Theory of solids I.

Proposed Topics.

I) Fermi statistics, second quantization and Sommerfeld theory of metals.

II) The Lattice. Bands. Metals and insulators.

III) Electron-Electron correlations.

IV) Magnetism. Itinerant and localized.

V) Electron-phonon interaction.

Theory of solids I. Summary sheets.

I) Second quantization.

Spin and statistics.

The wave function of identical fermions (bosons) is totally antisymmetric (symmetric).

Let $|\Psi\rangle$ be the wave function of N identical bosons or fermions and $P_{i,j}$ an operator which interchanges particle i and j. Then

$$\boxed{P_{i,j}|\Psi\rangle = \epsilon|\Psi\rangle \quad \text{with} \quad \epsilon = \begin{cases} 1 & \text{for bosons} \\ -1 & \text{for fermions} \end{cases}}$$

Slater determinants. (Totally antisymmetric states for identical fermions)

Let $\mathcal{H}$ be the Hilbert space of a single particle.

For the electron: $\mathcal{H} = \mathcal{L}^2(\mathbb{R}^3) \otimes \mathbb{C}^2$

The N-particle Hilbert space is then given by: $\mathcal{H}_N = \underbrace{\mathcal{H} \otimes \mathcal{H} \otimes \cdots \otimes \mathcal{H}}_{\text{N times}}$

Let $|E\rangle$ be a basis of $\mathcal{H}$: $\sum_E |E\rangle\langle E| = 1$ and $\langle E|E'\rangle = \delta_{E,E'}$

→ $|E_1, E_2, \cdots E_N\rangle \equiv |E_1\rangle \otimes |E_2\rangle \cdots \otimes |E_N\rangle$ is a basis of $\mathcal{H}_N$. That is:

$$\boxed{\begin{gathered}\sum_{E_1, E_2, \cdots E_N} |E_1, E_2, \cdots E_N\rangle\langle E_1, E_2, \cdots E_N| = 1 \text{ and} \\ \langle E_1, E_2, \cdots E_N | E'_1, E'_2, \cdots E'_N\rangle = \delta_{E_1, E'_1} \cdots \delta_{E_N, E'_N}\end{gathered}}$$

<u>Slater determinant.</u>

$$\boxed{\begin{aligned}|\Psi_{E_1, E_2, \cdots E_N}\rangle &= \frac{1}{\sqrt{N!}} \sum_{P \in \mathbb{S}(N)} (-1)^P P|E_1, , \cdots E_N\rangle = \\ &= \frac{1}{\sqrt{N!}} \sum_{P \in \mathbb{S}(N)} (-1)^P |E_{P(1)}, , \cdots E_{P(N)}\rangle\end{aligned}}$$

P is a permutation of N objects. $(-1)^P$ is the sign of the permutation.

Notes / Comments.

a) To uniquely define the phase of a Slater determinant, and ordering of single particle eigenstates has to be adopted. For example: $E_1 > E_2 > \cdots > E_N$

(Important since the state $|\Psi\rangle = |\Psi_{E_1,E_2}\rangle + e^{i\varphi}|\Psi_{E_3,E_4}\rangle$ differs from the state $|\Psi\rangle = |\Psi_{E_1,E_2}\rangle - e^{i\varphi}|\Psi_{E_3,E_4}\rangle$)

b) The Slater dets build a basis of the physical Hilbert space of N identical particles.

$$|\Psi\rangle = \sum_{E_1,E_2,\cdots E_N} f(E_1, E_2, \cdots E_N)|\Psi_{E_1,E_2,\cdots E_N}\rangle$$

$$\langle\Psi_{E'_1,E'_2,\cdots E'_N}|\Psi_{E_1,E_2,\cdots E_N}\rangle = \delta_{E'_1,E_1}\delta_{E'_2,E_2}\cdots\delta_{E'_N,E_N}$$

c) Real space representation of Slater determinant.

$$\langle x_1, x_2, \cdots x_N | \Psi_{E_1, E_2, \cdots E_N} \rangle = \Psi_{E_1, E_2, \cdots E_N}(x_1, x_2, \cdots x_N) =$$

$$= \frac{1}{\sqrt{N!}} \sum_{P \in \mathbb{S}(N)} (-1)^P \langle x_1, x_2, \cdots x_N | E_{P(1)}, , \cdots E_{P(N)} \rangle$$

$$= \frac{1}{\sqrt{N!}} \sum_{P \in \mathbb{S}(N)} (-1)^P \overbrace{\langle x_1 | E_{P(1)}}^{\equiv \Psi_{E_{P(1)}}(x_1)} \rangle \cdots \langle x_N | E_{P(N)} \rangle$$

$$= \frac{1}{\sqrt{N!}} \det \begin{pmatrix} \Psi_{E_1}(x_1) & \Psi_{E_1}(x_2) & \cdots & \Psi_{E_1}(x_N) \\ \vdots & \vdots & \vdots & \vdots \\ \Psi_{E_N}(x_1) & \Psi_{E_N}(x_2) & \cdots & \Psi_{E_N}(x_N) \end{pmatrix}$$

Position and spin

Note: $x = (\vec{x}, s)$, $\sum_x \equiv \int_{\mathbb{R}^3} d^3\vec{x} \sum_s$

c) Expectation value of operators between Slater determinants.

Let.

$$\langle x'_1, x'_2, \cdots x'_N | H | x_1, x_2, \cdots x_N \rangle = \delta_{x_1, x'_1} \cdots \delta_{x_N, x'_N} \left(\sum_n \overset{\text{One part. Op.}}{\overset{\downarrow}{H_0(x_n)}} + \frac{1}{2} \sum_{n \neq m} \overset{\text{Two part. Op.}}{\overset{\downarrow}{V(x_n, x_m)}} \right)$$

$$\langle \Psi_{E'_1, E'_2, \cdots E'_N} | H | \Psi_{E_1, E_2, \cdots E_N} \rangle =$$

$$\sum_P (-1)^P \sum_n \prod_{s \neq m} \langle E'_{P(s)} | E_s \rangle \langle E'_{P(m)} | H_0 | E_m \rangle +$$

$$\frac{1}{2} \sum_P (-1)^P \sum_{n \neq m} \prod_{s \neq m, n} \langle E'_{P(s)} | E_s \rangle \langle E'_{P(n)}, E'_{P(m)} | V | E_n, E_m \rangle$$

Note that:

$$\langle E'_{P(n)}, E'_{P(m)} | V | E_n, E_m \rangle = \sum_{x_1, x_2} \Psi^\star_{E'_{P(n)}}(x_1) \Psi^\star_{E'_{P(m)}}(x_2) V(x_1, x_2) \Psi_{E_n}(x_1) \Psi_{E_m}(x_2)$$

Example: For two particles

$$\begin{aligned}\langle \Psi_{E_1',E_2'}|H|\Psi_{E_1,E_2}\rangle =& \delta_{E_1,E_1'}\langle E_2'|H_0|E_2\rangle + \delta_{E_2,E_2'}\langle E_1'|H_0|E_2\rangle - \\ & \delta_{E_2,E_1'}\langle E_2'|H_0|E_1\rangle - \delta_{E_1,E_2'}\langle E_1'|H_0|E_2\rangle + \\ & \langle E_1', E_2'|V|E_1, E_2\rangle - \underbrace{\langle E_1', E_2'|V|E_2, E_1\rangle}_{\text{Exchange Interaction.}}\end{aligned}$$

The occupation number space.

Let $|n_1, n_2, n_3, \cdots n_\infty\rangle$ define a physical state with n_i particles in the single particle state i . We will again assume an ordering of the single particle states. (According to energy for example)

The states $|n_1, n_2, n_3, \cdots n_\infty\rangle$ build a basis of the Fock space.

$$\mathcal{H}_F = \oplus_{N=0}^{\infty} \mathcal{H}_N, \quad \mathcal{H}_N = \underbrace{\mathcal{H} \otimes \cdots \otimes \mathcal{H}}_{\text{N times}}$$

$$\sum_{n_1, n_2, \cdots, n_\infty} |n_1, n_2, n_3, \cdots n_\infty\rangle\langle n_1, n_2, n_3, \cdots n_\infty| = 1$$

$$\langle n_1', n_2', n_3', \cdots n_\infty' | n_1, n_2, n_3, \cdots n_\infty\rangle = \delta_{n_1', n_1} \delta_{n_2', n_2} \cdots \delta_{n_\infty', n_\infty}$$

For fermions: $n_i = 0, 1$

For Bosons: $n_i = 0, \cdots, \infty$

Fermionic creation and annihilation operators.

Let $\hat{c}_i^\dagger$ ($\hat{c}_i$) denote fermionic creation (annihilation) operators. These operators are defined through the anticommutation relations.

$$\left\{\hat{c}_i^\dagger, \hat{c}_j\right\} \equiv \hat{c}_i^\dagger \hat{c}_j + \hat{c}_j \hat{c}_i^\dagger = \delta_{i,j} \qquad \left\{\hat{c}_i^\dagger, \hat{c}_j^\dagger\right\} = \left\{\hat{c}_i, \hat{c}_j\right\} = 0$$

The vacuum state $|0\rangle$ is defined by: $c_i|0\rangle = \quad \forall\, i$

With the above definitions:

$$|n_1, n_2, n_3, \cdots n_\infty\rangle = \left(\hat{c}_1^\dagger\right)^{n_1} \left(\hat{c}_2^\dagger\right)^{n_2} \cdots \left(\hat{c}_\infty^\dagger\right)^{n_\infty} |0\rangle$$

Properties.

a) Two fermions cannot be in the same sate since $\hat{c}_i^\dagger \hat{c}_i^\dagger = 0$

b)

$$\hat{c}_s^\dagger|n_1, n_2, n_3, \cdots n_\infty\rangle = \begin{cases} (-1)^{n_1+n_s\cdots n_{s-1}}|n_1, \cdots, n_s+1, \cdots n_\infty\rangle & \text{if } \; n_s = 0 \\ 0 & \text{if } \; n_s = 1 \end{cases}$$

$$\hat{c}_s|n_1, n_2, n_3, \cdots n_\infty\rangle = \begin{cases} (-1)^{n_1+n_s\cdots n_{s-1}}|n_1, \cdots, n_s-1, \cdots n_\infty\rangle & \text{if } \; n_s = 1 \\ 0 & \text{if } \; n_s = 0 \end{cases}$$

c) The particle number operator. $\hat{n}_s \equiv \hat{c}_s^\dagger \hat{c}_s$

$$\hat{n}_s|n_1, n_2, n_3, \cdots n_\infty\rangle = n_s|n_1, n_2, n_3, \cdots n_\infty\rangle$$

$$\hat{n}_s\hat{n}_s = \hat{n}_s$$

d) $\langle n_1', n_2', n_3', \cdots n_\infty'|n_1, n_2, n_3, \cdots n_\infty\rangle = \delta_{n_1',n_1}\delta_{n_2',n_2}\cdots\delta_{n_\infty',n_\infty}$

Operators in the occupation number representation.

The first quantized operators A act on the space of Salter determinants.

The second operators $\hat{A}$ act on the occupation number states.

Let $|\Psi_{E'_1,E'_2,\cdots E'_N}\rangle$ and $|\Psi_{E_1,E_2,\cdots E_N}\rangle$ be two Slater determinants. The second

quantized form of the operator A is defined by:

$$\langle\Psi_{E'_1,E'_2,\cdots E'_N}|A|\Psi_{E_1,E_2,\cdots E_N}\rangle \equiv \langle 0|\hat{c}_{E'_N}\cdots\hat{c}_{E'_1}\,\hat{A}\,\hat{c}^{\dagger}_{E_1}\cdots\hat{c}^{\dagger}_{E_N}|0\rangle$$

To give an explicit form of the second quantized operator it is convenient to introduce field operators:

$$\hat{\Psi}^{\dagger}(x) = \sum_E \hat{c}^{\dagger}_E\langle x|E\rangle^{\dagger} = \sum_E \hat{c}^{\dagger}_E\Psi^{\dagger}_E(x)$$

The field operator creates a particle at *position* x since:

$$\hat{\Psi}^{\dagger}(x)|0\rangle = \sum_E \hat{c}^{\dagger}_E|0\rangle\langle E|x\rangle = \sum_E |E\rangle\langle E|x\rangle = |x>$$

Let the first quantized form of a Hamiltonian in real space read:

$$\langle x'_1, x'_2, \cdots x'_N | H | x_1, x_2, \cdots x_N \rangle = \delta_{x_1, x'_1} \cdots \delta_{x_N, x'_N} \left(\sum_n H_0(x_n) + \frac{1}{2} \sum_{n \neq m} V(x_n, x_m) \right)$$

Then:

$$\hat{H} = \sum_x \hat{\Psi}^\dagger(x) H_0(x) \hat{\Psi}\ (x) - \frac{1}{2} \sum_{x_1, x_2} \hat{\Psi}^\dagger(x_1) \hat{\Psi}^\dagger(x_2) V(x_1, x_2) \hat{\Psi}\ (x_1) \hat{\Psi}\ (x_2)$$

For:

$$\hat{\Psi}^\dagger(x) = \sum_E \hat{c}_E^\dagger \langle x | E \rangle^\dagger = \sum_E \hat{c}_E^\dagger \Psi_E^\dagger(x)$$

$$\hat{H} = \sum_{E, E'} \langle E | H_0 | E' \rangle \hat{c}_E^\dagger \hat{c}_{E'} - \frac{1}{2} \sum_{E, E', E'', E'''} \langle E, E' | V | E'', E''' \rangle \hat{c}_E^\dagger \hat{c}_{E'}^\dagger \hat{c}_{E''} \hat{c}_{E'''}$$

II) Sommerfeld theory of Metals. (Fermi liquid fix-point.)

$$H = \sum_i \frac{\vec{P}_i^2}{2m} \otimes 1_i \qquad \mathcal{H}_N = \otimes_{i=1}^{N} \mathcal{H}^{(i)} \qquad \mathcal{H}^{(i)} = \mathcal{L}^2(\mathbb{R}^3) \otimes \mathbb{C}^2$$

One-particle states:

$$|\Psi\rangle = |\vec{p}\rangle \otimes |s\rangle \equiv |\vec{p}, s\rangle \qquad H|\Psi\rangle = \frac{\vec{p}^2}{2m}|\Psi\rangle$$

$$\Psi'_s(x) = \langle \vec{x}, s' | \vec{p}, s\rangle = \langle \vec{x}|\vec{p}\rangle\langle s|s'\rangle = Ce^{i\vec{p}\cdot\vec{x}/\hbar}\delta_{s,s'}$$

Spinor:

$$\vec{\Psi}(x) = \begin{pmatrix} \langle x, \uparrow |\Psi\rangle \\ \langle x, \downarrow |\Psi\rangle \end{pmatrix}$$

Periodic boundary conditions in a box of linear length L yields the quantization

$$\vec{p} = \hbar\frac{2\pi}{L}(n_1, n_2, n_3) \quad n_i \in \mathbb{Z}$$ and $$C = \frac{1}{\sqrt{V}} = \frac{1}{\sqrt{L}^3}$$

Field operators: $$\hat{\Psi}_s^\dagger(\vec{x}) = \sum_{\vec{p},s'} \langle \vec{p}, s' | \vec{x}, s \rangle \hat{c}^\dagger_{\vec{p},s'} = \frac{1}{\sqrt{V}} \sum_{\vec{p}} e^{-i\vec{p}\cdot\vec{x}/\hbar} \hat{c}^\dagger_{\vec{p},s}$$

Commutation rules:

$$\left\{ \hat{c}^\dagger_{\vec{p},s}, \hat{c}_{\vec{p}',s'} \right\} = \delta_{\vec{p},\vec{p}'} \delta_{s,s'} \qquad \left\{ \hat{c}^\dagger_{\vec{p},s}, \hat{c}^\dagger_{\vec{p}',s'} \right\} = \left\{ \hat{c}_{\vec{p},s}, \hat{c}_{\vec{p}',s'} \right\} = 0$$

$$\left\{ \hat{\Psi}_s(\vec{x})^\dagger, \hat{\Psi}_{s'}(\vec{x}') \right\} = \delta^{(3)}(\vec{x} - \vec{x}') \delta_{s,s'} \qquad \left\{ \hat{\Psi}_s(\vec{x})^\dagger, \hat{\Psi}_{s'}(\vec{x}')^\dagger \right\} = \left\{ \hat{\Psi}_s(\vec{x}) \ , \hat{\Psi}_{s'}(\vec{x}') \ \right\} = 0$$

Hamiltonian in second quantized form:

$$\hat{H} = \sum_{\vec{p},s} \epsilon(\vec{p}) \hat{c}^\dagger_{\vec{p},s} \hat{c}_{\vec{p},s}, \quad \epsilon(\vec{p}) = \frac{\vec{p}^2}{2m}$$

Ground state wave function.

$$|\Psi_0\rangle = \prod_{\substack{\vec{p},\sigma \\ \epsilon(\vec{p})<\epsilon_F}} \hat{c}^\dagger_{\vec{p},\sigma}|0\rangle$$

The locus of momenta with $\epsilon(\vec{p}) = \epsilon_F$ defines the Fermi surface.

1d: two points
2d: a circle
3d: the surface of a sphere

$$|\vec{k}_F| = \frac{\sqrt{2m\epsilon_F}}{\hbar} \qquad \vec{p} = \hbar\vec{k}$$

Ground state energy.

$$E_0 = \langle\Psi_0|\hat{H}|\Psi_0\rangle = 2\sum_{|\vec{k}|<k_F}\epsilon(\vec{k}) = V2\int_0^{\epsilon_F} \mathrm{d}\epsilon g(\epsilon)\epsilon$$

Density of states:

$$g(\epsilon) = \frac{1}{(2\pi)^d}\int d^d\vec{k}\ \delta^{(d)}\left(\epsilon(\vec{k}) - \epsilon\right) = \underbrace{\frac{(2m)^{d/2-1}}{2(2\pi\hbar)^d}}_{\alpha_d}\epsilon^{d/2-1}$$

$$E_0 = \frac{2V\alpha_d}{d/2+1}{\epsilon_F}^{d/2+1}$$

Particle Number: $$N = \langle\Psi_0|\sum_{\vec{p},\sigma}\hat{n}_{\vec{p},\sigma}|\Psi_0\rangle = 2V\int_0^{\epsilon_F} d\epsilon g(\epsilon) = \frac{4V\alpha_d}{d}{\epsilon_F}^{d/2}$$

Thus: $$E_0(N,V) \propto N\rho^{2/d} \quad \text{where} \quad \rho = N/V$$

Hence and as required by thermodynamics $E_0(N,V)$ is a homogeneous function,

$$E_0(\lambda N, \lambda V) = \lambda E_0(N,V)$$

and

$$\left.\frac{\partial^2 E_0(N,V)}{\partial N^2}\right|_V > 0 \qquad\qquad \left.\frac{\partial^2 E_0(N,V)}{\partial V^2}\right|_N > 0$$

Thermodynamics:

Density matrix in grand canonical ensemble: (Mixed state) $\hat{\rho} = \frac{1}{Z} e^{-\beta\left(\hat{H} - \mu \hat{N}\right)}$

$$Z = \mathrm{Tr} e^{-\beta\left(\hat{H} - \mu \hat{N}\right)}$$

Partition function.

$$\hat{N} = \sum_{\vec{p},\sigma} \hat{n}_{\vec{p},\sigma}$$

Particle number operator.

$$\beta = \frac{1}{k_B T}$$

Inverse temperature.

$$\mu$$

Chemical potential.

Expectation value of an observable: $\langle \hat{O} \rangle = \mathrm{Tr} \hat{\rho}\, \hat{O}$

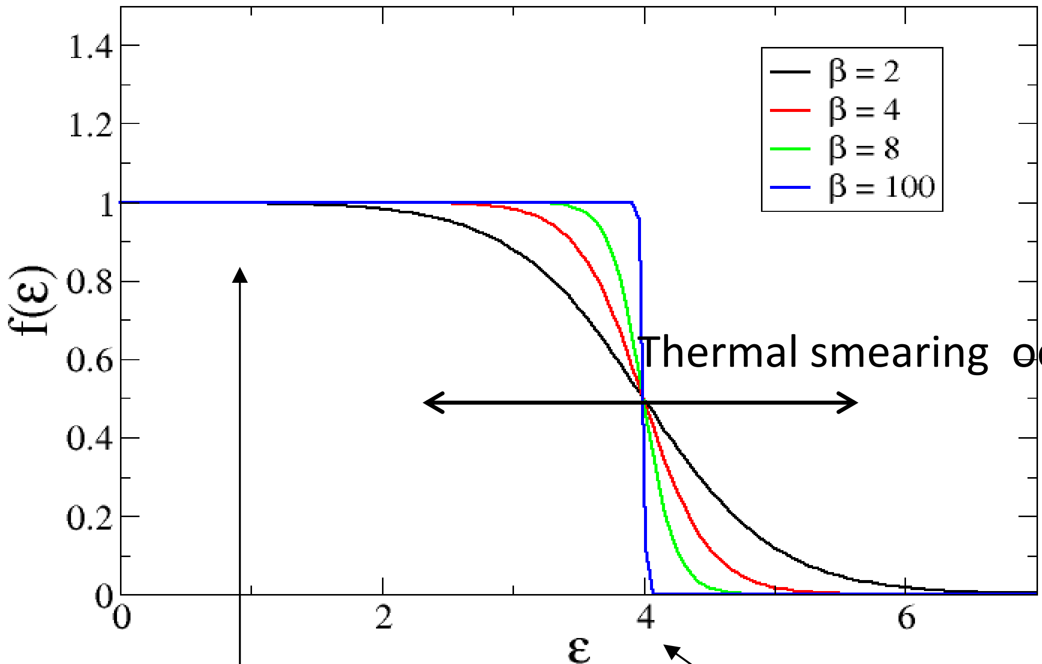
Properties for free electrons:

$$Z = \prod_{\vec{p},\sigma} \left(1 + e^{-\beta[\epsilon(\vec{p}) - \mu]}\right)$$

$$\langle \hat{n}_{\vec{p},\sigma} \rangle = \frac{1}{1 + e^{-\beta[\epsilon(\vec{p}) - \mu]}}$$

Fermi-function.

The Fermi Function.



Thermal smearing occurs on the scale $k_B T$

Chemical potential: $\mu = 4$

Electrons at energies $k_B T$ below the chemical potential are frozen out !

Specific heat.

Using the Sommerfeld expansion:

$$\int_{-\infty}^{\infty} d\epsilon \quad h(\epsilon) f(\epsilon) = \int_{-\infty}^{\mu} \quad h(\epsilon) \quad + h'(\mu)\,(k_B T)^2\,\frac{\pi^2}{6} \quad + \quad \mathcal{O}(k_B T^4)$$

One will show that the specific heat is given by:

$$\frac{1}{V}\left.\frac{\partial E}{\partial T}\right|_{V,N} = \frac{2\pi^2}{3} k_B^2 g(\epsilon_f) T + \mathcal{O}(T^3)$$

Each electron acquires a thermal energy $k_B T$

# of particles which acquire this energy (Fermi statistics) is $k_B T g(\epsilon_f)$

$$E \propto (k_B T)^2 g(\epsilon_f)$$

Pauli spin susceptibility.

First quantized form of Hamiltonian:

$$H = \frac{\vec{P}^2}{2m} \otimes 1 - \frac{g\mu_B}{\hbar} \sum_{i=1}^{3} B_i \otimes S_i \quad \text{with} \quad S_i = \frac{\hbar}{2}\sigma_i$$

σ_i are the Pauli spin matrices and: $$[S_i, S_j] = i \sum_{k=1}^{3} \epsilon^{i,j,k} S_k$$

Second quantized form:

$$\hat{H} = \sum_{\vec{p},s} \epsilon(\vec{p}) \hat{c}^\dagger_{\vec{p},s} \hat{c}_{\vec{p},s} - \frac{g\mu_B}{\hbar} \vec{B} \cdot \hat{\vec{S}}$$

$$\hat{\vec{S}} = \sum_{\vec{p}} \hat{\vec{S}}_{\vec{p}} \quad \text{and} \quad \hat{\vec{S}}_{\vec{p}} = \frac{\hbar}{2} \sum_{s,s'} \hat{c}^\dagger_{\vec{p},s} \vec{\sigma}_{s,s'} \hat{c}_{\vec{p},s'}$$

Magnetic field in z-direction:

$$\hat{H} = \sum_{\vec{p},s=\pm 1} \left(\epsilon(\vec{p}) - \mu_B B s\right) \hat{c}^{\dagger}_{\vec{p},s} \hat{c}_{\vec{p},s}$$

Induced magnetization of the electron gas: $\hat{M} = \sum_{\vec{p}} \hat{c}^{\dagger}_{\vec{p},\uparrow} \hat{c}_{\vec{p},\uparrow} - \hat{c}^{\dagger}_{\vec{p},\downarrow} \hat{c}_{\vec{p},\downarrow}$

$$\chi = \frac{1}{V} \left. \frac{\partial \langle \hat{M} \rangle}{\partial B} \right|_{B=0} = -2\mu_B \int \mathrm{d}\epsilon \;\; g(\epsilon) \frac{\partial f(\epsilon)}{\partial \epsilon}$$

With the Sommerfeld expansion:

$$\frac{\chi}{2\mu_B} = g(\mu) + g''(\mu)(k_B T)^2 \frac{\pi^2}{6} + \mathcal{O}(k_B T^4)$$

THE SPECIFIC HEATS OF METALS AT LOW TEMPERATURES

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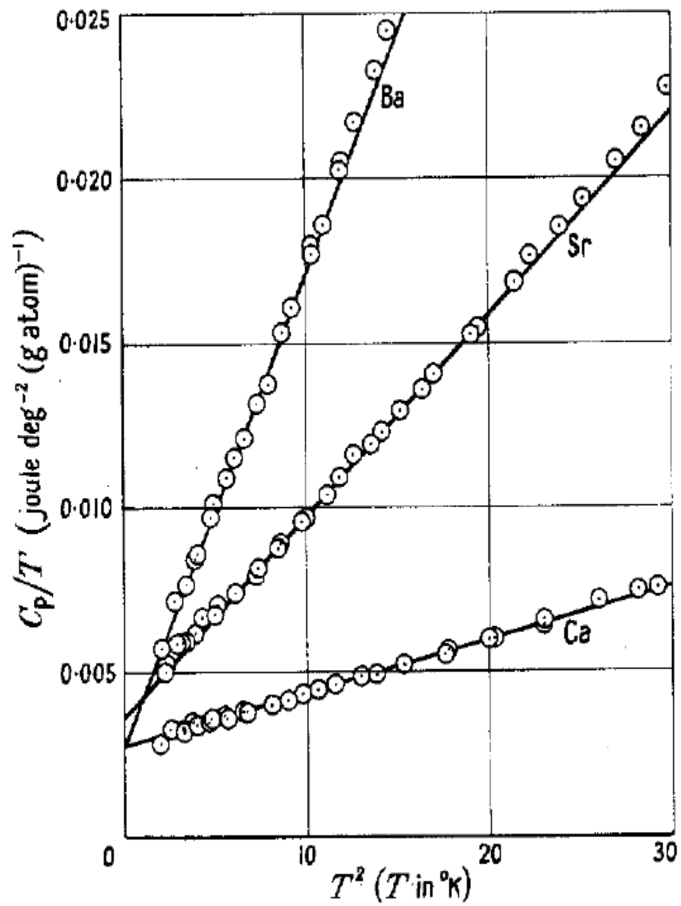

Figure 16. Experimental results for the alkaline earth metals. Plot of C_p/T against T^2.

1958 Rep. Prog. Phys. 21 226

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Specific heat of normal liquid ^{3}He

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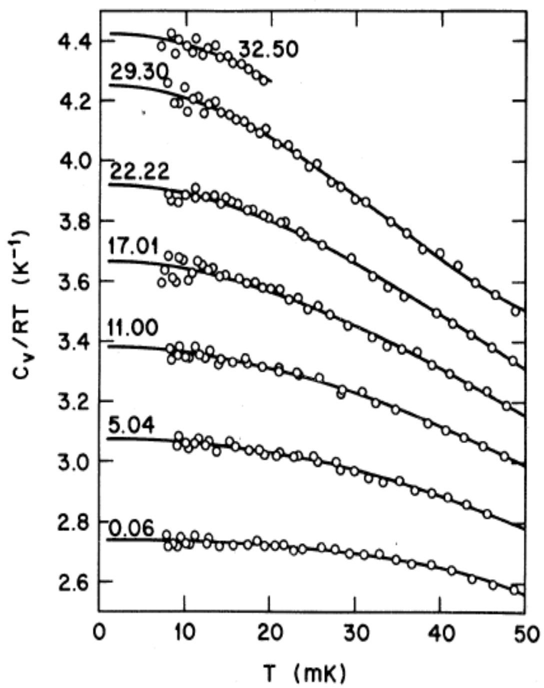

FIG. 14. Specific-heat measurements plotted as C_V/RT vs T. Numbers give the sample pressures in bars at 0.1 K. Solid curves are least-squares fits of the data using Eq. (11).

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Effective mass, spin fluctuations, and zero sound in liquid ^{3}He

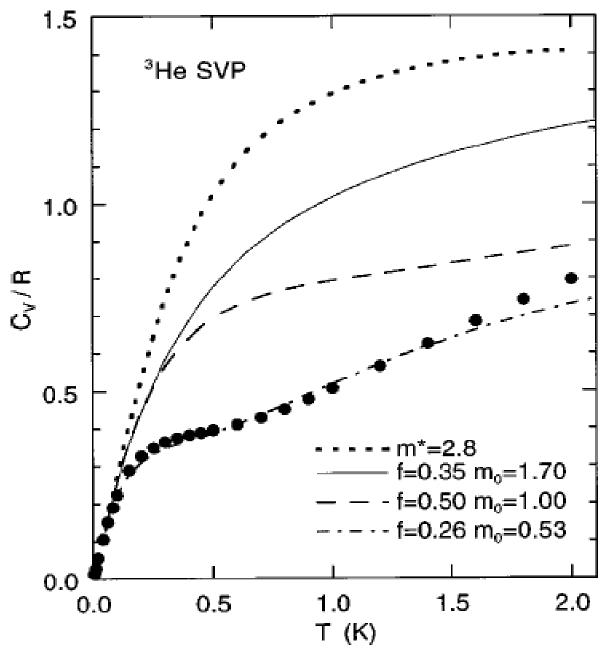


FIG. 10. Measured specific heat $C_V(T)$ (Ref. 19) (dots) as a function of temperature compared with $C_V(T)$ calculated using a free Fermi gas model $m^*=2.8$ (dotted line) and with the mass-enhanced model $m^*(k)$, Eq. (8), with $f=0.35$ and $m_0=1.7$ (solid line), with $f=0.5$ and $m_0=1$ (dashed line), and with best-fit values $f=0.26$ and $m_0=0.53$ (dash-dotted line).

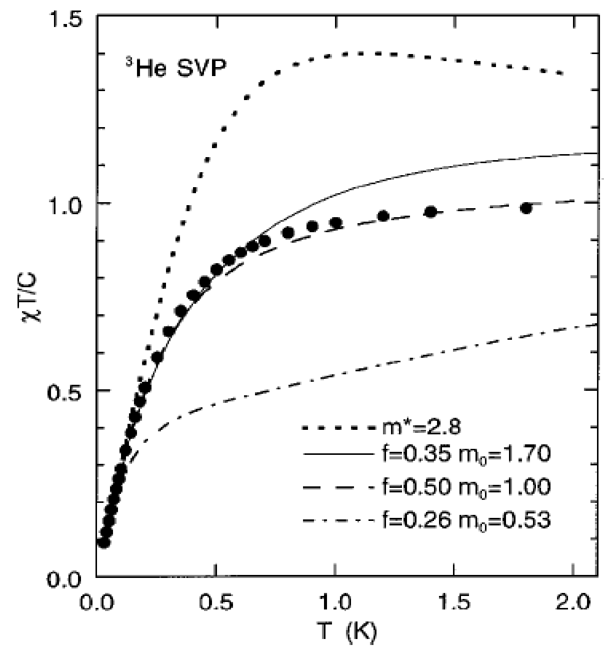


FIG. 11. Measured static magnetic susceptibility $\chi(T)$ (Ref. 47) (dots) multiplied by the temperature compared with $\chi(T)T$ calculated using a free Fermi gas model $m^*=2.8$ (dotted line) and with the mass-enhanced model $m^*(k)$, Eq. (8), with $f=0.35$ and $m_0=1.7$ (solid line), with $f=0.5$ and $m_0=1$ (dashed line), and with $f=0.26$ and $m_0=0.53$ (dash-dotted line), the values that give a good description of the specific heat.

II) The Lattice.

Electrons are subject to a periodic potential. Let

$\vec{R}_{\vec{n}} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$ denote the unit cells of the crystal structure.

$\vec{a}_i$ are the lattice vectors.

For N-ions per unit cell of net charge Z_μ and located at the positions $\vec{r}_\mu$ with respect to $\vec{R}_{\vec{n}}$ the ionic potential reads:

$$V_{e-ion}(\vec{x}) = -e^2 \sum_{\vec{n}} \sum_{\mu=1}^{N} \frac{Z_\mu}{|\vec{x} - (\vec{R}_{\vec{n}} + \vec{r}_\mu)|}$$

Hence $H = \frac{\vec{P}^2}{2m} + V_{e-ion}(\vec{x})$ is invariant under translations $\vec{x} \rightarrow \vec{x} + \vec{R}_{\vec{n}}$

→ Crystal momentum conservation and Bloch theorem.

The translation Operator.

Def: $$\hat{\boldsymbol{T}}_{\vec{\boldsymbol{a}}}|\vec{\boldsymbol{x}}\rangle = |\vec{\boldsymbol{x}}+\vec{\boldsymbol{a}}\rangle$$

Properties.

$$\hat{T}^{\dagger}_{\vec{a}}\hat{T}_{\vec{a}} = 1$$ Unitary.

$$\hat{T}_{\vec{a}}\hat{T}_{\vec{b}} = \hat{T}_{\vec{a}+\vec{b}} = \hat{T}_{\vec{b}}\hat{T}_{\vec{a}}$$ Abelian group.

For $\hat{T}_{\vec{a}}|\lambda\rangle = \lambda(\vec{a})|\lambda\rangle \quad |\lambda(\vec{a})| = 1 \quad \text{and} \quad \lambda(\vec{a})\lambda(\vec{b}) = \lambda(\vec{a}+\vec{b})$

$$\hat{T}^{\dagger}_{\vec{a}}\hat{\vec{X}}\hat{T}_{\vec{a}} = \hat{\vec{X}} + \vec{a}$$ Transformation of position operator

$$\hat{T}^{\dagger}_{\vec{a}}\hat{\vec{P}}\hat{T}_{\vec{a}} = \hat{\vec{P}}$$ Transformation of momentum operator

Symmetry. $$\left[\hat{\boldsymbol{T}}_{\vec{\boldsymbol{a}}}, \hat{\boldsymbol{H}}\right] = 0$$

→ Eigenvectors of $\hat{H}$ can be chosen to be also eigenvectors of $\hat{T}_{\vec{a}}$

Bloch $\exists \; |\Psi_n\rangle$

$$\boldsymbol{H|\Psi_n\rangle = E_n|\Psi_n\rangle}$$
$$\boldsymbol{T_{\vec{R}_{\vec{n}}}|\Psi_n\rangle = \lambda(\vec{R}_{\vec{n}})|\Psi_n\rangle}$$

Since: $\vec{R}_{\vec{n}} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$, $\lambda(\vec{R}_{\vec{n}}) = \lambda^{n_1}(\vec{a}_1)\lambda^{n_2}(\vec{a}_2)\lambda^{n_3}(\vec{a}_3)$

Let $\lambda(\vec{a}_j) = e^{2\pi i x_j}$ $j = 1, 2, 3$ $x_j \in \mathbb{R}$ and $\boldsymbol{\vec{b}_i \cdot \vec{a}_j = 2\pi\delta_{i,j}}$

Then: $\lambda(\vec{R}_{\vec{n}}) = e^{i\vec{k}\cdot\vec{R}_{\vec{n}}}$ with $\vec{k} = x_1\vec{b}_1 + x_2\vec{b}_2 + x_3\vec{b}_3$

Reciprocal Lattice. $\vec{G} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$ $m_i \in \mathbb{Z}$

Bloch, rewritten

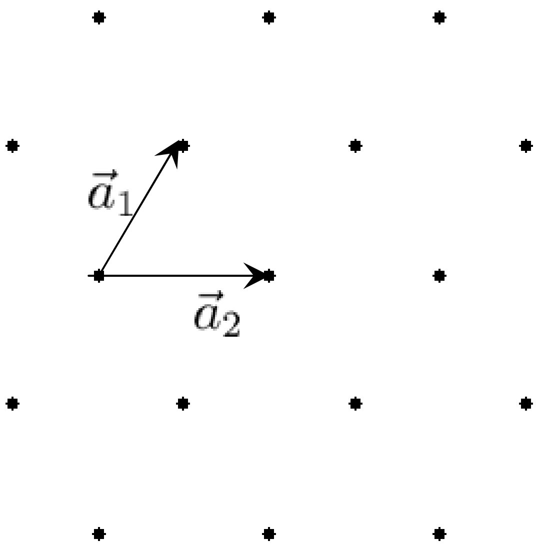
$$\boldsymbol{H|n,\vec{k}\rangle = E_n(\vec{k})|n,\vec{k}\rangle}$$
$$\boldsymbol{T_{\vec{R}_{\vec{n}}}|n,\vec{k}\rangle = e^{i\vec{k}\cdot\vec{R}_{\vec{n}}}|n,\vec{k}\rangle}$$

- $|n,\vec{k}\rangle = |n,\vec{k}+\vec{G}\rangle$ The crystal momentum can be restricted to the Brillouin zone (Wigner Seitz cell of the reciprocal lattice.)
- $$\boldsymbol{\sum_{n,\vec{k}\in BZ} |n,\vec{k}\rangle\langle n,\vec{k}| = 1}$$

Example of Brillouin zone: Triangular lattice.

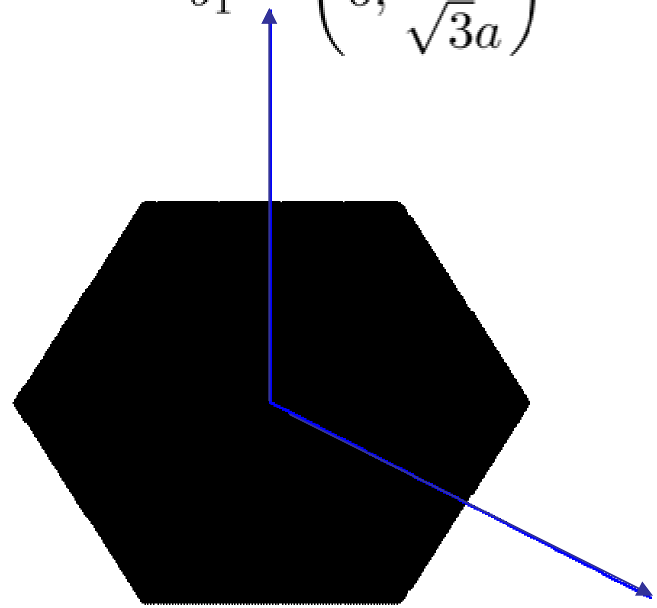
Real space.

$$\vec{a}_1 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right) \quad \vec{a}_2 = a\,(1,0)$$



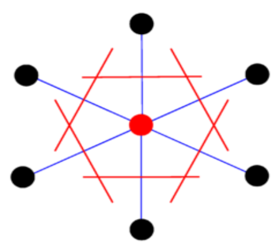
Brillouin Zone. Wigner Seitz cell of the reciprocal lattice.

$$\vec{b}_1 = \left(0, \frac{4\pi}{\sqrt{3}a}\right)$$



$$\vec{b}_2 = \left(\frac{2\pi}{a}, -\frac{2\pi}{\sqrt{3}a}\right)$$

Construction of the Wigner-Seitz cell.



Bloch states.

- Real space representation.

$$\langle\vec{x}|n,\vec{k}\rangle = \Psi_{n,\vec{k}}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}}u_{n,\vec{k}}(\vec{x})$$

$$u_{n,\vec{k}}(\vec{x}+\vec{R}_{\vec{n}}) = u_{n,\vec{k}}(\vec{x})$$

- Extended states.

- Quantization of crystal momentum follows from boundary condition.

$$\Psi_{n,\vec{k}}(\vec{x}+L\vec{a}_j) = \Psi_{n,\vec{k}}(\vec{x}) \qquad \vec{k} = \frac{m_1}{L}\vec{b}_1 + \frac{m_2}{L}\vec{b}_2 + \frac{m_3}{L}\vec{b}_3 \quad m_j \in \mathbb{Z}$$

- Field operators.

$$\hat{\Psi}^\dagger_s(\vec{x})|0\rangle \equiv |\vec{x},s\rangle = \sum_{n,\vec{k}\in BZ,s'} |n,\vec{k},s'\rangle\langle n,\vec{k},s'|\vec{x},s\rangle = \sum_{n,\vec{k}\in BZ} \Psi^\dagger_{n,\vec{k}}(\vec{x})\;\hat{c}^\dagger_{n,\vec{k},s}|0\rangle$$

- Second quantized Hamiltonian

$$\hat{H} = \sum_{s,s'}\int d^3\vec{x}\int d^3\vec{x}'\,\hat{\Psi}^\dagger_s(\vec{x})\langle\vec{x},s|H|\vec{x}',s'\rangle\hat{\Psi}_{s'}(\vec{x}')$$

$$= \sum_{n,\vec{k}\in BZ,s} E_n(\vec{k})\hat{c}^\dagger_{n,\vec{k},s}\hat{c}_{n,\vec{k},s}$$

Wannier Functions.

- Let N be the number of unit cells and let us assume periodic boundary conditions. Then

$$\frac{1}{N}\sum_{\vec{R}_{\vec{n}}} e^{i\vec{k}\cdot\vec{R}_{\vec{n}}} = \delta_{\vec{k},\vec{0}}$$

$$\vec{k} = \frac{m_1}{L}\vec{b}_1 + \frac{m_2}{L}\vec{b}_2 + \frac{m_3}{L}\vec{b}_3 \quad m_j \in \mathbb{Z}$$

$\vec{k} \in BZ$

$\vec{R}_{\vec{n}}$ Runs over all unit cells.

$$|n\vec{k}\rangle = \frac{1}{\sqrt{N}}\sum_{\vec{R}_{\vec{n}}} e^{i\vec{k}\cdot\vec{R}_{\vec{n}}} \underbrace{\frac{1}{\sqrt{N}}\sum_{\vec{k}\in BZ} e^{-i\vec{k}'\cdot\vec{R}_{\vec{n}}}|n,\vec{k}'\rangle}_{\equiv |n,\vec{R}_{\vec{n}}\rangle}$$

$\equiv |n,\vec{R}_{\vec{n}}\rangle$ Wannier state.

- Bloch → Delocalized
  Wannier → Localized.

- Completeness: $\displaystyle\sum_{n,\vec{R}_{\vec{n}}} |n,\vec{R}_{\vec{n}}\rangle\langle n,\vec{R}_{\vec{n}}| = 1$

- Real space representation. $\langle\vec{x}|n,\vec{R}_{\vec{n}}\rangle = \Phi(\vec{x}-\vec{R}_{\vec{n}})$

- Note. The Wannier states are not uniquely defined. Let U be a unitary transformation which rotates the band index. Then,

$$|n, \vec{R}_{\vec{n}}\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{k}\in BZ} \sum_{m=1}^{N_{bands}} e^{-i\vec{k}'\cdot\vec{R}_{\vec{n}}} U_{n,m} |m, \vec{k}'\rangle$$

equally defines a Wannier state.

- Field Operators.

$$\hat{\Psi}_s^\dagger(\vec{x})|0\rangle \equiv |\vec{x}, s\rangle = \sum_{n,\vec{R}_{\vec{n}},s'} |n, \vec{R}_{\vec{n}}, s'\rangle\langle n, \vec{R}_{\vec{n}}, s'|\vec{x}, s\rangle$$

$$= \sum_{n,\vec{R}_{\vec{n}}} \Phi_n^\dagger(\vec{x} - \vec{R}_{\vec{n}})\, \hat{c}^\dagger_{n,\vec{R}_{\vec{n}},s}|0\rangle$$

<u>Fermionic commutation rules.</u>

$$\left\{\hat{c}^\dagger_{n,\vec{R},s}, \hat{c}_{n',\vec{R},s'}\right\} = \delta_{n,n'}\delta_{\vec{R},\vec{R}'}\delta_{s,s'} \text{ and } \left\{\hat{c}^\dagger_{n,\vec{R},s}, \hat{c}^\dagger_{n',\vec{R},s'}\right\} = \left\{\hat{c}_{n,\vec{R},s}, \hat{c}_{n',\vec{R},s'}\right\} = 0$$

- Second quantized Hamiltonian (tight binding)

$$\hat{H} = \sum_{s,s'} \int d^3\vec{x} \int d^3\vec{x}' \, \hat{\Psi}_s^\dagger(\vec{x}) \langle \vec{x}, s | H | \vec{x}', s' \rangle \hat{\Psi}_{s'}(\vec{x}')$$

$$= \sum_{n,n',\vec{R},\vec{R}',s} t_{n,n'}(\vec{R} - \vec{R}') \hat{c}^\dagger_{n,\vec{R},s} \hat{c}_{n',\vec{R}',s}$$

Hopping matrix element between Wannier states centered around R and R' .

$$t_{n,n'}(\vec{R} - \vec{R}') = \int \mathrm{d}\vec{x} \, \Phi_n^\dagger(\vec{x} - \vec{R}) H(\vec{P}, \vec{x}) \Phi_{n'}(\vec{x} - \vec{R}')$$

Example. One dimensional chain.

$$\hat{H} = -t \sum_{\vec{i}=\vec{a}\cdots L\vec{a},\sigma} \left(\hat{c}^{\dagger}_{\vec{i},\sigma} \hat{c}_{\vec{i}+\vec{a},\sigma} + \hat{c}^{\dagger}_{\vec{i}+\vec{a},\sigma} \hat{c}_{\vec{i},\sigma} \right)$$

$\vec{i} = n\vec{a}$ Direct lattice.

$\vec{G} = n\frac{\vec{a}}{|\vec{a}|}\frac{2\pi}{|\vec{a}|}$ Reciprocal lattice.

Periodic Boundary.

$$\hat{c}^{\dagger}_{\vec{i}+L\vec{a},\sigma} = \hat{c}^{\dagger}_{\vec{i},\sigma}$$

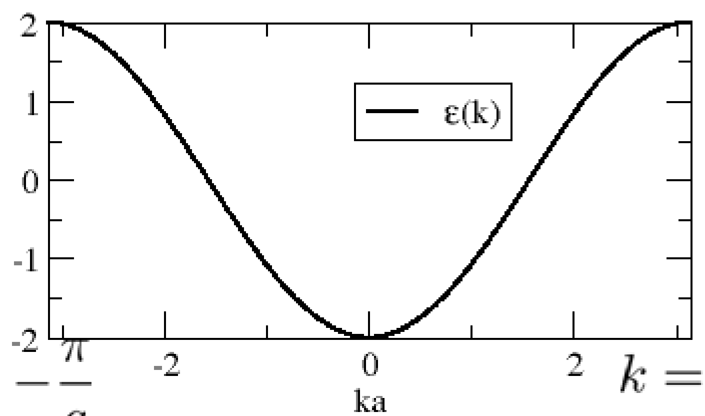
$$\vec{k} = m\frac{\vec{G}}{L}$$

Bloch. $\hat{c}^{\dagger}_{\vec{k},\sigma} = \frac{1}{\sqrt{L}} \sum_{\vec{i}} e^{i\vec{k}\cdot\vec{i}} \hat{c}^{\dagger}_{\vec{i},\sigma}$

$$\hat{H} = \sum_{\vec{k}\in BZ,\sigma} \epsilon(\vec{k}) \hat{c}^{\dagger}_{\vec{k},\sigma} \hat{c}_{\vec{k},\sigma}$$

$\epsilon(\vec{k}) = -2t\cos(\vec{k}\cdot\vec{a})$

For $\vec{a} = a\vec{e}_x$



$k = -\frac{\pi}{a}$ $k = \frac{\pi}{a}$

BZ. $k \in \left[-\frac{\pi}{a}, \frac{\pi}{a} \right[$

III) Electron-electron correlations.

a) Coulomb repulsion in second quantization.

General form. Hubbard model. Gellium.

a) Kubo Linear response.
Zero temperature, Finite temperature.
Response to an eternal potential.

c) The dielectric constant.
Screening, Plasmons, Friedel oscillations.

d) Lifetime of a quasi-particle

e) Landau theory of Fermi liquids.

III a Coulomb repulsion in second quantization.

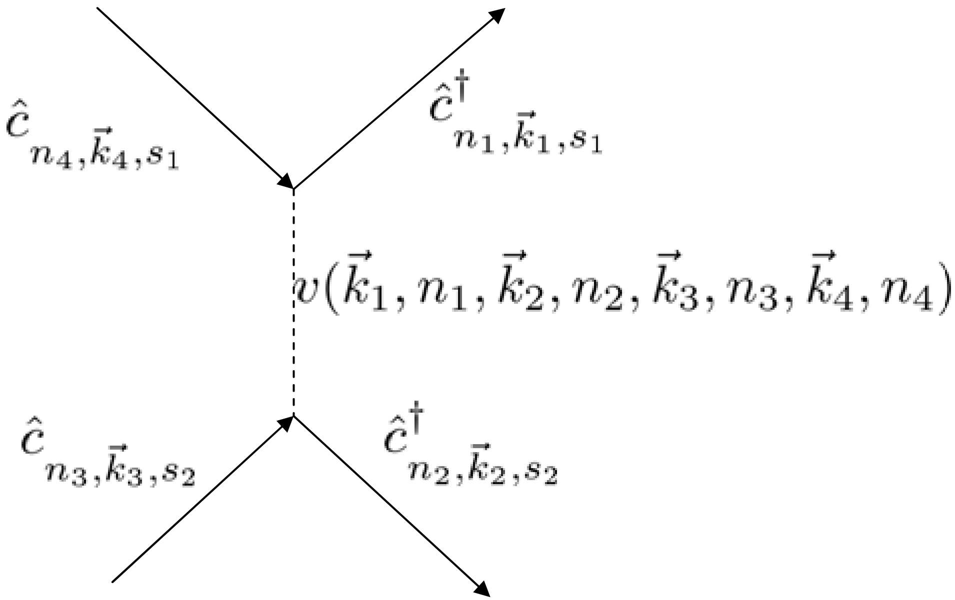
$$H = \sum_i \left[\frac{\vec{P}_i^2}{2m} + V_{e-ion}(\vec{x}_i) \right] + \frac{1}{2} \sum_{i \neq j} V(\vec{x}_i - \vec{x}_j)$$ with $$V(\vec{x}) = \frac{e^2}{|\vec{x}|}$$

Field operators: $$\hat{\Psi}_s^\dagger(\vec{x}) = \sum_{n,\vec{k} \in BZ} \Psi^\dagger_{n,\vec{k}}(\vec{x})\, \hat{c}^\dagger_{n,\vec{k},s}$$ Bloch representation.

$$\hat{H} = \sum_{\vec{k} \in BZ,\sigma,n} \epsilon_n(\vec{k}) \hat{c}^\dagger_{n,\vec{k},s} \hat{c}_{n,\vec{k},s} + \frac{1}{2N} \sum_{s_1,s_2} \sum_{\substack{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4 \\ n_1,n_2,n_3,n_4}} \Delta(\vec{k}_1 + \vec{k}_2 - \vec{k}_3 - \vec{k}_4) \times$$
$$v(\vec{k}_1, n_1, \vec{k}_2, n_2, \vec{k}_3, n_3, \vec{k}_4, n_4) \hat{c}^\dagger_{n_1,\vec{k}_1,s_1} \hat{c}^\dagger_{n_2,\vec{k}_2,s_2} \hat{c}_{n_3,\vec{k}_3,s_2} \hat{c}_{n_4,\vec{k}_4,s_1}$$

$$\Delta(\vec{k}) = \frac{1}{N} \sum_{\vec{R}} e^{i\vec{k}\vec{R}}$$ Laue function. Crystal momentum conservation up to reciprocal lattice vector

$$v(\vec{k}_1, n_1, \vec{k}_2, n_2, \vec{k}_3, n_3, \vec{k}_4, n_4) = N^2 \sum_{\vec{R}} e^{i\vec{R}(\vec{k}_4 - \vec{k}_1)} \int_\Omega d\vec{y}_1 d\vec{y}_2 \Psi^\dagger_{\vec{k}_1,n_1}(\vec{y}_1) \Psi^\dagger_{\vec{k}_2,n_2}(\vec{y}_2) V(\vec{y}_1 - \vec{y}_2 + \vec{R}) \Psi_{\vec{k}_3,n_3}(\vec{y}_2) \Psi_{\vec{k}_4,n_4}(\vec{y}_1)$$



Crystal momentum conservation.

$$\vec{k}_1 - \vec{k}_4 = \vec{k}_3 - \vec{k}_2 = \vec{q}$$

<u>Question:</u> $\frac{e^2}{r} \simeq 10eV$ for $r = 10^{-10}m$ $\qquad \epsilon_F \simeq 7eV \;\; Cu$

a) Is the Fermi surface stable against correlation effects ?
b) Are aspects of the Sommerfeld theory of metals still applicable?

<u>For example 1D</u> → Fermi liquid is unstable to so called Luttinger liquid
(Possible theme for Seminar.).

Simplifications:

a) Narrow bands: (i.e. Wannier wave functions have little overlap)

$$v(\vec{k}_1, n_1, \vec{k}_2, n_2, \vec{k}_3, n_3, \vec{k}_4, n_4) \equiv v(\vec{q}, \vec{k}_1, \vec{k}_2, n_1, n_2, n_3, n_4) \simeq v(\vec{q}, n_1, n_2, n_3, n_4)$$

$$\vec{k}_1 - \vec{k}_4 = \vec{k}_3 - \vec{k}_2 = \vec{q}$$

Single Band:

$$\hat{H} = \sum_{\vec{k} \in BZ, s} \epsilon(\vec{k}) \hat{c}^\dagger_{\vec{k},s} \hat{c}_{\vec{k},s} + \frac{1}{2} \sum_{\vec{q}} v(\vec{q})\, \hat{n}(\vec{q})\, \hat{n}(-\vec{q})$$

$$\hat{n}(\vec{q}) = \frac{1}{\sqrt{N}} \sum_{\vec{k},s} \hat{c}^\dagger_{\vec{k},s} \hat{c}_{\vec{k}+\vec{q},s} = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{-i\vec{q}\cdot\vec{R}} \sum_{s} \hat{c}^\dagger_{\vec{R},s} \hat{c}_{\vec{R},s}$$

Strong screening: $v(\vec{q}) = U$

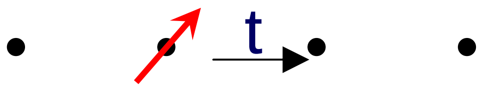
$$\hat{H} = \sum_{\vec{k} \in BZ, s} \epsilon(\vec{k}) \hat{c}^\dagger_{\vec{k},s} \hat{c}_{\vec{k},s} + U \sum_{\vec{R}} \hat{n}_{\vec{R},\uparrow}\, \hat{n}_{\vec{R},\downarrow}$$

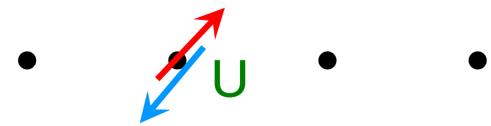
Hubbard model.

$\hat{n}_{\vec{R},s} = \hat{c}^\dagger_{\vec{R},s} \hat{c}_{\vec{R},s}$ Spin-s particle number count in Wannier state centered at R.

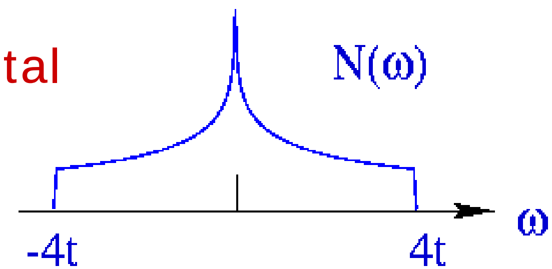
Hubbard and Heisenberg models *(Possible theme for Seminar.)*

$$\hat{H} = -t \sum_{<i,j>,\sigma} \hat{c}^{+}_{i,\sigma} \hat{c}_{j,\sigma} \quad + \sum_{i} U\,(\hat{c}^{+}_{i,\uparrow}\hat{c}_{i,\uparrow} - 1/2)(\hat{c}^{+}_{i,\downarrow}\hat{c}_{i,\downarrow} - 1/2)$$

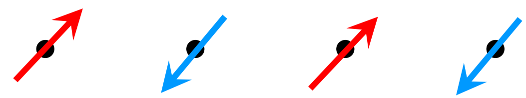




Metal

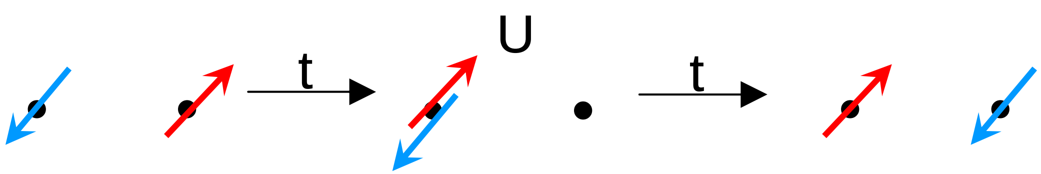


Half-filling: Insulator. Charge scale **U**



Charge is localized spin is still active.

Strong coupling: U/t >>1, Half-filling.



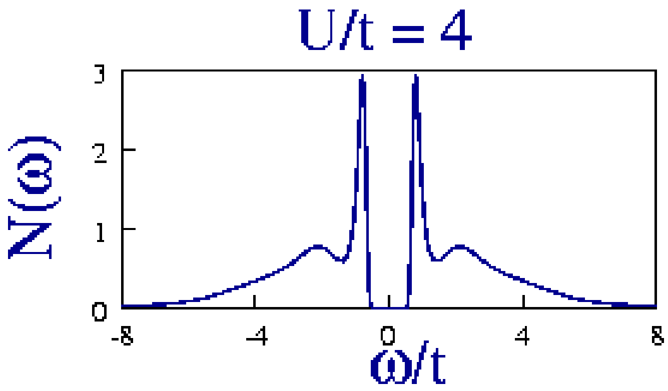
Magnetic scale: $J \sim t^2/U$

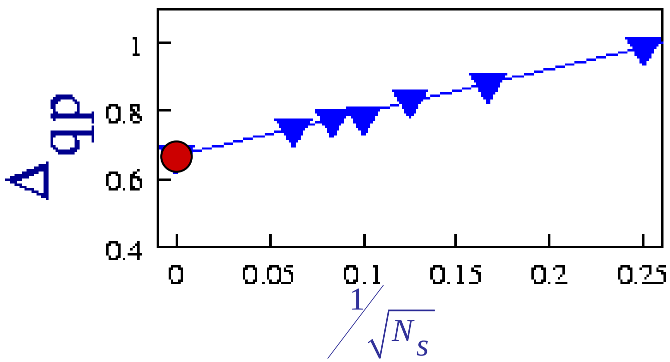
$$H = J \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j$$

Heisenberg model.

The Mott Insulator. Half-band filling (2D square lattice)

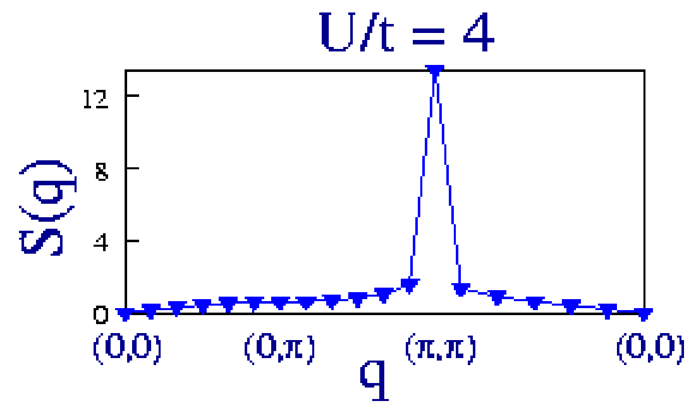
Charge.

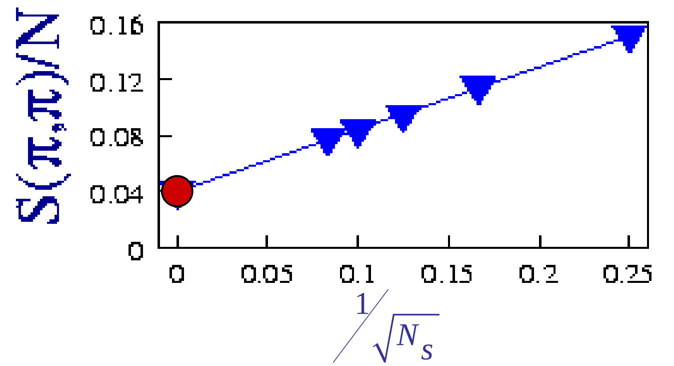




Quasiparticle gap > 0

Spin.



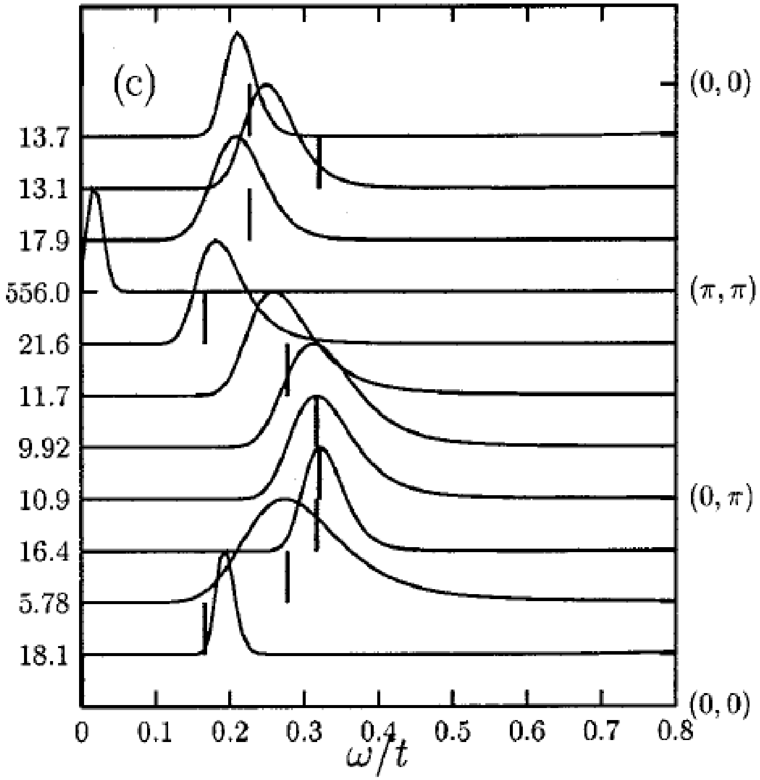


Long-range antiferromagnetic order.
Gapless spin excitations: Spin waves.

F.F. Assaad M. Imada JPSJ 95. (Auxiliary field QMC)

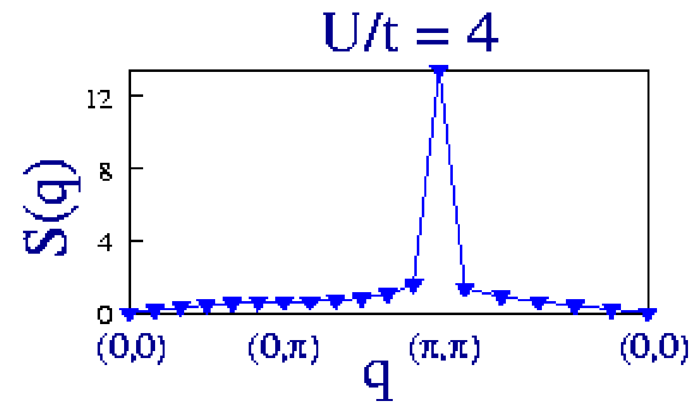
The Mott Insulator. Half-band filling (2D square lattice)

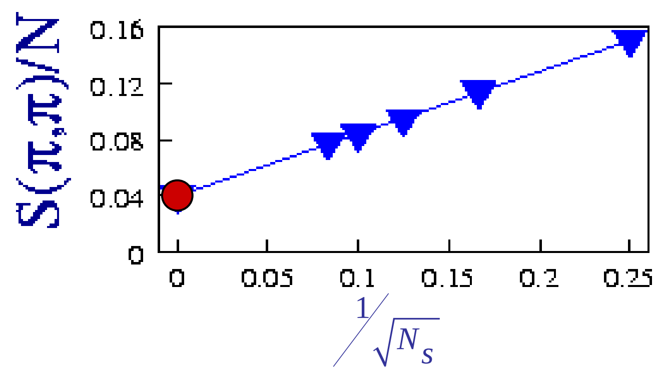
Spin excitations are present below the charge gap (1.3 t)



$$S(\vec{q},\omega) = \sum_n |\langle n|\hat{S}^+(\vec{q})|0\rangle|^2 \delta(\omega - (E_n - E_0))$$

Spin.

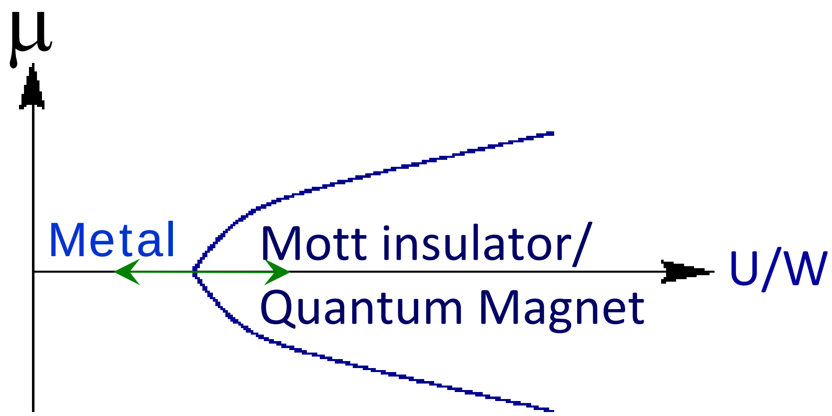




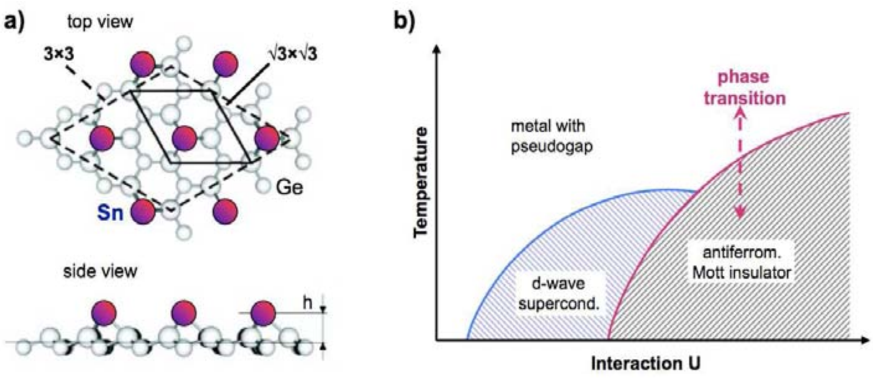
Long-range antiferromagnetic order.
Gapless spin excitations: Spin waves.

F.F. Assaad M. Imada JPSJ 95.   (Auxiliary field QMC)

The metal insulator transition and correlated states in the vicinity of the Mott insulator.



Sn/Si(111): A half-filled Hubbard model on a triangular lattice. P1.



Bandwidth controlled (2D)

Doping induced (2D)

→ high-temperature superconductivity.

2D Organics. (Kagawa et al. Nature 05)

LETTERS

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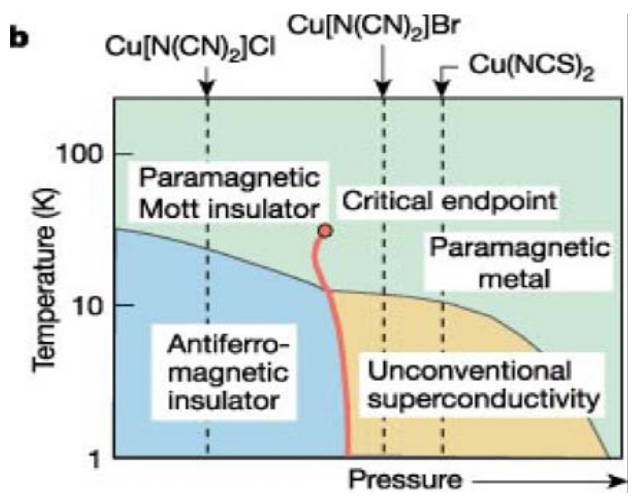
nature physics

Superconductivity in one-atomic-layer metal films grown on Si(111)

Tong Zhang[1,2], Peng Cheng[1], Wen-Juan Li[1,2], Yu-Jie Sun[1], Guang Wang[1], Xie-Gang Zhu[1], Ke He[2], Lili Wang[2], Xucun Ma[2], Xi Chen[1]*, Yayu Wang[1], Ying Liu[3], Hai-Qing Lin[4], Jin-Feng Jia[1] and Qi-Kun Xue[1,2]*



Opposite limit. Nearly free electrons → Gellium.

The lattice of ions is replaced by a homogeneous background of charge density ρ

$$H = \sum_i \left[\frac{\vec{P}_i^2}{2m} - \int_V \mathrm{d}\vec{R} \frac{|e|\rho}{|\vec{x}_i - \vec{R}|} \right] + \frac{1}{2} \sum_{i \neq j} V(\vec{x}_i - \vec{x}_j) \quad \text{with} \quad V(\vec{x}) = \frac{e^2}{|\vec{x}|}$$

Field operators: $$\hat{\Psi}_s^\dagger(\vec{x}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{x}} \hat{c}_{\vec{k},s}^\dagger$$ Plane wave representation.

$$\hat{H} = \sum_{\vec{k},s} \epsilon(\vec{k}) \hat{c}_{\vec{k},s}^\dagger \hat{c}_{\vec{k},s} + \frac{1}{2} \sum_{\vec{q} \neq \vec{0}} v(\vec{q})\, \hat{n}(\vec{q})\, \hat{n}(-\vec{q})$$

$$\epsilon(\vec{k}) = \frac{\hbar^2 \vec{k}^2}{2m} \ , \quad v(\vec{q}) = \frac{4\pi e^2}{\vec{q}^2}$$ and $$\hat{n}(\vec{q}) = \frac{1}{\sqrt{N}} \sum_{\vec{k},s} \hat{c}_{\vec{k},s}^\dagger \hat{c}_{\vec{k}+\vec{q},s}$$