INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
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SMR. 758 - 7

SPRING COLLEGE IN CONDENSED MATTER
ON QUANTUM PHASES
(3 May - 10 June 1994)

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INFRARED SINGULARITIES:

X-RAY EDGE, KONDO EFFECT, HEAVY PARTICLES etc.

LECTURES 1 AND 2

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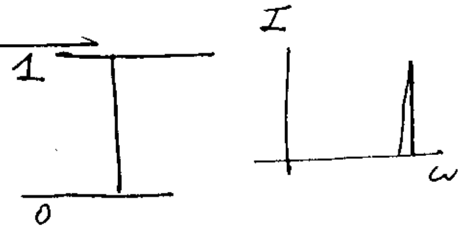
Elemental edge singularities



[redacted] state interactions,

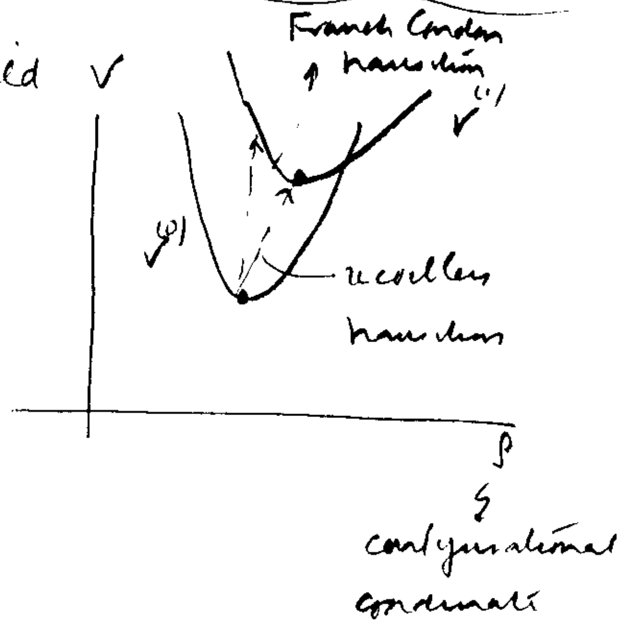
— Localized entity → transition between two discrete states

$$|\Psi^{(0)}\rangle \longrightarrow |\Psi^{(1)}\rangle$$

Coupled to a heat bath → different hamiltonians in states $|0\rangle$ and $|1\rangle$

$\boxed{H^{(0)} \to H^{(1)}}$ → inelastic scattering

Example : coupling to phonon field V



$V^{(1)} - V^{(0)}$ may correspond to a shift of the equilibrium position

$$\begin{cases} H^{(0)} = \sum_q \omega_q b_q^* b_q \\ H^{(1)} - H^{(0)} = \sum_q \alpha_q \left[b_q^* + b_{-q} \right] \end{cases}$$

Sudden approximation

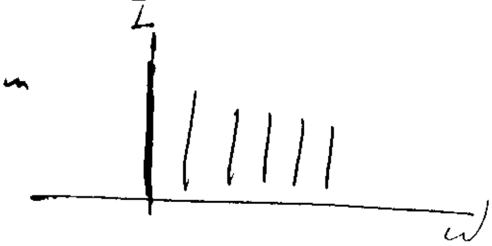
$$\begin{cases} \Psi^{(0)} = \varphi \to \text{eigenstates } \varphi_n , \xi_n \\ \Psi^{(1)} = \psi \to \text{eigenstates } \psi_\alpha , E_\alpha \end{cases}$$

$|\varphi_0\rangle = \sum_\alpha C_\alpha |\psi_\alpha\rangle$ → spectrum $I(\omega) = \sum_\alpha |C_\alpha|^2 \delta(\omega - E_\alpha + \xi_0)$

Fourier transform $\Rightarrow$ $I(t) = |\langle \varphi_0 | \psi_\alpha \rangle|^2 e^{i(E_\alpha - \xi_0)t}$

$$= \langle \varphi_0 | e^{i(H_1 - H_0)t} | \varphi_0 \rangle$$

↳ shape of spectrum



— Recoilless "Mossbauer" line:

↳ Amplitude $|\langle \varphi_0 | \psi_0 \rangle|^2$: finite for coupling to phonons

↓

$\boxed{\text{Zero for coupling to a Fermi liquid: orthogonality catastrophe}}$

$$\begin{cases} H^{(0)} = \sum_i \frac{p_i^2}{2m} \\ H^{(1)} = H^{(0)} + \sum V(R_0 - r_i) \end{cases}$$

(impurity located at R_0)

Second order perturbation calculation

$$\underbrace{\psi_0 = \frac{1}{A}}_{\text{normalization}} \left\{ \varphi_0 + \sum_n \frac{V_{on}}{\underbrace{W_{no}}_{E_n - E_0 = \omega}} \varphi_n \right\}$$

$$A = 1 + \sum_n \frac{|V_{n0}|^2}{\omega_{n0}^2} = \int_0^\infty \frac{d\omega}{\omega^2}\,\overline{V^2}\rho(\omega)$$

$$\overline{V^2}\rho(\omega) = \sum_n |V_{n0}|^2\,\delta(\omega-\omega_{n0})$$

average final state potential

density of electron-hole excitations

In practice $\rho(\omega) \sim \omega$ (exclusion principle: the hole is within ω from E_F)

↳ $\boxed{\text{A logarithmically divergent}}$

↓

<u>NO Mössbauer line</u>

<u>Summation → power law</u>

– <u>Determinantal calculation</u>

(i) Impurity at origin in free fermion gas

⇓

Consider one particular channel, say $\ell=0$

↓

k is an <u>energy</u> variable

($d\varepsilon = k v_F$)

↳ rotational invariance

↓

partial wave analysis

↓

phase shifts of V $\delta_\ell(k)$

for each channel ℓm

energy

We want to calculate $I(t) = \langle \varphi_0 | e^{iHt} | \varphi_0 \rangle \, e^{-iE_0 t}$

Slater determinant of filled unperturbed states

N×N

$\mathrm{Det}\left[\chi_k(r_i)\right]$

Sum of one body hamiltonians

$H = \sum_i h_i$

When expanding determinants, only overlaps for the same particle r_i enter

$$\Lambda_{kk'}(t) = \int d\tau_i \, \chi_k^*(r_i) \, e^{ih_i t} \, \chi_{k'}(r_i)$$

filled states in $|\varphi_0\rangle$

$k < k_F$

N×N matrix

one electron matrix element

Recombining the terms →

$$\boxed{e^{iE_0 t} I(t) = \mathrm{Det}\left[\underline{\Lambda}(t)\right]}$$

Exact result as long as V is a one body potential

But $\mathrm{Log}\left[\mathrm{Det}\,\underline{\Lambda}\right] = \mathrm{Log}\left[\prod \text{eigenvalues}\right] = \mathrm{Tr}\,\mathrm{Log}\,\underline{\Lambda}$

EXPONENTIATION

$$\boxed{e^{iE_0 t} I(t) = \exp\left[\mathrm{tr}\left\{\log \underline{\Lambda}(t)\right\}\right]}$$

(ii) Phase shift algebra

• Bare state χ_k, energy ε_k

↓

Partial wave analysis: one channel $lm\sigma$ (say $l=0$)

↓

only one variable $|k|$ → energy.

Consider a spherical box with radius R $\Rightarrow$ $\psi(R)=0$.

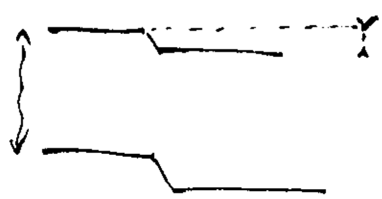
↓

Quantization condition
$$\begin{cases} kR = n\pi & \text{without potential} \\ \bar{k}R = n\pi - \delta & \text{with potential} \end{cases}$$

(Actually extra shifts due to Bessel functions: only the difference matters)

• δ is a function of k.

$\Delta k = \frac{\pi}{R}$



$\bar{k} - k = -\frac{\delta}{R}$, $\Rightarrow$ $\Delta\bar{k} = \frac{\pi}{R}\left[1 - \frac{1}{R}\frac{\partial\delta}{\partial k}\right]$

• The energy (kinetic at infinity) is

$$\bar{\varepsilon}_k = \varepsilon_k - \frac{\delta}{\pi}\Delta\varepsilon = \varepsilon_k - \frac{\delta}{\pi\nu}$$

level spacing

↳ density of states in one rotational channel

↓

Density of states in the presence of impurity

$$\bar{\nu} = \frac{1}{v_k\,\Delta\bar{k}} \simeq \frac{R}{\pi v_k}\left[1 + \frac{1}{R}\frac{\partial\delta}{\partial k}\right]$$

$\Downarrow$

$$\boxed{\bar{\nu} - \nu = \frac{1}{\pi}\frac{\partial\delta}{\partial\varepsilon}}$$

Corollary: Friedel sum rule for displaced charge

$$Q_I = \int_{-\infty}^{\varepsilon_F} (\bar{\rho} - \rho)\, d\varepsilon = \frac{\delta_F}{\pi} \quad \text{per channel}$$

- The same asymptotic behaviour yields the overlap of wave functions with and without potential

$$\begin{matrix} \bar{\chi}_k & & \chi_k \end{matrix}$$

$$\downarrow$$

$$\langle \chi_k | \bar{\chi}_{k'} \rangle = \frac{\sin \delta_k}{\pi \rho_k} \frac{1}{\bar{\varepsilon}_{k'} - \varepsilon_k} = x_{kk'}$$

ensures normalization via Poisson's formula

(iii) Application to determinantal calculations

$$\Lambda_{kk'}(t) = \sum_p x^*_{kp}\, x_{k'p}\, e^{i \bar{\varepsilon}_p t}$$

k and k' are filled ($< k_F$), p is anything

For long time, the summation is dominated by $k \simeq k' \simeq p$
(destructive interference)

$$\downarrow$$

$$e^{-i\varepsilon_k t} \Lambda_{kk'} = \frac{\sin^2 \delta_k}{\pi^2} \sum_m \frac{\exp[\,i m t / \rho_k]}{\left(m - n - \frac{\delta}{\pi}\right)\left(m - n' - \frac{\delta}{\pi}\right)}$$

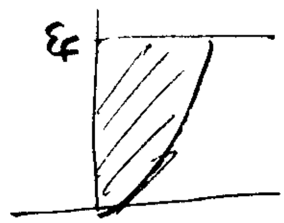
(m, n, n' integers, all energies are measured from ε_k)

Summation carried out with Poisson's formula

$$\boxed{\begin{aligned} \Lambda &= 1 - X \\ X_{kk'} &= \frac{\sin\delta_k \, e^{-i\delta_k}}{\pi \rho_k} \left[\frac{1 - e^{i(\varepsilon_k - \varepsilon_{k'})t}}{\varepsilon_k - \varepsilon_{k'}} \right] \end{aligned}}$$

(iii) Asymptotic long times behaviour

Destructive interference → drop the exponential term and cut the integrals at $\varepsilon_k - \varepsilon_{k'} \propto 1/t$.



$\Downarrow$

Weak Coupling limit

$$\log[1 - X] = -X - \frac{X^2}{2} \; - - - -$$

$$\mathrm{Tr}\, X = it \sum_k \frac{\delta_k}{\pi \rho_k}$$

level shift $e^{i\Delta E_0 t} \sim I(t)$

(E_0 is shifted by the final potential V)

$$\sum_{kk'} \frac{[1 - \cos(\varepsilon_k - \varepsilon_{k'})t]}{(\varepsilon_k - \varepsilon_{k'})^2}$$

logarithmic divergence at Fermi level

$$\log I \sim \frac{\delta^2}{\pi^2} \log t$$

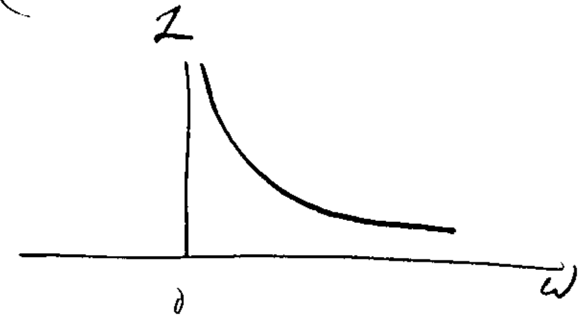
$\boxed{\text{Conclusions}}$

$$Z(t) = \frac{e^{i\bar{E}_0 t}}{t^{\alpha}} \qquad \left(\alpha = \frac{\delta^2}{\pi^2} \text{ in Born approx.}\right)$$

$\downarrow$

$$Z(\omega) = \frac{1}{\omega^{1-\alpha}}$$

ω measured from $\bar{E}_0$



- No Mossbauer peak
- Power law singularity with exponent α depending on V
- If $\frac{1}{t} \sim$ level spacing $\sim \frac{1}{N}$, then $Z(t) \sim |\langle\varphi_0|\psi_0\rangle|^2$

$\downarrow$

orthogonality catastrophe $\langle\varphi_0|\psi_0\rangle = \left(\frac{1}{N}\right)^{\delta^2/2\pi^2}$

one channel

(iv) Generalization to strong coupling

Mathematical problem of calculating $\mathrm{Tr}\,\mathrm{Log}(1 - \underset{\sim}{X})$ exact

$\Downarrow$

- level shift ΔE_0 given by Friedel rule
- $\alpha = \delta^2/\pi^2$ with true phase shift

$\downarrow$

Back to other formulation

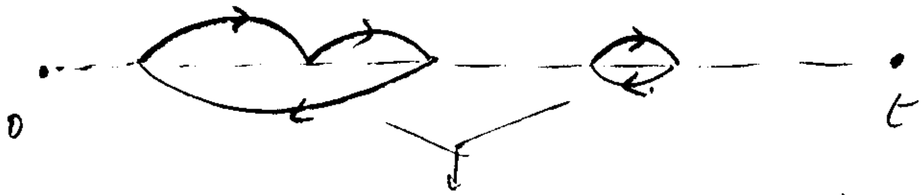
~~[redacted] theory of the x-ray edge~~

– Perturbation theory in real time space:

$$I(t) = \langle \varphi_0 | e^{iHt} | \varphi_0 \rangle$$

$$= \langle \varphi_0 | U(t) | \varphi_0 \rangle$$

↳ evolution operator in the transient potential V between times 0 and t



transient response of the fermion gas to V

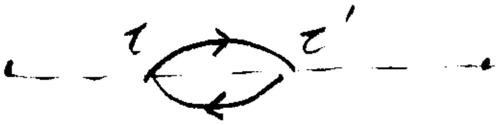
But V is structureless: excitation of electron-hole pairs does not modify the potential

$\boxed{\text{Exponentiation}}$

(linked cluster expansion)

$$\begin{cases} G(t) = e^{iE_0 t} I(t) = \exp\left[C(t)\right] \\ C = \text{single closed loop where } \underline{\text{all}} \text{ vertices are between } 0 \text{ and } t \end{cases}$$

• Born approximation with a contact potential $V(r) = \delta_{r,0}$



$$C(t) = \int_0^t d\tau \, d\tau' \; g_0(\tau'-\tau)\, g_0(\tau-\tau')$$

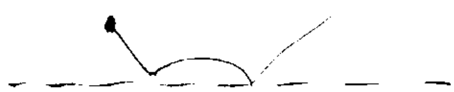
Local fermion propagator $g_0 = \sum_k e^{i E_k \tau} \begin{cases} 1-n_k & \text{if } \tau>0 \\ -n_k & \text{if } \tau<0 \end{cases}$

$$\boxed{g_0 \sim \frac{i}{\sqrt{\tau}}}$$

•

Two integrations → $C \sim \log t$ → $I \sim \frac{1}{t^{\alpha}}$ (M1)

• Exact solution for large t (ND 1968).



(i) $g[\tau,\tau']$

$$= g_0(\tau-\tau') + \int_0^t d\tau'' \; g_0(\tau-\tau'')\, V\, g(\tau'',\tau')$$

free propagator

Muskhelishvili singular integral equation: exact solutions

Power law singularities when τ or τ' approach 0 and t

More exactly, the following asymptotic form holds

$$g(\tau,\tau') = g_0(\tau-\tau')\left[\frac{(t-\tau')\,\tau}{\tau'(t-\tau)}\right]^{\delta/\pi}$$

δ is the phase shift at Fermi level for the channel considered

Valid if all time differences > cut off $\eta \sim \Lambda^{-1}$ where Λ is band width

(ii) The closed loop contribution involves $g(\tau,\tau)$. More exactly, if $V \to \lambda V$, then

$$\lambda \frac{\partial C}{\partial \lambda} = -i \int_0^t d\tau \; V g(\tau,\tau)$$

We expand $g(\tau,\tau')$ in the limit $\tau-\tau' \to 0$

regular terms

Vg = const

$\downarrow$

Energy shift ΔE_0

edge correction

(expansion of brackets

$\downarrow$

factor $(\tau-\tau')$ which balances that of g_0)

$\downarrow$

$g \sim \frac{t}{\tau(t-\tau)}$ $\to$ logarithmic divergence cutoff at η.

$$\boxed{C = -\alpha \operatorname{Log} t}$$

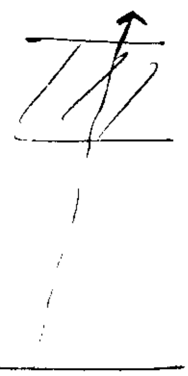
→ Exact expression of $\boxed{\alpha = \dfrac{\delta^2}{\pi^2}}$

(Determination of δ obtained by continuity starting from the line $V=0$, $\delta=0$: see discussion of bound states!)

• Can be extended to band spectra, in which the transition creates or destroys an electron in the conduction band ("fermions")

↓

• open line in the spectrum



The "photoelectron" may scatter any number of times on the transient impurity

↳ exponentiation unaffected

$$e^{iE_0 t} I(t) = L(t)\, e^{C(t)}$$

$$L(t) \sim t^{2\delta/\pi - 1} \qquad e^{C(t)} \sim \frac{1}{t^{\delta^2/\pi^2}}$$

(comes from expression of $g(0,t)$)

The resulting spectrum is

$$I(\omega) = \frac{1}{\omega^{2\delta/\pi - \delta^2/\pi^2}}$$

(Combination of a vertex correction L and self energy G)

Remarks

(i) All results are asymptotic, valid if $\omega \ll \Lambda$

(i.e. $t \gg \tau = \Lambda^{-1}$)

- The cut off enters in the ~~[illegible]~~ form of $Z(\omega)$

$$\begin{cases} \text{Line spectrum} & Z \sim \frac{1}{\omega}\left(\frac{\omega}{\Lambda}\right)^{\delta^2/\pi^2} \\ \text{Band spectrum} & Z \sim \left(\frac{\Lambda}{\omega}\right)^{2\delta/\pi - \delta^2/\pi^2} \end{cases}$$

(ii) The extension to all rotational channels is easy, since the rotational index (l, m, σ) is conserved along any electron line

Summation over $(l m \sigma)$ in closed loops

Specific l for the open line

$$\alpha_c = \sum_l \underset{\text{spin}}{2}\,\underset{m\text{ index}}{(2l+1)}\,\frac{\delta_l^2}{\pi^2}$$

– For band spectra, the photoelectron belongs to a specific l_0 channel fixed by symmetry

(e.g. $l_0 = 1$ for a dipole transition between two s states)

$$\downarrow$$

$$\alpha = \alpha_c = \frac{2\delta_{l_0}}{\pi}$$

l_0 may be varied by changing the spectrum studied

CONCLUSION. – ~~Maxima~~ Edge singularities occur when a Fermi system with a linear excitation spectrum ($\rho(\omega) \sim \omega$) is subject to a discontinuous perturbation

$\rightarrow$ $\boxed{\text{power laws with non universal exponents}}$

– They disappear at finite T, or if the perturbation is progressive → effect of recoil ?

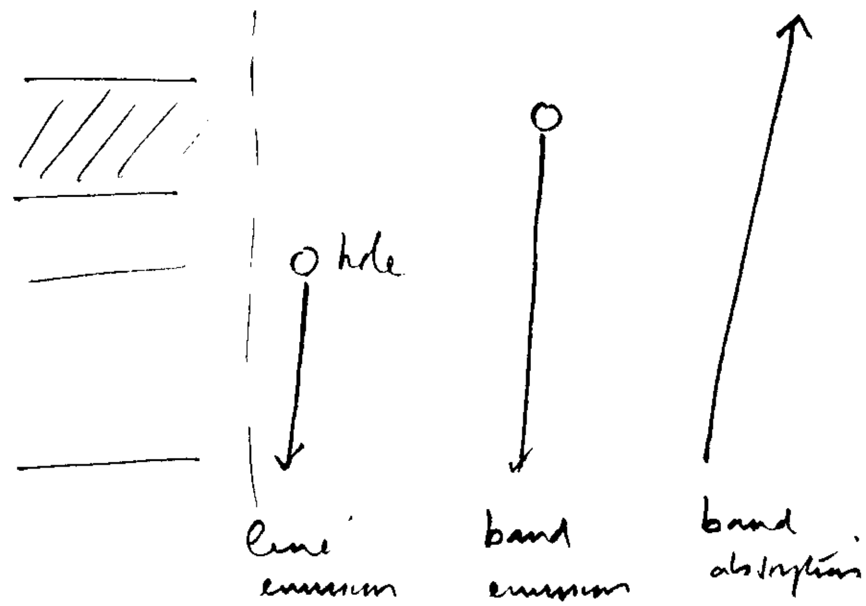
For details, see original paper

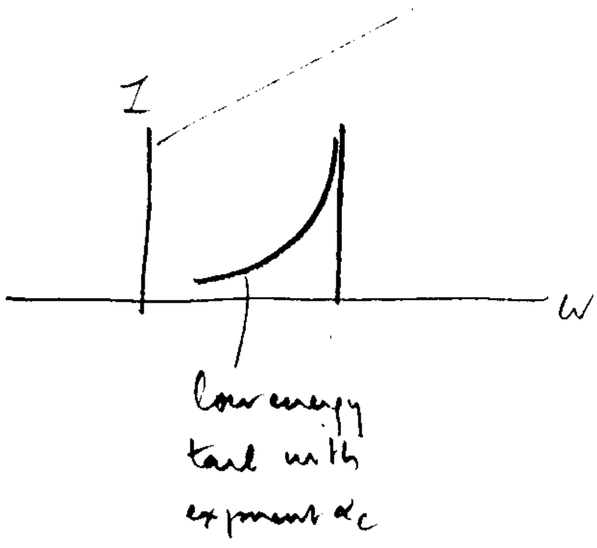
PN-CD Phys Rev 178 1097 (1969)

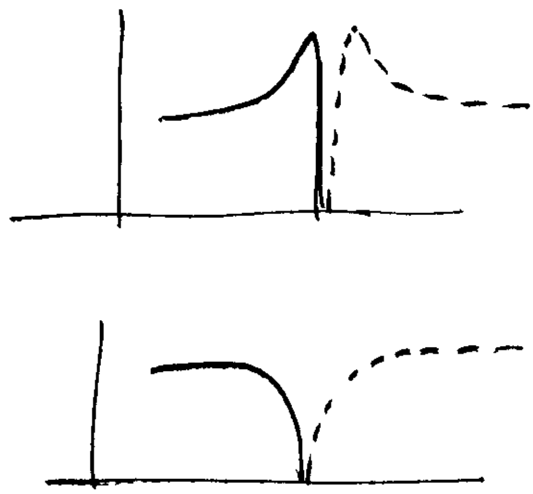
NC-PN Journal de P, 32, 913 (1971)

– Physical examples

(i) X-ray emission and absorption







enhancement or depression of spectrum depending on whether closed loops or L dominate

Enhancement likely if $l_0 = 0$
L_0 dipole spectrum between p and s states: $L_{II\,III}$ spectra

Observed since before [illegible] in Magnesium, etc...
But comparison with experiment delicate, as the asymptotic range may be narrow

↳ (Singularities hidden by other effects)

↓

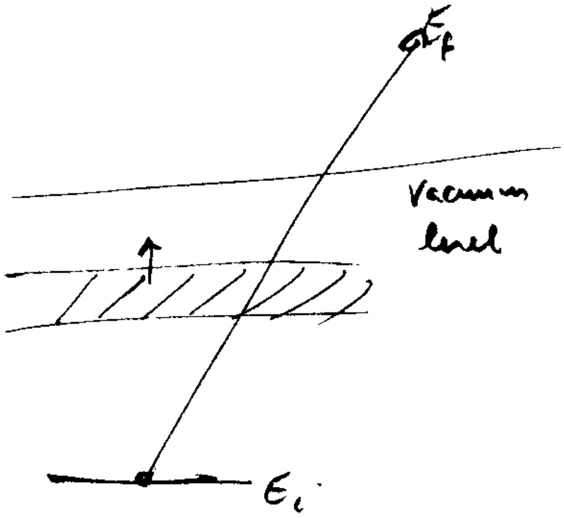
<u>Crusade in the seventies</u> (cf present situation for RVB, ...).

⇓

Beware of experimental arguments (no doubt on the existence of singularities: <u>consistent</u> theory), but need a <u>quantitative</u> theory in order to fit experiments

(ii) <u>Photoemission from deep states</u>

$$E_f = E_i + \underbrace{\omega_0}_{\text{photon}} - \underbrace{\omega}_{\text{inelastic excitation of conduction band}}$$



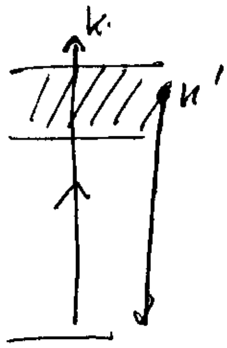
↓

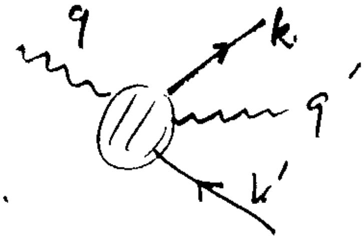
- Closed loop contribution (no input in conduction band)

- low energy tail of photoelectron spectrum

(iii) Resonant Raman Scattering

- Photon q, ω $\rightarrow$ excitation of deep core state $\rightarrow$ deexcitation, emission of $q' \omega'$





Raman scattering with excitation of one electron hole pair

let $\mu - \varepsilon_c = \omega_0$: Absorption threshold

$$\hookrightarrow \omega = \omega_0 + \bar{\omega}, \quad \varepsilon_k = \mu + \bar{\varepsilon}_k$$

$$\boxed{\bar{\omega} = \bar{\omega}' + \bar{\varepsilon}_k - \bar{\varepsilon}_{k'}}$$

Resonant scattering if all energies $\bar{\omega}, \bar{\varepsilon}$ are small

$\downarrow$

2^{nd} order transition probability

$$\boxed{w(\omega, \omega') = 2\pi\, n_k' (1 - n_k) \left| \frac{W_k W_{k'}}{\bar{\omega} - \bar{\varepsilon}_k} \right|^2 \delta(\bar{\omega} - \bar{\varepsilon}_k - \bar{\omega}' + \bar{\varepsilon}_{k'})}$$

(Near resonance, this second order process $(J.A)^2$, dominates the usual first order quadratic term ρA^2)

- Final and intermediate state interactions
  ↳ further electron hole pairs : edge singularities?

Because one must sum over intermediate states before squaring, must account for interference effects between different intermediate states

⇓

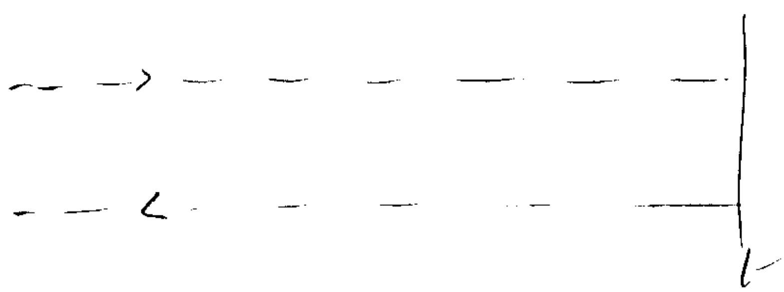
Need for a density matrix calculation of intensity rather than a Schrödinger equation for amplitude

⇓

Keldysh perturbation expansion

Probability of a final state Ψ_f at time t

$$P_f = \langle \Psi_i | U(-\infty, t) | \Psi_f \rangle \langle \Psi_f | U(t, -\infty) | \Psi_i \rangle$$



Two time axis, one for bra, one for ket

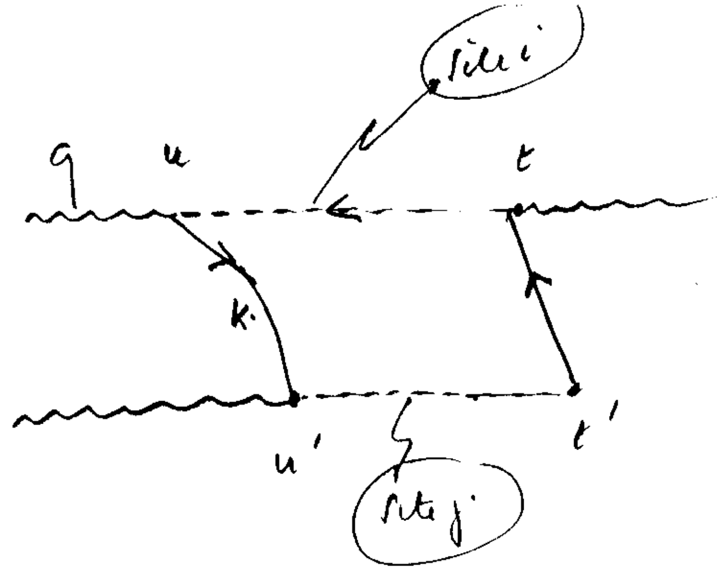
↓

2x2 matrix for Green's function

↓

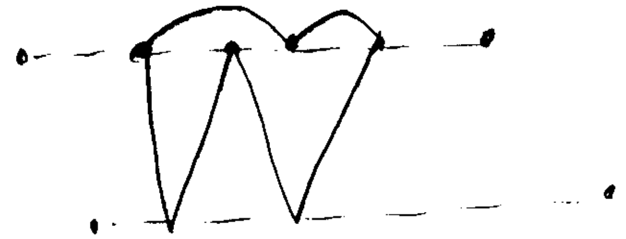
Separate information on statistics and dynamics

Here



$u-u'$ = Fourier transform of incoming frequency ω
$t-t'$ = " " outgoing " ω'
$t-u$ = basis for transition probability

Final state interactions come from multiple scattering of the two open lines on the holes, and from closed loops



- No interference between sites : $i=j$.

~~[illegible]~~ with some manipulation, reduction to a single Muskhelishvili equation → exact solution

$$W(\omega,\omega') = \underbrace{\left(\frac{\Lambda}{\overline{\omega}}\right)^{\alpha}}_{\text{edge exponent}} \underbrace{f\left(\frac{\overline{\omega}}{\overline{\omega}'}\right)}_{\text{universal function}}$$

$2^{\text{ème}}$ cours

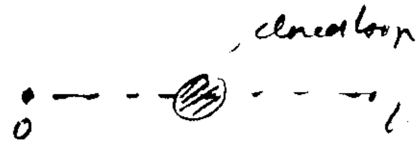
Transition from state $\left\{ \begin{array}{l} 0 \text{ to state } 1 \\ H \to \bar{H} = H + V \end{array} \right.$

Transient one body potential

$$I(t) = \langle \varphi_0 | e^{i\bar{H}t} | \varphi_0 \rangle e^{-iE_0 t}$$

↳ spectrum $I(\omega)$

Perturbative approach $\quad I(t) = e^{C(t)}$



$$C(t) = -\alpha_c \log t$$

$$\alpha_c = \sum_{\ell m \sigma} \left(\frac{\delta_\ell}{\pi} \right)^2 = \sum_\ell 2(\ell+1) \frac{\delta_\ell^2}{\pi^2}$$

phase shift at Fermi level

Determinantal approach

$$e^{iE_0 t} I(t) = \mathrm{Det}\left[\underset{\sim}{\Lambda}(t) \right] = \exp\left[\mathrm{Tr} \log \underset{\sim}{\Lambda} \right]$$

$$\underset{\sim}{\Lambda}_{kk'} = \sum_p \langle k | \bar{p} \rangle \langle \bar{p} | k' \rangle e^{i\bar{E}_p t}$$

k ↳ filled initial state $\quad \bar{p}$ ↳ any final eigenstate

Same type of exponentiation

Band spectra

one additional open line with channel l_0

$$\begin{cases} I(t) = e^{C(t)}\, L(t) \\ L(t) = \dfrac{1}{t^{1-2\delta_{l_0}/\pi}} \end{cases}$$

Additional note : relation to orthogonality catastrophy

$$I(t) = \sum_{\bar{n}} \left|\langle 0 | \bar{n} \rangle\right|^2 e^{i(\bar{E}_n - E_0)t} = \frac{1}{(Dt)^\alpha}$$

level spacing $\sim \dfrac{D}{N}$ → Band width

If $t \sim \dfrac{N}{D}$, only one state contributes

$$I(t) \sim \left|\langle 0 | \bar{0} \rangle\right|^2 \sim \left(\frac{1}{N}\right)^\alpha$$

$$\downarrow$$

$$\boxed{\langle 0 | \bar{0} \rangle \sim \frac{1}{N^{\alpha/2}}}$$

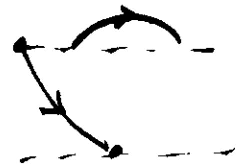
Anderson orthogonality catastrophy with half exponent

Here again $\alpha = \delta^2/\pi^2$

Calculation of f messy, but possible

- Interference effects $i \neq j$

Two coupled equations for G_{ii} and G_{ij}



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The Muskhelishvili method does not work (due to non commutativity of G 2×2 matrices

↓

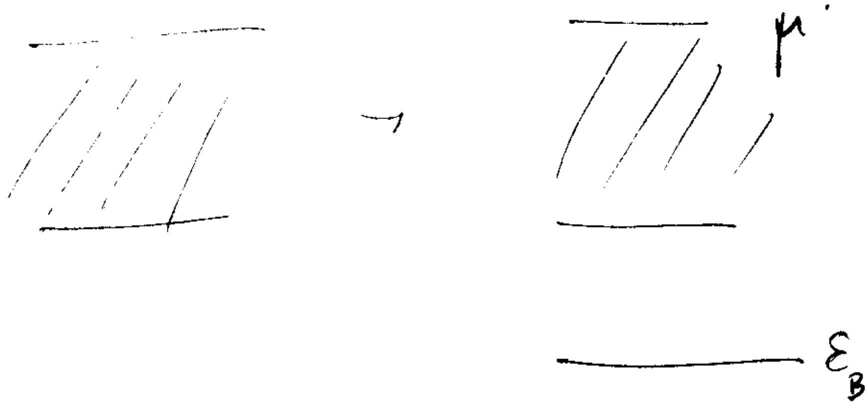
Physical effect unchanged

But theory at a loss: important to be aware

Ref PN-EA Phys. Rev. B10 3099 (1974)

– The problem of bound states

Final state potential strong enough to bind one particle



(For simplicity, consider spinless particles)

(i) Line spectrum

In the final state, the bound state is either full or empty

$\Downarrow$

Two thresholds

Bound state full

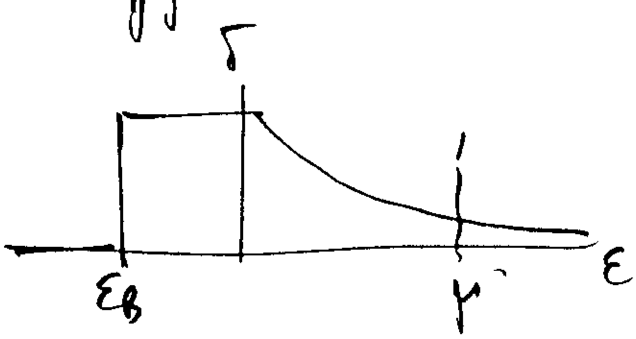
absolute threshold ω_0

$\downarrow$

usual exponent

$$Z(t) = \frac{1}{t^{\delta^2/\pi^2}}$$

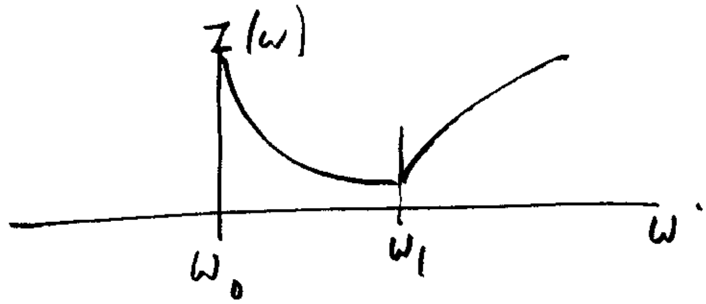
with δ obtained by continuity from the high energy limit



Bound state empty

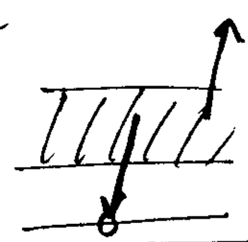
Secondary thresholds

$\omega_0 + \mu - \varepsilon_B$.



Remark: the secondary threshold is blurred by particle interactions which give a finite lifetime to the bound state hole

$\boxed{\text{Auger process}}$



In order to consider the secondary exponent, two methods

Phenomenology

The bound electron is excited to the valence band

$\downarrow$

equivalent to a photoelectron

$\Downarrow$

$$I(t) = \frac{1}{t^{\delta^2/\pi^2 + 1 - \frac{2\delta}{\pi}}}$$

$$= \frac{1}{t^{\left(\frac{\delta}{\pi}-1\right)^2}}$$

Exact

Determinantal calculation

$$e^{iE_0 t} I(t) = \mathrm{Det}\left[\Lambda(t)\right]$$

$$\Lambda_{kk'} = \langle \chi_k | e^{iht} | \chi_{k'} \rangle$$

$$= \sum_n \langle \chi_k | n \rangle \langle n | \chi_{k'} \rangle e^{iE_n t}$$

$\Downarrow$

$$\underbrace{\Lambda = \Lambda_S}_{\text{old calculation}} + \underbrace{\Lambda_B}_{\text{Bound state contribution separable}} = 1 - X + \Lambda_B$$

Use the fact that $\mathrm{Det}\left[A\,B\right] = \mathrm{Det}\,A \;\mathrm{Det}\,B$

$\Downarrow$ $\quad \log\left[\mathrm{Det}\,\Lambda\right] = \log \mathrm{Det}(1-X) + \mathrm{Tr}\log\left[1 + \frac{1}{1-X}\Lambda_B\right]$

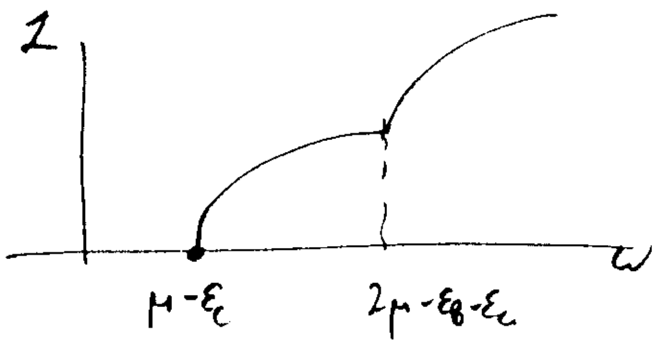
$$I(t) = \underbrace{I_S}_{\substack{\text{secondary threshold} \\ \text{(Bound state empty)}}} \Big[\underbrace{1 + \langle B | \tfrac{1}{1-X} | B \rangle e^{iE_B t}}_{\substack{\text{absolute threshold} \\ \text{(Bound state full)}}} \Big]$$

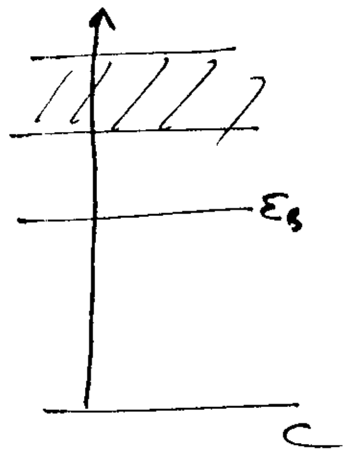
Detailed calculation delicate (the phase shift in Z_δ is shifted by π once the bound state is singled out).

↳ confirmation of naive phenomenology.

(ii) Band spectrum

ε_B full or empty





old experiment

$$Z(t) = \frac{1}{t^\alpha}$$

$$\alpha = \left(\frac{\delta}{\pi} - 1\right)^2.$$

The bound state is frozen, and it does not enter anywhere

Two results

1971

Determinantal analysis

$$\alpha = \left(\frac{\delta}{\pi} - 2\right)^2.$$

confirmed by Ohtaka + Tanabe

?

1994

Two photoelectrons (one from C, one from B)

$$Z = L^2 e^{c}$$

$$L^2 \to \frac{1}{t^{2-4\delta/\pi}} \qquad c \to \frac{1}{t}\,\delta^2/\pi^2.$$

α decreases by 2.

Remarks

- For two photoelectrons, the spectrum is

$$I(\omega) \sim \int_0^\infty d\omega_1 d\omega_2 \, \delta(\omega - \omega_1 - \omega_2) \sim \omega \implies I(t) \sim \frac{1}{t^2}.$$

No ambiguity

- Only questionable point is the interpretation of a bound state hole as another photoelectron

(iii) The Hopfield rule of thumb

- $\frac{\delta}{\pi}$ is the charge that must be brought from ∞ in order to achieve the ground state in the presence of the final state potential. For a line spectrum, there is no input in the conduction band: one must indeed bring $n = \delta/\pi$ from infinity (in each rotational channel)

$$\hookrightarrow \boxed{I(t) \sim \frac{1}{t^{n^2}}}$$

- Also works for a band spectrum

$$n = \underbrace{\frac{\delta}{\pi} - 1}_{\text{photoelectron}}$$

or for a line spectrum with empty bound state

$$\Downarrow$$

$$\boxed{\text{Hopfield rule}}$$

Widely accepted

• In fact, very likely wrong.

(i) Two photoelectrons → clear counterexample

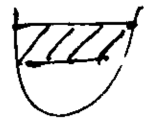
$$\alpha = 2 - 4\frac{\delta}{\pi} + \frac{\delta^2}{\pi^2} \neq \left(\frac{\delta}{\pi} - 2\right)^2 .$$

(ii) Anyhow, if no real rotational symmetry, the channels may "communicate"

↓

"short circuit" for bringing charge from infinity

(iii) Analysis by Combescot and Tanguy of excited "Slice" distribution with two Fermi levels (obtained by optical pumping)



↓

Counterexample

My conclusion: the Hopfield rule of thumb is incorrect.
(Two functions $f(x)$ and $g(x)$ that coincide at two points are not necessarily equal)!

[redacted] Questions

– Validity of preceding discussion

Assumptions
- non interacting fermions
- decoupled scalar channels $l\,m\,\sigma$
- structureless final state scalar potential

Does edge singularity survive these assumptions ?

(i) Effect of interactions

. Negligible because everything occurs near the Fermi level, where particle interactions reduce to a mean field Hartree Fock like self energy (Landau theory).

↳ "effective free particles" with renormalized phase shifts δ_l

(Can be formalized with a poor man's scaling argument

Formal perturbation treatment by Yamada and Yosida

(ii) Channel coupling

Physically important, as it questions the Hopfield rule.

↓

Best studied for the orthogonality catastrophe

$$\langle 0 | \Phi_0 \rangle \sim \frac{1}{N^{\alpha/2}} \quad , \; \alpha = \sum_{lms} \left(\frac{\delta_l}{\pi}\right)^2 .$$

Extensively discussed by Yamada and Yosida

- Formally, α is related to the S matrix at Fermi level

$$\alpha = \mathrm{Tr}\left[\frac{\log S(\mu)}{2\pi}\right]^2 \qquad (1)$$

$S(\mu)$ is the elastic scattering matrix at Fermi level

S diagonal $= e^{2i\delta}$

when channels are decoupled

$$\alpha = \sum_{\ell m s} \left(\frac{\delta_\ell}{\pi}\right)^2$$

(1) provides a generalization to the coupled case

More precise discussion

Treatment of one body scattering at energy z

$$g^r = \frac{1}{H_0 - z + i\eta} = g_1 - i g_2$$

$$S(z) = 1 - 2i\pi \int dz \; \delta(z - H_0)\, t^R(z)\, \delta(z - H_0)$$

$$t^R(z) = V \frac{1}{1 - g^r V} \qquad t\text{-matrix}$$

$$\boxed{\alpha = \operatorname{Tr}\left[\left(\frac{\operatorname{Log}\left(1 - 2i\pi\,\delta(z - H_0)\,t^{e}(z)\right)}{2\pi}\right)^2\right]_{z=\mu}}$$

- Perturbation calculation of $Y \cdot Y_1$: very tricky, as the propagators becomes non commuting channel matrices

$$(n) \longrightarrow (n')$$

cf Raman scattering

Formal demonstration very complicated

- Poor man's scaling

Reduce band width Λ

$\downarrow$

effective scattering matrix

$\downarrow$

asymptotic decoupling of channels close to Fermi level

(eigenvalues of S matrix)

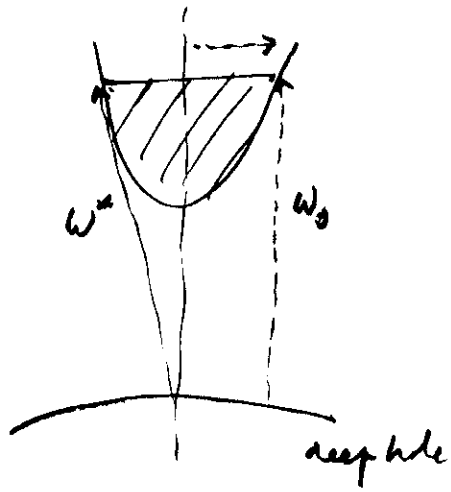
Convincing, but not rigorous

(iii). Final state exchange scattering

Interplay of X-ray edge + Kondo : still largely open problem (very difficult). → Scaling argument?

- Recoil of the Scatterer : lethal to edge singularity if it goes to infinity

(i) Qualitative argument



- Translational invariance

↓

k conservation in optical transition ("vertical")

↓

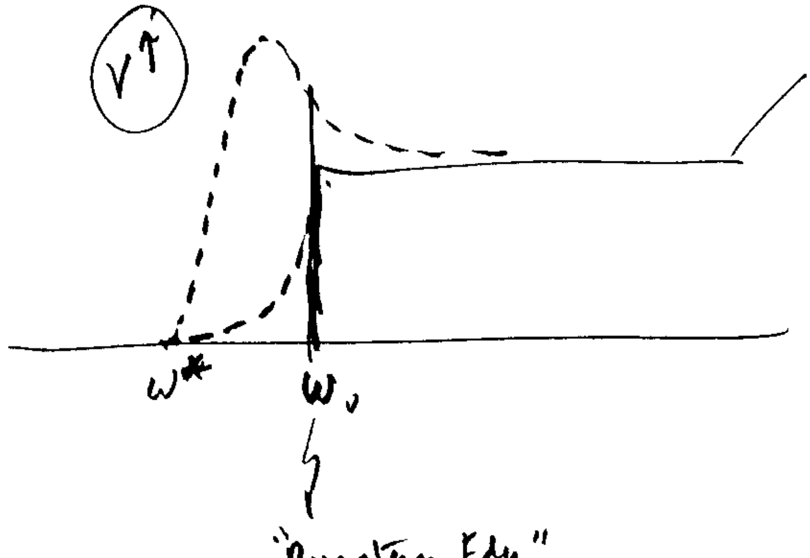
Threshold for direct transition ω_0

- But interactions allow for inelastic Auger processes

↓

absolute threshold ω^* if $d \geq 2$

$(\omega_0 - \omega^*)$ is the recoil energy of the hole, $E_h(k_F)$.

- 

Continuous evolution of spectrum

↓

X ray-edge if $\omega^* - \omega_0 \to 0$

(ii) Characteristic energies

- Final state attraction $V \rightarrow \quad g = \underbrace{\nu}_{\text{density of states}} V$

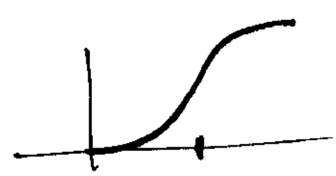
If Fermi sea is frozen,
"Mahan bound state" $\left\{ \begin{array}{l} \varepsilon = \mu - \delta \\ \delta \sim \varepsilon_F \exp(-1/g) \end{array} \right.$

- (cf analogy with Cooper states in superconductors)

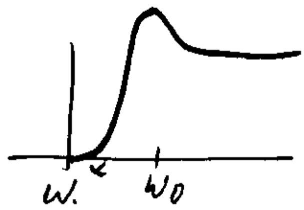
That bound state is below μ and it cannot be observed — but δ fixes an energy scale which should be compared to ε_h.

- $\boxed{\delta \ll \varepsilon_h}$ (i.e. $g \log \underbrace{\frac{m_h}{m_e}}_{\text{mass ratio}} \ll 1$)

Final state interactions are weak: the "Mahan mode" disappears in the broad Auger tail



• $\boxed{\delta \gtrsim \varepsilon_n}$ $\left(g \log \beta \gtrsim 1 \right)$



A peak appears between ω_0 and ω_1^*, but there is no singularity

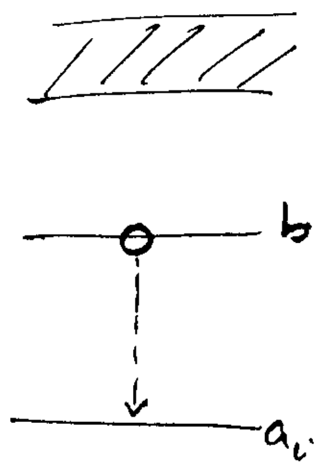
• $\boxed{\delta \gg \varepsilon_n}$.

The peak evolves towards the edge singularity

CONCLUSION : edge singularities are washed out by recoil

(at least if $d \geq 2$: continuum of Auger processes)

(iii) A perturbative argument



• local perturbation on an impurity (line spectrum) → exciting hamiltonian

$A_i \, \beta_i^*$

A_i: external field localized at site i

β_i^*: core transition $= b_i^* a_i$

(i) The core excitation β_i^* creates a local state perturbation in the conduction band

$$V\, c_i^* c_i$$

Old : known

(ii) The new feature is that the excitation can move.

$$t\, \beta_i^* \beta_j \qquad \text{(site representation)}$$

(bandwidth ~ ε_h in the former ξ)

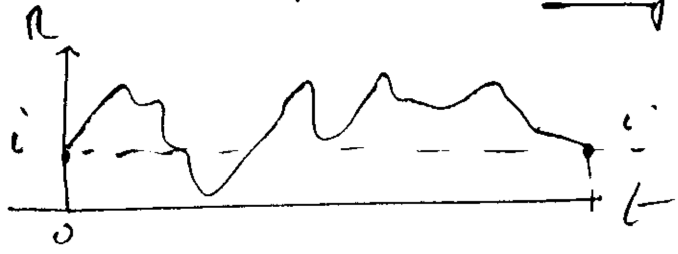
↓

Absorption $I(\omega)$ Fourier transform of $Z(t)$

hopping from site to site

Perturbation expansion in t = sum over histories

CONCLUSION : The valence band responds to a <u>moving</u> transient impurity



$$G(t) = \langle d_o(t)\, d_o^*(0) \rangle \quad .$$

In real time, a <u>transient</u> potential is felt by the light particles. If the heavy particle does not recoil, it stays at the origin 0, and G is just the exponential of closed loop contributions

$$G(t) = \exp\,[C(t)]$$

In Born approximation

$$C(t) = U^2 \int_0^t d\tau\, d\tau'\, g_{oo}(\tau - \tau')\, g_{oo}(\tau' - \tau) \quad .$$

Since $g_{oo}(\tau) \sim 1/\tau$, $C(t) \sim \text{Log } t$, yielding the usual power law of G. The calculation beyond Born approximation does not change the physics.

Assume now that the particle recoils : Between its creation and destruction ar $r = 0$, it <u>wanders</u> : G is a sum over histories of the heavy particles

$$G(t) = \sum_{r(t)} G[r(t)\,,t] \quad .$$

<u>For a given history</u>, the light gas is subject to a transient <u>time dependent</u> potential (monitored by the position r). The closed loop decoupling remains valid, and

$$\left\{ \begin{aligned} & G[r(t)\,,t] = \exp[\, C((r(t), t] \\ & C[r(t)\,,t] = \int_0^t d\tau\, d\tau'\, U^2 g\,[r(\tau) - r(\tau'), \tau - \tau'] \\ & \qquad\qquad\qquad\qquad g\,[r(\tau') - r(\tau), \tau' - \tau] \end{aligned} \right.$$

The only difference is the presence of <u>non local</u> propagators g (still within Born approximation). Of course, the calculation must be done for <u>each</u> history r(t), and the hard step is the sum over paths, which I cannot carry exactly (cf. Anderson-Yuval in the Kondo problem !).

The only ingredient is the non local g.

$$g[\rho,\tau] = \int v d\varepsilon_k \, e^{i\varepsilon_k \tau} e^{i\vec{k}\cdot\vec{\rho}} \, .$$

One can easily find an explicit expression, but I will focus on the limit $\tau >> \rho/v_F$ where v_F is the light particle Fermi velocity. That certainly holds if d is "heavy". It seems to me that even with equal masses, long time diffusion like motion will always generate a recoil $\rho << v_F \tau$. Then the integral over $|k|$ is dominated by the time phase (easy to check).

$$g(\rho,\tau) = -\frac{iv}{\tau} < e^{i\vec{k}_F \cdot \vec{\rho}} >$$

where the average is over the Fermi surface (angular average). If $\rho = 0$ (no recoil), you recover the usual result.

The effect of dimensionality is then straightforward

$$< e^{i\vec{k}_F \cdot \vec{\rho}} > = \begin{cases} \dfrac{\sin k_F\rho}{k_F\rho} & \text{cf} \quad d = 3 \\ J_o(k_F\rho) & \text{cf} \quad d = 2 \\ \cos k_F\rho & \text{cf} \quad d = 1 \end{cases}$$

The closed loop contribution involves the <u>square</u> of that angular average, hence an extra factor in C.

Important in 1-d metal
↓
critical exponent
$\frac{1}{8}, \frac{1}{2}\left(\frac{\delta}{\pi}\right)^2$
for $\delta = \pi h$?

For a non localized particle the recoil ρ diverges when τ goes to ∞ (I suspect that $\rho \sim \tau^{1/2}$, diffusive like, but I am not sure). When d = 1, the average $<\cos^2 k_F(\rho)> = 1/2$: the $1/\tau^2$ behaviour remains upon averaging (althoug[redacted]The infrared catastrophy is still there, despite recoil. That is consistent with standard wisdom.

When d = 2 or 3, however, the extra factor goes to zero when $\rho \to \infty$, respectively as $1/\rho$ and $1/\rho^2$. Hence the closed loop contribution is no longer logarithmically divergent

$$C \sim \int_0^t d\tau \, d\tau' \, \frac{1}{(\tau - \tau')^2 \, \rho^n_{\tau\tau'}}$$

(n = 1, 2). I cannot carry an exact calculation further, since it involves the summation over paths. But it seems clear that C is <u>finite</u>. If this is so, there is no infrared catastrophy.

CONCLUSION

- No edge singularity if particles wanders to ∞ for infinite t except for $d = 1$

  ↳ Note crucial role of dimensions

Nothing in $d = 2$, contrary to PWA statements

- Reduced singularity if localization. But what does that mean

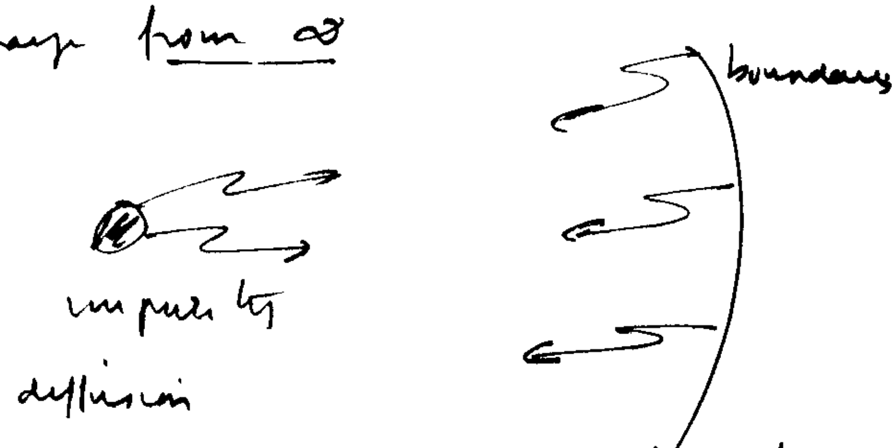
  { localized coherent states?

  { Possibility of incoherent diffusion that would also wash out the singularity?

  (Localization is induced by edge singularity)

?

- Note that the argument is consistent with the Hopfield argument, that puts emphasis from the input of charge from ∞



Screening is achieved either by moving charge towards impurity or vice versa

The real problem is that of localization

- The problem is related to that of diffusion of heavy particles discussed in chapter V

If diffusion anomalous, does $f \to \infty$?

— As of now, questions raised in a simple model, which is highly questionable, but which should lead to something

Local excitations

$$g_{ij} = 0 \quad \forall\, i \neq 0$$

Unusual, opposite to the physical case, where the bath moves easily while the scatterer moves slowly. But it allows to raise the issue

Simplified model

— light Fermi gas replaced by a set of boson modes with a linear spectral density (Caldeira - Leggett model)

Such a spectrum exists on <u>each</u> <u>site</u> i. The bosons are assumed <u>not</u> to propagate

↳ $D_{ii}(\omega)$ localized

— The propagator for a heavy particle is

where the cross denotes a hopping t. A phonon line must begin and end <u>on the same site</u>

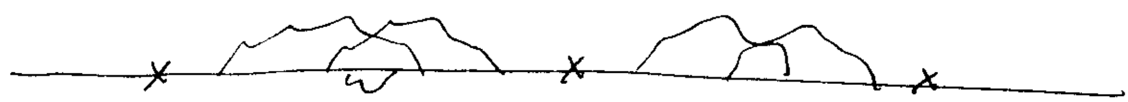
— <u>Key approximation</u>: G_{ij} implies a succession of hoppings from i to j

⇓

→ { We assume that the heavy particle never returns
→ { twice to the same site

I believe that such an approximation is equivalent to infinite dimension

Then the propagator is a sequence of renormalized <u>local</u> G_0, separated by t



$$\downarrow$$

$$G(k,\omega) = \frac{1}{\varepsilon_k - g^{-1}(\omega)}$$

g = localized propagator with phonons

— For a single particle, g is a standard X-ray problem, solved in time space

$$\left.\begin{aligned} g(t) &= e^{C(t)} \\ C &= -\frac{\delta^2}{\pi^2} \cdot \log t \end{aligned}\right\} \quad g(\omega) = \frac{1}{\omega}\left(\frac{\omega}{D}\right)^{\alpha} \qquad \alpha = \frac{\delta^2}{\pi^2}$$

$$\Downarrow$$

<u>Guess</u> : for a finite filling n of the heavy band, the branch cut of g is split on the $\omega > 0$ side (weight $(1-n)$), and on the negative ω side (weight n).

(?) $$g = \frac{1}{\omega}\left|\frac{\omega}{D}\right|^{\alpha} \begin{cases} (1-n) + n\, e^{\pm i\pi\alpha} & (\omega < 0) \\ (1-n)\, e^{\pm i\pi\alpha} + n & (\omega > 0) \end{cases}$$

altogether, my guess is
$$\boxed{\begin{array}{l} g(\omega) = \dfrac{1}{-f(\omega) + \varepsilon_k} \\ f(\omega) \sim \bar{f}\,\omega\left(\dfrac{D}{\omega}\right)^{\alpha} \end{array}}$$

— Consequences

(i) The local density of states is unchanged
$$\rho = \sum_k \frac{f_2}{(f_1 - \varepsilon_k)^2 + f_2^2}.$$

(ii) The renormalization constant is
$$\frac{1}{z} = \frac{\partial f_1}{\partial \omega} \sim \omega^{\alpha}$$

(iii) The quasiparticle energy is a root of
$$f_1(\omega) = \varepsilon_k \quad \rightarrow \quad \omega \sim \varepsilon_k^{\frac{1}{1-\alpha}}$$

(iv) The width of the resonance is
$$\Gamma = z f_2 \sim \omega^{\alpha} \frac{\omega}{\omega^{\alpha}} \sim \omega$$

(v) As in 1d, the Fermi level is well defined; but n_k is continuous with a power law. $\delta n_k \sim \left(\frac{\varepsilon_k}{D}\right)^{\frac{\alpha}{1-\alpha}}$

— Comparison with the recoil argument

(i) One history in time space

$$g(t) \sim_{L} \frac{1}{t^{\alpha}}$$

$$G = \prod \left(\frac{1}{\tau_{i+1} - \tau_i} \right)^{\alpha}$$

The lack of long loops does not preclude the existence of a power law.

Exponential behaviour when the overall t goes to ∞ (more and more stretches).

(ii) But apparently the summation over τ_i restores an anomalous behaviour

QUESTION: will the propagation of bosons wash the singularity out ?

— More generally, the model is pathologic (nothing on dimension, mass ratio m/M): where is pathology.

(i) No return ($d = \infty$) : 2 doubts

(ii) local phonons : no way to relax when the particle is gone

QUESTION : is the "travelling along" of particle and boson a general claim ?

(probably yes).

Open problem. · My guess is that localization will not occur if the mass ratio is ~ 1 and the coupling weak.

No edge singularity

- Possibility of localization for strong coupling (see chapter 5)
- In the silly model, it seems that localization always occurs

lack of a lower cut off ?

?