50 years of BCS School

Basics of pairing

Ilya Vekhter

*Louisiana State University, USA*
Timescale

H. Kamerlingh-Onnes
1911, Nobel Prize 1913

G. Holst
“carefully carried out all the measurements”

J. Bardeen, L. Cooper and R. Schrieffer
1957, Nobel Prize 1972

\[ \Psi = \prod_k \left( 1 - h_k \right)^{\frac{1}{2}} + h_k^{\frac{1}{2}} b_k^* \Phi_0, \]

Why so long?
Solids: 1900 -- 1925

- **1897 J.J. Thomson**: discovery of an electron
- **1900 P. Drude**: transport theory
  - classical electrons scatter on atoms. Wiedemann-Franz ratio.

\[
\sigma = \frac{ne^2 \tau}{m} \quad \kappa = \frac{v^2 c \tau}{3}
\]

\[
\frac{\kappa}{\sigma T} = \frac{c_v m v^2}{3 ne^2}
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\]

\[
\frac{\kappa}{\sigma T} = \frac{c_v m v^2}{3 n e^2}
\]

\[
c_v = \frac{3 n k_B}{2}
\]

\[
m v^2 = 3 k_B T
\]
Solids: 1900 -- 1925

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- 1900 P. Drude: transport theory

Classical electrons scatter on atoms. Wiedemann-Franz.

\[ \sigma = \frac{ne^2\tau}{m} \]
\[ \kappa = \frac{v^2c_v\tau}{3} \]

\[ \frac{\kappa}{\sigma T} = \frac{c_vmv^2}{3ne^2} = \frac{3}{2} \left( \frac{k_B}{e} \right)^2 \approx 1.11 \times 10^{-8} W\Omega / K^2 \]

- 1904 H. Lorentz: Maxwell-Boltzmann to treat electron-atom collisions. Wrong temperature dependence, wrong WF
- No understanding of metal physics
- 1911: superconductivity... what is it about?
Missing specific heat

1912: P. Debye: specific heat of lattice vibrations (phonons),

No trace of classical electronic specific heat

http://hyperphysics.phy-astr.gsu.edu/hbase/solids/phonon.html
Metals: 1925 -- 1930

- W. Pauli exclusion principle, beginning of solid state theory

Then he said, "Who are you?" "I am Weisskopf, you asked me to be your assistant."
"Yes," he said, "first I wanted to take Bethe, but he works on solid state theory, which I don't like, although I started it."
Metals: 1925 -- 1930

- W. Pauli: exclusion principle
- Fermi-Dirac statistics

Fermi energy $E_F \approx 10000K$
Metals: 1925 -- 1930

- W. Pauli: exclusion principle
- Fermi-Dirac statistics

Fermi energy $E_F \sim 10000 K$

Absorbed energy $\Delta E \sim n(k_BT)^2/E_F \sim (k_BT)^2N_0$

Specific heat $C_V \sim nk_B (k_BT/E_F) \ll nk_B$
Metals: 1925 -- 1930

- **W. Pauli**: exclusion principle
- **Fermi-Dirac statistics**: $C_V \sim k_B^2 N_0 kT \ll nk_B$
- **Sommerfeld** theory of conductivity

\[
\frac{k}{\sigma T} = \frac{c_v m v^2}{3n e^2}
\]

\[
c_v = \frac{3nk_B}{2}
\]

\[
mv^2 = 3k_B T
\]
Metals: 1925 -- 1930

- **W. Pauli**: exclusion principle
- **Fermi-Dirac statistics**: \( C_V << n k_B \)
- **Sommerfeld** theory of conductivity

\[
\begin{align*}
\kappa / \sigma T &= \frac{c_v m v^2}{3 n e^2} \\
\kappa &= c_v m v^2 / \sigma T \\
\frac{c_v}{3 k_B} &= m v^2 / 3 k_R T \\
\frac{c_v}{k_B} &= m v_F^2 = k_B T (2 E_F / k_B T)
\end{align*}
\]
Metals: 1925 -- 1930

- W. Pauli: exclusion principle
- Fermi-Dirac statistics: \( C_V << n k_B \) measurable at low \( T \)
- Sommerfeld theory of conductivity

\[
\frac{\kappa}{\sigma T} = \frac{\pi^2}{3} \left( \frac{k_B}{e} \right)^2 \approx 2.44 \times 10^{-8} W \Omega / K^2
\]
Metals: 1925 -- 1930

- W. Pauli: exclusion principle
- Fermi-Dirac statistics: $C_V \ll nk_B$ measurable at low $T$
- Sommerfeld theory of conductivity

$$\frac{\kappa}{\sigma T} = \frac{\pi^2}{3} \left( \frac{k_B}{e} \right)^2 \approx 2.44 \times 10^{-8} W\Omega / K^2$$

- Problem: Mean free path too long
- Bloch’s theorem for a crystal
- Infinite mean free path in a periodic lattice


Metals: summary

\[ a_B = \frac{\hbar^2}{m e^2} \]

\[ \varepsilon = \frac{e^2}{a} \approx \frac{\hbar^2}{ma^2} \]

Debye frequency:

\[ \frac{1}{2} M \omega_D^2 \left( \frac{a}{2} \right)^2 \approx \frac{\hbar^2}{ma^2} \]

\[ \hbar \omega_D \approx \varepsilon \sqrt{\frac{m}{M}} \]

Electron momenta:

\[ k_F \approx \frac{2 \pi n_{\text{max}}}{L} \approx \frac{2 \pi N}{Na} = \frac{1}{a} \]

\[ v_F \approx \frac{\hbar}{ma} \approx 10^{-2} c \]

Energy scales:

\[ E_F \approx \frac{\hbar^2}{ma^2} \approx 10^4 K \]

\[ \beta = \sqrt{\frac{M}{m}} \approx 300 \]

\[ \hbar \omega_D \approx 300 K \]

\[ T_c \leq 10 K << E_F, \omega_D \]

Very small scale
later work in this field, particularly that on ferromagnetism, I shall add an epilogue concerning my unsuccessful encounter with superconductivity. It started right after I had my Ph.D. and returned to Zurich as Pauli’s assistant for the academic year 1928–9. Pauli thought that superconductivity was the only remaining matter of some interest in the theory of metals and that I should get on with it so as to be finally done with all these ‘dirt-effects’. Actually, I had already started to think about the problem and had realized that the explanation of persistent currents required a consideration of the previously neglected interaction between electrons. The idea, independently expressed by Landau, was that it should thus be possible at low temperatures to obtain a minimum of the free energy in a state of the metal with finite current. My own confidence in the idea was supported by the analogy I therefore started industriously to consider various types of interaction, regardless of their possible origin, and to look whether the Schrödinger equation would allow stationary states of the electrons with non-vanishing current and a minimum of the energy. Once in a while I thought that I had indeed found such states but it never took Pauli long to point to some error in the calculations. While he did not object to my approach he became rather annoyed at my continued failure to come out with the desired answer to such a simple question. It finally turned out that

After the fog, which so long enveloped the phenomenon, had begun to lift many years later, I could not resist reminding Pauli that the problem was not quite as easy to solve as he thought when he gave it to me. Since that time he had become more mellow – so much more, in fact, that he agreed.

F. Bloch 1980
Second Bloch’s theorem

in a system of macroscopic dimensions as a continuously variable quantity. Indeed, I was so discouraged by my negative result that I saw no further way to progress and for a considerable time there was for me only the dubious satisfaction to see that others, without noticing it, kept on falling into the same trap. This brought me to the facetious statement that all theories of superconductivity can be disproved, later quoted in the more radical form of ‘Bloch’s theorem’: ‘Superconductivity is impossible’!
Second Bloch’s theorem

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**Flaw:** thinking of a superconductor as a state of a metal with finite current
Superconductivity: 1930-1937

- **1932 Keesom, Kok**: specific heat anomaly in tin

J. C. McLennan 1934
Superconductivity: 1930-1937

- 1932 Keesom, Kok: specific heat anomaly in tin

Superconductivity is a stable thermodynamic phase different from the usual metallic state.
Superconductivity: 1930-1937

- 1933 Meissner-Ochsenfeld: Meissner effect

Superconductors are not just perfect conductors
Superconductivity: 1930-1937

- Gorter: $B=0$ inside a superconductor
- London equations: zero resistivity and Meissner effect

\[ m \frac{dv}{dt} = eE \quad j = n_s ev \]

\[ \frac{\partial}{\partial t} \left( \frac{m}{n_s e^2} j \right) = E \]

\[ \nabla \times E = -c^{-1} \frac{\partial H}{\partial t} \]

\[ \frac{m}{n_s e^2} \nabla \times j = -c^{-1} H \]

- Penetration depth

\[ \nabla \times H = \frac{4\pi}{c} j \]

\[ \nabla^2 H - \lambda_L^{-2} H = 0 \]

\[ B = H_0 \exp(-x / \lambda_L) \]

\[ \lambda_L^2 = \frac{mc^2}{4\pi n_s e^2} \]
Rigidity of wave function and gap

\[ \frac{\partial}{\partial t} \left( \frac{m}{n_s e^2} \mathbf{j} \right) = \mathbf{E} \]

\[ \frac{m}{n_s e^2} \nabla \times \mathbf{j} = -c^{-1} \mathbf{H} \]

\[ \mathbf{H} = \nabla \times \mathbf{A} \]

\[ \mathbf{E} = -c^{-1} \frac{\partial \mathbf{A}}{\partial t} \]

\[ \mathbf{j} = -\frac{n_s e^2}{mc} \mathbf{A} \]

\[ \nabla \cdot \mathbf{j} = 0 \]

\[ \nabla \cdot \mathbf{A} = 0 \]

But gauge invariance?

Conductor with all its various possible currents. It would be sufficient to show that this state has the following properties:

1. Its energy is separated by a finite interval from that of the ordinary Bloch states and lies lower than those.

2. Its eigenfunction is nondegenerate and in a weak magnetic field it undergoes no stronger perturbation than one proportional to \( H^2 \).

F. London 1937
Rigidity of wave function and gap

\[ \frac{\partial}{\partial t} \left( \frac{m}{n_s e^2} j \right) = E \]

\[ \frac{m}{n_s e^2} \nabla \times j = -c^{-1} H \]

\[ H = \nabla \times A \]

\[ E = -c^{-1} \frac{\partial A}{\partial t} \]

\[ j = -\frac{n_s e^2}{mc} A \]

\[ \nabla \cdot j = 0 \]

\[ \nabla \cdot A = 0 \]

- **Rigidity**: wave function does not respond to \( A \) (phase coherence over large distances)

\[ j_p \propto -\frac{e\hbar}{2m} \left[ \Psi^* \nabla \Psi - \Psi \nabla \Psi^* \right] \]

\[ j_d \propto -\frac{e^2}{mc} |\Psi|^2 A \]

- **Energy gap** between continuum and superconducting state

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Superconductivity: 1939-1949

- **Pippard**: there is another scale besides $\lambda_L$
- **Non-local electrodynamics**: current averaged over $\xi_0$
- **Ginzburg-Landau**: effective theory for order parameter
- **Discussed in other lectures**
Isotope effect: 1950

data, and we feel that these experiments firmly establish the relation

$$M^4 T_e = \text{const}$$

in mercury.

Reynolds, Serin, Nesbitt 1950
Maxwell 1950
It should perhaps be mentioned in this context that before 1950, every ‘expert’ knew that ions, being so heavy, would have nothing to do with superconductivity. In fact Kammerling Onnes, using mercury from meteors, seemed to have shown that the transition temperature does not depend on the isotopic composition, and a laboratory had rejected an offer from Harwell of isotopes for the measurement of superconductive transition temperatures as a waste of time.

H. Frohlich 1980

Reynolds, Serin, Nesbitt 1950
Maxwell 1950
Isotope effect: 1950

Reynolds, Serin, Nesbitt 1950
Maxwell 1950

Ionic motion is important for superconductivity
Phonon attraction: formalism

Amplitudes of processes:

\[ \frac{|V|^2}{E(p_1) - E(p_1 - \hbar k) - \hbar \omega(k)} + \frac{|V|^2}{E(p_2) - E(p_2 + \hbar k) - \hbar \omega(k)} \]

\[ \frac{|V|^2 \hbar \omega(k)}{[E(p_1) - E(p_1 - \hbar k)]^2 - [\hbar \omega(k)]^2} \]

Phonon-mediated attractive e-e interaction for electrons within \( \omega_D \) of the Fermi surface

H. Fröhlich 1952
Phonon attraction: simple picture

- Time electron spends near an atom: \( \tau \approx a / v_F \)
- Typical momentum transfer: \( p \approx F \tau \approx (e^2 / a^2) \tau \)
- Typical atomic displacement: \( M \omega_D^2 x^2 \approx p^2 / M \)

\[
x \approx \frac{p}{M \omega_D} \approx \frac{a}{v_F} \frac{e^2}{a^2} \frac{1}{M \omega_D} \approx \frac{a}{\hbar / (ma)} \frac{e^2}{a^2} \frac{\hbar \sqrt{M / m}}{M (e^2 / a)} \approx \frac{a}{\beta}
\]
Phonon attraction: simple picture

Time electron spends near an atom
\[ \tau \approx a / v_F \]

Typical momentum transfer
\[ p \approx F \tau \approx (e^2 / a^2) \tau \]

Typical atomic displacement
\[ x \approx a / \beta \quad \beta = \sqrt{M / m} \]

Change in potential
\[ \Delta U \approx -\frac{e^2 x}{a a} \approx -\frac{e^2}{a \beta} \approx -\hbar \omega_D \]
Phonon attraction: simple picture

Time electron spends near an atom
\[ \tau \approx a / v_F \]

Typical momentum transfer
\[ p \approx F \tau \approx (e^2 / a^2) \tau \]

Typical atomic displacement
\[ x \approx a / \beta \quad \beta = \sqrt{M / m} \]

Change in potential
\[ \Delta U \approx -\hbar \omega_D \]

Time before atoms relax back
\[ \tau_M \approx \omega_D^{-1} \]

Displacement trail length
\[ l \approx v_F \tau_M \approx \beta a \]
Phonon attraction: simple picture

Time electron spends near an atom \( \tau \approx a / v_F \)

Typical momentum transfer \( p \approx F \tau \approx (e^2 / a^2) \tau \)

Typical atomic displacement \( x \approx a / \beta \quad \beta = \sqrt{M / m} \)

Change in potential \( \Delta U \approx -\hbar \omega_D \)

Time before atoms relax back \( \tau_M \approx \omega_D^{-1} \approx (a / v_F) \beta \)

Displacement trail length \( l \approx v_F \tau_M \approx \beta a \)

“Tube” of attractive potential: most advantageous for electrons moving in opposite directions

V. Weisskopf 1979
and still

I also tried the same thing as Frohlich and Bardeen, which is to solve the Frohlich and Bardeen model with such precision that the estimated errors in the calculation are less than the difference in energy one is looking for. I made diagrams and loops. When one is working with partition functions, it turns out there are all kinds of wonderful tricks that one can do with the diagrams. I calculated the specific heat to enormous precision, and the specific heat was still proportional to $T$. 
and still

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R. Feynman 1956
I also tried the same thing as Frohlich and Bardeen, which is to solve the Frohlich and Bardeen model with such precision that the estimated errors in the calculation are less than the difference in energy one is looking for. I made diagrams and loops. When one is working with partition functions, it turns out there are all kinds of wonderful tricks that one can do with the diagrams. I calculated the specific heat to enormous precision, and the specific heat was still proportional to $T$. However, a student of mine, Michael Cohen, pointed out that the series expansion which I was carrying out may not lead to the lowest state at all. Suppose, for example, that one has a harmonic oscillator and considers the effect of a small perturbation, $e x^3$, on the ground-state energy. Regardless of how small $\epsilon$ is, one can never derive the answer from perturbation theory even though the series appears to be nicely convergent. The reason, of course, is that if one goes far enough from the origin the potential becomes arbitrarily large and negative, and hence no lowest state exists. In other words, what happens is that one starts with a function which is qualitatively different from the correct function and the right answer lies in a qualitatively different place. Thus when one starts with
Cooper phenomenon

Bound states of two electrons near the Fermi surface:

$$\left[ -\frac{\hbar^2}{2m} \left( \nabla_1^2 + \nabla_2^2 \right) + V(r_1, r_2) \right] \Psi(r_1, r_2) = \left( E + 2E_F \right) \Psi(r_1, r_2)$$

Our “interaction tube”: CM at rest

$$\Psi(r_1, r_2) = \sum_k \psi(k) \exp[ik \cdot (r_1 - r_2)]$$

What is the matrix element?

$$V_{kk'} = L^{-3} \int V(r) \exp[ir \cdot (k - k')] dr$$
Both electrons near the Fermi surface: *rapidly oscillating phases*

\[ V_{kk'} \approx -U_0 L^3 \int_0^l \exp[ir \cdot |k - k'|] dr \]

\[ |E - E'| \approx \hbar v_F |k - k'| \leq \frac{\hbar v_F}{a \beta} \approx \frac{\hbar^2}{m a^2 \beta} \approx \hbar \omega_D \]

\[ V_{kk'} = \begin{cases} -V, & \text{if } |E(k) - E(k')| < \hbar \omega_D, \\ 0, & \text{otherwise} \end{cases} \]
Bound State

\[ 2E(k)\psi(k) + \sum_{k} V_{kk'} \psi(k') = (E + 2E_F)\psi(k) \]

Key: filled Fermi sea

\[ \psi(k) = 0 \text{ for } k < k_F \]

Solution:

\[ \psi(k) = \frac{\sum_{k} V_{kk'} \psi(k')}{E - 2(E(k) - E_F)} \]

Self-consistency:

\[ 1 = V \sum_{k} \frac{1}{2(E(k) - E_F) - E} \approx VN_0 \int_0^{\hbar \omega_D} d\xi (2\xi - E)^{-1} \]

Bound state of two electrons with opposite momenta:

Cooper pair

\[ E_0 = -2\hbar \omega_D \exp[-2 / N_0V] \]

NB: \[ E_0 \approx \Delta_0 \]

L. N. Cooper 1956
Importance of the Fermi surface

• Same problem without FS:

\[ \psi(k) = \sum_k \frac{V_{kk} \psi(k')}{E - 2E(k)} = \frac{C}{E - 2E(k)} \]

• Self-consistency on \( C \) is equation for energy \( E \)

\[ \frac{1}{V} = \sum_k \frac{1}{\hbar^2 k^2 / m + |E|} \]

Is there a bound state for a small attractive potential?

For small \( E \) integral finite: need critical potential value

3D

\[ \frac{1}{V} = \int \frac{4\pi k^2 dk}{\hbar^2 k^2 / m + |E|} \]

2D

\[ \frac{1}{V} = \int \frac{2\pi k dk}{\hbar^2 k^2 / m + |E|} \approx N_0 \ln \frac{W}{|E|} \]

\[ E = -W \exp(-1/VN_0) \]

Fermi surface makes it “2D”
Comments

- Non-perturbative result: *no expansion* $V \sim 0$
- Cooper pairs: *bosonic objects*
- Bose condensation of pairs leads to superconductivity.  
  
  *M. Schafroth, S. Butler, J. Blatt 1957*

---

$^4$He is also a collection of bound fermions (6, not 2).

**What is special about gas of Cooper pairs?**
Cooper pair gas

**Spread of momentum**
\[ \Delta_0 \approx v_F \Delta p \]
\[ \frac{\Delta p}{p_F} \approx \frac{\Delta_0}{E_F} \]

**Cooper pair size**
\[ \xi_0 \approx \hbar v_F / \Delta_0 \approx a(E_F / \Delta_0) \]

**Electron density**
\[ n \approx a^{-3} \]

**Cooper pair density**
\[ n_c \approx a^{-3} \left( \frac{\Delta_0}{E_F} \right) \approx a^{-2} \xi_0^{-1} \]

**Distance between pairs**
\[ d \approx n_c^{-1/3} \approx a \left( \frac{E_F}{\Delta_0} \right)^{1/3} \ll \xi_0 \]

**Strongly overlapping gas of Cooper pairs**
Dilute Bose gas

Single-particle states

Ensemble states

$\xi n^3 < < 1$

$\xi$

condensate

$\xi$

excited

$\xi$

ground state

Gapless spectrum: when one particle is excited (starts moving) it has little chance of scattering off the particles in the condensate
Dense neutral Bose gas

Single-particle states

\[ n_0 \xi^3 \sim 1 \]

\( k \neq 0 \)

\( k = 0 \)

condensate

Ensemble states

excited

gap \( \Delta \)

ground state

Low energy excitation: rotation of atoms relative to one another: typical energy

\[ \Delta \approx \hbar^2 / M_0 \xi^2 \]

Rotons
Cooper pair gas

Ensemble states

Overlapping charged pairs:
roton energy high

Energy gap=energy to
dissociate a pair

How to describe such a state?
What is the “right” combination?
BCS wave function

Reduced Hamiltonian:
electron pairing

Not the usual bosonic operators!
BCS wave function

Reduced Hamiltonian: electron pairing

\[ H = \sum_{k\sigma} 2\varepsilon_k b_k^+ b_k + \sum_{kk'} V_{kk'} b_{k'}^+ b_k \]

Not the usual bosonic operators!

\[ n_{k\sigma} = c_{k\sigma}^+ c_{k\sigma} \]
\[ b_k^+ = c_{k\uparrow}^+ c_{-k\downarrow} \]
\[ \{c_{k\sigma}, c_{k'\sigma'}\} = \delta_{kk'} \delta_{\sigma\sigma'} \]
\[ [b_k, b_k^+] = 1 - n_{k\uparrow} - n_{-k\downarrow} \]
\[ (b_k^+)^2 = 0 \]
\[ (b_k)^2 = 0 \]

Variational approach: unoccupied / doubly occupied states, no single occupancy

Inspiration: polaron
BCS wave function

Reduced Hamiltonian: electron pairing

\[ H = \sum_{k\sigma} 2\varepsilon_k b^+_k b_k + \sum_{kk'} V_{kk'} b^+_k b_k \]

Not the usual bosonic operators!

\[
\begin{align*}
n_{k\sigma} &= c^{+\sigma}_{k\sigma} c^{-\sigma}_{k\sigma} \\
 b^+_k &= c^+_k c^-_{-k} \\
 [b_k, b^+_k] &= 1 - n_{k\uparrow} - n_{k\downarrow} \\
 (b^+_k)^2 &= 0 \\
 (b_k)^2 &= 0
\end{align*}
\]

Variational approach: unoccupied / doubly occupied states, no single occupancy

Inspiration: polaron

Static distortion of the lattice around an electron: emission of multiple phonons into the same state

\[
\Psi \propto \prod_k \exp[g_k (a^+_k + a^-_{-k})] |\text{vac}\rangle
\]

T.D. Lee, F. Low, D. Pines 1953
BCS wave function II

\[ \Psi \propto \prod_k e^{g_k b_k^+} |vac\rangle \equiv \prod_k (1+g_k b_k^+) |vac\rangle \]

Normalization:

\[ \Psi_{BCS} = \prod_k (u_k + v_k c_k^+ c_{-k}^+) |vac\rangle \]

Probability empty:

\[ u_k^2 + v_k^2 = 1 \]

Probability occupied

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Ground state energy

\[ E_g = \langle \Psi_{BCS} | H - \mu N | \Psi_{BCS} \rangle = \sum_{kk'} V_{kk'} u_k v_{k'} + \sum_{kk'} \sum_{\sigma} 2\varepsilon_k v_k^2 \]

Choice of coefficients: variational method

\[ u_k = \sin \theta_k \]
\[ v_k = \cos \theta_k \]

\[ \frac{\partial E_g}{\partial \theta} = 0 \]

Excitation energy

\[ E_k = \sqrt{\varepsilon_k^2 + \Delta^2} \]
\[ \Delta_k = -\sum_{k'} V_{kk'} u_{k'} v_k \]
\[ \Delta \approx 2\hbar \omega_D \exp\left(-1/N_0V\right) \approx E_0 \]

Condensation energy

\[ E_g(\Delta) - E_g(\Delta = 0) = -N_0\Delta^2 / 2 \]
Occupation numbers

Probability that the states with momenta $k$ and $-k$ are occupied

$$\nu_k^2 = \frac{1}{2} \left( 1 - \frac{\epsilon_k}{E_k} \right)$$

At $T=0$ looks like thermally smeared Fermi distribution

No discontinuity in occupation numbers: no gap in momentum space

Gap in excitations that are not coherent with the pairs: different phase
Particle number

\[ \Psi_{BCS} = \prod_k (u_k + v_k c_{k\uparrow} c_{-k\downarrow}) |\text{vac}\rangle \]

Particle number is not conserved!

\[ \langle N \rangle = 2 \sum_k \langle \Psi_{BCS} | c_{k\uparrow} c_{k\uparrow} | \Psi_{BCS} \rangle = 2 \sum_k v_k^2 \]

\[ \delta N^2 = \langle (N - \langle N \rangle)^2 \rangle = 4 \sum_k u_k^2 v_k^2 \]

Small relative fluctuations of the particle number
Particle number II

Project on a state with a definite $N$ of electrons

State with $N$ electrons has phase $iN\varphi/2$

$$\Psi_B CS = \sum \lambda_N \Psi_N$$

$$\Psi_\varphi = \prod_k \left( u_k + v_k e^{i\varphi} c_k^+ c_{-k}^+ \right) | vac \rangle$$

$$\Psi_N = \int_0^{2\pi} d\varphi e^{-iN\varphi/2} \prod_k \left( u_k + v_k e^{i\varphi} c_k^+ c_{-k}^+ \right) | vac \rangle = \int_0^{2\pi} d\varphi e^{-iN\varphi/2} \Psi_\varphi$$

All phases needed for definite particle number

Number and phase are conjugate variables

$$N \leftrightarrow -i \partial / \partial \varphi$$

$$\varphi \leftrightarrow i \partial / \partial N$$

$$\Delta N \Delta \varphi \approx 1$$

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Cargese
Summary I

- Reduction of the problem to essential physics, and then trial for new ground states/excitations
- Solve problems even seemingly difficult ones: electrons form pairs despite Coulomb repulsion
Summary I

- Reduction of the problem to essential physics, and then trial for new ground states/excitations
- Solve problems even seemingly difficult ones: electrons form pairs despite Coulomb repulsion
- Works for other complicated problems: Laughlin wave function for fractional quantum Hall.
\[ \Psi(z_1, \ldots, z_n) = \prod_{ij} (z_i - z_j)^3 e^{-|z|^2}, z = x + iy \]
- Does the reduction method always work?
Extension of BCS: AFM, RVB and all that

- Doped Hubbard systems (High-$T_c$, cobaltates)
  \[ H = \sum_{\langle ij \rangle} t c_{i\sigma}^+ c_{j\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow} \]
  double occupancy expensive \( U \gg t \)

- Superexchange: AFM interaction
  \[ H = \sum_{\langle ij \rangle} t c_{i\sigma}^+ c_{j\sigma} + \sum_i J S_i S_j \]

- If not 1 electron per site: vacancies that move

C. Gros 2007
Resonating valence bonds

- Form singlets on neighboring sites
  \[ \begin{align*}
  \frac{J}{4} & \quad \frac{J}{4} & \quad \frac{J}{4} \\
  -3 \frac{J}{4} & \quad -3 \frac{J}{4}
\end{align*} \]

- Look at 1D chain, compare energy
  valence bond wins in 1D
  energies may be close in 2D, with frustration...

- Make a linear superposition of bonds:
  allow them to resonate to lower the kinetic energy: mobile singlets
  \[ \text{Anderson, Anderson and Fazekas, 1973} \]
RVB trial wave function

- Two electrons on a *mobile* valence bond of length $r$

\[ b_r^+ = \sum_i c_{i\uparrow}^+ c_{i+r\downarrow}^+ = \sum_k c_{k\uparrow}^+ c_{-k\downarrow}^+ e^{ikr} \]

- Vary bond length/no double occupancy

\[ b^+ = \sum_k a(k) c_{k\uparrow}^+ c_{-k\downarrow}^+ \quad \sum_k a(k) = 0 \]

- Bonds condense/resonate

\[ (b^+)^{N/2} |\text{vac}\rangle \quad \text{double occupancy} \]

- Project out doubly occupied (Gutzwiller)

\[ \Psi_{RVB} = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})(b^+)^{N/2} |\text{vac}\rangle \]

*Anderson, 1987*
BCS and RVB

- Consider an unusual pairing
  \[ b_k^+ = a(k)c_{k\uparrow}^+c_{-k\downarrow}^+ \]

- Construct a BCS wave function
  \[ \Psi \propto \prod_k e^{g_k b_k^+} |vac\rangle = \exp(\sum g_k b_k^+) |vac\rangle \]

- Project a fixed number
  \[ \Psi_{BCS,N} = \left[ \sum_k \nu_k b_k^+ \right]^{N/2} |vac\rangle \]

- Prohibit double occupancy
  \[ \Psi_{RVB} = \prod_i (1 - n_i^\uparrow n_i^\downarrow) \Psi_{BCS,N} \]

Resonating valence bonds and Cooper pairs look similar: basis for theories of exotic SC


…
Summary and challenge

- (Correctly) guessing a wave function remains the best way to solve a strongly correlated problem

- **Challenge**: wave function describing an electronic system with most exotic properties.

- **Bonus points**: Hamiltonian for which this wave function is a good variational ground state

- **Prize**: TBD