Quantum Many-Body Theory
Two Lectures

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1 Usefull Books

Many Electron Theory S.Raims

This is the most elementary book on the market.Pedagogically sound but does not cover very much.

Methods of Quantum Field Theory in Statistical Physics A.A.Abrikosov,L.P.Gorkov and I.E.Dzyloshinskii

Pioneered the use of quantum field theory methods in condesed matter physics.A classic.Very Russian, Landau School, in style.'64

Theory of Interacting Fermi Systems P.Nozière

Elegant in a very precise , french, way but very abstract and does not teckle many physically interesting problems.'63

Quantum Theory of Many-Particle Systems A.Fetter and J.D.Walecka

AGD made readable for American graduate students

A guide to Feynman diagrams in Many-Body Theory R.D. Mattuck

Fun.Gives good 'feel' for using digrams but short on physics.'76

Statistical Physics Part 2 Landau and Lifschitz + Pitaevskii

Not as good as the earlier L+L books but covers more physics then the other many-body books.

Greens Functions and Condensed Matter G.Rickayzen

A modern, pedagogically carefull text but very introductory.'80

Quantum Many-Particle Systems J.W.Negele and H.Orland

The first truely modern text book on the subject.It uses path integrals both for fields and particles. It covers a lot of ground but it is ters .It is a hard read for the uninitiated.Paperback '98

Basic Notions of Condensed Matter Physics P.W.Anderson of 'more is different'

Brilliant but idiosyncratic.Definitely for further reading.

Quantum Field Theory in Condensed Matter Physics (second edition) Alexei M. Tsvelik

The last hurrah of the Landau School.Selected acheavments of sophisticated field theory in solving condensed matter physics problems.

Not for beginners.

Quantum Theory of Many-Body Systems A.M.Zagoskin

The best modern introductory text.Strong on Superconductivity but there is little on magnetism.

Quantum Liquids A.J.Leggett

A book which treats many of the deepest problems in non-relativistic quatum many-body theory without significant use of field theoretical

methods.A most worthwhile read.

2 'Many-Body Theory' is not needed in:

- Introducing electron-electron interaction in the description of atoms, molecules and solids

- Taking into account electron-electron correlations in the description of atoms, moleculs and solids

Both of these effects are catered for, albeit approximately, in a **selfconsistant one electron calculation** based on the LDA presciption for the exchange correlation functional $E_{xc}[n(\overrightarrow{r})]$.

'Many-Body Theory' is useful in describing **highly correlated systems**

3 The Many-Body Wavefunction

3.1 Schrödingers equation

$$\widehat{H}(\overrightarrow{r}_1, \overrightarrow{r}_2, ...)\psi(\overrightarrow{r}_1, \overrightarrow{r}_2, ...\overrightarrow{r}_N) = E\psi(\overrightarrow{r}_1, \overrightarrow{r}_2, ...\overrightarrow{r}_N) \tag{1}$$

$$\widehat{H} = \widehat{H}_0 + \hat{V} \tag{2}$$

$$\widehat{H}_0 = \sum_{i=1}^{N} -\frac{\hbar^2}{2m}\nabla_i^2 + V^{ext}(\overrightarrow{r}_i) \tag{3}$$

$$\widehat{V} = V(\overrightarrow{r}_1, \overrightarrow{r}_2, ...) = \frac{1}{2}\sum_{i \neq j}^{N} V(\overrightarrow{r}_i - \overrightarrow{r}_j) \tag{4}$$

3.2 Non-interacting particles: $\widehat{V} = 0$

A solution of the Schrödingers equation is the simple product state:

$$\psi(\overrightarrow{r}_1, \overrightarrow{r}_2, ... \overrightarrow{r}_N) = \phi(\overrightarrow{r}_1)\phi(\overrightarrow{r}_2)\phi(\overrightarrow{r}_3)..\phi(\overrightarrow{r}_N) = \prod_{i}^{N} \phi(\overrightarrow{r}_i) \tag{5}$$

3.3 Symmetry under premutation: the dogma or indistinguishability

$$\widehat{\wp}_{i\to j}\psi(\overrightarrow{r}_1,\overrightarrow{r}_2,.\overrightarrow{r}_i..\overrightarrow{r}_j..\overrightarrow{r}_N)=e^{i\theta}\psi(\overrightarrow{r}_1,\overrightarrow{r}_2,.\overrightarrow{r}_j.\overrightarrow{r}_i..\overrightarrow{r}_N) \qquad (6)$$

3.3.1 Bosons:$\theta=0$

$$\psi(\overrightarrow{r}_1,\overrightarrow{r}_2,...\overrightarrow{r}_N)=\frac{\sqrt{N!}}{\sqrt{n_1!n_2!..n_N!}}\sum_{\wp}\widehat{\wp}\phi_{\lambda_1}(\overrightarrow{r}_1)\phi_{\lambda_2}(\overrightarrow{r}_2)\phi_{\lambda_3}(\overrightarrow{r}_3)..\phi_{\lambda_N}(r_N) \qquad (7)$$

3.3.2 Fermions $\theta = \pi$

$$\psi(\overrightarrow{r}_1, \overrightarrow{r}_2, ...\overrightarrow{r}_N) = \frac{1}{\sqrt{N}} \sum_{\wp} (-1)^{\mathbb{N}_{\wp}\widehat{\wp}} \phi_{\lambda_1}(\overrightarrow{r}_1)\phi_{\lambda_2}(\overrightarrow{r}_2)\phi_{\lambda_3}(\overrightarrow{r}_3)..\phi_{\lambda_N}(r_N) \tag{8}$$

This can be written as a Slater determinant

$$\psi(\overrightarrow{r}_1, \overrightarrow{r}_2, ...\overrightarrow{r}_N) = \frac{1}{\sqrt{N}} \left\| \begin{array}{ccc} \phi_{\lambda_1}(\overrightarrow{r}_1) & \phi_{\lambda_1}(\overrightarrow{r}_2) & \phi_{\lambda_1}(\overrightarrow{r}_N) \\ \phi_{\lambda_2}(\overrightarrow{r}_1) & \phi_{\lambda_2}(\overrightarrow{r}_2) & \phi_{\lambda_2}(\overrightarrow{r}_N) \\ & & \\ \phi_{\lambda_N}(\overrightarrow{r}_1) & \phi_{\lambda_N}(\overrightarrow{r}_2) & \phi_{\lambda N}(\overrightarrow{r}_N) \end{array} \right\| \tag{9}$$

3.3.3 Spin Statistics theorem:

- Half integer spin particles like electrons or ^{3}He atoms are **Fermions**
- Integer spin particles like ^{4}He atoms or photons are *Bosons*

3.3.4 Example:

Two spin 1/2 electrons

$$\psi(\overrightarrow{r}, \sigma_1; \overrightarrow{r}_2, \sigma_2) = \frac{1}{\sqrt{2}} \left(\phi_1(\overrightarrow{r}_1, \sigma_1)\, \phi_2(\overrightarrow{r}_2, \sigma_2) - \phi_1(\overrightarrow{r}_2, \sigma_2)\phi_2(\overrightarrow{r}_1, \sigma_1)\right) \tag{10}$$

3.3.5 The two electron Slater determinant:

$$\psi(\overrightarrow{r}_{1,}\sigma_1;\overrightarrow{r}_{2,}\sigma_2)=\frac{1}{\sqrt{2}}\begin{vmatrix}\phi_1(\overrightarrow{r}_{1,}\sigma_1) & \phi_1(\overrightarrow{r}_{2,}\sigma_2)\\ \phi_2(\overrightarrow{r}_{1,}\sigma_1) & \phi_2(\overrightarrow{r}_{2,}\sigma_2)\end{vmatrix} \tag{11}$$

$$=\frac{1}{\sqrt{2}}\Big(\phi_1(\overrightarrow{r}_{1,}\sigma_1)\phi_2(\overrightarrow{r}_{2,}\sigma_2)-\phi_1(\overrightarrow{r}_{2,}\sigma_2)\phi_2(\overrightarrow{r}_{1,}\sigma_1)\Big) \tag{12}$$

Take the one particle states to be of the form $\phi(\overrightarrow{r},\sigma)=\varphi(\overrightarrow{r})\chi(\sigma)$ and show that

$$\begin{aligned}\psi(\overrightarrow{r}_{1,}\sigma_1;\overrightarrow{r}_{2,}\sigma_2) \quad = \quad & \tfrac{1}{2\sqrt{2}}[(\varphi_1(\overrightarrow{r}_1)\varphi_2(\overrightarrow{r}_2)-\varphi_1(\overrightarrow{r}_2)\varphi_2(\overrightarrow{r}_1)) \\ & (\chi_1(\sigma_1)\chi_2(\sigma_2)+\chi_1(\sigma_2)\chi_2(\sigma_1))] \qquad (13) \\ & +\tfrac{1}{2\sqrt{2}}[(\varphi_1(\overrightarrow{r}_1)\varphi_2(\overrightarrow{r}_2)+\varphi_1(\overrightarrow{r}_2)\varphi_2(\overrightarrow{r}_1)) \\ & (\chi 1(\sigma_1)\chi_2(\sigma_2)-\chi_1(\sigma_2)\chi_2(\sigma_1))] \qquad (14)\end{aligned}$$

Triplet : (the spin component is symmetric and the orbital component is anti-symmetric)

- $\chi_1(\sigma) = \chi_2(\sigma) = \chi(\sigma)$ (either $\chi_\uparrow(\sigma)$ or $\chi\downarrow(\sigma)$)

$$\frac{1}{\sqrt{2}}\left[\left(\varphi_1(\overrightarrow{r}_1)\varphi_2(\overrightarrow{r}_2) - \varphi_1(\overrightarrow{r}_2)\varphi_2(\overrightarrow{r}_1)\right)\chi(\sigma_1)\chi(\sigma_2)\right] \tag{15}$$

- $\chi_1(\sigma) \neq \chi_2(\sigma)$ (namely 1=↑ and 2=↓)

$$\begin{gathered}\tfrac{1}{2\sqrt{2}}[\left(\varphi_1(\overrightarrow{r}_1)\varphi_2(\overrightarrow{r}_2) - \varphi_1(\overrightarrow{r}_2)\varphi_2(\overrightarrow{r}_1)\right) \\ \Big(\chi_\uparrow(\sigma_1)\chi_\downarrow(\sigma_2) + \chi_\uparrow(\sigma_2)\chi_\downarrow(\sigma_1)\Big)]\end{gathered} \tag{16}$$

- Singlet : (the spin component is anti-symmetric and the orbital component is symmetric)

$$\begin{gathered}\frac{1}{2\sqrt{2}}[(\varphi_1(\overrightarrow{r}_1)\varphi_2(\overrightarrow{r}_2)+\varphi_1(\overrightarrow{r}_2)\varphi_2(\overrightarrow{r}_1)) \\ \Big(\chi_\uparrow(\sigma_1)\chi_\downarrow(\sigma_2)-\chi_\uparrow(\sigma_2)\chi_\downarrow(\sigma_1)\Big)]\end{gathered} \tag{17}$$

3.4 Perturbation Theory

As in single-body quantum mechanics it fallows from

$$\widehat{H}=\widehat{H_0}+\hat{V} \tag{18}$$

that

$$E_0 - E_0^{(0)} = \langle \boldsymbol{\Psi}_0^{(0)} \mid \widehat{V} \mid \boldsymbol{\Psi}_0^{(0)} \rangle + \tag{19}$$

$$\sum_{n \neq 0}^{\infty} \frac{\langle \boldsymbol{\Psi}_0^{(0)} \mid \widehat{V} \mid \boldsymbol{\Psi}_n^{(0)} \rangle \langle \boldsymbol{\Psi}_n^{(0)} \mid \widehat{V} \mid \boldsymbol{\Psi}_0^{(0)} \rangle}{E_0^{(0)} - E_n^{(0)}} + \ldots \tag{20}$$

where $\mid \boldsymbol{\Psi}_0^{(0)} \rangle$ and $\mid \boldsymbol{\Psi}_n^{(0)} \rangle$ are the ground state and an excited state of the non-interacting system.

Note that

$$\psi_n^{(0)}(\overrightarrow{r}_1, \overrightarrow{r}_2, \ldots \overrightarrow{r}_N) = \langle \overrightarrow{r}_1, \overrightarrow{r}_2 \ldots . \overrightarrow{r}_N \mid \boldsymbol{\Psi}_n^{(0)} \rangle \tag{21}$$

and bellow is an example of how to calculate matrix elements

$$\langle \boldsymbol{\Psi}_{\lambda_1,\lambda_2} \mid V(\overrightarrow{r}_1 - \overrightarrow{r}_2) \mid \boldsymbol{\Psi}_{\lambda_1,\lambda_2} \rangle = \int d^3 r_1 \int d^3 r_2 \boldsymbol{\Psi}^{\times}_{\lambda_1,\lambda_2}(\overrightarrow{r}_1, \overrightarrow{r}_2) \tag{22}$$

$$V(\overrightarrow{r}_1 - \overrightarrow{r}_2)\Psi_{\lambda_1,\lambda_2}(\overrightarrow{r}_1, \overrightarrow{r}_2) = \tag{23}$$

$$+\int d^3r_1 \int d^3r_2 \left|\phi_{\lambda_1}(\overrightarrow{r}_1)\right|^2 \left|\phi_{\lambda_2}(\overrightarrow{r}_2)\right| V(\overrightarrow{r}_1 - \overrightarrow{r}_2)\,\{\Longleftarrow Coulomb\} + \tag{24}$$

$$-\int d^3r_1 \int d^3r_2 \phi^{\times}_{\lambda_1}(\overrightarrow{r}_2)\phi^{\times}_{\lambda_2}(\overrightarrow{r}_1)\phi_{\lambda_1}(\overrightarrow{r}_1)\phi_{\lambda_2}(\overrightarrow{r}_2)V(\overrightarrow{r}_1 - \overrightarrow{r}_2)\,\{\Longleftarrow Exchange\} \tag{25}$$

The point of the above brief discussion is that the non interacting wavefunctions $\psi_n^{(0)}(\overrightarrow{r}_1, \overrightarrow{r}_2, ...\overrightarrow{r}_N)$ form a complete set and hence the perturbation theory can, in principle, be carried out to all orders in the interaction $\widehat{V}$.**If** this procedure converges it leads to an exact solution for $E_0 - E_0^{(0)}$.Other questions of non-relativistic many-body theory can be can be tackled similarly.Clearly, to make headway you need good book-keeping.This is what Quantum Field Theory provides

3.5 Correlated wave functions:

Instead of proceeding systematically sometimes it is better to guess the answer: Take the wavefunction to be in the form;

$$\boldsymbol{\Psi}(\overrightarrow{r}_1, \overrightarrow{r}_2, ...\overrightarrow{r}_N) \simeq e^{-\frac{1}{2}\sum\limits_{i,j} u(\overrightarrow{r} i - \overrightarrow{r}_j)} \left\| \begin{array}{ccc} \phi_{\lambda_1}(\overrightarrow{r}_1) & \phi_{\lambda_1}(\overrightarrow{r}_2) & \phi_{\lambda_1}(\overrightarrow{r}_N) \\ \phi_{\lambda_2}(\overrightarrow{r}_1) & \phi_{\lambda_2}(\overrightarrow{r}_2) & \phi_{\lambda_2}(\overrightarrow{r}_N) \\ & & \\ \phi_{\lambda_N}(\overrightarrow{r}_1) & \phi_{\lambda_N}(\overrightarrow{r}_2) & \phi_{\lambda N}(\overrightarrow{r}_N) \end{array} \right\| \tag{26}$$

and find the orbitals $\phi_{1,}\phi_{2,}\phi_{3...}\phi_N$ u$(\overrightarrow{r}_{i-}\overrightarrow{r}_j)$ by minimizing $\langle \boldsymbol{\Psi} \mid \widehat{H} \mid \boldsymbol{\Psi} \rangle$.This is the variational method.Examples of its efficacy is the BCS wavefunction (for superconductivity, Nobel prize) and the Laughlin wave function(for fractional Quantum Hall state,Nobel prize.)

4 Second Quatization as a good bookkeeping system:

4.1 Occupation number representation

$\psi_n^{(0)}(\overrightarrow{r}_1, \overrightarrow{r}_2, ... \overrightarrow{r}_N)$ is completely determned by the one particle orbitals defined by

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V^{ext}(\overrightarrow{r})\right)\phi_\lambda(\overrightarrow{r}) \;=\; \epsilon_\lambda\phi_\lambda(\overrightarrow{r}) \tag{27}$$

$$\langle\phi_\lambda \;\;|\;\; \phi_{\lambda'}\rangle = \delta_{\lambda,\lambda'} \tag{28}$$

and the **occupation numbers** n_{λ_1},n_{λ_2},$\mathsf{n}_{\lambda_3}, \ldots.\mathsf{n}_{\lambda_N} \equiv \{n_\lambda\}$ .Thus, it is worthwhile to define $\mid \{n_\lambda\}\rangle$ as

$$\psi_n^{(0)}(\overrightarrow{r}_1, \overrightarrow{r}_2, \ldots \overrightarrow{r}_N) = \langle \overrightarrow{r}_1, \overrightarrow{r}_2 \ldots \overrightarrow{r}_N \mid n_{\lambda_1,} n_{\lambda_2} \ldots n_{\lambda_N}\rangle \tag{29}$$

The way a determinental wavefunction can change is by the removal of one orbital, say $\phi_{\lambda'}$, and the introduction of an other, say $\phi_{\lambda''}$.In the occupation number representation this means reducing n_λ by 1 and increasing $\mathsf{n}_{\lambda'}$ by 1.One can conveniently implement these operation in the Hilbert space spanned by the states $\mid \{n_\lambda\}\rangle$ called Fock-Space.In this space a general state vector has the fallowing form

$$\mid \ \boldsymbol{\Psi}\rangle = \sum_{\lambda} A_\lambda^{(1)} \mid n_{\lambda'}\rangle + \sum_{\lambda_1,\lambda_2} A_{\lambda_1,\lambda_2}^{(2)} \mid n_{\lambda_1}, n_{\lambda_2}\rangle \tag{30}$$

$$\sum_{\lambda_1,\lambda_2,\lambda_3} A_{\lambda_1,\lambda_2,\lambda_3}^{(3)} \ \mid \ n_{\lambda_1}, n_{\lambda_2} n_{\lambda_3}\rangle + \ldots. \tag{31}$$

4.2 Creation and Annihilation Operators:

$$c_\lambda^\dagger \mid ...n_\lambda...\rangle = (-1)^{\sum_{\lambda'}^{\lambda'\langle\lambda} n_{\lambda'}} (1 - n_\lambda) \mid ...n_\lambda + 1...\rangle \tag{32}$$

$$c_\lambda \mid ...n_\lambda...\rangle = (-1)^{\sum_{\lambda'}^{\lambda'\langle\lambda} n_{\lambda'}} (n_\lambda) \mid ...n_\lambda - 1...\rangle \tag{33}$$

$$c_\lambda^\dagger \mid ...n_\lambda = 1...\rangle = 0 \tag{34}$$

$$c_\lambda \mid ...n_\lambda = 0...\rangle = 0 \tag{35}$$

$$c_\lambda^2 = 0, \quad c\dagger^2 = 0 \tag{36}$$

$$c_\lambda c_{\lambda'}^\dagger = -c_{\lambda'}^\dagger c_\lambda \tag{37}$$

Finally with a bit more algebra (see books, Riems for exemple) we have the **Fermionic commutation relations**

$$\begin{array}{c} c_\lambda c_{\lambda'}^\dagger + c_{\lambda'}^\dagger c_\lambda = \delta_{\lambda,\lambda'} \\ c\dagger_\lambda c_{\lambda'}^\dagger + c_{\lambda'}^\dagger c_\lambda^\dagger = 0 \quad c_\lambda c_{\lambda'} + c_{\lambda'} c_\lambda = 0 \end{array} \tag{38}$$

For **bosons** one finds (in books)

$$\begin{aligned} a_\lambda a^\dagger_{\lambda'} - a^\dagger_{\lambda'} a_\lambda &= \delta_{\lambda,\lambda'} \\ a\dagger_\lambda a^\dagger_{\lambda'} - a^\dagger_{\lambda'} a^\dagger_\lambda &= 0 \quad a_\lambda a_{\lambda'} - a_{\lambda'} a_\lambda = 0 \end{aligned} \tag{39}$$

The purpose of these manipulations is to pose the whole many-body problem in a new framework.Noting that the states $\mid \{n_\lambda\}\rangle$ are eigen tates of the 'number operator'$\widehat{n}_\lambda \equiv c^\dagger_\lambda c_\lambda$,whose eigenvalues are the occupation numbers n_λ we may wriet the Hamiltonian $\widehat{H}_0$ as

$$\widehat{H}_0 = \sum_\lambda \epsilon_\lambda c^\dagger_\lambda c_\lambda \tag{40}$$

Evidently,

$$\langle \Psi \mid \widehat{H}_0 \mid \Psi \rangle = \sum_\lambda \epsilon_\lambda n_\lambda \tag{41}$$

as it should be. It takes longer but it can also be shown that

$$\widehat{V} = \sum_{\lambda_1,\lambda_{2,\lambda_3\lambda_4}} V_{\lambda_1,\lambda_{2,\lambda_3\lambda_4}} c^\dagger_{\lambda_1} c^\dagger_{\lambda_2} c_{\lambda_3} c_{\lambda_4} \tag{42}$$

where $V_{\lambda_1,\lambda_{2,\lambda_3\lambda_4}}$ is a matrix element involving only the 4 orbitals $\phi_{\lambda_1}, \phi_{\lambda_2}, \phi_{\lambda_2}, \phi_{\lambda_4}$ Thus, we have eliminated all references to specific particles, namely their 'names' i in $\overrightarrow{r}_i$ .EUREKA.

4.2.1 Quantum Fields

Let us now introduce the field operators

$$\psi^{\dagger}(\overrightarrow{r}) = \sum_{\lambda} \phi_{\lambda}^{\times}(\overrightarrow{r}) c_{\lambda}^{\dagger} \tag{43}$$

$$\psi(\overrightarrow{r}) = \sum_{\lambda} \phi_{\lambda}(\overrightarrow{r}) c_{\lambda} \tag{44}$$

which creat and annihilate, respectively, particles at $\overrightarrow{r}$.From the Fermionic commutation relations $c_{\lambda} c_{\lambda'}^{\dagger} + c_{\lambda'}^{\dagger} c_{\lambda} = \delta_{\lambda,\lambda'}$ it fallows that

$$\psi_{\sigma'}(\overrightarrow{r}') \psi_{\sigma}^{\dagger}(\overrightarrow{r}) + \psi_{\sigma}^{\dagger}(\overrightarrow{r}) \psi_{\sigma'}(\overrightarrow{r}') = \delta_{\sigma,\sigma'} \delta(\overrightarrow{r} - \overrightarrow{r}') \tag{45}$$

$$\psi_{\sigma'}(\overrightarrow{r}') \psi_{\sigma}(\overrightarrow{r}) + \psi_{\sigma}(\overrightarrow{r}) \psi_{\sigma'}(\overrightarrow{r}') = 0 \tag{46}$$

$$\psi_{\sigma'}^{\dagger}(\overrightarrow{r}') \psi_{\sigma}^{\dagger}(\overrightarrow{r}) + \psi_{\sigma}^{\dagger}(\overrightarrow{r}) \psi_{\sigma'}^{\dagger}(\overrightarrow{r}') = 0 \tag{47}$$

It turns out that all operators in Fock-Space can be written in terms of these field operators:

$$\widehat{\rho}_\sigma(\overrightarrow{r}) = \psi_\sigma^\dagger(\overrightarrow{r})\psi_\sigma(\overrightarrow{r}) \tag{48}$$

$$\rho_\sigma(\overrightarrow{r}) = \langle \mathbf{\Psi} \mid \psi_\sigma^\dagger(\overrightarrow{r})\psi_\sigma(\overrightarrow{r}) \mid \mathbf{\Psi}\rangle \tag{49}$$

where $\widehat{\rho}_\sigma(\overrightarrow{r})$ is the density operator and $\rho_\sigma(\overrightarrow{r})$ is the phsical particle density of the sytem.Similarly, the corresponding particle current operator and current is given by

$$\widehat{\overrightarrow{j}}_\sigma(\overrightarrow{r}) = \frac{\hbar}{i2m}\left(\psi_\sigma^\dagger(\overrightarrow{r})\overrightarrow{\nabla}\psi_\sigma(\overrightarrow{r}) - \overrightarrow{\nabla}\psi_\sigma^\dagger(\overrightarrow{r})\psi_\sigma(\overrightarrow{r})\right) \tag{50}$$

$$\overrightarrow{j}_\sigma(\overrightarrow{r}) = \langle \mathbf{\Psi} \mid \widehat{\overrightarrow{j}}_\sigma(\overrightarrow{r}) \mid \mathbf{\Psi}\rangle \tag{51}$$

Finally, and most importantly,

$$\widehat{H}_0 = \sum_{\sigma} \int d^3 r \psi^{\dagger}_{\sigma}(\overrightarrow{r}) \left(-\frac{\hbar^2}{2m} \nabla^2 + V^{ext}(\overrightarrow{r}) \right) \psi_{\sigma}(\overrightarrow{r}) \tag{52}$$

$$\widehat{V} = \frac{1}{2} \int d^3 r \int d^3 r' \psi^{\dagger}_{\sigma'}(\overrightarrow{r}) \psi^{\dagger}_{\sigma}(\overrightarrow{r}') \mathsf{v}^{e-e}(\overrightarrow{r} - \overrightarrow{r'}) \psi_{\sigma'}(\overrightarrow{r}') \psi_{\sigma}(\overrightarrow{r}) \tag{53}$$

EUREKA again as we have eliminated and referece to the one particle states which appeared in the Slater determinants.What is left looks like a one patricle (Schrödinger) theory except now the 'wave functions' $\psi(\overrightarrow{r})$ and $\psi^{\dagger}(\overrightarrow{r})$ are non commuting operators.This non commuting algebra in Fock-Space takes care of the permutation symmetry requirement on the many body wavefunction $\psi(\overrightarrow{r}_1, \overrightarrow{r}_2, ... \overrightarrow{r}_N)$. In fact it is this that makes the many body problem difficult.

5 Quatizing the Schrödingers equation

5.0.2 The Lagrangian

Fallowing P.Jordan and E.P.Wigner (Z.Physik 47,631 '28) regard the usual Schrödingers equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2+V^{ext}(\overrightarrow{r})\right)\psi(\overrightarrow{r},t)=i\hbar\dot{\psi}(\overrightarrow{r},t) \tag{54}$$

for one particle as the Euler-Lagrange equation for the classical fields $\psi(\overrightarrow{r}, t)$ and $\psi^{\times}(\overrightarrow{r}, t)$.As will be shown bellow it fallows from the Lagrangian:

$$L(t) = \int d^3r \left[i\hbar\psi^{\times}\dot{\psi} - \frac{\hbar^2}{2m}\overrightarrow{\nabla}\psi^{\times} \cdot \overrightarrow{\nabla}\psi - V^{ext}\psi^{\times}\psi \right] \tag{55}$$

The action corresponding to this L is defined as

$$S(t_1, t_2) = \int\limits_{t_1}^{t_2} dt' L(t') \tag{56}$$

According to the Principle of Least Action ψ and $\psi^{\times}$ will evolve in time in such way as to minimize the action .Namely,

$$\delta S(t_1, t_2) = 0 \tag{57}$$

where δ implies infitecimal variations due to idependent changes $\psi + \delta\psi$ and $\psi^{\times} + \delta\psi^{\times}$.

Varying $\psi^{\times}$

$$\delta \int\limits_{t_1}^{t_2} dt' L(t') = \int\limits_{t_1}^{t_2} dt' \int d^3r \left[i\hbar\dot{\psi}\delta\psi^{\times} - \frac{\hbar^2}{2m}\overrightarrow{\nabla}\delta\psi^{\times} \cdot \overrightarrow{\nabla}\psi - V^{ext}\delta\psi^{\times}\psi \right] \tag{58}$$

$$\int\limits_{t_1}^{t_2} dt' \int d^3r \left[i\hbar\dot{\psi} + \frac{\hbar^2}{2m}\overrightarrow{\nabla} \cdot \overrightarrow{\nabla}\psi - V^{ext}\psi \right] \delta\psi^{\times} - \int\limits_{t_1}^{t_2} dt' \int\limits_{\mathbf{\Sigma}} \overrightarrow{d\mathbf{\Sigma}} \cdot \frac{\hbar^2}{2m}\overrightarrow{\nabla}\psi\delta\psi^{\times} = 0 \tag{59}$$

Sice the surface term vanishes at infinity the above relations can only holds iff

$$i\hbar\dot{\psi} + \frac{\hbar^2}{2m}\overrightarrow{\nabla} \cdot \overrightarrow{\nabla}\psi - V^{ext}\psi = 0 \tag{60}$$

Problem 1: By varying ψ show that $\psi^{\times}$ satisfies the complex conjugate of the Schrödingers equation.

5.0.3 The Hamiltonian:

The point of finding L is that it leads to a canonical momentum $\pi(\overrightarrow{r}, t)$ and a Hamiltonian H for the 'classical' Schrödinger Field $\psi(\overrightarrow{r}, t)$:

$$\pi(\overrightarrow{r}, t) \equiv \frac{\delta L}{\delta \dot{\psi}} = \psi^{\times}(\overrightarrow{r}, t) \tag{61}$$

Now, using H=$\pi\dot{\psi} - L$ (H=p$\dot{q} - L$) we find

$$H_0 = \int d^3r \left(\frac{\hbar^2}{2m} \overrightarrow{\nabla}\psi^{\times} \cdot \overrightarrow{\nabla}\psi + V^{ext}\psi^{\times}\psi \right) \tag{62}$$

5.0.4 Canonical Quatization:

In analogy with the convetional rule that p and q become operators $\widehat{p}, \widehat{q}$ such that $[\widehat{q}, \widehat{p}] = i\hbar$ we make $\psi^{\times}$ and ψ operators

$$\left(\psi(\overrightarrow{r}, t)\psi^{\dagger}(\overrightarrow{r}', t') \pm \psi\dagger(\overrightarrow{r}', t')\psi(\overrightarrow{r}, t)\right) = \delta(t - t')\delta(\overrightarrow{r} - \overrightarrow{r}') \tag{63}$$

$$\left(\psi\dagger(\overrightarrow{r}, t)\psi^{\dagger}(\overrightarrow{r}', t') \pm \psi\dagger(\overrightarrow{r}', t')\psi\dagger(\overrightarrow{r}, t)\right) = 0 \tag{64}$$

$$\left(\psi(\overrightarrow{r}, t)\psi(\overrightarrow{r}', t') \pm \psi(\overrightarrow{r}', t')\psi(\overrightarrow{r}, t)\right) = 0 \tag{65}$$

where $+$ describes fermions and - bosons.

Note that

$$i\hbar\dot{\psi} = \left[\psi, \widehat{H}_0\right] = -\frac{\hbar^2}{2m}\overrightarrow{\nabla} \cdot \overrightarrow{\nabla}\psi - V^{ext}\psi \tag{66}$$

is now an operator equation.

It is natural to define the particle number operator $\widehat{N}$ as

$$\widehat{N} = \int d^3 r \psi\dagger(\overrightarrow{r}, t)\psi(\overrightarrow{r}, t) \tag{67}$$

Reassuringly,

$$i\hbar\dot{\widehat{N}} = \left[\widehat{N}, \widehat{H}_0\right] = 0 \tag{68}$$

namely $\widehat{N}$ is a constant of the motion.Furthermore, if we expand the field operators $\psi^\dagger(\overrightarrow{r}, t)$and $\psi(\overrightarrow{r}, t)$ in a complete set of one particle, c-number, orbitals $\{\phi_\lambda(\overrightarrow{r})\}$

with operator coefficients$c_\lambda(t)$, $c_\lambda^\dagger(t)$

$$\psi(\overrightarrow{r},t) = \sum_\lambda \phi_\lambda(\overrightarrow{r})c_\lambda(t) \tag{69}$$

$$\psi^\dagger(\overrightarrow{r},t) = \sum_\lambda \phi_\lambda(\overrightarrow{r})c_\lambda^\dagger(t) \tag{70}$$

we can define an occupation number operator

$$\widehat{n}_\lambda \equiv c_\lambda^\dagger c_\lambda \tag{71}$$

As can be readily shown the operators c$_\lambda$ and c$_\lambda^\dagger$ inheret the commutation relations of $\psi^\dagger(\overrightarrow{r},t)$ $\psi(\overrightarrow{r},t)$ $e.g.$

$$c_\lambda c_{\lambda'}^\dagger \pm c_{\lambda'}^\dagger c_\lambda = \delta_{\lambda,\lambda'} \tag{72}$$

$$c_\lambda^\dagger c_{\lambda'}^\dagger \pm c_{\lambda'}^\dagger c_\lambda^\dagger = 0 \tag{73}$$

$$c_\lambda c_{\lambda'} \pm c_{\lambda'} c_\lambda = 0 \tag{74}$$

and by substituting Eqs 69 and 70 into Eqs 62,67 using Eq.27 one finds

$$\widehat{H}_0 = \sum_\lambda \epsilon_\lambda \widehat{n}_\lambda \tag{75}$$

$$\widehat{N} = \sum_\lambda \widehat{n}_\lambda \tag{76}$$

It then fallows that all theoccupation number operators $\widehat{n}_\lambda$ correspond to constants of the motion $\left[\widehat{n}_\lambda, \widehat{H}_0\right] = 0$.Consequently, the eigentates of $\widehat{H}_0$ can be labeled by the eigenvalues n$_\lambda$ of $\widehat{n}_\lambda$:

$$\widehat{n}_\lambda \mid ....n_\lambda..\rangle = n_\lambda \mid ....n_\lambda..\rangle \tag{77}$$

and for the fermionic commutation relation n_λ can take only the values 0 and 1 due to the fact that

$$\widehat{n}_\lambda \widehat{n}_\lambda = c_\lambda^\dagger c_\lambda c_\lambda^\dagger c_\lambda = c_\lambda^\dagger c_\lambda - c_\lambda^\dagger c_\lambda^\dagger c_\lambda c_\lambda = \widehat{n}_\lambda \tag{78}$$

Thus, remarkably, the canonical quantization of the Schrödingers fields $\psi^\dagger, \psi$ reproduces the same many-body Fock-Space as our consideration of antisymetrized many body wave functions written as Slater determinants.In fact, for a non-ineratcting collection of paticles

$$\psi(\overrightarrow{r}_1, \overrightarrow{r}_2, ... \overrightarrow{r}_N) = \langle \overrightarrow{r}_N ... \overrightarrow{r}_2 \overrightarrow{r}_1 \mid \psi \rangle \tag{79}$$

$$\mid \overrightarrow{r}_1, \overrightarrow{r}_2, ... \overrightarrow{r}_N \rangle = \psi^\dagger(\overrightarrow{r}_N) .. \psi^\dagger(\overrightarrow{r}_2) \psi^\dagger(\overrightarrow{r}_1) \mid 0 \rangle . \tag{80}$$

$$\langle \overrightarrow{r}_N ...... \overrightarrow{r}_2 \overrightarrow{r}_1 \mid = \langle 0 \mid \psi(\overrightarrow{r}_N) ..... \psi(\overrightarrow{r}_2) \psi(\overrightarrow{r}_1) \tag{81}$$

$$\psi(\overrightarrow{r}_1, \overrightarrow{r}_2, ... \overrightarrow{r}_N) = \langle 0 \mid \psi(\overrightarrow{r}_N) ..... \psi(\overrightarrow{r}_2) \psi(\overrightarrow{r}_1) \mid \psi \rangle \tag{82}$$

where $\mid 0 \rangle$ is the ground state with no particles (*vacume*).Clealy, the above set of arguments deserve the name *second quatization.*

For bosons similar argument apply and due to the different commutation relations n_λ may take on any value between 0 and ∞.

In conclusion it should be stressed *second quatization* gives nothing new, in the above sense only in non relativistic quatum mechanics.In the case of the Dirac equation or indeed of the Maxwells equation the *vacume* brings in new physics namely v*acume fluctuations*

5.0.5 Particle-Particle interaction:

$$L(t) = \int d^3r \left[i\hbar\psi^\times \dot{\psi} - \frac{\hbar^2}{2m}\overrightarrow{\nabla}\psi^\times \cdot \overrightarrow{\nabla}\psi - V^{ext}\psi^\times\psi - eV\psi^\times\psi - \left|\overrightarrow{\nabla}V\right|^2 \right] \tag{83}$$

where V is a variable (electrostatic) field , note that -$\overrightarrow{\nabla} V(\overrightarrow{r}) = \overrightarrow{E}(\overrightarrow{r})$. We now must minimize the action S(t_1, t_2) with respect to V as well as ψ and $\psi\times$:

$$\frac{\delta S}{\delta V} = \int_{t_1}^{t_2} dt \left[e\psi^{\times}(\overrightarrow{r})\psi(\overrightarrow{r}) - \frac{1}{4\pi}\nabla^2 V(\overrightarrow{r}) \right] = 0 \tag{84}$$

Thus

$$e\psi^{\times}(\overrightarrow{r})\psi(\overrightarrow{r}) = \frac{1}{4\pi}\nabla^2 V(\overrightarrow{r}) \tag{85}$$

which is Gausses equation whose solution is:

$$V(\overrightarrow{r}) = e\int d^3r' \frac{\psi^{\times}(\overrightarrow{r}')\psi(\overrightarrow{r}')}{|\overrightarrow{r} - \overrightarrow{r}'|} \tag{86}$$

Using this result we can eliminate V from the Lagrangian and therefore from the Hamiltonian to find

$$\begin{aligned} H &= \int d^3r(-\frac{\hbar^2}{2m}\overrightarrow{\nabla}\psi^\times \cdot \overrightarrow{\nabla}\psi + V^{ext}\psi^\times\psi && (87) \\ &+\frac{e^2}{2}\int d^3r \int d^3r' \frac{\psi^\times(\overrightarrow{r})\psi(\overrightarrow{r})\psi^\times(\overrightarrow{r}')\psi(\overrightarrow{r}')}{|\overrightarrow{r}-\overrightarrow{r}'|}) && (88) \end{aligned}$$

Quatizing this Hamiltonian yealds the *interaction Hamiltonian*

$$\widehat{V} = \frac{e^2}{2}\int d^3r \int d^3r' \frac{\psi^\dagger(\overrightarrow{r})\psi^\dagger(\overrightarrow{r}')\psi(\overrightarrow{r}')\psi(\overrightarrow{r})}{|\overrightarrow{r}-\overrightarrow{r}'|} \qquad (89)$$

Clearly, as far as condesed matter physics is concerned, the resulting $\widehat{H}=\widehat{H}_0+\widehat{V}$ is , more or less, **the theory of everything**

6 So, where do the models such as the Hubbard or Anderson models come in

- As the temperature T$\Rrightarrow$ 0 **degrees of freedoms freeze out**

- Neer the low temperature **fixed point** only a few degees of freedom remains

- These degrees of freedoms are described by an effective Hamiltonian H$_{eff}$ which involves only their coordinats and momenta as variables

- The effecctive Hamiltonian, H$_{eff}$, also includes parameters such as effective mass m$_{eff}$,coupling constants like U, J,g etc.. which are determined by the deegrees of freedoms which have been frozen out

- The form of such effective Hamiltonians are not known and they may ,and do, differ from system to system.this is what is meant by **More is different**

7 The Greens Functions of Many-Body Theory (at T=0)

7.1 Definition:

$$G_{\sigma,\sigma'}(\overrightarrow{r},t\,;\overrightarrow{r}',t') = -i\langle \Phi_0 \mid T\left\{\psi_\sigma(\overrightarrow{r},t)\psi^\dagger_\sigma(\overrightarrow{r}',t')\right\} \mid \Phi_0\rangle \tag{90}$$

$$i\hbar\partial_t\psi = [\psi, H] \quad \Rrightarrow \psi_\sigma(\overrightarrow{r},t) = e^{\frac{i}{\hbar}Ht}\psi_\sigma(\overrightarrow{r})e^{-\frac{i}{\hbar}Ht} \tag{91}$$

$$G_{\sigma,\sigma'}(\overrightarrow{r},t\ ;\overrightarrow{r}',t') = -i\begin{pmatrix} \langle\Phi_0 \mid \psi_\sigma(\overrightarrow{r},t)\psi^\dagger_\sigma(\overrightarrow{r}',t') \mid \Phi_0\rangle & t > t' \\ \pm\langle\Phi_0 \mid \psi^\dagger_\sigma(\overrightarrow{r}',t')\psi_\sigma(\overrightarrow{r},t) \mid \Phi_0\rangle & t < t' \end{pmatrix} \tag{92}$$

7.2 Observables

$$n_\sigma(\overrightarrow{r},t) = -i\lim_{\overrightarrow{r}\longrightarrow\overrightarrow{r}'} G_{\sigma,\sigma'}(\overrightarrow{r},t\ ;\overrightarrow{r}',t^+)\text{ where t}^+ = t+0^+ \tag{93}$$

$$\overrightarrow{m}(\overrightarrow{r},t) = -i\lim_{\overrightarrow{r}\longrightarrow\overrightarrow{r}'}\sum_{\alpha,\beta}\overrightarrow{\sigma}_{\alpha,\beta}G_{\beta,\alpha}(\overrightarrow{r},t\ ;\overrightarrow{r}',t^+) \tag{94}$$

7.3 Equation of motion:

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2m}\nabla^2 - V^{ext}(\overrightarrow{r})\right) G_{\sigma,\sigma'}(\overrightarrow{r}, t\ ; \overrightarrow{r}', t') = \hbar\delta\left(\overrightarrow{r} - \overrightarrow{r}'\right)\delta\left(t - t'\right) \tag{95}$$

$$-i\langle \Phi_0 \mid T\left\{\left[\psi_\sigma(\overrightarrow{r}, t), \widehat{V}\right]\psi^\dagger_\sigma(\overrightarrow{r}', t')\right\} \mid \Phi_0\rangle \tag{96}$$

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2m}\nabla^2 - V^{ext}(\overrightarrow{r})\right) G_{\sigma,\sigma'}(\overrightarrow{r}, t\ ; \overrightarrow{r}', t') = \hbar\delta\left(\overrightarrow{r} - \overrightarrow{r}'\right)\delta\left(t - t'\right) \tag{97}$$

$$-i \int d\overrightarrow{r}'' \langle \Phi_0 \mid T\left\{\psi^\dagger_\sigma(\overrightarrow{r}'', t)\psi_\sigma(\overrightarrow{r}'', t)v(\overrightarrow{r}'' - \overrightarrow{r})\psi_\sigma(\overrightarrow{r}, t)\psi^\dagger_\sigma(\overrightarrow{r}', t')\right\} \mid \Phi_0\rangle \tag{98}$$

$$\left(i\hbar\partial_t + \frac{\hbar^2}{2m}\nabla^2 - V^{ext}(\overrightarrow{r})\right) G_{\sigma,\sigma'}(\overrightarrow{r}, t\ ;\overrightarrow{r}', t') \tag{99}$$

$$-\sum_{\sigma''} \int d\overrightarrow{r}'' \int dt'' \boldsymbol{\Sigma}_{\sigma,\sigma''}(\overrightarrow{r}, t; \overrightarrow{r}'', t'') G_{\sigma,\sigma'}(\overrightarrow{r}'', t''; \overrightarrow{r}', t') = \hbar\delta\left(\overrightarrow{r} - \overrightarrow{r}'\right)\delta\left(t - t'\right) \tag{100}$$

where by definition

$$
\begin{aligned}
-i\int d\overrightarrow{r}''\langle\Phi_0 \quad &| \quad T\left\{\psi^\dagger_\sigma(\overrightarrow{r}'',t)\psi_\sigma(\overrightarrow{r}'',t)v(\overrightarrow{r}''-\overrightarrow{r})\psi_\sigma(\overrightarrow{r},t)\psi^\dagger_\sigma(\overrightarrow{r}',t')\right\}|\Phi_0\rangle \quad (101)\\
&= \quad \sum_{\sigma''}\int d\overrightarrow{r}''\int dt''\Sigma_{\sigma,\sigma''}(\overrightarrow{r},t\;;\overrightarrow{r}'',t'')G_{\sigma,\sigma'}(\overrightarrow{r}'',t''\;;\overrightarrow{r}',t') \quad (102)
\end{aligned}
$$

7.4 Free electron Greens function:

$$
\psi_\sigma(\overrightarrow{r},t)=\frac{1}{L^{3/2}}\sum_{\overrightarrow{k}}e^{i\overrightarrow{k}\cdot\overrightarrow{r}}c_{\overrightarrow{k},\sigma}(t) \quad \text{etc...} \qquad (103)
$$

$$
\begin{aligned}
G^{0}_{\sigma,\sigma'}(\overrightarrow{r},t\;;\overrightarrow{r}',t') &= -i\delta_{\sigma,\sigma'}\frac{1}{L^{3}}\sum_{\overrightarrow{k}} e^{i\overrightarrow{k}\cdot(\overrightarrow{r}-\overrightarrow{r}')-i\epsilon_{\overrightarrow{k}}t} && (104)\\
& \Big[\Theta(t-t')\Theta(k-k_F)-\Theta(t'-t)\Theta(k_F-k)\Big] && (105)
\end{aligned}
$$

Using the indentity

$$
\Theta(t-t') = -\int\limits_{-\infty}^{\infty} d\epsilon \frac{1}{2\pi i}\frac{e^{i\epsilon(t-t')}}{\epsilon+i\eta} \qquad (106)
$$

$$G^0_{\sigma,\sigma'}(\overrightarrow{r},t\ ;\overrightarrow{r}',t') = \frac{1}{(4\pi)^4}\int d\overrightarrow{k}\int d\epsilon e^{i\overrightarrow{k}\cdot(\overrightarrow{r}-\overrightarrow{r}')-i\epsilon_{\overrightarrow{k}}t} \tag{107}$$

$$\delta_{\sigma,\sigma'}\left[\frac{\Theta(k-k_F)}{\epsilon-\epsilon_{\overrightarrow{k}}+i\eta}+\frac{\Theta(k_F-k)}{\epsilon-\epsilon_{\overrightarrow{k}}-i\eta}\right] \tag{108}$$

$$\frac{1}{(4\pi)^4}\int d\overrightarrow{k}\int d\epsilon e^{i\overrightarrow{k}\cdot(\overrightarrow{r}-\overrightarrow{r}')-i\epsilon_{\overrightarrow{k}}t}G^0_{\sigma,\sigma'}(\overrightarrow{k},\epsilon) \tag{109}$$

$$G^0_{\sigma,\sigma'}(\overrightarrow{k},\epsilon) = \delta_{\sigma,\sigma'}\left[\frac{1}{\epsilon-\epsilon_{\overrightarrow{k}}+i\eta sign(k-k_F)}\right] \tag{110}$$

The real part of the poles et $\epsilon = \epsilon_{\overrightarrow{k}} \pm i\eta$ are the dispersion relations

$$\epsilon_{\overrightarrow{k}} = \frac{\hbar^2 k^2}{2m} - \epsilon_F \tag{111}$$

7.5 Fermi Liquid Theory:

For a homogeneous system the exact Greensfunctio is an analytic function of the complex energy varaiable z:

$$G_{\sigma,\sigma}(\overrightarrow{k}, z) = \left[\frac{1}{\epsilon - \epsilon_{\overrightarrow{k}} - \Sigma_\sigma(\overrightarrow{k}, z)} \right] \tag{112}$$

$$\lim_{\epsilon \longrightarrow \mu} \boldsymbol{\Sigma}_\sigma(\overrightarrow{k}, z) = sign(\mu - \epsilon) C_k (\epsilon - \mu)^2 \tag{113}$$

and therefore

$$\lim_{\epsilon \longmapsto \mu} G(\overrightarrow{k}, \epsilon) = \frac{1}{\epsilon - \epsilon_{\overrightarrow{k}} - \boldsymbol{\Sigma}_R(\overrightarrow{k}, \epsilon) - i sign(\mu - \epsilon) C_k (\epsilon - \mu)^2} \tag{114}$$

Take the quasi-particle energy $E_{\overrightarrow{k}}$ to be such that

$$E_{\overrightarrow{k}} - \epsilon_{\overrightarrow{k}} - \boldsymbol{\Sigma}_R(\overrightarrow{k}, E_{\overrightarrow{k}}) = 0 \tag{115}$$

Then

$$G(\overrightarrow{k},\epsilon) = \frac{Z_k}{\epsilon - E_{\overrightarrow{k}} - i\frac{1}{\tau_{\overrightarrow{k}}}} + f(\overrightarrow{k},\epsilon) \tag{116}$$

where bthe' life-time'

$$\frac{1}{\tau_{\overrightarrow{k}}} = Z_k C_k (E_{\overrightarrow{k}} - \mu)^2 \tag{117}$$

This result translates to a low temperature resistivity :

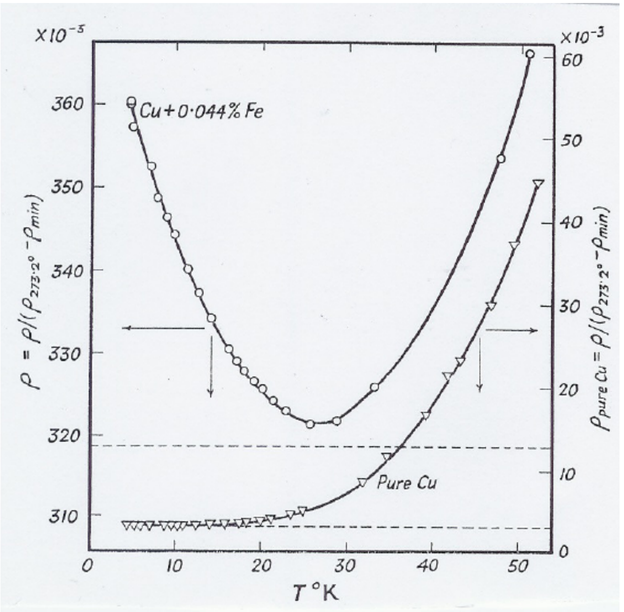
$$R(T) \sim \left(\frac{k_B T}{\epsilon_F}\right)^2 \tag{118}$$

Experimental observation of such temrperature dependence is widly regarded as the finger print of beeing neer a Fermi-Liquid fixed point.An alternative fixed point is the **Luttinger Liquid:**

$$\frac{1}{\tau_{\overrightarrow{k}}} \sim (E_{\overrightarrow{k}} - \mu) \tag{119}$$

8 The Kondo Effect

The resistivity minimum:


×10⁻⁵
360
350
340
330
320
310
ρ = ρ/(ρ273·2° − ρmin)
Cu+0·044% Fe
Pure Cu
×10⁻³
60
50
40
30
20
10
0
ρpure Cu = ρ/(ρ273·2° − ρmin)
0
10
20
30
40
50
T °K

8.1 Transport Theory:

$$\sigma = -\frac{2e^2}{3V}\int d\epsilon_{\overrightarrow{k}}\tau_{\overrightarrow{k}}v^2_{\overrightarrow{k}}n(\epsilon_{\overrightarrow{k}})\frac{\partial f}{\partial \epsilon_{\overrightarrow{k}}} \tag{120}$$

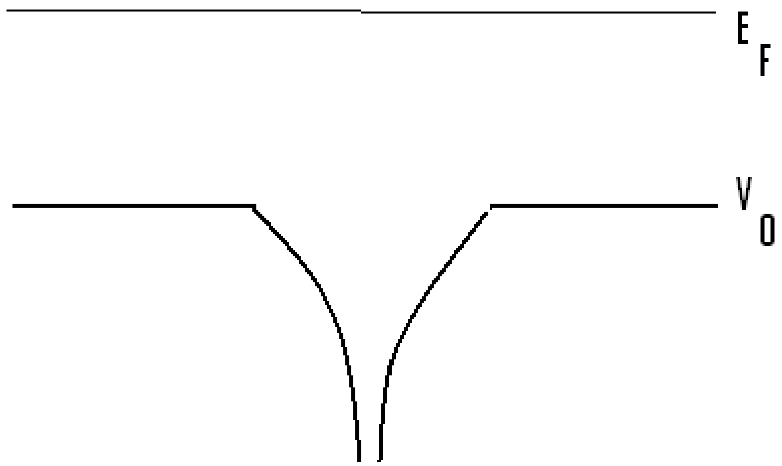
$$\frac{1}{\tau_{\overrightarrow{k}}} = \frac{2\pi}{\hbar}\sum_f \left|\langle f \mid \widehat{t}(\epsilon) \mid i\rangle\right|^2 \delta\left(\epsilon - \epsilon_f + \epsilon_i\right) \tag{121}$$

$$\widehat{t} = \mathsf{V}+\mathsf{V}\mathsf{G}^0\mathsf{V}+\mathsf{V}\mathsf{G}^0\mathsf{V}\mathsf{G}^0\mathsf{V}\ \ldots \tag{122}$$

$$t_{\overrightarrow{k},\overrightarrow{k}'}(\epsilon) = \mathsf{V}_{\overrightarrow{k},\overrightarrow{k}'} + \int d\overrightarrow{k}''\mathsf{V}_{\overrightarrow{k},\overrightarrow{k}''}\frac{1}{\epsilon - \epsilon_{\overrightarrow{k}''} + i\eta}\mathsf{V}_{\overrightarrow{k}'',\overrightarrow{k}'} + .. \tag{123}$$

8.2 Many-Particle Single Scatterer Theory

A single (muffin-tin type) potential well scatters a degenerate system of non-interacting electrons:



Scattering of a degenerate electron sytem from a potential well

The ususal one-particle t-matrix t$_{\vec{k}\,',\vec{k}}(\epsilon)$ generalizes to

$$T_{\overrightarrow{k}'s';\overrightarrow{k},s}(E) =< \Psi_{\overrightarrow{k}',s'} \mid \widehat{T}(E) \mid \Psi_{\overrightarrow{k},s} >$$

where

$$\widehat{T}(E) = \widehat{V} + \widehat{V}\widehat{G}_0(E)\widehat{T}(E)$$

$$\widehat{G}_0(E) = \frac{1}{E - \widehat{H_0}}$$

$$\widehat{H_0} = \sum_{\widehat{k},s} \epsilon_{\overrightarrow{k},s} c^{\dagger}_{\widehat{k},s} c_{\overrightarrow{k},s}$$

$$| \boldsymbol{\Psi}_{\overrightarrow{k},s} >= c^{\dagger}_{\overrightarrow{k},s} \mid \boldsymbol{\Psi}_0 >$$

$$\widehat{V} = \sum_{\overrightarrow{k},\overrightarrow{k}'} \mathsf{V}_{\overrightarrow{k},\overrightarrow{k}'} c^{\dagger}_{\widehat{k}} c_{\overrightarrow{k}'} \tag{124}$$

or

$$\widehat{V} = \sum_{\overrightarrow{k},\alpha,m;\overrightarrow{k}'\beta m'} \left(J_{||} S^{z}_{imp} \cdot \sigma^{z}_{\alpha,\beta} + J_{\perp} \left(S^{+}\sigma^{-} + S^{-}\sigma^{+} \right)_{\alpha m;\beta m'} c^{\dagger}_{\widehat{k},\alpha} c_{\overrightarrow{k}',\beta} \right) \tag{125}$$

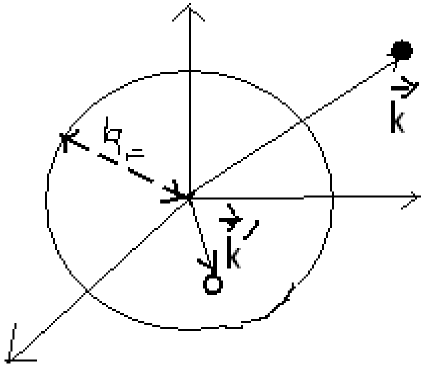
.

Perturbation theory::

$$\widehat{T}(E) = \widehat{V} + \widehat{V}\frac{1}{E-\widehat{H}_0}\widehat{V} + \widehat{V}\frac{1}{E-\widehat{H}_0}\widehat{V}\frac{1}{E-\widehat{H}_0}\widehat{V}.....$$

8.2.1 Particles and holes (spinless)

$$\begin{aligned}
c^{\dagger}_{\overrightarrow{k}} &= \alpha^{\dagger}_{\overrightarrow{k}} \quad \text{for } \left|\overrightarrow{k}\right| > \text{ k}_F \\
c^{\dagger}_{\overrightarrow{k}} &= \beta_{-\overrightarrow{k}} \quad \text{for } \left|\overrightarrow{k}\right| < \text{ k}_F \\
c_{\overrightarrow{k}} &= \alpha_{\overrightarrow{k}} \quad \text{for } \left|\overrightarrow{k}\right| > \text{ k}_F \\
c_{\overrightarrow{k}} &= \beta^{\dagger}_{-\overrightarrow{k}} \quad \text{for } \left|\overrightarrow{k}\right| < \text{ k}_F
\end{aligned}$$



$E_{\vec{k}} > E_F$

$E_{\vec{k}'} < E_F$

Particles Holes

$$\begin{aligned}
\widehat{H}_{\mathsf{0}} - \mu\widehat{N} &= \sum_{\overrightarrow{k}} \epsilon_{\overrightarrow{k}} c^{\dagger}_{\overrightarrow{k}} c_{\overrightarrow{k}} - \mu \sum_{\overrightarrow{k}} c^{\dagger}_{\overrightarrow{k}} c_{\overrightarrow{k}} = \sum_{\overrightarrow{k}\,.>k_F} \epsilon_{\overrightarrow{k}} \alpha^{\dagger}_{\overrightarrow{k}}\, \alpha_{\overrightarrow{k}} \\
+ \sum_{\overrightarrow{k}\,.<k_F} \epsilon_{\overrightarrow{k}} \beta_{\overrightarrow{k}}\, \beta^{\dagger}_{\overrightarrow{k}} & \quad - \mu \sum_{\overrightarrow{k}\,.>k_F} \alpha^{\dagger}_{\overrightarrow{k}}\, \alpha_{\overrightarrow{k}} \; - \mu \sum_{\overrightarrow{k}\,.<k_F} \beta_{\overrightarrow{k}}\, \beta^{\dagger}_{\overrightarrow{k}} \\
&= \sum_{\overrightarrow{k}\,<k_F} (\epsilon_{\overrightarrow{k}} - \mu) + \sum_{\overrightarrow{k}\,.>k_F} (\epsilon_{\overrightarrow{k}} - \mu) \alpha^{\dagger}_{\overrightarrow{k}}\, \alpha_{\overrightarrow{k}} \\
& \quad - \sum_{\overrightarrow{k}\,.<k_F} (\mu - \epsilon_{\overrightarrow{k}}) \beta^{\dagger}_{\overrightarrow{k}}\, \beta_{\overrightarrow{k}}
\end{aligned}$$

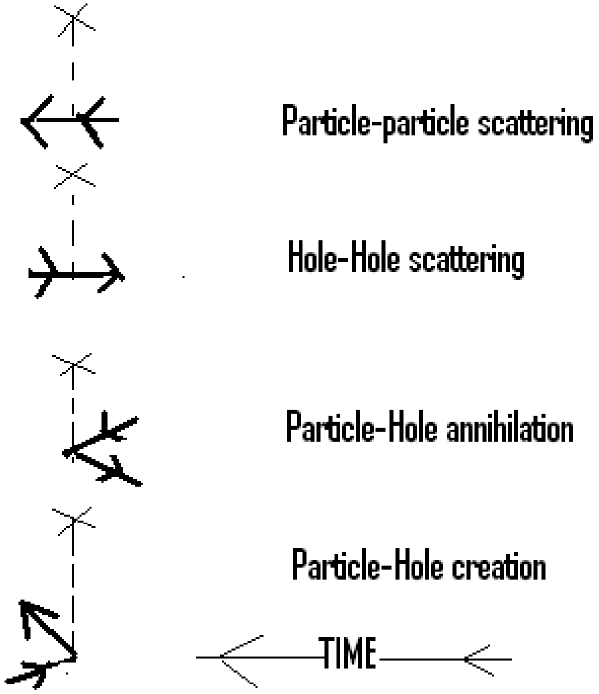
$$\widehat{V} = \sum_{\overrightarrow{k}\,,\overrightarrow{k}\,'} \mathsf{V}_{\overrightarrow{k}\,,\overrightarrow{k}\,'} c^{\dagger}_{\widehat{k}} c_{\overrightarrow{k}\,'} = \widehat{V}^{pp} + \widehat{V}^{ph} + \widehat{V}^{hp} + \widehat{V}^{hh}$$

Diagrammatically

$$\widehat{V}^{pp} = \sum_{\vec{k} > \vec{k_F}, \vec{k}' > \vec{k_F}} \mathsf{V}_{\vec{k}, \vec{k}'} \alpha^{\dagger}_{\hat{k}} \alpha_{\vec{k}'}$$

$$\widehat{V}^{ph} = \sum_{\vec{k} > \vec{k_F}, \vec{k}' < \vec{k_F}} \mathsf{V}_{\vec{k}, \vec{k}'} \alpha^{\dagger}_{\hat{k}} \beta \dagger_{\vec{k}'} \quad \widehat{V}^{hp} = \sum_{\vec{k} < \vec{k_F}, \vec{k}' > \vec{k_F}} \mathsf{V}_{\vec{k}, \vec{k}'} \beta_{\hat{k}} \alpha_{\vec{k}}$$

$$\widehat{V}^{hh} = \sum_{\vec{k} > \vec{k_F}, \vec{k}' > \vec{k_F}} \mathsf{V}_{\vec{k}, \vec{k}'} \alpha^{\dagger}_{\hat{k}} \alpha_{\vec{k}'}$$

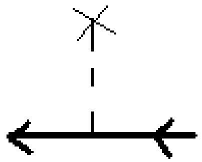

Particle-particle scattering
Hole-Hole scattering
Particle-Hole annihilation
Particle-Hole creation
TIME

8.2.2 Scattering from a static potential $\mathbf{v}_{\vec{k}',\vec{k}}$:

For spinless 'particle-particle'scattering

$$\mid \Psi_{\vec{k}} >= \alpha^{\dagger}_{\vec{k}} \mid \Psi_0 >$$

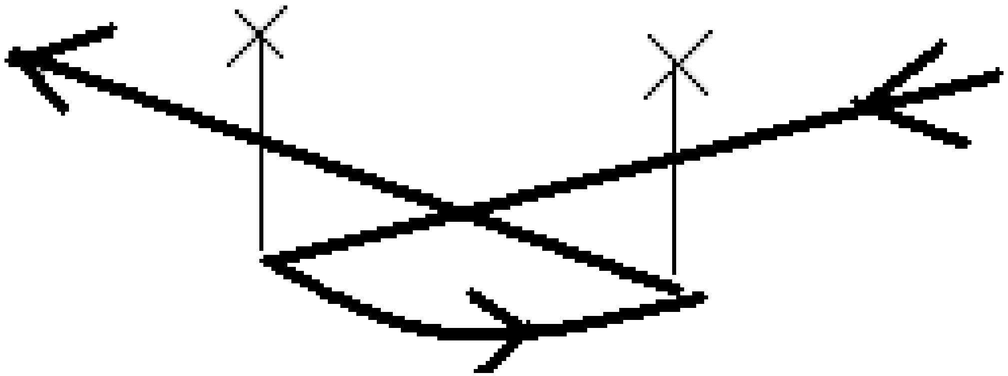
$$T^{(1)}_{\vec{k}',\vec{k}}(\epsilon_{\vec{k}}) =$$



$$= \mathrm{v}_{\vec{k}',\vec{k}}$$

$$T^{2a}_{\overrightarrow{k}', \overrightarrow{k}}(\epsilon_{\overrightarrow{k}}) =$$

$$= \sum_{\overrightarrow{k}''} \mathsf{v}_{\overrightarrow{k}', \overrightarrow{k}''} \frac{1 - f_{\overrightarrow{k}''}}{\epsilon_{\overrightarrow{k}} - \epsilon_{\overrightarrow{k}''}} \mathsf{v}_{\overrightarrow{k}'', \overrightarrow{k}}$$



$$T^{2b)}_{\overrightarrow{k}\,',\overrightarrow{k}}(\epsilon_{\overrightarrow{k}}) \;=\; -\sum_{\overrightarrow{k}\,''} \mathsf{v}_{\overrightarrow{k}\,'',\overrightarrow{k}} \frac{f_{\overrightarrow{k}\,''}}{-\epsilon_{\overrightarrow{k}\,'}, + \epsilon_{\overrightarrow{k}\,''}} \mathsf{v}_{\overrightarrow{k}\,',\overrightarrow{k}\,''}$$

$$T^{2a}_{\overrightarrow{k}',\overrightarrow{k}}(\epsilon_{\overrightarrow{k}}) + T^{2b)}_{\overrightarrow{k}',\overrightarrow{k}}(\epsilon_{\overrightarrow{k}}) =$$

$$\int d^3k'' \mathsf{v}_{\overrightarrow{k}',\overrightarrow{k}''} \frac{1}{\epsilon_{\overrightarrow{k}} - \epsilon_{\overrightarrow{k}''}} \mathsf{v}_{\overrightarrow{k}'',\overrightarrow{k}}$$

because

$$\int d^3k'' \left(\mathsf{v}_{\overrightarrow{k}',\overrightarrow{k}''} \mathsf{v}_{\overrightarrow{k}'',\overrightarrow{k}} - \mathsf{v}_{\overrightarrow{k}'',\overrightarrow{k}} \mathsf{v}_{\overrightarrow{k}',\overrightarrow{k}''} \right) f_{\overrightarrow{k}''} \Longrightarrow 0]$$

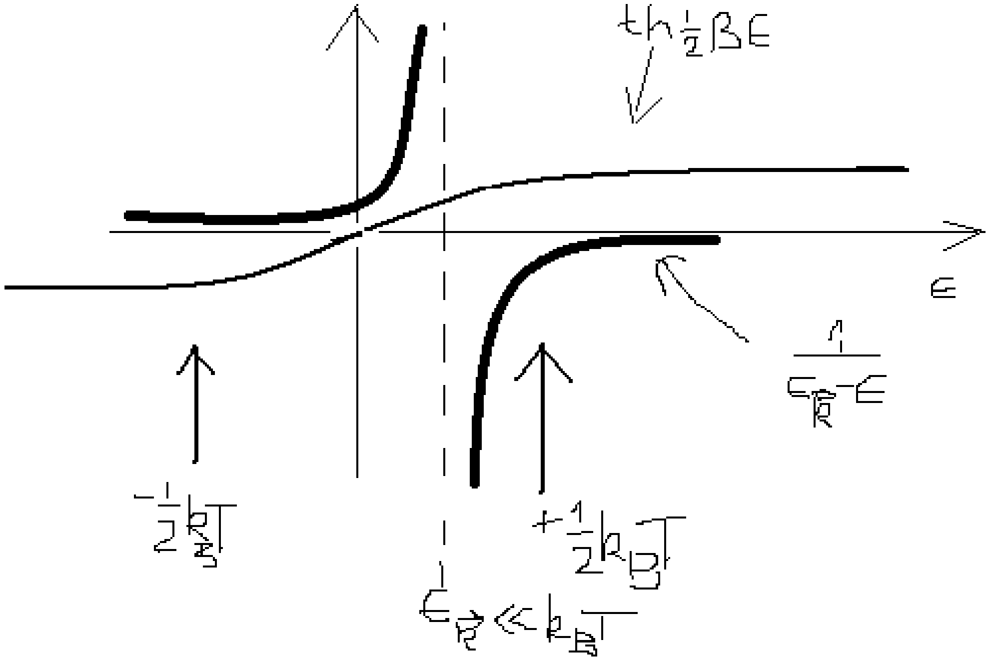
This happens to all orders and hence $\mathsf{T}_{\overrightarrow{k}',\overrightarrow{k}}(\epsilon_{\overrightarrow{k}})$ is given by the convetional Born series for one particle scattering.If the **target can change ist state** and therefore, in general,its energy the scattering electon will be knocked off the energy shell .Namely, electron hole pairs will be created resulting in the famous Kondo divergences.

8.2.3 The break down of the Born peturbation series

For

$$\widehat{V} = \sum_{\overrightarrow{k},\alpha,m;\overrightarrow{k}'\beta m'} \left(J_{\shortparallel} S^{z}_{imp} \cdot \sigma^{z}_{\alpha,\beta} + J_{\perp} \left(S^{+}\sigma^{-} + S^{-}\sigma^{+} \right)_{\alpha m;\beta m'} c^{\dagger}_{\widehat{k},\alpha} c_{\overrightarrow{k}',\beta} \right) \tag{126}$$

$$\sum_{\overrightarrow{k}''} \left(\frac{P}{\epsilon_{\overrightarrow{k}} - \epsilon_{\overrightarrow{k}''}} \right) \left(1 - 2f_{\overrightarrow{k}''} \right) = n(\epsilon_F) \int_{-D}^{D} d\epsilon \frac{P}{\epsilon_{\overrightarrow{k}} - \epsilon} th \left(\frac{1}{2} \beta \epsilon \right) \tag{127}$$


$\text{th}\,\frac{1}{2}\beta\epsilon$
ϵ
$\frac{1}{\epsilon_{\vec{k}}-\epsilon}$
$-\frac{1}{2}k_BT$
$+\frac{1}{2}k_BT$
$\epsilon_{\vec{k}} \ll k_BT$

For $\epsilon_{\overrightarrow{k}} << k_B T$

$$\approx 2 \ln \frac{k_B T}{D}$$

For $\epsilon_{\overrightarrow{k}} >> k_B T$

$$\approx 2 \ln \frac{\epsilon_{\overrightarrow{k}}}{D}$$

Finally

$$T^{(1)}_{i,f} = J_\perp \left(S^+ \sigma^- + S^- \sigma + \right) + J_\| S^z \sigma^z \tag{128}$$

$$T^{(2)}_{i,f}(\epsilon) = \left(J_{\|} J_{\perp}\left(S^{+}\sigma^{-} + S^{-}\sigma+\right) + J_{\perp}^{2} S^{z}\sigma^{z}\right) \ln(\frac{\epsilon}{D}) \tag{129}$$

which , for J$_{\|} = J_{\perp}$=J, leads to

$$R(T) = R_B(1 + \frac{2Jn(\epsilon_F)}{N} \ln \frac{k_B T}{D}) \tag{130}$$

This diverges at at the **Kondo temparature T$_K$** defined by

$$\frac{2Jn(\epsilon_F)}{N} \ln \frac{k_B T}{D} = 1 \tag{131}$$

$$k_B T_K = D e^{-\frac{N}{|Jn(0)|}} \tag{132}$$

Typically the Kondo temperature is small $T_K \sim 10 - 100K$. Having calculated the Curie temperature T$_C$ and the superconducting transition temperature T$_c$ with considerable success **it** is one of the **outstanding** chalanges to the first principles methods to calulate T_K

Finally

Evidently the perturbation series diverges.A way to summ up such logarithmically divergent series is to use scaling arguments as fallows

8.3 Poorman Scaling:

$$T(\epsilon; V_1 + \delta V_1, V_2 + \delta V_2, V_3 + \delta V_3; D + \delta D) = 0$$

In the case of magnetic impurities

$$\mathsf{T}_{\vec{k}\,', \vec{k}}(z) = [J_\perp (S^+\sigma^- + S^-\sigma^+) + J_\parallel S^z \sigma^z] - [J_\parallel J_\perp (S^+\sigma^- + S^-\sigma^+) + J_\parallel^2 S^z \sigma^z] n(\epsilon_F) \ln \frac{z}{D} + ...$$

$$\begin{aligned}\delta J \quad \perp \quad &= -J_\perp J_\| n(\epsilon_f)\delta \ln \frac{z}{D} = -J_\perp J_\| N(\epsilon_F)\delta \ln \frac{\delta D}{D} \\ \delta J \quad \| \quad &= -J_\|^2 N(\epsilon_F)\delta \ln \frac{z}{D} = -J_\|^2 N(\epsilon_F)\delta \ln \frac{\delta D}{D}\end{aligned}$$

$$\frac{\partial J \perp}{\partial \ln D} = -nJ_\| J_\perp \ , \quad \frac{\partial J_\|}{\partial \ln D} = -nJ_\|^2 \tag{133}$$

For $J_\| = J_\perp = -J$ (J>0)

$$
\begin{aligned}
\frac{dJ}{dD} &= n\frac{J^2}{D} \\
\int_{J_0}^{J} dJ' \frac{1}{J'^2} &= n \int_{D_0}^{D} \frac{dD}{D} \\
-\frac{1}{J} + \frac{1}{J_0} &= n \ln \frac{D}{D_0} \\
J &= \frac{nJ_0}{1 - nJ_0 \ln \frac{D}{D_0}} \\
k_B T_K &= D_0 e^{-\frac{1}{nJ_0}} \\
k_B T_K &= D e^{-\frac{1}{nJ}}
\end{aligned}
$$

So K$_B T_K$ is a scale invariant low energy scale

As the temperature is lowered

nJ(T)=

$$t_{\overrightarrow{k},\overrightarrow{k}'} = J + J^2 N(\epsilon_F) \ln \frac{W}{k_B T} + ..$$

The Kondo Temperature

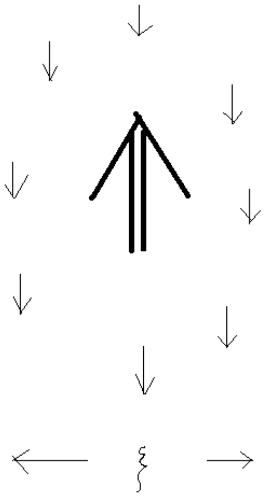
$$T_K = W e^{-\frac{1}{J N(\epsilon_F)}}$$

The Resistivity:

$$R_K = R_B(1 + \frac{2Jn(\epsilon_F)}{N} \ln \frac{k_B T}{W} + ...)$$

$$R_B = \frac{3}{2}\frac{m\pi}{e^2\hbar}\frac{\Omega}{\epsilon_F}\left(\frac{J}{2N}\right)^2 S(S+1)$$

The Ground state is a spin singlet:



The compemsation Claude

$$\xi_K = \frac{\hbar V_F}{k_B T_K}$$