}'} c^\dagger_{\mathbf{k}'\uparrow} c^\dagger_{-\mathbf{k}'\downarrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$$

## Lecture XIII: BCS theory of Superconductivity

▷ From Cooper argument, two electrons above Fermi sea can form a bound state

$$|\phi\rangle = \frac{1}{L^d}\int_0^L d^d r_1 \int_0^L d^d r_2\, g(\mathbf{r}_1-\mathbf{r}_2) c^\dagger_\uparrow(\mathbf{r}_1) c^\dagger_\downarrow(\mathbf{r}_2)|\Omega\rangle$$

$$= \sum_{\mathbf{k},\mathbf{k}'} \overbrace{\frac{1}{L^{2d}}\int_0^L d^d r_1 \int_0^L d^d r_2\, g(\mathbf{r}_1-\mathbf{r}_2) e^{i\mathbf{k}\cdot\mathbf{r}_1} e^{i\mathbf{k}'\cdot\mathbf{r}_2}}^{\delta_{\mathbf{k}+\mathbf{k}',0}\, g_\mathbf{k}}\, c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{\mathbf{k}'\downarrow}|\Omega\rangle = \sum_\mathbf{k} g_\mathbf{k} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}|\Omega\rangle$$

where $g_\mathbf{k} = \frac{1}{L^d}\int d^d r\, g(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}$ denotes pair wavefunction

To develop insight into the many-body system, consider effective theory involving only interaction between pairs: <u>BCS Hamiltonian</u>

$$\hat{H} = \sum_\mathbf{k} \epsilon_\mathbf{k} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \frac{V}{L^d}\sum_{\mathbf{k}\mathbf{k}'} c^\dagger_{\mathbf{k}'\uparrow} c^\dagger_{-\mathbf{k}'\downarrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$$

Transition to condensate signalled by development of "anomalous average" $\bar{b}_\mathbf{k} = \langle \text{g.s.}|c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}|\text{g.s.}\rangle$, i.e. $|\text{g.s.}\rangle$ is not an eigenstate of particle number!

Since we expect quantum fluctuations of $\bar{b}_\mathbf{k}$ to be small, we may set

$$c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} = \bar{b}_\mathbf{k} + \overbrace{c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} - \bar{b}_\mathbf{k}}^{\text{small}}$$

(cf. approach to BEC where $a^\dagger_0$ replaced by a C-number) so that

$$\begin{aligned}
\hat{H} - \mu\hat{N} &= \sum_{\mathbf{k}\sigma} \overbrace{(\epsilon_\mathbf{k}-\mu)}^{\xi_\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \frac{V}{L^d}\sum_{\mathbf{k}\mathbf{k}'} c^\dagger_{\mathbf{k}'\uparrow} c^\dagger_{-\mathbf{k}'\downarrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}, \\
&\simeq \sum_{\mathbf{k}\sigma} \xi_\mathbf{k} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \frac{V}{L^d}\sum_{\mathbf{k}\mathbf{k}'} \left(\bar{b}_\mathbf{k} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} + b_{\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} - \bar{b}_\mathbf{k} b_{\mathbf{k}'}\right) + O(\text{small})^2
\end{aligned}$$

Setting $\frac{V}{L^d}\sum_\mathbf{k} b_\mathbf{k} \equiv \Delta$, obtain the "Bogoliubov-de Gennes" or "Gor'kov" Hamiltonian

$$\begin{aligned}
\hat{H} - \mu\hat{N} &= \sum_{\mathbf{k}\sigma} \xi_\mathbf{k} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \sum_\mathbf{k}\left(\bar{\Delta} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow} + \Delta c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}\right) + \frac{L^d|\Delta|^2}{V} \\
&= \sum_\mathbf{k} \begin{pmatrix} c^\dagger_{\mathbf{k}\uparrow} & c_{-\mathbf{k}\downarrow} \end{pmatrix} \begin{pmatrix} \xi_\mathbf{k} & -\Delta \\ -\bar{\Delta} & -\xi_\mathbf{k} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix} + \sum_\mathbf{k} \xi_\mathbf{k} + \frac{L^d|\Delta|^2}{V}
\end{aligned}$$

For simplicity, let us for now assume that $\Delta$ is real (soon we will see that global phase is arbitrary...)

*Bilinear in fermion operators,* $\hat{H} - \mu\hat{N}$ diagonalised by transformation

$$\begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix} = \overbrace{\begin{pmatrix} u_{\mathbf{k}} & v_{\mathbf{k}} \\ -v_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix}}^{\mathrm{O}^T} \begin{pmatrix} \gamma_{\mathbf{k}\uparrow} \\ \gamma^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix}$$

where anticommutation relations require $O^T O = \mathbf{1}$,
i.e. $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$ (orthogonal transformations)

Substituting, transformed Hamiltonian $OHO^T$ diagonalised if (Ex.)

$$2\xi_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} + \Delta(v_k^2 - u_{\mathbf{k}}^2) = 0$$

i.e. setting $u_k = \sin\theta_{\mathbf{k}}$ and $v_{\mathbf{k}} = \cos\theta_{\mathbf{k}}$,

$$\tan 2\theta_{\mathbf{k}} = -\frac{\Delta}{\xi_{\mathbf{k}}}, \qquad \sin 2\theta_{\mathbf{k}} = \frac{\Delta}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}}, \qquad \cos 2\theta_{\mathbf{k}} = -\frac{\xi_{\mathbf{k}}}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}}$$

(N.B. for complex $\Delta = |\Delta| e^{i\phi}$, $v_{\mathbf{k}} = e^{i\phi}\cos\theta_{\mathbf{k}}$)

As a result,

$$\hat{H} - \mu\hat{N} = \sum_{\mathbf{k}} \xi_{\mathbf{k}} + \frac{L^d \Delta^2}{V} + \sum_{\mathbf{k}} \begin{pmatrix} \gamma^\dagger_{\mathbf{k}\uparrow} & \gamma_{-\mathbf{k}\downarrow} \end{pmatrix} \begin{pmatrix} (\xi_{\mathbf{k}}^2 + \Delta^2)^{1/2} & \\ & -(\xi_{\mathbf{k}}^2 + \Delta^2)^{1/2} \end{pmatrix} \begin{pmatrix} \gamma_{\mathbf{k}\uparrow} \\ \gamma^\dagger_{-\mathbf{k}\downarrow} \end{pmatrix}$$

$$= \sum_{\mathbf{k}} (\xi_{\mathbf{k}} - (\xi_{\mathbf{k}}^2 + \Delta^2)^{1/2}) + \frac{L^d \Delta^2}{V} + \sum_{\mathbf{k}\sigma} (\xi_{\mathbf{k}}^2 + \Delta^2)^{1/2} \gamma^\dagger_{\mathbf{k}\sigma} \gamma_{\mathbf{k}\sigma}$$

Quasi-particle excitations, created by $\gamma^\dagger_{\mathbf{k}\sigma}$, have minimum energy $\Delta$

g.s. identified as state annihilated by all the quasi-particle operators $\gamma_{\mathbf{k}\sigma}$, i.e.

$$|\text{g.s.}\rangle \equiv \prod_{\mathbf{k}} \gamma_{-\mathbf{k}\downarrow}\gamma_{\mathbf{k}\uparrow}|\Omega\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} c_{-\mathbf{k}\downarrow} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow})(u_{\mathbf{k}} c_{\mathbf{k}\uparrow} - v_{\mathbf{k}} c^\dagger_{-\mathbf{k}\downarrow})|\Omega\rangle$$

$$= \prod_{\mathbf{k}} v_{\mathbf{k}} (u_{\mathbf{k}} c_{-\mathbf{k}\downarrow} c^\dagger_{-\mathbf{k}\downarrow} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})|\Omega\rangle = \text{const.} \times \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})|\Omega\rangle$$

in fact, const. = 1

Note that global phase of $\Delta$ is arbitrary, i.e. $|\text{g.s.}\rangle$ continuously degenerate (cf. BEC)

▷ Self-consistency condition: BCS gap equation

$$\Delta \equiv \frac{V}{L^d} \sum_{\mathbf{k}} \bar{b}_{\mathbf{k}} = \frac{V}{L^d} \sum_{\mathbf{k}} \langle \text{g.s.}| c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} |\text{g.s.}\rangle = \frac{V}{L^d} \sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}}$$

$$= \frac{V}{2L^d} \sum_{\mathbf{k}} \sin 2\theta_{\mathbf{k}} = \frac{V}{2L^d} \sum_{\mathbf{k}} \frac{\Delta}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}}$$

i.e. $$1 = \frac{V}{2L^d}\sum_{\mathbf{k}}\frac{1}{\sqrt{\xi_{\mathbf{k}}^2+\Delta^2}} = \frac{V\nu(\mu)}{2}\int_{-\omega_D}^{\omega_D} d\xi \frac{1}{\sqrt{\xi^2+\Delta^2}} = V\nu(\mu)\sinh^{-1}(\omega_D/\Delta)$$

if $\omega_D \gg \Delta$, $\Delta \simeq 2\omega_D e^{-\frac{1}{\nu(\mu)V}}$

▷ In limit $\Delta \to 0$, $v_{\mathbf{k}}^2 = \cos^2\theta_{\mathbf{k}} = \frac{1}{2}(\cos 2\theta + 1) = \frac{1}{2}\left(1 - \frac{\xi_k}{\sqrt{\xi_{\mathbf{k}}^2+\Delta^2}}\right) \mapsto \theta(\mu - \epsilon_{\mathbf{k}})$,

and $|\text{g.s.}\rangle$ collapses to filled Fermi sea with chemical potential $\mu$

For $\Delta \neq 0$, states in vicinity of $\mu$ rearrange into condensate of Cooper pairs

▷ Spectrum of quasi-particle excitations $\sqrt{\xi_{\mathbf{k}}^2+\Delta^2}$ shows rigid energy gap $\Delta$

▷ Density of quasi-particle states:

$$\begin{aligned}\rho(\epsilon) &= \frac{1}{L^d}\sum_{\mathbf{k}\sigma}\delta(\epsilon - \sqrt{\xi_{\mathbf{k}}^2+\Delta^2}) = \int d\xi\,\nu(\xi)\delta(\epsilon - \sqrt{\xi^2+\Delta^2}) \\ &\approx \nu(\mu)\sum_{s=\pm 1}\int_{-\infty}^{\infty} d\xi \frac{\delta\left(\xi - s(\epsilon^2-\Delta^2)^{1/2}\right)}{\left|\frac{\partial}{\partial\xi}(\xi^2+\Delta^2)^{1/2}\right|} = 2\nu(\mu)\Theta(\epsilon-\Delta)\frac{\epsilon}{(\epsilon^2-\Delta^2)^{1/2}}\end{aligned}$$

i.e. spectral weight transferred from Fermi surface to interval $[\Delta, \infty]$

▷ <u>Field Theory of Superconductivity</u>

Starting point is Hamiltonian for local (contact) pairing interaction:

$$\hat{H} = \int d^d r \left[\sum_\sigma c_\sigma^\dagger(\mathbf{r})\frac{\hat{\mathbf{p}}^2}{2m}c_\sigma(\mathbf{r}) - V\, c_\uparrow^\dagger(\mathbf{r})c_\downarrow^\dagger(\mathbf{r})c_\downarrow(\mathbf{r})c_\uparrow(\mathbf{r})\right]$$

▷ Quantum partition function: $\mathcal{Z} = \operatorname{tr} e^{-\beta(\hat{H}-\mu\hat{N})}$

$$\mathcal{Z} = \int_{\psi(\beta)=-\psi(0)} D(\bar\psi,\psi)\exp\Big\{-\overbrace{\int_0^\beta d\tau\int_0^L d^d r}^{x\equiv(\tau,\mathbf{r})\quad \int dx}\Big[\sum_\sigma \bar\psi_\sigma\left(\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu\right)\psi_\sigma - V\bar\psi_\uparrow\bar\psi_\downarrow\psi_\downarrow\psi_\uparrow\Big]\Big\}$$

where $\psi_\sigma(\mathbf{r},\tau)$ denote Grassmann (anticommuting) fields

Options for analysis:

- perturbative expansion in $V$? No — transition to condensate non-perturbative in $V$
- Mean-field (saddle-point) analysis

To prepare for s.p. analysis, it is useful to trade Grassmann fields for "slow fields" that parameterise the low-energy fluctuations of condensed phase

This is achieved by a general technique known as...

▷ Hubbard-Stratonovich decoupling:

Introduce complex commuting field $\Delta(\mathbf{r},\tau)$ whose expectation value translates to that of "anomalous average" $\langle c_\uparrow^\dagger c_\downarrow^\dagger\rangle$

$$e^{V\int dx\,\bar\psi_\uparrow\bar\psi_\downarrow\psi_\downarrow\psi_\uparrow} = \int D(\bar\Delta,\Delta)\exp\Big\{-\int dx\,\overbrace{\left[\frac{|\Delta(\mathbf{r},\tau)|^2}{V}+(\bar\Delta\psi_\downarrow\psi_\uparrow+\Delta\bar\psi_\uparrow\bar\psi_\downarrow)\right]}^{\frac{1}{V}(\bar\Delta+V\bar\psi_\uparrow\bar\psi_\downarrow)(\Delta+V\psi_\downarrow\psi_\uparrow)-V\bar\psi_\uparrow\bar\psi_\downarrow\psi_\downarrow\psi_\uparrow}\Big\}$$

Using identity $\int_0^\beta d\tau\,\bar\psi_\downarrow\partial_\tau\psi_\downarrow = -\int_0^\beta(\partial_\tau\bar\psi_\downarrow)\psi_\downarrow = \int_0^\beta \psi_\downarrow\partial_\tau\bar\psi_\downarrow$

$$\int_0^\beta d\tau\int_0^L d^dr\,\bar\psi_\downarrow\overbrace{\left(\partial_\tau-\frac{\hbar^2\partial^2}{2m}-\mu\right)}^{[\hat G_0^{(\mathrm{p})}]^{-1}}\psi_\downarrow = \int_0^\beta d\tau\int_0^L d^dr\,\psi_\downarrow\overbrace{\left(\partial_\tau+\frac{\hbar^2\partial^2}{2m}+\mu\right)}^{[\hat G_0^{(\mathrm{h})}]^{-1}}\bar\psi_\downarrow$$

where $\hat G_0^{(\mathrm{p/h})}$ denotes GF or propagator of free particle/hole Hamiltonian,

$$\mathcal{Z} = \int D(\bar\psi,\psi)\int D(\bar\Delta,\Delta)e^{-\int dx\frac{|\Delta|^2}{g}}$$

$$\times\exp\left[-\int dx\,\overbrace{(\bar\psi_\uparrow\quad\psi_\downarrow)}^{\text{Nambu spinor }\bar\Psi}\overbrace{\begin{pmatrix}[\hat G_0^{(\mathrm{p})}]^{-1} & \Delta\\ \bar\Delta & [\hat G_0^{(\mathrm{h})}]^{-1}\end{pmatrix}}^{\text{Gorkov Hamiltonian }\hat{\mathcal{G}}^{-1}}\begin{pmatrix}\psi_\uparrow\\ \bar\psi_\downarrow\end{pmatrix}\right]$$

$$= \int D(\bar\psi,\psi)\int D(\bar\Delta,\Delta)e^{-\int dx\frac{|\Delta|^2}{g}}\exp\left[-\int dx\,\bar\Psi\hat{\mathcal{G}}^{-1}\Psi\right]$$

Using Gaussian Grassmann field integral:

$$\int D(\bar\Psi,\Psi)\exp\left[-\sum_{ij}\bar\Psi_i A_{ij}\Psi_j\right] = \det\mathbf{A} = \exp[\ln\det\mathbf{A}] = \exp[\mathrm{tr}\ln\,\mathbf{A}]$$

$$\mathcal{Z} = \int D(\bar\Delta,\Delta)\exp\Big[-\overbrace{\int dx\frac{|\Delta|^2}{V}+\mathrm{tr}\ln\,\hat{\mathcal{G}}^{-1}[\Delta]}^{\text{Effective action }S[\Delta]}\Big]$$

*meaning of trace*

i.e. $\mathcal{Z}$ expressed as functional field integral over complex scalar field $\Delta(x)$

Formal expression is exact; but to proceed, we must invoke some approximation:

▷ Examples of Hubbard-Stratonovich decoupling

e.g. (1) weakly interacting electron gas: $\mathcal{Z} \equiv \text{tr}\, e^{-\beta(\hat{H}-\mu\hat{N})} = \int_{\substack{\bar{\psi}(0)=-\bar{\psi}(\beta)\\ \psi(0)=-\psi(\beta)}} D(\bar{\psi},\psi) e^{-S[\bar{\psi},\psi]}$

$$S = \int_0^\beta d\tau \left[ \int d^d r \sum_\sigma \bar{\psi}_\sigma(\mathbf{r},\tau) \left( \partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu \right) \psi_\sigma(\mathbf{r},\tau) \right.$$
$$\left. + \frac{1}{2} \int d^d r d^d r' \sum_{\sigma,\sigma'} \bar{\psi}_\sigma(\mathbf{r},\tau) \bar{\psi}_{\sigma'}(\mathbf{r}',\tau) \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \psi_{\sigma'}(\mathbf{r}',\tau) \psi_\sigma(\mathbf{r},\tau) \right]$$

Coulomb interaction decoupled by scalar field, $\mathcal{Z} = \int D(\bar{\psi},\psi) \int D\phi\, e^{-S_{\text{eff}}}$

$$S_{\text{eff}} = \int_0^\beta d\tau \left[ \int d^d r \sum_\sigma \bar{\psi}_\sigma(\mathbf{r},\tau) \left( \partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu + ie\phi \right) \psi_\sigma(\mathbf{r},\tau) + \frac{1}{8\pi}(\partial\phi)^2 \right]$$

Physically: $\phi$ represents bosonic photon field that mediates Coulomb interaction

e.g. (2) itinerant ferromagnetism in Hubbard model

$$S = \int d\tau \sum_{\mathbf{k}\sigma} \bar{\psi}_{\mathbf{k}\sigma}(\partial_\tau + \epsilon_\mathbf{k} - \mu)\psi_{\mathbf{k}\sigma} + 3U \int d\tau \sum_\mathbf{m} \overbrace{\bar{\psi}_{\mathbf{m}\uparrow}\bar{\psi}_{\mathbf{m}\downarrow}\psi_{\mathbf{m}\downarrow}\psi_{\mathbf{m}\uparrow}}^{-2\mathbf{S}_\mathbf{m}^2}$$

where $\mathbf{S}_\mathbf{m} = \frac{1}{2}\sum_{\alpha\beta} \bar{\psi}_{\mathbf{m}\alpha}\sigma_{\alpha\beta}\psi_{\mathbf{m}\beta}$ (cf. electron spin operator)

Hubbard interaction decoupled by vector field, $\mathcal{Z} = \int D(\bar{\psi},\psi) \int DM\, e^{-S_{\text{eff}}}$

$$S_{\text{eff}} = \int d\tau \sum_{\mathbf{k}\sigma} \bar{\psi}_{\mathbf{k}\sigma}(\partial_\tau + \epsilon_\mathbf{k} - \mu)\psi_{\mathbf{k}\sigma} + \int d\tau \sum_\mathbf{m} \left[ \frac{\mathbf{M}_\mathbf{m}^2}{2U} - \sum_{\alpha\beta} \bar{\psi}_{\mathbf{m}\alpha} \mathbf{M}_\mathbf{m} \cdot \sigma_{\alpha\beta} \psi_{\mathbf{m}\beta} \right]$$

Physically: $\vec{M}$ represents bosonic magnetisation field

## Lecture XIV: Field Theory of Superconductivity

Recap: Cast as field integral

$$\mathcal{Z} = \int_{\psi(\beta)=-\psi(0)} D(\bar{\psi},\psi)\exp\Big\{-\overbrace{\int_0^\beta d\tau\int_0^L d^d r}^{x\equiv(\tau,\mathbf{r})\quad \int dx}\Big[\sum_\sigma \bar{\psi}_\sigma\overbrace{\left(\partial_\tau+\frac{\hat{\mathbf{p}}^2}{2m}-\mu\right)}^{[\hat{G}_0^{(\mathrm{p})}]^{-1}}\psi_\sigma - V\bar{\psi}_\uparrow\bar{\psi}_\downarrow\psi_\downarrow\psi_\uparrow\Big]\Big\}$$

local pair interaction may be decoupled by Hubbard-Stratonovich field, $\Delta(x)$

Integrating over the Grassmann fields, $\bar{\psi}_\sigma$, and $\psi_\sigma$, $\mathcal{Z} = \int D(\bar{\Delta},\Delta)e^{-S[\Delta]}$ with

$$S[\Delta] = \int dx\,\frac{|\Delta|^2}{V} - \overbrace{\mathrm{tr}\ln\hat{\mathcal{G}}^{-1}[\Delta]}^{\int dx\,\langle x|\mathrm{tr}_2\ln\hat{\mathcal{G}}^{-1}[\Delta]|x\rangle},\qquad \hat{\mathcal{G}}^{-1} = \begin{pmatrix}[\hat{G}_0^{(\mathrm{p})}]^{-1} & \Delta\\ \bar{\Delta} & [\hat{G}_0^{(\mathrm{h})}]^{-1}\end{pmatrix}$$

$$[\hat{G}_0^{\mathrm{p/h}}]^{-1} = \partial_\tau\,{}^{+}/_{-}\left(\frac{\hat{\mathbf{p}}^2}{2m}-\mu\right)$$

To proceed further, it was necessary to invoke some approximation

▷ <u>I. Mean-field theory:</u> far from critical temperature, $T_c$, we expect field integral to be dominated by saddle-point:

$$\begin{aligned}\delta S \equiv S[\Delta+\delta\Delta]-S[\Delta] &= \int dx\frac{1}{V}(\bar{\Delta}\,\delta\Delta+\delta\bar{\Delta}\,\Delta+|\delta\Delta|^2)\\ &\quad -\mathrm{tr}\ln\left[\hat{\mathcal{G}}^{-1}+\begin{pmatrix}0 & \delta\Delta\\ \delta\bar{\Delta} & 0\end{pmatrix}\right]+\mathrm{tr}\ln\left[\hat{\mathcal{G}}^{-1}\right]\\ &= (\cdots)-\mathrm{tr}\ln\left[1+\hat{\mathcal{G}}\begin{pmatrix}0 & \delta\Delta\\ \delta\bar{\Delta} & 0\end{pmatrix}\right]\\ &= \int dx\frac{1}{V}(\bar{\Delta}\,\delta\Delta+\delta\bar{\Delta}\,\Delta)-\mathrm{tr}\left[\hat{\mathcal{G}}\begin{pmatrix}0 & \delta\Delta\\ \delta\bar{\Delta} & 0\end{pmatrix}\right]+O(|\delta\Delta|^2)\\ &= (\cdots)-\int dx\,\big(\mathcal{G}_{21}(x,x)\delta\Delta(x)+\mathcal{G}_{12}(x,x)\delta\bar{\Delta}(x)\big)+O(|\delta\Delta|^2)\end{aligned}$$

where $\mathrm{tr}[\hat{\mathcal{G}}_{21}\delta\Delta] = \int dx\,\langle x|\hat{\mathcal{G}}_{21}\delta\Delta|x\rangle = \int dx\,\mathcal{G}_{21}(x,x)\delta\Delta(x)$

i.e. $\Delta(x)$ obeys the saddle-point condition: $\dfrac{\delta S}{\delta\bar{\Delta}} = \dfrac{\Delta(x)}{V}-\mathcal{G}_{12}(x,x) = 0$

With the Ansatz $\Delta(x)=\Delta$ const., $\hat{\mathcal{G}}|k\rangle = \mathcal{G}(k)|k\rangle$, with $|k\rangle\equiv|\omega_n,\mathbf{k}\rangle$ and

$$\mathcal{G}^{-1}(k) = \begin{pmatrix}-i\omega_n+\xi_k & \Delta\\ \bar{\Delta} & -i\omega_n-\xi_k\end{pmatrix},\qquad \xi_k = \frac{\hbar^2k^2}{2m}-\mu$$

$$\mathcal{G}(k) = \frac{1}{-\omega_n^2-\xi_k^2-|\Delta|^2}\begin{pmatrix}-i\omega_n-\xi_k & -\Delta\\ -\bar{\Delta} & -i\omega_n+\xi_k\end{pmatrix}$$

i.e. $\Delta$ obeys the gap equation:

$$\frac{\Delta}{V} = \langle x|\hat{\mathcal{G}}_{12}|x\rangle = \sum_k \overbrace{\langle x|k\rangle}^{e^{-ik\cdot x}/\sqrt{\beta L^{d/2}}} \mathcal{G}_{12}(k)\langle k|x\rangle = \frac{1}{\beta L^d}\sum_k \mathcal{G}_{12}(k) = \frac{1}{\beta L^d}\sum_{\omega_n,\mathbf{k}} \frac{\Delta}{\omega_n^2 + E_k^2}$$

with $E_k = \sqrt{\xi_k^2 + |\Delta|^2}$ and $k\cdot x = \omega_n\tau - \mathbf{k}\cdot\mathbf{r}$

Using (fermionic) Matsubara frequency summation

$$\sum_{\omega_n} h(\omega_n) = \sum_p \mathrm{Res}\left[h(-iz)\frac{\beta}{e^{\beta z}+1}\right]_{z=z_p}$$

with $h(-iz) = \dfrac{1}{(z-E_k)(-z-E_k)}$, $z_p = \pm E_k$ with residue $h(z_p) = \pm\dfrac{1}{2E_k}$ and

$$\frac{\Delta}{V} = \frac{1}{L^d}\sum_{\mathbf{k}}\left(\frac{1}{e^{-\beta E_k}+1} - \frac{1}{e^{\beta E_k}+1}\right)\frac{\Delta}{2E_k} = \frac{1}{L^d}\sum_{\mathbf{k}}\tanh(\beta E_k/2)\frac{\Delta}{2E_k}$$

For $T=0$, $\beta\to\infty$,

$$\frac{1}{V} = \frac{1}{L^d}\sum_{\mathbf{k}}\frac{1}{2E_k} = \int\frac{d\xi\,\nu(\xi)}{2\sqrt{\xi^2+|\Delta|^2}} \simeq \frac{\nu(0)}{2}\int_{-\hbar\omega_D}^{\hbar\omega_D}\frac{d\xi}{\sqrt{\xi^2+|\Delta|^2}} = \nu(0)\sinh^{-1}\left(\frac{\hbar\omega_D}{|\Delta|}\right),$$

i.e. $|\Delta| \simeq 2\hbar\omega_D \exp\left[-\dfrac{1}{\nu(0)V}\right]$

For $T=T_c$, $\Delta=0$,

$$\frac{1}{V} \simeq \nu(0)\int_{-\hbar\omega_D}^{\hbar\omega_D} d\xi\frac{\tanh(\beta_c\xi/2)}{2\xi} \simeq \nu(0)\ln(1.14\beta_c\hbar\omega_D), \qquad k_{\mathrm{B}}T_c \simeq 1.14\hbar\omega_D\exp\left[-\frac{1}{\nu(0)V}\right]$$

▷ <u>II. Ginzburg-Landau theory</u>: since $\Delta$ develops continuously from zero, close to $T_c$, we may develop perturbative expansion in (small) $\Delta(x)$

$$\text{Noting}: \qquad \hat{\mathcal{G}}^{-1}[\Delta] = \hat{\mathcal{G}}_0^{-1}\left[1 + \hat{\mathcal{G}}_0\begin{pmatrix}0 & \Delta\\ \bar{\Delta} & 0\end{pmatrix}\right], \qquad \hat{\mathcal{G}}_0 \equiv \hat{\mathcal{G}}(\Delta=0)$$

$$\mathrm{tr}\ln\hat{\mathcal{G}}^{-1}[\Delta] = \mathrm{tr}\ln\hat{\mathcal{G}}_0^{-1} - \frac{1}{2}\mathrm{tr}\left[\hat{\mathcal{G}}_0\begin{pmatrix}0 & \Delta\\ \bar{\Delta} & 0\end{pmatrix}\right]^2 + \cdots, \qquad \ln(1+z) = -\sum_{n=1}^{\infty}\frac{(-z)^n}{n}$$

- Zeroth order term in $\Delta \rightsquigarrow$ 'free particle' contribution, viz. $\mathcal{Z}_0 = e^{\mathrm{tr}\ln\hat{\mathcal{G}}_0^{-1}} = \det\hat{\mathcal{G}}_0^{-1}$
- First (and all odd) order term(s) absent

- Second order term:

$$\text{Noting } \hat{G}_0^{(\text{p/h})} \overbrace{|k\rangle}^{|\omega_n,\mathbf{k}\rangle} = \overbrace{(-i\omega_n + (\hbar^2\mathbf{k}^2/2m - \mu))^{-1}}^{G_0^{(\text{p/h})}(k)} |k\rangle$$

$$\text{and using id.} = \sum_k |k\rangle\langle k|, \qquad \Delta_k = \frac{1}{\sqrt{\beta L^d}} \int dx\, e^{-ik\cdot x}\Delta(x)$$

$$\begin{aligned} \text{tr}[\hat{G}_0^{(\text{p})}\Delta\hat{G}_0^{(\text{h})}\bar{\Delta}] &= \sum_{kk'} G_0^{(\text{p})}(k) \overbrace{\langle k|\Delta|k'\rangle}^{\Delta_{k'-k}/\sqrt{\beta L^d}} G_0^{(\text{h})}(k')\langle k'|\bar{\Delta}|k\rangle \\ &\overset{q=k'-k}{=} \sum_q \Delta_q \bar{\Delta}_q \overbrace{\frac{1}{\beta L^d}\sum_k G_0^{(\text{p})}(k) G_0^{(\text{h})}(k+q)}^{\text{pairing susceptibility } \Pi(q)} \end{aligned}$$

$$\text{i.e.} \quad \Pi(\omega_m, \mathbf{q}) = \frac{1}{\beta L^d}\sum_{\omega_n,\mathbf{k}} \frac{1}{-i\omega_n + \xi_{\mathbf{k}}} \frac{1}{-i(\omega_n+\omega_m) - \xi_{\mathbf{k}+\mathbf{q}}}, \qquad \xi_{\mathbf{k}} = \frac{\hbar^2\mathbf{k}^2}{2m} - \mu$$

Combined with bare term,

$$S[\Delta] = \sum_q \left[\frac{1}{V} + \Pi(q)\right] \bar{\Delta}_q \Delta_q + O(|\Delta|^4)$$

In principle, one can evaluate $\Pi(q)$ explicitly;
however we can proceed more simply by considering a...

▷ 'Gradient expansion':

$$\begin{aligned} \Pi(\mathbf{q},\omega_m) &= \Pi(0) + i\omega_m \overbrace{\frac{\partial}{\partial(i\omega_m)}\Pi(0)}^{\tau} + q_\alpha \overbrace{\frac{\partial}{\partial q_\alpha}\Pi(0)}^{=0} + \frac{1}{2}q_\alpha q_\beta \overbrace{\frac{\partial^2}{\partial q_\alpha \partial q_\beta}\Pi(0)}^{K\delta_{\alpha\beta},\quad K = \frac{1}{d}\partial_{\mathbf{q}}^2\Pi(0)} + O(\omega_m^2, \mathbf{q}^4) \\ &= \Pi(0) + i\omega_m\tau + \frac{K}{2}\mathbf{q}^2 + O(\omega_m^2, \mathbf{q}^4) \end{aligned}$$

At large enough temperatures, $k_\text{B}T_c \gg 1/\tau$, dynamics may be neglected
altogether (viz. $\Delta(x) \equiv \Delta(\mathbf{r})$) and one obtains

▷ <u>Ginzburg-Landau action</u>

$$\begin{aligned} S[\Delta] &= \int_0^\beta d\tau \sum_{\mathbf{q}} \left(\frac{t}{2} + K\mathbf{q}^2\right) \bar{\Delta}_{\mathbf{q}}\Delta_{\mathbf{q}} + O(|\Delta|^4) \\ &= \beta \int d^d r \left[\frac{t}{2}|\Delta|^2 + \frac{K}{2}|\partial\Delta|^2 + u|\Delta|^4 + \cdots\right] \end{aligned}$$

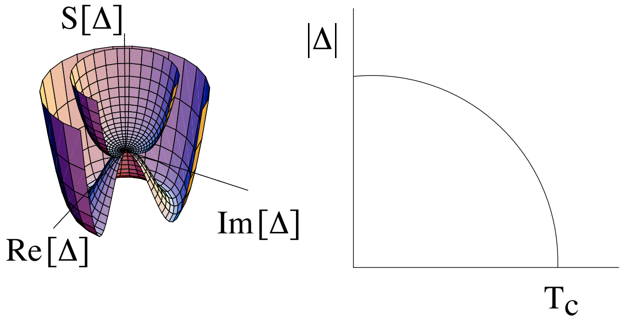
where $\frac{t}{2} = \frac{1}{V} + \Pi(0)$, and $K, u > 0$ (cf. weakly interacting Bose gas)

▷ <u>Landau Theory</u>: If we assume that dominant contribution to $\mathcal{Z} = e^{-\beta F}$ arises from minumum action, i.e. spatially homogeneous $\Delta$ that minimises

$$\frac{S[\Delta]}{\beta L^d} = \frac{t}{2}|\Delta|^2 + u|\Delta|^4$$

one obtains $|\Delta|\left(t + 4u|\Delta|^2\right) = 0,\qquad |\Delta| = \begin{cases} 0 & t > 0 \\ \sqrt{-t/4u} & t < 0 \end{cases}$

i.e. for $t < 0$, spontaneous breaking of continuous U(1) symmetry associated with phase $\rightsquigarrow$ gapless fluctuations — Goldstone modes




With $\Pi(0) \simeq -\nu(0)\ln(1.14\beta\hbar\omega_D)$ (as before), $T_c$ fixed by condition $\frac{t}{2} \equiv \frac{1}{V} + \Pi(0)|_{T=T_c} = 0$, i.e. $\frac{1}{V} = \nu(0)\ln(1.14\beta_c\hbar\omega_D)$

Therefore

$$\frac{t}{2} = \frac{1}{V} + \Pi(0,T) = \nu(0)\ln\left(\frac{\beta_c}{\beta}\right) = \nu(0)\ln\left(\frac{T}{T_c}\right) = \nu(0)\ln\left(1 + \frac{T - T_c}{T_c}\right) \simeq \nu(0)\left(\frac{T - T_c}{T_c}\right)$$

i.e. physically $t$ is a 'reduced temperature'

## Lecture XV: Superconductivity and Gauge Invariance

▷ Recall: Starting with Hamiltonian for electrons with local (contact) pairing interaction:

$$\hat{H} = \int d^d r \left[ \sum_\sigma c_\sigma^\dagger(\mathbf{r}) \frac{\hat{\mathbf{p}}^2}{2m} c_\sigma(\mathbf{r}) - V\, c_\uparrow^\dagger(\mathbf{r}) c_\downarrow^\dagger(\mathbf{r}) c_\downarrow(\mathbf{r}) c_\uparrow(\mathbf{r}) \right]$$

quantum partition function can be expressed as field integral involving complex field

$$\mathcal{Z} = \int D[\bar{\Delta}, \Delta] e^{-S[\bar{\Delta},\Delta]}, \qquad S = \sum_q \left[ \frac{1}{V} + \Pi(q) \right] |\Delta_q|^2 + O(\Delta^4)$$

where pair susceptibility

$$\Pi(q) = \frac{1}{\beta L^d} \sum_k G_0^{(\mathrm{p})}(k) G_0^{(\mathrm{h})}(k+q), \qquad G_0^{(\mathrm{p/h})}(k) = \frac{1}{-i\omega_n {}^{+}/_{-} (\hbar^2 \mathbf{k}^2/2m - \mu)}$$

Gradient expansion of action $\rightsquigarrow$ Ginzburg-Landau theory

$$S[\Delta] = \beta \int d^d r \left[ \frac{t}{2} |\Delta|^2 + \frac{K}{2} |\partial \Delta|^2 + u|\Delta|^4 + \cdots \right]$$

where $\frac{t}{2} = \frac{1}{V} + \Pi(0) \simeq \nu(0) \frac{T - T_c}{T_c}$, and constants $K, u > 0$

▷ What about the physical properties of the condensed phase?

To establish origin of perfect diamagnetism (and zero resistance), one must accommodate electromagnetic field in Ginzburg-Landau action

▷ Inclusion of EM field into action requires minimal substitution: $\hat{\mathbf{p}} \to \hat{\mathbf{p}} - e\mathbf{A}$ and addition of action for photon field ($\hbar = 1$, $c = 1$, $4\pi\epsilon_0 = 1$, $\mu_0 = 1/\epsilon_0 c^2 = 4\pi$. )

$$S_{\mathrm{EM}} = -\int dx\, \frac{1}{4\mu_0} F_{\mu\nu} F^{\mu\nu}, \qquad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$$

Repitition of field theory in presence of vector field obtains generalised Ginzburg-Landau theory: $\mathcal{Z} = \int D\mathbf{A} \int D[\Delta, \bar{\Delta}] e^{-S}$

$$S = \beta \int d^d r \Big[ \frac{t}{2} |\Delta|^2 + \frac{K}{2} |(\partial - i2e\mathbf{A})\Delta|^2 + u|\Delta|^4 + \overbrace{\frac{1}{8\pi} (\partial \times \mathbf{A})^2}^{\mathcal{L}_{\mathrm{EM}}} \Big]$$

Factor of 2 due to pairing *(focusing only on spatial fluctuations of* $\mathbf{A}$*)*

▷ Gauge Invariance: Action invariant under local gauge transformation

$$\mathbf{A} \mapsto \mathbf{A}' = \mathbf{A} - \partial\phi(\mathbf{r}), \qquad \Delta \mapsto \Delta' = e^{-2ie\phi(\mathbf{r})} \Delta$$

$$(\partial - i2e\mathbf{A})\Delta \mapsto (\partial - i2e(\mathbf{A} - \partial\phi))e^{-2ie\phi(\mathbf{r})}\Delta = e^{-2ie\phi(\mathbf{r})}(\partial - i2e\mathbf{A})\Delta$$

i.e. $|(\partial - i2e\mathbf{A})\Delta|^2$ (as well as $\partial \times \mathbf{A}$) invariant

▷ "Anderson-Higgs mechanism": phase of complex order parameter $\Delta = |\Delta|e^{-2ie\phi(\mathbf{r})}$ can be absorbed into $\mathbf{A} \mapsto \mathbf{A}' = \mathbf{A} - \partial\phi(\mathbf{r})$

$$S = \beta \int d^d r \left[\frac{t}{2}|\Delta|^2 + \frac{K}{2}(\partial|\Delta|)^2 + \frac{m_\nu^2}{2}\mathbf{A}^2 + u|\Delta|^4 + \frac{1}{8\pi}(\partial \times \mathbf{A})^2\right]$$

where $m_\nu^2 = 4e^2K|\Delta|^2$

i.e. massless phase degree of freedom $\phi(\mathbf{r})$ has disappeared and photon field $\mathbf{A}$ has acquired a 'mass'!

Example of a general principle:

"Below $T_c$, Goldstone bosons ($\phi$) and gauge field $\mathbf{A}$ conspire to create massive excitations, and massless excitations are unobservable", cf. electroweak theory

Coherence (healing) length $\xi = \sqrt{K/t}$ describes scale over which fluctuations are correlated – diverges on approaching transition

▷ Meissner effect: minimisation of action w.r.t. $\mathbf{A}$

$$\frac{1}{4\pi}\partial\times \overbrace{(\partial \times \mathbf{A})}^{\mathbf{B}} - m_\nu^2\mathbf{A} = 0 \qquad \mapsto \qquad (\partial^2 - 4\pi m_\nu^2)\mathbf{B} = 0$$

$\mathbf{B} = 0$ is the only constant uniform solution $\rightsquigarrow$ perfect diamagnetism

$1/m_\nu$ provides the length scale (London penetration depth), over which a magnetic field can penetrates the superconductor at the boundary

Free energy of superconductor first proposed on phenomenological grounds — how? ...& why is crude gradient expansion so successful?

▷ **Statistical Field Theory**

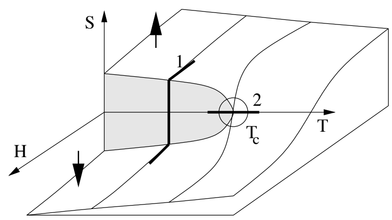
Superconducting transition is an example of a "critical phenomena"

Close to critical point $T_c$, the thermodynamic properties of a system are dictated by "universal" characteristics

To understand why, consider a simpler prototype: the *classical* Ising (i.e. one-component) ferromagnet:

$$H = -J\sum_{\langle ij\rangle} S_i^z S_j^z + B\sum_i S_i^z, \qquad S_i^z = \pm 1$$

Equilibrium Phase diagram?




What happens in the vicinity of critical point?

1. 1st order transition — order parameter (magnetisation) changes discontinuously; correlation length (scale over which fluctuations correlated) remains finite

2. 2nd order transition — order parameter changes continuously; correlation length diverges ($\xi \sim 1/t^{1/2}$)

...motivates consideration of "hydrodynamic" theory which surrenders information about microscopic length scales and involves a coarse-grained order parameter field

$$\mathcal{Z} = e^{-\beta F} = \int DS(\mathbf{r})\; e^{-\beta H_{\text{eff}}[S(\mathbf{r})]}$$

with $\beta H_{\text{eff}}[S]$ constrained (only) by fundamental symmetry (translation, rotation, etc.)

$$\beta H_{\text{eff}}[S(\mathbf{r})] = \int d^d r \left[\frac{t}{2}S^2 + \frac{K}{2}(\partial S)^2 + uS^4 + \cdots + BS\right]$$

cf. Ginzburg-Landau Theory

▷ Landau theory: $S(\mathbf{r}) = S$ const.

$$\frac{\beta F}{L^d} = \min_S \left[\frac{t}{2}S^2 + uS^4\right], \qquad \text{etc.}$$

▷ Continuous phase transitions separate into Universality classes with the same characteristic critical behaviour

E.g. (1) Ising model – liquid/gas: $S \to$ density $\rho$, $B \to$ pressure $P$

E.g. (2) Superconductivity – classical XY ferromagnet: $\Delta' + i\Delta'' \to (S_x, S_y)$