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SUMMER SCHOOL on LOW-DIMENSIONAL QUANTUM SYSTEMS: Theory and Experiment (16 - 27 JULY 2001)

PLUS

PRE-TUTORIAL SESSIONS (11 - 13 JULY 2001)

CONDUCTIVITY OF A LONG CLEAN WIRE

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These are preliminary lecture notes, intended only for distribution to participants

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Conductivity of a clean 1-d wire

- Transport and weakly violated conservation laws
- Interacting electrons (RG, Luttinger liquids, bosonization and all that)
- Interacting electrons in the presence of a periodic potentail
- Transport and the Memory Functional Formalism
- Computation of the conductivity
- Complex dependence on Filling and Temperature

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An ideal 1d wire: carbon nanotube

nanotubes: rolled up graphite sheets



Atomic resolution on the nanotubes



mK experiments on an individual nanotube



Tans, Devoret, These, Smalley, Georilgs, Deiker, Nature 386, 474 (1987)

Weakly coupled 1d wires: Bechgaard salts

TMTSF



stacked molecules



(TMTSF)2X

X∓(PF6)- ,.... by D. Jerome



Correlation gap and dimensional cross-over





open Fermi surface: two Fermi-sheets

Historical remarks

• most papers:

neglect Umklapp away from 1/2 filling - (irrelevant operator)

- $\rightarrow \sigma(T > 0) = \sigma_{\text{bulk}} = \infty$ $\rightarrow G = G_{\text{contact}} = \frac{2e^2}{h} \text{ (conductance)}$
- Giamarchi (91), $(4k_F G)$ -Umklapp

- perturbation theory (memory functional)

$$ightarrow \sigma(T>0)<\infty$$

- Luther-Emery transformation

 $\rightarrow \sigma = \infty$

- many papers: using PT result of Giamarchi or same result with different PT
- Giamarchi, Millis (92) (band structure effects) $\infty > \sigma(T > 0) > T^{-n}$
- Castella, Zotos *et al.* (95-97): *integrable* systems - infinite number of conserved quantities. Select $Q_1...Q_N$, $(\langle Q_n Q_m \rangle = \delta_{nm} \langle Q_n^2 \rangle)$ then:

$$\sigma(T > 0, \omega) = 2\pi D(T)\delta(\omega) + \dots$$
$$D(T) \geq \frac{1}{2} \sum_{n=1}^{N} \frac{(\chi_{JQ_n})^2}{\chi_{Q_nQ_n}}$$

Gedankenexperiment I

• \tilde{P} exactly conserved:



How much $\lim_{t\to\infty} \langle J \rangle$ is induced by $\langle \tilde{P} \rangle$?

 $\frac{\langle J(t \to \infty) \rangle}{\langle \tilde{P} \rangle} = \frac{\chi_{J\tilde{P}}}{\chi_{\tilde{P}\tilde{P}}} \quad \Rightarrow \quad \frac{\langle J(t \to \infty) \rangle}{\langle J(t = 0) \rangle} = \frac{\chi_{J\tilde{P}}^2}{\chi_{\tilde{P}\tilde{P}}\chi_{JJ}}$

infinite conductivity at T > 0

$$\operatorname{Re}\sigma(\omega) = 2\pi D\delta(\omega) + \sigma_{\operatorname{reg}}(\omega)$$

Drude weight
$$D = \frac{1}{2} \frac{\chi^2_{J\tilde{P}}}{\chi_{\tilde{P}\tilde{P}}}$$

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(exact if only \tilde{P} conserved (Suzuki 71))

Gedankenexperiment II



peak in $\sigma(\omega)$, decay-rate of \tilde{P} determines $\sigma(0)$

$$D = \frac{1}{2} \frac{\chi_{J\tilde{P}}^2}{\chi_{\tilde{P}\tilde{P}}}$$

From the lattice to the continuum A general Hamiltonian on a lattice

$$H = H_0 + H_{e-e} + H_{lat}$$

$$H_0 = \sum \epsilon_k c_k^{\dagger} c_k$$

 $H_{e-e} = \sum_{k \in BZ} V_{k_1,k_2} c_{k_1}^{\dagger} c_{k_2} c_{k_3}^{\dagger} c_{k_4} \delta_G(k_1 - k_2 + k_3 - k_4)$

 H_{lat} = some periodic lattice potential

with $\delta_G(k) = \sum_G \delta(k-G)$

• How do we study low-energy, long-distance behaviour?

- Do RG to obtain low-energy effective hamiltonian

- Alternatively, build effective hamiltonian "by hand"

From the lattice to the continuum



• keep modes: $k = \pm k_F + q$, $q \leq \Lambda$ $c_{n,\alpha} = \sum_k c_{k,a} e^{ikna} \approx e^{ik_F x} \psi_{R,\alpha}(x) + e^{-ik_F x} \psi_{L,\alpha}(x)$ with:

-
$$\psi^{\dagger}_{R}(x) = \sum e^{-iqx} c^{\dagger}_{k_{F}+q}$$

-
$$\psi^{\dagger}_L(x) = \sum e^{-iqx} c^{\dagger}_{-k_F+q}$$

low - energy effective Hamiltonian:
 Fixed point Hamiltonian + correction terms

- Fixed point Hamiltonian: $H^* = H_{LL}$ (Luttinger liquid) - Correction Terms: $H^{corrections} = H_{irr} + H_{umklapp}$

From the lattice to the continuum

The Luttinger liquid



separate in slowly varying left- and right moving electrons:

- $egin{array}{rl} \Psi_{\uparrow/\downarrow}(x) &=& \Psi_{L,\uparrow/\downarrow}(x)e^{-ik_Fx} \ &+ \Psi_{R,\uparrow/\downarrow}(x)e^{ik_Fx} \end{array}$
- lowest energies: linearize around Fermi energy fixed point: Luttinger liquid

$$H_{LL} = v_F \int \left(\Psi_{R\sigma}^{\dagger} i \partial_x \Psi_{R\sigma} - \Psi_{L\sigma}^{\dagger} i \partial_x \Psi_{L\sigma} \right) + g \int \rho(x)^2$$

= $\frac{1}{2} \int \frac{dx}{2\pi} \sum_{\nu=\sigma,\rho} v_{\nu} \left(K_{\nu} (\partial_x \theta_{\nu})^2 + \frac{1}{K_{\nu}} (\partial_x \phi_{\nu})^2 \right)$

- bosonization: $\Psi_{L/R,\uparrow/\downarrow}(x) \propto e^{-i\Phi_{L/R,\uparrow/\downarrow}(x)}$
- spin-charge separation, non-Fermi liquid: power-laws
- deviation from H_{LL} irrelevant: perturbation theory convergent, effects small at low temperature (exception: half-filling)

• dangerously irrelevant for conductivity

From the lattice to the continuum Classify deviations from LL-Hamiltonian

$$H = H_{LL} + H_{\rm irr} + \sum_{n=\infty}^{\infty} H_{n,m}^U$$

Luttinger liquid + irrelevant terms + Umklapp with:

$$P_{T} = \sum_{\sigma} \int dx \left(\Psi_{R\sigma}^{\dagger} i \partial_{x} \Psi_{R\sigma} + \Psi_{L\sigma}^{\dagger} i \partial_{x} \Psi_{L\sigma} \right)$$

$$J_{0} = N_{R} - N_{L} = \sum_{\sigma} \int dx \left(\Psi_{R\sigma}^{\dagger} \Psi_{R\sigma} - \Psi_{L\sigma}^{\dagger} \Psi_{L\sigma} \right)$$

$$H_{LL} = v_{F} \int \left(\Psi_{R\sigma}^{\dagger} i \partial_{x} \Psi_{R\sigma} - \Psi_{L\sigma}^{\dagger} i \partial_{x} \Psi_{L\sigma} \right) + g \int \rho(x)^{2}$$

$$[H_{irr}, P_{T}] = [H_{irr}, J_{0}] = 0$$

$$Umklapp: H_{n,m}^{U}$$

$$n \text{ fermions from L to R} + lattice momentum} \Delta k_{n,m} = n2k_{F} - mG$$

$$H_{1,m}^{U} \approx g_{1,m}^{U} \sum_{\sigma} \int e^{i\Delta k_{1,m}x} \Psi_{R\sigma}^{\dagger} \Psi_{L\sigma} \rho_{-\sigma} + h.c.$$

$$H_{2,m}^{U} \approx g_{2,m}^{U} \int e^{i\Delta k_{2,m}x} \Psi_{R\uparrow}^{\dagger} \Psi_{R\downarrow}^{\dagger} \Psi_{L\downarrow} \Psi_{L\uparrow} + h.c.$$

$$H^{U}_{3,m} \approx g^{U}_{3,m} \int e^{i \Delta k_{3,m}x} \Psi^{\dagger}_{R\uparrow} \Psi^{\dagger}_{R\uparrow} \Psi^{\dagger}_{R\downarrow} \Psi_{L\downarrow} \Psi_{L\downarrow} \Psi_{L\uparrow} \Psi_{L\uparrow} + h.c.$$

From the lattice to the continuum The continuum Hamiltonian

$$\boldsymbol{H} = H_{LL} + H_{\mathrm{irr}} + \sum_{n,m}^{\infty} H_{n,m}^{U}$$

• The fixed point Hamiltonian

$$H_{LL} = v_F \int \left(\Psi_{R\alpha}^{\dagger} i \partial_x \Psi_{R\alpha} - \Psi_{L\alpha}^{\dagger} i \partial_x \Psi_{L\alpha} \right) + g \int \rho^2$$
$$= \frac{1}{2} \int \frac{dx}{2\pi} \sum_{\nu=\sigma,\rho} v_{\nu} \left(K_{\nu} (\partial_x \theta_{\nu})^2 + \frac{1}{K_{\nu}} (\partial_x \phi_{\nu})^2 \right)$$

- H_{irr} band structure terms etc. (need not be specified.)
- Umklapp terms $H_{n,m}^U$

- transfer n fermions from L to R (and vice versa) and lattice momentum $mG = m\frac{2\pi}{a}$

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- dangerously irrelevant

From the lattice to the continuum

Umklapp terms are of the form:

$$\begin{split} H^{U}_{0,m} &\approx g^{U}_{0,m} \int e^{i\Delta k_{0,m}x} (\rho_{L} + \rho_{R})^{2} + h.c. \\ H^{U}_{1,m} &\approx g^{U}_{1,m} \sum_{\sigma} \int e^{i\Delta k_{1,m}x} \Psi^{\dagger}_{R\sigma} \Psi_{L\sigma} \rho_{-\sigma} + h.c. \\ H^{U}_{2,m} &\approx g^{U}_{2,m} \int e^{i\Delta k_{2,m}x} \Psi^{\dagger}_{R\uparrow} \Psi^{\dagger}_{R\downarrow} \Psi_{L\downarrow} \Psi_{L\uparrow} + h.c. \\ H^{U}_{2n,m} &\approx g^{U}_{2n,m} \int e^{i\Delta k_{2n,m}x} \\ &\times \prod_{j=0}^{n-1} \frac{\partial_{x}^{j} \Psi^{\dagger}_{R\uparrow} \partial_{x}^{j} \Psi^{\dagger}_{R\downarrow} \partial_{x}^{j} \Psi_{L\downarrow} \partial_{x}^{j} \Psi_{L\uparrow}}{(j!/\alpha^{j})^{4}} + h.c. \end{split}$$

Momentum transfer:

$$\Delta k_{n,m} = n2k_F - mG$$

Bosonized Umklapp term

$$H_{n,m,n_s}^U = \frac{g_{n,m,n_s}^U}{(2\pi\alpha)^n} \int e^{i\Delta k_{n,m}x} e^{i\sqrt{2}(n\phi_\rho + n_s\phi_\sigma)}$$

Transfers:

- n electrons with n_S total spin
- mG momentum absorbed by lattice

Weakly violated conservation laws

Operators:

$$P_T = -i\sum_{\sigma} \int dx \left(\Psi_{R\sigma}^{\dagger} \partial_x \Psi_{R\sigma} + \Psi_{L\sigma}^{\dagger} \partial_x \Psi_{L\sigma} \right)$$
$$J_0 = N_R - N_L = \sum_{\sigma} \int dx \left(\Psi_{R\sigma}^{\dagger} \Psi_{R\sigma} - \Psi_{L\sigma}^{\dagger} \Psi_{L\sigma} \right)$$

- conserved on the Fermi-surface. Note $P \approx k_F J_0 + P_T$

- violation leads to degrading of electric current
 - terms in H_{irr} commute with both, $[H_{irr}, P_T] = [H_{irr}, J_0] = 0$
 - terms in H^U
 - do not commute with either P_T or J_0
 - dangerously irrelevant

Observation: $[H_{2n,m}^U, \Delta k_{n,m}J_o + 2nP_T]$

- single Umklapp does not degrade the current completely
- need at least two Umklapps to have finite conductivity

From the lattice to the continuum

Define pseudo-momentum $\tilde{P}_{n,m}$ with $\Delta k_{n,m} = n \cdot 2k_F - mG$

$$\tilde{P}_{n,m} = \frac{\Delta k_{n,m}}{2n} (N_R - N_L) + P_T$$

(without Umklapp: $\tilde{P}_{n,0}$ =usual momentum)

• Hamiltonian with single type of Umklapp conserves pseudo-momentum $\Rightarrow \infty$ conductivity

$$\left[H_{LL}+H_{irr}+H_{n,m}^U, \tilde{P}_{n,m}\right]=0$$

- interplay of two independent Umklapps $H^U_{n,m}, H^U_{n',m'}$ renders σ finite
- second strongest Umklapp determines $\sigma(\omega = 0)$

How to calculate $\sigma(\omega)$ perturbatively?

- Problem: σ and $1/\sigma$ singular function of perturbations for $\omega \to 0$
- full quantum-transport equations?
 ⇒ difficult (highly non-linear interaction of LL bosons)
- approximate conservation laws known
 ⇒ "hydrodynamic" description possible
- use Memory Matrix Formalism in space of slow modes (Mori (65), Zwanzig (61))
 - combined short-time and perturbative expansion for slow decay rates
 - short-time dynamics of slowest modes = long time behavior
 - weights of low-frequency peak exactly reproduced if time-scales well separated

Transport and the Memory Function Formalism I

- Memory Functional Formalism: study transport in the presence of approximate conserved quantities.

Mori (65), Zwanzig (61), Götze Wölfle (72), Giamarchi (91)

• Scalar product in *operator* space

$$(A(t)|B) \equiv \frac{1}{\beta} \int_0^\beta d\lambda \left\langle A(t)^{\dagger} B(i\lambda) \right\rangle$$

• Static susceptibility

$$\chi_{AB} = \beta(A|B) \qquad t = 0$$

• Dynamic Correlation function

$$C_{AB}(z) \equiv \int_{0}^{\infty} e^{izt} \left(A(t)|B\right) dt$$
$$= \left(A \left|\frac{i}{z-L}\right|B\right), \quad LA = [H, A]$$
$$= \frac{i}{\beta z} \int_{0}^{\infty} e^{izt} \left\langle [A(t), B] \right\rangle - \frac{(A|B)}{iz}$$

• Conductivity

$$\sigma(\omega, T) = \beta C_{JJ}(\omega) = \beta (J | \frac{i}{\omega - L} | J)$$

Transport and the Memory Function Formalism II

Transport in the presence of several "slow" variables: $j_1 = J, j_2, \ldots, j_N$

• The conductivity

$$\sigma(\omega,T) = [(\hat{M}(\omega,T) - i\omega)^{-1}\hat{\chi}(T)]_{1,1}$$

• The susceptibility matrix

$$\hat{\chi}_{pq} = \beta(j_p|j_q)$$

• The memory matrix

$$\hat{M}_{pq}(\omega) = \beta \sum_{r} \left(\partial_t j_q \left| Q \frac{i}{\omega - QLQ} Q \right| \partial_t j_r \right) (\hat{\chi}^{-1})_{rp}.$$

• The projection away from slow modes

$$Q = 1 - \sum_{pq} |j_q| \beta(\hat{\chi}^{-1})_{qp} (j_p).$$

Philosophy:

 \hat{M} non-singular in P.T.

- P.T. valid for short-time behavior

- P.T. also valid for long-time behavior of slowest modes (provided slow modes dynamics projected out - Q.)

- If there are linear combination of $\{j_p\}$ that are conserved: $\tilde{J}_1, \ldots, \tilde{J}_S$

Intermezzo - conserved quantities

 \rightarrow expect ∞ dc - conductivity.

Indeed, carry out matrix inversion, project out zero - modes etc.

$$\sigma(\omega \to 0, T > 0) = i \frac{(\hat{\chi}\hat{\chi}_c^{-1}\hat{\chi})_{11}}{\omega + i0} + \sigma_{\text{reg}}(\omega, T)$$

where:

•
$$\hat{\chi}_c^{-1} = \mathcal{P}_c (\mathcal{P}_c \hat{\chi} \mathcal{P}_c)^{-1} \mathcal{P}_c$$

- \mathcal{P}_c projection on space of conserved variables
- $\sigma_{reg}(\omega, T)$ regular as long as all conserved currents are included.

Thus

• Re
$$\sigma(\omega \to 0) = 2\pi D(T)\delta(\omega) = \pi(\hat{\chi}\hat{\chi}_c^{-1}\hat{\chi})_{1,1}\delta(\omega)$$

Determined by the overlaps of the current J with conserved quantities, $\tilde{\chi}_{1,s}$

The generic case

- All variables j_1, \ldots, j_N decay slowly
- Restrict to two dimensional space

 $j_1 = J \approx v_F J_0$ $j_2 = P_T$

- commute with all scattering processes on Fermi-surface

- longest decay rate, exponential in T, dominate transport

- can neglect other slow quantities at low - T,

decay as powers of T (unless model is integrable e.g. $H_{LL} + H_{21}^U$ relevant at 1/2 filling)

The calculation I

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We can approximate:

• $L_{LL} = [H_{LL}]$. $\partial_t v_F J_0$ and $\partial_t P_T$ linear in $g_{n,m}^U$

• $L_{LL}P_T = L_{LL}J_0 = 0$, so no contribution from QThus

$$\hat{M} \approx \sum_{nm} M_{nm}(\omega, T) \begin{pmatrix} v_F^2 (2n)^2 & -2nv_F \Delta k_{nm} \\ -2nv_F \Delta k_{nm} & (\Delta k_{nm})^2 \end{pmatrix} \hat{\chi}^{-1}$$

where

$$\hat{\chi} \approx \begin{pmatrix} 2v_F/\pi & 0\\ 0 & \frac{\pi T^2}{3} \left(\frac{1}{v_{\rho}^3} + \frac{1}{v_{\sigma}^3}\right) \end{pmatrix}$$
$$M_{nm} \equiv (g_{nm}^U)^2 M_n(\Delta k_{n,m},\omega) \equiv \frac{\langle F;F \rangle_{\omega}^0 - \langle F;F \rangle_{\omega=0}^0}{i\omega}.$$

with

- $F = [J_0, H_{nm}^U]/(2n)$
- $\langle F:F\rangle^0_{\omega}$ retarded correlation function of Fwith respect to H_{LL} .

The calculation II

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For *n* arbitrary and $n_S = 0$, $(M_2$, Giamarchi 91)

$$M_{n}(\Delta k,\omega) = \frac{2\sin 2\pi K_{\rho}^{n}}{\pi^{4}\alpha^{2n-2}v_{\rho}} \left[\frac{2\pi\alpha T}{v_{\rho}}\right]^{4K_{\rho}^{n}-2} \frac{1}{i\omega} \times \left[B(K_{\rho}^{n}-iS_{+},1-2K_{\rho}^{n})B(K_{\rho}^{n}-iS_{+},1-2K_{\rho}^{n}) -B(K_{\rho}^{n}-iS_{+},1-2K_{\rho}^{n})B(K_{\rho}^{n}-iS_{+}^{n},1-2K_{\rho}^{n})\right]$$

where

-
$$K_{\rho}^{n} = (n/2)^{2} K_{\rho}$$

- $S_{\pm} = (\omega \pm v_{\rho} \Delta k)/(4\pi T)$

Approximate forms:

$$\approx \frac{\alpha^{2-2n}}{\pi^2 \Gamma^2 (2K_{\rho}^n) v_{\rho} T} \left(\frac{\alpha \Delta k}{2}\right)^{4K_{\rho}^n - 2} e^{-v_{\rho} \Delta k/(2T)}$$

$$M_n \approx \frac{(\alpha T/v_{\rho})^{n^2 K_{\rho} - 1} (\alpha \Delta k)^{n_s^2 K_{\sigma} - 2}}{\Gamma^2 (n_s^2 K_{\sigma}/2) v_{\sigma}^2 \alpha^{2n - 3}} e^{-v_{\sigma} \Delta k/(2T)}$$

$$\approx T^{n^2 K_{\rho} + n_s^2 K_{\sigma} - 3}$$

One Umklapp, two Umklapps..

One Umklapp term (insufficient to degrade current)

 → finite Drude peak, infinite dc - conductivity

$$D(T) \approx \frac{v_{\rho} K_{\rho}}{\pi} \frac{1}{1 + T^2 \frac{2\pi^2 n^2 K_{\rho}}{3(v_{\rho} \Delta k_{nm})^2} \left(1 + \frac{v_{\rho}^3}{v_{\sigma}^3}\right)}.$$
 (1)

• Two Umklapp terms $(H^U_{n,m}, H^U_{n',m'})$ \rightarrow finite dc - conductivity

$$\sigma(T,\omega=0) = \frac{(\Delta k_{nm})^2 / M_{n'm'} + (\Delta k_{n'm'})^2 / M_{nm}}{\pi^2 (n\Delta k_{n'm'} - n'\Delta k_{nm})^2} \quad (2)$$



Conductivity for two Umklapp terms H_{21}^U and H_{20}^U $\Delta k_{21} = -1.5 \Delta k_{20}, K_{\rho} = 0.7, K_{\sigma} = 1.3, g_{20} = g_{21} = 1,$ T = 0.18, 0.20.

Commensurate filling

- Commensurate filling:

 $filling = \frac{m}{n} \rightarrow \Delta k_{nm} = 0.$ Recall $k_F = (filling) \frac{\pi}{a}$

- Does dominant scattering process H_{nm}^U relax the current?
- Depends on the overlap χ_{JP_T}
 - Identity $\chi_{JP_T} = \Delta \rho + o(e^{-\beta E_F})$

 $\Delta \rho = 2\Delta n/a$ - electron density deviation from commensurate filling.

- 3d array of wires - $\Delta \rho$ is T - independent, determined by charge neutrality
- single wire -

 $\Delta
ho(T) \sim T^2/(mv^3)$

PH sym breaking $\sim k2/(2m)$

• Replace

 Δk by $(\pi \Delta \rho)$.

The conductivity

Which of the scattering processes will dominate? - <u>intermediate T</u> : small n (low order) - Pauli

- <u>lower T</u> : exponential factor prevails, smallest Δk_{nm}
 - Close to commensurate filling $k_F \approx G \frac{m_0}{n_0}$ dominant processes $H_{n_0 m_0}^U$, $H_{n_1 m_1}^U$ where $\Delta k_{n_0, m_0} \approx 0$, $\Delta k_{n_1, m_1} = \pm G/n_0$ $\rightarrow (n_1 m_0 = \pm 1 \mod n_0)$ $\rightarrow n_1 = \gamma n_0$, $\gamma \sim 1$

We find: The conductivity close to commensurability: $\sigma(k_F \approx Gm_0/(2n_0)) \sim (\Delta n(T))^2 \exp[\beta v G/(2n_0)]$ $\sigma(k_F = Gm_0/(2n_0)) \sim T^{-n_0^2 K_\rho - (n_0 \mod 2)^2 K_\sigma + 3}$

• At typical incommensurate filling Do saddle-point approximation with respect to n of: $-\beta v G/(2N) + (\gamma N)^2 K \log[T]$

We find: Typical conductivity:

 $\sigma_{\rm typical} \sim \exp[c(\beta v G)^{2/3}]$

Filling dependence of the conductivity



- Enhancement at commensurate filling n
- Dip at commensurate point: overlap of current J and approx. conserved current $J_c = \Delta k_{nm}J_0 + P_T$ given by $\chi_{JJ_c} = n n_{\text{commensurate}}$

$$\sigma(n \sim M/N) pprox \max\left[(\Delta n)^2 e^{\beta v G/N}, T^{-N^2 K_{
ho}}
ight]$$