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Electrical conductivity of charged particle systems and the Zubarev NSO method

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Outline

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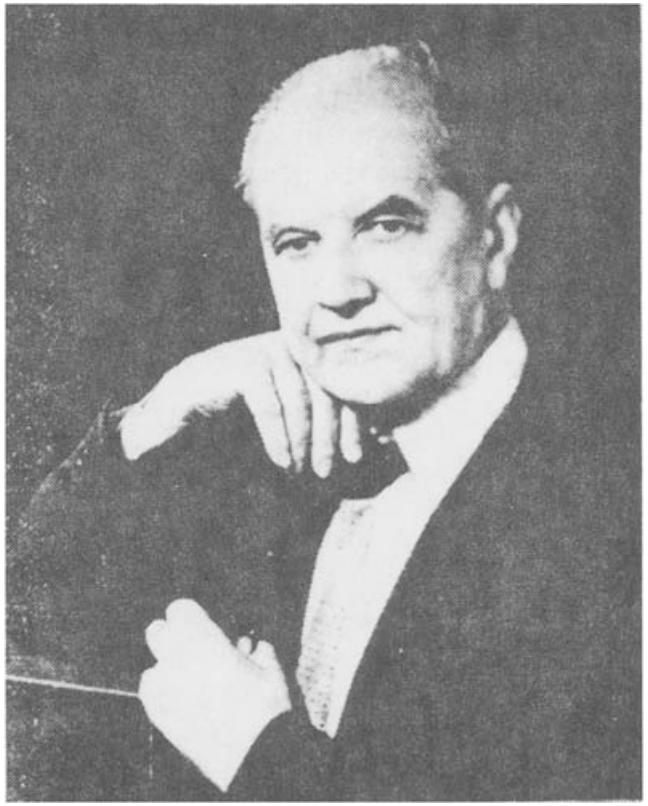

- Plasma conductivity, kinetic theory
- Generalized linear response theory
- Perturbation expansions
- Entropy production
- Recent work

Ohm’s law

Charged particle system: electrons and protons, external electric field E

Voltage U electrical current I

Resistivity $R = U/I$

current density $j = I/A$ $j = \sigma E_{\mathrm{intrinsic}}$

conductivity $\sigma = 1/R$

transport coefficient

heat production $dQ/dt = j \cdot E$ entropy production $dS_{\mathrm{intr.}}/dt$

Thermodynamics of irreversible processes

Microscopic approach

microscopic (atomistic) model

Hamiltonian

$$\mathrm{H_S} = \mathrm{H_0} + \mathrm{H_{int}} = \sum_{c,\boldsymbol{p}} E_{c,\boldsymbol{p}} \mathrm{a}^{\dagger}_{c,\boldsymbol{p}} \mathrm{a}_{c,\boldsymbol{p}} + \frac{1}{2} \sum_{c,d,\boldsymbol{k},\boldsymbol{p},\boldsymbol{q}} \frac{e_c e_d}{\epsilon_0 \Omega q^2} \mathrm{a}^{\dagger}_{c,\boldsymbol{p}+\boldsymbol{q}} \mathrm{a}^{\dagger}_{d,\boldsymbol{k}-\boldsymbol{q}} \mathrm{a}_{d,\boldsymbol{k}} \mathrm{a}_{c,\boldsymbol{p}}$$

c, d : electrons, protons

$$E_{c,\boldsymbol{p}} = \frac{\hbar^2 p^2}{2 m_c}$$

Coulomb interaction

$$\mathrm{H_F} = -\sum_c e_c E \mathrm{X_c}$$

$$\mathrm{X_c} = \sum_i^{N_c} \mathrm{x}_{c,i}$$

$$H = \mathrm{H_S} + \mathrm{H_{field}}$$

bath??? open system, stationary state

Lorentz plasma

neglect e-e interaction, only mean field. neutralizing background, adiabatic limit, ions at fixed positions Ri

Lorentz plasma model (condensed matter) isotropic system

Hamiltonian for the electron subsystem

$$\mathrm{H_S} = \mathrm{H_0} + \mathrm{H_{int}} = \sum_{\boldsymbol{p}} E_{\boldsymbol{p}} \mathrm{a}^{\dagger}_{\boldsymbol{p}} \mathrm{a}_{\boldsymbol{p}} + \sum_{\boldsymbol{p},\boldsymbol{q}} V(q) \mathrm{a}^{\dagger}_{\boldsymbol{p}+\boldsymbol{q}} \mathrm{a}_{\boldsymbol{p}}$$

statically screened Coulomb potential

$$V(\boldsymbol{r}) = \sum_i V_{\mathrm{ei}}(\boldsymbol{r} - \boldsymbol{R}_i)$$

Boltzmann equation

single-particle distribution function $f_1(\mathbf{r}, \mathbf{p}, t)$

low-density limit

$$\frac{\partial}{\partial t} f_1 + \mathbf{v} \frac{\partial}{\partial \mathbf{r}} f_1 + \mathbf{F}^{\text{external}} \frac{\partial}{\partial \mathbf{p}} f_1 = \left(\frac{\partial}{\partial t} f_1 \right)_{\text{St}}$$

Collision integral

$$\left(\frac{\partial}{\partial t} f_1 \right)_{\text{St}} = \int d^3\mathbf{v}_2 \int d\Omega \frac{d\sigma}{d\Omega} |\mathbf{v}_1 - \mathbf{v}_2| \{ f_1(\mathbf{r}, \mathbf{p}_1', t) f_1(\mathbf{r}, \mathbf{p}_2', t) - f_1(\mathbf{r}, \mathbf{p}_1, t) f_1(\mathbf{r}, \mathbf{p}_2, t)$$

Degeneration

ideal gas as equilibrium solution
implementation of correlations, conservation of energy

Dense, strongly interacting systems?

Solution

Coulomb plasma (Spitzer) Fokker-Planck equation

$$\sigma(n,T) = 0.591 \frac{(k_B T)^{3/2} (4\pi\epsilon_0)^2}{m^{1/2} e^2} \frac{1}{(-1/2)\ln[n] + c(T) + d(T) n^{1/2} \ln[n] \dots}$$

Lorentz plasma model relaxation time ansatz

$$\sigma(n,T) = 2^{5/2} \pi^{-3/2} \frac{(k_B T)^{3/2} (4\pi\epsilon_0)^2}{m^{1/2} e^2} \frac{1}{(-1/2)\ln[n] + c'(T) + d'(T) n^{1/2} \ln[n] \dots}$$

virial expansions

$$\sigma^{-1}(T,n) = A(T)\log n + B(T) + C(T) n^{1/2} \log n \pm \dots$$

$$A(T) = -\frac{1}{2s} \frac{e^2 m^{1/2}}{(4\pi\epsilon_0)^2 (k_B T)^{3/2}},$$

$$\sigma_{dc} = s \frac{(k_B)^{3/2} (4\pi\epsilon_0)^2}{m^{1/2} e^2} \frac{1}{\Lambda(p_{therm})}$$

Coulomb: s = 0.591

Lorentz: s = 1.0159

The Zubarev NSO method

principle of weakening of initial correlations (Bogoliubov)

$$\rho_\epsilon(t) = \epsilon \int_{-\infty}^{t} e^{\epsilon(t_1 - t)} U(t,t_1) \rho_{\rm rel}(t_1) U^\dagger(t,t_1)\, dt_1$$

time evolution operator $U(t,t_0)$

relevant statistical operator: maximum of information entropy

Selection of the set of relevant observables $\{B_n\}$

self-consistency relations $\mathrm{Tr}\{\rho_{\rm rel}(t) B_n\} \equiv \langle B_n \rangle^t_{\rm rel} = \langle B_n \rangle^t$

Extended von Neumann equation

$$\frac{\partial}{\partial t}\varrho_\varepsilon(t) + \frac{i}{\hbar}\left[H, \varrho_\varepsilon(t)\right] = -\varepsilon\left(\varrho_\varepsilon(t) - \varrho_{\rm rel}(t)\right)$$

$\varrho(t) = \lim_{\varepsilon \to 0} \varrho_\varepsilon(t)$ after thermodynamic limit

Thermodynamic equilibrium

$$\frac{\partial}{\partial t}\rho(t) + \frac{i}{\hbar}[H^t, \rho(t)] = 0$$

equilibrium
$$\frac{\partial}{\partial t}\rho_{\rm eq}(t) = 0$$

$$\langle H \rangle_{\rm eq} = U(\Omega, \beta, \mu_c), \qquad \langle N_c \rangle_{\rm eq} = \Omega n_c(T, \mu_c)$$

Extremum of information entropy

$$S_{\rm inf}[\rho] = -\,{\rm Tr}\{\rho \log \rho\} \qquad {\rm Tr}\{\rho\, C_n\} = \langle C_n \rangle$$

Gibbs distribution

$$\rho_{\rm eq} = \frac{\exp\{-\beta(H - \sum_c \mu_c N_c)\}}{{\rm Tr}\exp\{-\beta(H - \sum_c \mu_c N_c)\}}$$

entropy

$$S_{\rm eq}[\rho_{\rm eq}] = -k_{\rm B}\,{\rm Tr}\{\rho_{\rm eq} \log \rho_{\rm eq}\}$$

not valid in nonequilibrium
$$\frac{d}{dt}[{\rm Tr}\{\rho(t) \log \rho(t)\}] = 0.$$

Relevant statistical operator

State of the system in the past $\mathrm{Tr}\{\rho(t) B_n\} = \langle B_n \rangle^t$

Construction of the relevant statistical operator at time t

$$S_{\mathrm{rel}}(t) = -k_{\mathrm{B}}\, \mathrm{Tr}\{\rho_{\mathrm{rel}}(t) \log \rho_{\mathrm{rel}}(t)\}$$

$$\delta[\mathrm{Tr}\{\rho_{\mathrm{rel}}(t) \log \rho_{\mathrm{rel}}(t)\}] = 0$$

$$\mathrm{Tr}\{\rho_{\mathrm{rel}}(t) B_n\} \equiv \langle B_n \rangle^t_{\mathrm{rel}} = \langle B_n \rangle^t$$

Generalized Gibbs distribution

$$\rho_{\mathrm{rel}}(t) = \exp\left\{-\Phi(t) - \sum_n \lambda_n(t) B_n\right\}$$

$$\Phi(t) = \log \mathrm{Tr} \exp\left\{-\sum_n \lambda_n(t) B_n\right\}$$

$$\frac{\partial S_{\mathrm{rel}}(t)}{\partial t} = \sum_n \lambda_n(t) \langle \dot{B}_n \rangle^t$$

But: von Neumann equation?
Entropy?

The Zubarev solution of the initial value problem

Use the relevant statistical operator as initial state,
The missing correlations are produced dynamically

$$\rho_{t_0}(t) = U(t,t_0)\rho_{\mathrm{rel}}(t_0)U^\dagger(t,t_0)$$

$$i\hbar\frac{\partial}{\partial t}U(t,t_0) = H^t U(t,t_0) \qquad U(t,t_0) = \exp\left\{-\frac{i}{\hbar}H(t-t_0)\right\}$$

Abel's theorem

$$\rho_\epsilon(t) = \epsilon\int_{-\infty}^{t} e^{\epsilon(t_1-t)}U(t,t_1)\rho_{\mathrm{rel}}(t_1)U^\dagger(t,t_1)\,dt_1$$

$$\rho_{\mathrm{NSO}}(t) = \lim_{\epsilon\to 0}\rho_\epsilon(t)$$

Generalized linear response theory

External field

$$H^t = H_S + H_F^t \qquad H_F^t = -\sum_j h_j e^{-i\omega t} A_j$$

response: currents etc. $\qquad \langle B_n \rangle^t = \mathrm{Tr}\{\rho(t) B_n\} \propto h_j$

$$\rho_{\mathrm{rel}}(t) = \exp\left\{-\Phi(t) - \beta\left(\mathcal{H} - \sum_n F_n(t) B_n\right)\right\} \qquad \mathcal{H} = H_S - \sum_c \mu_c N_c$$

$$\Phi(t) = \log \mathrm{Tr} \exp\left\{-\beta\left(\mathcal{H} - \sum_n F_n(t) B_n\right)\right\}$$

Elimination of the response parameters F_n

$$\langle B_n \rangle^t_{\mathrm{rel}} = \mathrm{Tr}\{\rho_{\mathrm{rel}}(t) B_n\} = \mathrm{Tr}\{\rho(t) B_n\} = \langle B_n \rangle^t$$

$$\rho_{\mathrm{irrel}}(t) = \rho(t) - \rho_{\mathrm{rel}}(t) \qquad \mathrm{Tr}\{\rho_{\mathrm{irrel}}(t) B_n\} = 0$$

Elimination of the Lagrange multipliers

h(t), F(t) small, expand all, linearization

$$\rho_{\rm rel}(t) = \rho_{\rm eq} + \beta \int_0^1 d\lambda \sum_n F_n(t) B_n(i\hbar\beta\lambda)\rho_{\rm eq}$$

$$\rho_\epsilon(t) = \rho_{\rm rel}(t) - \beta\, e^{-i\omega t}\int_{-\infty}^0 dt_1\, e^{-i(\omega+i\epsilon)t_1}\int_0^1 d\lambda \Big[-\sum_j h_j \dot{A}_j(i\lambda\beta\hbar + t_1)\rho_{\rm eq} +$$

$$+\sum_n \big(F_n \dot{B}_n(i\lambda\beta\hbar + t_1)\rho_{\rm eq} - i\omega F_n B_n(i\lambda\beta\hbar + t_1)\rho_{\rm eq}\big)\Big].$$

Response equations

$$\langle B_n\rangle^t_{\rm rel} = {\rm Tr}\{\rho_{\rm rel}(t) B_n\} = {\rm Tr}\{\rho(t) B_n\} = \langle B_n\rangle^t$$

$$\sum_n \{\langle B_m; \dot{B}_n\rangle_z - i\omega\langle B_m; B_n\rangle_z\} F_n = \sum_j \langle B_m; \dot{A}_j\rangle_z h_j$$

$$\sum_n P_{mn} F_n = \sum_j D_{mj} h_j.$$

$$(A|B) = \int_0^1 d\lambda\ {\rm Tr}\{A e^{-\lambda\beta\mathcal{H}} B e^{\lambda\beta\mathcal{H}}\rho_{\rm eq}\} = \int_0^1 d\lambda\ {\rm Tr}\{A B(i\lambda\beta\hbar)\rho_{\rm eq}\}$$

$$\langle A; B\rangle_z = \int_{-\infty}^0 dt\, e^{-izt}(A|B(t)) \qquad z = \omega + i\epsilon$$

Kubo formula

$$\sigma_{\mathrm{dc}}^{\mathrm{Kubo}} = \frac{e^2\beta}{m^2\Omega}\langle P; P\rangle_{i\epsilon}^{\mathrm{irred}}$$

numerical simulations

thermodynamic Green’s functions, and
Feynman diagrams, path integral methods

Other expressions: integration by parts

$$-iz\langle A; B\rangle_z = (A|B) + \langle \dot{A}; B\rangle_z = (A|B) - \langle A; \dot{B}\rangle_z$$

Force–force correlation function

Relevant observable $B = P = m\dot{X}$ $\quad j_{\rm el} = (e/m\Omega)P = (e/\Omega)\dot{X}$

Response equation

$$F[(\dot{P}|P) + \langle \dot{P};\dot{P}\rangle_{i\epsilon}] = \frac{e}{m}E\{(P|P) + \langle P;\dot{P}\rangle_{i\epsilon}\}$$

$$R = \frac{1}{\sigma_{\rm dc}} = \frac{\Omega\beta}{e^2N^2}\frac{\langle \dot{P};\dot{P}\rangle_{i\epsilon}}{1 + \frac{\beta}{mN}\langle P;\dot{P}\rangle_{i\epsilon}}$$

Ziman formula

$$R = \frac{m^2\Omega^3}{12\pi^3\hbar^3e^2N^2}\int_0^\infty dE(p)\left(-\frac{df(E)}{dE}\right)\int_0^{2p} dq\, q^3|V_q|^2$$

$$\sigma_{\rm dc} = \frac{3}{4\sqrt{2\pi}}\frac{(k_{\rm B})^{3/2}(4\pi\epsilon_0)^2}{m^{1/2}e^2}\frac{1}{\Lambda(p_{\rm therm})}$$

Extended set of relevant observables

arbitrary moments of the single- particle distribution function

$$P_n = \sum_{\mathbf{p}} \hbar p_x (\beta E_p)^{n/2} a^\dagger_{\mathbf{p}} a_{\mathbf{p}}$$

$$\sigma_{\rm dc} = s \frac{(k_{\rm B})^{3/2}(4\pi\epsilon_0)^2}{m^{1/2}e^2} \frac{1}{\Lambda(p_{\rm therm})}$$

one-moment approach $s = 3/(4\sqrt{2\pi})$

exact $s = 2^{5/2}/\pi^{3/2}$

Single-particle distribution function

and the general form of the linearized Boltzmann equation

$$\frac{e}{m}\mathbf{E} \cdot [(\mathbf{P}|n_\nu) + \langle \mathbf{P}; \dot{n}_\nu \rangle_{\omega+i\epsilon}] = \sum_{\nu'} F_{\nu'} P_{\nu'\nu}$$

$$P_{\nu'\nu} = (\dot{n}_{\nu'}|\Delta n_\nu) + \langle \dot{n}_{\nu'}; \dot{n}_\nu \rangle_{\omega+i\epsilon} + i\omega\{(\Delta n_{\nu'}|\Delta n_\nu) - \langle \dot{n}_{\nu'}; \Delta n_\nu \rangle_{\omega+i\epsilon}\}$$

$$f_\nu(t) = \mathrm{Tr}\{\rho(t)\, n_\nu\} = f^0_\nu + \beta \sum_{\nu'} F_{\nu'} (\Delta n_{\nu'}|\Delta n_\nu)$$

Two-particle distribution function, bound states

Green's function approach for the Kubo formula

Correlation function

$$\sigma^{\mathrm{Kubo}}(\omega) = \frac{e^2\beta}{3m^2\Omega}\langle \mathbf{P};\mathbf{P}\rangle^{\mathrm{irred}}_{\omega+i\epsilon}$$

Green function

$$\sigma^{\mathrm{Kubo}}(\omega) = \frac{e^2\beta}{3m^2\Omega}\frac{\hbar}{\beta}\int\frac{d\omega'}{i\pi}\frac{1}{z-\omega'}\frac{1}{\omega'}\,\mathrm{Im}\,G_{\mathbf{P},\mathbf{P}}(0,\omega'+i\epsilon)$$

Polarization function

$$G_{\mathbf{P},\mathbf{P}}(\mathbf{Q},iZ_\lambda) = \hbar^2\sum_{\mathbf{p},\mathbf{p}'}\mathbf{p}\cdot\mathbf{p}'\sum_{z_\nu,z'_\nu}\Pi(\mathbf{p},iz_\nu,\mathbf{Q},iZ_\lambda,\mathbf{p}',iz'_\nu)$$

Zeroth order
with respect to the interaction

$$\sum_{z_\nu,z'_\nu}\Pi^{\mathrm{RPA}}(\mathbf{p},iz_\nu,\mathbf{Q},iZ_\lambda,\mathbf{p}',iz'_\nu) = \frac{f(E_p)-f(E_{\mathbf{p}+\mathbf{Q}})}{iZ_\lambda+E_p-E_{\mathbf{p}+\mathbf{Q}}}\delta_{\mathbf{p},\mathbf{p}'}$$

spectral density

$$I_{n_\mathbf{p},n_{\mathbf{p}'}}(\omega,Q) = 2\pi f(E_p)[1-f(E_p)]\,\delta_{\mathbf{p},\mathbf{p}'}\,\delta(\omega+E_p-E_{\mathbf{p}+\mathbf{Q}})$$

Fourier transform

$$\sigma^{\mathrm{Kubo},0}(\omega)\big|_{\omega=0} = \frac{e^2\beta\hbar^2}{3m^2\Omega}\sum_{\mathbf{p},\mathbf{p}'}\mathbf{p}\cdot\mathbf{p}'\frac{1}{\epsilon}f(E_p)[1-f(E_p)]\delta_{\mathbf{p},\mathbf{p}'}$$

$$\sigma^{\mathrm{Kubo},0}_{\mathrm{dc}} = \frac{ne^2}{m}\frac{1}{\epsilon}$$

Higher orders

Dressed propagators

$$G(\mathbf{p}, iz_\nu) = \int \frac{d\omega}{2\pi} \frac{1}{iz_\nu - \omega} A(\mathbf{p}, \omega) =$$

$$= \int \frac{d\omega}{2\pi} \frac{1}{iz_\nu - \omega} \frac{\mathrm{Im}\,\Sigma(\mathbf{p}, \omega)}{[\omega - E_p - \mathrm{Re}\,\Sigma(\mathbf{p}, \omega)]^2 + [\mathrm{Im}\,\Sigma(\mathbf{p}, \omega)]^2}$$

Self-energy

Electron-ion collisions, Born approximation

$$\Sigma(\mathbf{p}, E_p) = \sum_{\mathbf{q},\mathbf{k}} V^2(q) \frac{f(E_k^{\mathrm{ion}})}{E_p - E_{\mathbf{p}+\mathbf{q}}}$$

$$\mathrm{Im}\,\Sigma(\mathbf{p}, E_p) = \frac{\hbar}{2\tau_p} = N_{\mathrm{ion}} \sum_{\mathbf{q}} V^2(q)\, \pi\delta(E_p - E_{\mathbf{p}+\mathbf{q}})$$

$$\sigma^{\mathrm{Kubo},1}(0) = \frac{e^2\beta\hbar^2}{3m^2\Omega} \sum_{\mathbf{p}} \frac{1}{2} p^2 \tau_p f(E_p)[1 - f(E_p)] = \frac{ne^2}{m^2}\bar{\tau}$$

Instead of the total cross section $\bar{\tau}$ the transport cross section should appear.

Vertex contribution

$$\Pi(\mathbf{p}, iz_\nu, \mathbf{Q}, iZ_\lambda, \mathbf{p}', iz'_\nu) = \int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi} A(\mathbf{p}, \omega_1) A(\mathbf{p} - Q, \omega_2) \frac{1}{iz_\nu - \omega_1} \frac{1}{iz_\nu - iZ_\lambda - \omega_2} \times$$

$$\times \left\{ \delta_{\mathbf{p},\mathbf{p}'} \delta_{z_\nu, z'_\nu} + \sum_{\mathbf{p}_1, z_1} \Gamma(\mathbf{p}, iz_\nu, \mathbf{Q}, iZ_\lambda, \mathbf{p}_1, iz_1) \Pi(\mathbf{p}_1, iz_1, \mathbf{Q}, iZ_\lambda, \mathbf{p}', iz'_\nu) \right\}$$

$$\sigma^{\mathrm{Kubo},2}(0) = \frac{ne^2}{m} \bar{\tau}^{\mathrm{transp}}$$

Kubo–Greenwood approach

atoms (70) in a (periodic) box, Kohn-Sham: DFT-MD $H_{\rm KS}|\mathbf{k}\nu\rangle = E_{\mathbf{k}\nu}|\mathbf{k}\nu\rangle$

$$\mathbf{P}(t-i\hbar\tau) = \exp\left\{\frac{i}{\hbar}(t-i\hbar\tau)H_{\rm KS}\right\}\mathbf{P}\exp\left\{-\frac{i}{\hbar}(t-i\hbar\tau)H_{\rm KS}\right\}$$

$$\mathbf{P} = \sum_{\mathbf{k},\mathbf{k}',\nu,\nu'}\langle\mathbf{k}\nu|\mathbf{p}|\mathbf{k}'\nu'\rangle a^\dagger_{\mathbf{k}\nu}a_{\mathbf{k}'\nu'} \qquad \langle\mathbf{k}\nu|\mathbf{p}|\mathbf{k}'\nu'\rangle = \delta_{\mathbf{k},\mathbf{k}'}\left[\hbar\mathbf{k}\,\delta_{\nu,\nu'} + \frac{1}{\Omega_{\rm c}}\int_{\Omega_{\rm c}} d^3\mathbf{r}\,u^*_{\mathbf{k}\nu}(\mathbf{r})\frac{\hbar}{i}\frac{\partial}{\partial\mathbf{r}}u_{\mathbf{k}\nu'}(\mathbf{r})\right]$$

$$\mathrm{Re}\,\sigma^{\rm KG}_{\alpha\beta}(\omega) = \frac{2\pi e^2}{3\Omega_{\rm c}m^2\omega}\sum_{\mathbf{k},\nu,\nu'}\langle\mathbf{k}\nu|\mathbf{p}_\alpha|\mathbf{k}\nu'\rangle\cdot\langle\mathbf{k}\nu'|\mathbf{p}_\beta|\mathbf{k}\nu\rangle(f_{\mathbf{k}\nu}-f_{\mathbf{k}\nu'})\,\delta_\epsilon(E_{\mathbf{k}\nu}-E_{\mathbf{k}\nu'}-\hbar\omega)$$

For the dc conductivity $\lim_{\omega\to 0}\sigma^{\rm KG}_{\alpha\beta}(\omega)$ follows $0/0$. smearing $\delta_\epsilon(x) = \frac{1}{\pi}\frac{\epsilon}{x^2+\epsilon^2}$

Perturbation theory, Lorentz plasma $\langle\mathbf{k}_1|\mathbf{p}|\mathbf{k}_2\rangle = \hbar\mathbf{k}_1\,\delta_{\mathbf{k}_1,\mathbf{k}_2} + \frac{\langle\mathbf{k}_1|V|\mathbf{k}_2\rangle}{E_{\mathbf{k}_1}-E_{\mathbf{k}_2}}(\hbar\mathbf{k}_1-\hbar\mathbf{k}_2)$

$-1/A$

$$\tau^{\rm KG}(k) = \frac{1}{\epsilon} + \frac{1}{\epsilon^2}\frac{1}{k^3}\frac{n_{\rm ion}e^4m\pi}{\varepsilon_0^2\hbar^2}\int_0^{2k}\frac{dq}{(2\pi)^2}\frac{q^3}{(q^2+\kappa_{\rm D}^2)^2} + \mathcal{O}\left(\frac{e^8}{\epsilon^3}\right)$$

$$\frac{1}{\epsilon} + \frac{1}{\epsilon^2}A + \cdots = \frac{1}{\epsilon}\left(1+\frac{1}{\epsilon}A+\cdots\right) = \frac{1}{\epsilon}\frac{1}{1-A/\epsilon+\cdots} \qquad \text{limit } \epsilon\to 0$$

stochastic forces

$$R = \frac{1}{\sigma_{\mathrm{dc}}} = \frac{\Omega\beta}{e^2N^2}\frac{\langle \dot{\mathrm{P}};\dot{\mathrm{P}}\rangle_{\mathrm{i}\epsilon}}{1+\frac{\beta}{mN}\langle \dot{\mathrm{P}};\dot{\mathrm{P}}\rangle_{\mathrm{i}\epsilon}} \qquad \sigma_{\mathrm{dc}} = \frac{ne^2}{m}\frac{mN/\beta + \langle \mathrm{P};\dot{\mathrm{P}}\rangle_{\mathrm{i}\epsilon}}{\langle \dot{\mathrm{P}};\dot{\mathrm{P}}\rangle_{\mathrm{i}\epsilon}} = \frac{ne^2}{m}\frac{-\langle \mathrm{P};\mathrm{P}\rangle_{\mathrm{i}\epsilon}}{-(\mathrm{P}|\mathrm{P})+\epsilon\langle \mathrm{P};\mathrm{P}\rangle_{\mathrm{i}\epsilon}}$$

$$\frac{1}{\tau} = \Sigma = \frac{\langle \dot{\mathrm{P}};\dot{\mathrm{P}}\rangle_{\mathrm{i}\epsilon}}{(\mathrm{P}|\mathrm{P})} = \epsilon - \epsilon^2\frac{\langle \mathrm{P};\mathrm{P}\rangle_{\mathrm{i}\epsilon}}{(\mathrm{P}|\mathrm{P})} = \epsilon - \epsilon^2\frac{m}{ne^2}\sigma(0) \quad \longrightarrow 0 \text{ for } \epsilon \longrightarrow 0.$$

Markov limit: Plateau problem

$$R = \frac{m^2\Omega}{e^2\beta(\mathrm{P}|\mathrm{P})}\frac{\langle \dot{\mathrm{P}};\mathrm{P}\rangle_{\mathrm{i}\epsilon}}{\langle \mathrm{P};\mathrm{P}\rangle_{\mathrm{i}\epsilon}}$$

$$= \frac{m^2\Omega}{e^2\beta(\mathrm{P}|\mathrm{P})}\frac{1}{(\mathrm{P}|\mathrm{P})}\left\langle \left\{\dot{\mathrm{P}} - \frac{\langle \dot{\mathrm{P}};\mathrm{P}\rangle_{\mathrm{i}\epsilon}}{\langle \mathrm{P};\mathrm{P}\rangle_{\mathrm{i}\epsilon}}\mathrm{P}\right\};\left\{\dot{\mathrm{P}} - \frac{\langle \dot{\mathrm{P}};\mathrm{P}\rangle_{\mathrm{i}\epsilon}}{\langle \mathrm{P};\mathrm{P}\rangle_{\mathrm{i}\epsilon}}\mathrm{P}\right\}\right\rangle_{\mathrm{i}\epsilon}$$

stochastic forces: $\mathrm{F}_{\mathrm{st}} = \dot{\mathrm{P}} - \frac{\langle \dot{\mathrm{P}};\mathrm{P}\rangle_{\mathrm{i}\epsilon}}{\langle \mathrm{P};\mathrm{P}\rangle_{\mathrm{i}\epsilon}}\mathrm{P}$

V. P. Kalashnikov,
Linear relaxation equations in the nonequilibrium statistical operator method,
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Outlook

memory-function approach

$$\sigma^{\text{Kubo}}(\omega) = \frac{e^2\beta}{m^2\Omega}\langle P; P\rangle^{\text{irred}}_{\omega+i\epsilon}$$

$$\sigma^{\text{Kubo}}(\omega) = i\frac{ne^2}{m}\frac{1}{\omega + M(\omega)}$$

$$M(\omega) = i\langle \dot{P}; \dot{P}\rangle^{\text{proper}}_{\omega+i\epsilon}\frac{\beta}{mN} = M'(\omega) + iM''(\omega)$$

Defining the memory function as the “proper” part of the force– force correlation function corresponds to introducing the projected Liouville superoperator in the Mori approach

$$R = M''(0)m/ne^2$$

A.A. Vladimirov, D. Ihle, and N. M. Plakida, “Optical and dc conductivities of cuprates: Spin fluctuation scattering in the t–J model,” Phys. Rev. B, 85, 224536 (2012)

H. Mori, “A continued-fraction representation of the time-correlation functions,” Progr. Theoret. Phys., 34, 399–416 (1965).

Problems

- Is the virial expansion correct?
- Extension of the set of relevant observables
- Hopping conductivity
- Treatment of initial correlations
- Kinetic and hydrodynamic approaches

H. Reinholz, G. Ropke, S. Rosmej, and R. Redmer, “Conductivity of warm dense matter including electron– electron collisions,” Phys. Rev. E, 91, 043105 (2015).

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D. N. Zubarev, V. G. Morozov, I. P. Omelyan, and M. V. Tokarchuk, “Unification of the kinetic and hydrodynamic approaches in the theory of dense gases and liquids,” Theor. Math. Phys., 96, 997–1012 (1993).

Open systems

- Heat production and entropy (E^2)
- Coupling to the radiation field
- Slip
- Finite value of the source term
- Scattering theory

$$\frac{\partial}{\partial t}\psi_\epsilon(\mathbf{r},t) + \frac{i}{\hbar}H\psi_\epsilon(\mathbf{r},t) = -\epsilon[\psi_\epsilon(\mathbf{r},t) - \psi^{\hat{t}}_{\mathrm{rel}}(\mathbf{r},t)]$$

R. Der and G. Ropke, “Influence of infinitesimal source terms in the Liouville equation (Zubarev’s method) on macroscopic evolution equations,” Phys. Lett. A, 95, 347–349 (1983)

G. Ropke, A. Selchow, A. Wierling, and H. Reinholz, “Lindhard dielectric function in the relaxation-time approximation and generalized linear response theory,” Phys. Lett. A, 260, 365–369 (1999)

M. Gell-Mann and M. L. Goldberger,
“The formal theory of scattering,” Phys. Rev., **91**, 398–408 (1953).

Thanks for your attention !!!

evaluation of equilibrium correlation functions

numerical simulations

$$-iz\langle A;B\rangle_z = (A|B) + \langle \dot{A};B\rangle_z = (A|B) - \langle A;\dot{B}\rangle_z$$

thermodynamic Green's functions, and Feynman diagrams, path integral methods

$$N_{mn} = (B_m|B_n)$$

$$P_{mn} = (B_m|\dot{B}_n) + \langle \dot{B}_m;\dot{B}_n\rangle_{\omega+i\epsilon} - i\omega(B_m|B_n) - i\omega\langle \dot{B}_m;B_n\rangle_{\omega+i\epsilon}$$

$$D_{mj} = (B_m|\dot{A}_j) + \langle \dot{B}_m;\dot{A}_j\rangle_{\omega+i\epsilon}$$

$$\langle B_n\rangle^t = \langle B_n\rangle^t_{\rm rel} = -\beta\sum_m F_m e^{i\omega t} N_{mn}$$

Virial expansion of the resistivity

$$\sigma^{-1}(n,T) = A(T)\ln n + B(T) + C(T) n^{1/2} \ln n + \cdots$$

$$\Gamma = (4\pi/3)^{1/3} n^{1/3} (k_B T)^{-1} e^2 / 4\pi\epsilon_0$$
$$= 2.695 \times 10^{-5} n^{1/3}\ T^{-1} \mathrm{m\,K}\ .$$

$$\Theta = \frac{2 m k_B T}{\hbar^2} (3\pi^2 n)^{-2/3}$$

$$\sigma = 0.591 \frac{(4\pi\epsilon_0)^2 (k_B T)^{3/2}}{e^2 m^{1/2}} \left[\ln\Gamma^{-3/2} + 1.124 + \frac{1}{\sqrt{6}+\sqrt{3}} \Gamma^{3/2} \ln\Gamma^{-3/2} + \cdots \right]^{-1}$$

$$= 1.530 \times 10^{-2} T^{3/2} (\ln\Gamma^{-3/2} + 1.124 + 0.239 \Gamma^{3/2} \ln\Gamma^{-3/2})^{-1}\ (\Omega\,\mathrm{m\,K}^{3/2})^{-1}\ .$$

G.R., Phys. Rev. A **38**, 3001 (1988)

Virial expansion of the plasma conductivity

$$\sigma^{-1}(T,n) = A(T)\log n + B(T) + C(T)n^{1/2}\log n \pm \ldots$$

$$A(T) = -\frac{1}{2s}\frac{e^2 m^{1/2}}{(4\pi\epsilon_0)^2(k_{\rm B}T)^{3/2}},$$

$$\sigma_{\rm dc} = s\frac{(k_{\rm B})^{3/2}(4\pi\epsilon_0)^2}{m^{1/2}e^2}\frac{1}{\Lambda(p_{\rm therm})}$$

Quantum Statistical Approach to Nonequilibrium

Generalized Gibbs ensemble

$$\hat{\rho}_{\rm rel}(t) = \frac{1}{Z_{\rm rel}(t)} {\rm e}^{-\beta(\hat{H}_s - \mu\hat{N}) - \beta\sum_n F_n(t)\hat{B}_n}$$

from the maximum of entropy at given mean values

$$\mathrm{Tr}\left\{\hat{\rho}(t)\hat{B}_n\right\} = \langle\hat{B}_n\rangle^t = \mathrm{Tr}\left\{\hat{\rho}_{\rm rel}(t)\hat{B}_n\right\}$$

Equation of evolution for the nonequilibrium statistical operator (Zubarev)

$$\frac{\partial}{\partial t}\rho(t) + \frac{i}{\hbar}\left[H_s + H_f^t, \rho(t)\right] = -\varepsilon\left(\rho(t) - \rho_{rel}(t)\right)$$

Choice of the set of relevant observables:
fluctuation of the single-particle occupation number

$$\delta f_1(p,t) = f_1(p,t) - f_p^{(0)} = \langle\hat{n}_p - f_p^{(0)}\rangle^t = \langle\delta\hat{n}_p\rangle^t = \mathrm{Tr}\left\{\rho(t)\delta\hat{n}_p\right\}$$

D. Zubarev, V. Morozov, G. R., *Statistical Mechanics of Nonequilibrium Processes*, Berlin 1996

Kinetic Theory from Nonequilibrium QED

Path-ordered Green's function for Dirac field operators

$$G(\underline{1}\,\underline{2}) \;=\; -i\,\left\langle T_C[S\,\psi_I(\underline{1})\bar{\psi}_I(\underline{2})]\right\rangle / \left\langle S\right\rangle, \qquad S = T_C \exp\left\{-i\int d\underline{1}\,\hat{A}_I^{\mu}(\underline{1})\,J_{\mu}^{(\mathrm{ext})}(\underline{1})\right\},$$

and for the (transverse) fluctuations of the electromagnetic fields

$$D^{\mu\nu}(\underline{1}\,\underline{2}) \;=\; \frac{\delta A^{\mu}(\underline{1})}{\delta J_{\nu}^{(\mathrm{ext})}(\underline{2})} = -i\langle T_C\,\Delta\hat{A}^i(\underline{1})\,\Delta\hat{A}^j(\underline{2})\rangle$$

Equations of motion, self-energy, vertex functions and polarization matrix
Wigner transform (X,k) and decomposition $(d_s^{\gtrless}, d_s^{+})$
differences and sums: transport and mass shell equations

$$\left\{k^2 - \mathrm{Re}\,\pi_s^{+}, d_s^{\gtrless}\right\} + \left\{\mathrm{Re}\,d_s^{+}, \pi_s^{\gtrless}\right\} = i\left(\pi_s^{>}\,d_s^{<} - \pi_s^{<}\,d_s^{>}\right),$$

$$\left\{\mathrm{Im}\,\pi_s^{+}, d_s^{\gtrless}\right\} + \left\{\mathrm{Im}\,d_s^{+}, \pi_s^{\gtrless}\right\} = 2\left(k^2 - \mathrm{Re}\,\pi_s^{+}\right)\left(d_s^{\gtrless} - \left|\,d_s^{+}\right|^2\pi_s^{\gtrless}\right),$$

$$\left\{k^2 - \pi_s^{\pm}, d_s^{\pm}\right\} = 0, \qquad \left(k^2 - \pi_s^{\pm}\right) d_s^{\pm} = 1$$

with the four-dimensional Poisson bracket

$$\{F_1(X,k), F_2(X,k)\} \;=\; \frac{\partial F_1}{\partial X^{\mu}}\frac{\partial F_2}{\partial k_{\mu}} - \frac{\partial F_1}{\partial k^{\mu}}\frac{\partial F_2}{\partial X_{\mu}}$$

V.G. Morozov, G. Röpke: "Kinetic Theory of Radiation in Nonequilibrium Relativistic Plasmas"
Ann. Phys. (N.Y.) 324, 1261 (2009)

Linear Response Theory

Weak external fields h, $H_f^t = \sum_j h_j e^{i\omega t} A_j$

First order expansion with respect to the response parameter F

$$\sum_m F_m \left\{ (\dot{\hat{B}}_m, \hat{B}_n) + \left\langle \dot{\hat{B}}_m ; \dot{\hat{B}}_n \right\rangle_z - i\omega (\hat{B}_m, \hat{B}_n) - i\omega \left\langle \hat{B}_m ; \dot{\hat{B}}_n \right\rangle_z \right\} = \sum_j h_j \left\{ (\dot{\hat{A}}_j, \hat{B}_n) + \left\langle \dot{\hat{A}}_j ; \dot{\hat{B}}_n \right\rangle_z \right\}$$

Equilibrium correlation functions: Green's functions, MD simulations

$$\left\langle \hat{A}; \hat{B} \right\rangle_z = \int_{-\infty}^{0} \mathrm{d}t \ \mathrm{e}^{-izt} \left(\hat{A}(t), \hat{B} \right) \qquad \left(\hat{A}, \hat{B} \right) = \beta \int_0^1 \mathrm{d}\lambda \ \mathrm{Tr} \left\{ \hat{\rho}_0 \hat{A}(i\lambda\hbar\beta) \hat{B} \right\}$$

Fluctuation of the single-particle occupation number

$$\delta f_1(p,t) = f_1(p,t) - f_p^{(0)} = F_p(t) \beta f_p^{(0)} (1 - f_p^{(0)}) = -F_p(t) \frac{d}{dE_p} f_p^{(0)}$$

Response equation for the single-particle distribution function

$$\sum_{p'} F_{p'} \left\{ (\dot{\hat{n}}_{p'}, \delta\hat{n}_p) + \left\langle \dot{\hat{n}}_{p'} ; \dot{\hat{n}}_p \right\rangle_z - i\omega (\delta\hat{n}_{p'}, \delta\hat{n}_p) - i\omega \left\langle \delta\hat{n}_{p'} ; \dot{\hat{n}}_p \right\rangle_z \right\} = -\frac{eE}{m} \sum_{p''} \hbar\vec{p}'' \cdot \vec{e}_F \left\{ (\hat{n}_{p''}, \delta\hat{n}_p) + \left\langle \hat{n}_{p''} ; \dot{\hat{n}}_p \right\rangle_z \right\}$$

Linearized Boltzmann equation, Kubo formula, generalized FDT

Solutions: moment expansions, Kohler variational principle

Evaluation of transport coefficients

Evaluation of correlation functions, solution of the response equations

Electron-ion collisions, zero frequency limit: relaxation time ansatz

Electron-electron collisions, arbitrary frequencies: Kohler variational principle

Single moment approach: Kubo-Nakano formula

$$\sigma_{\alpha\beta}(\omega) = \frac{1}{V} \int_0^\infty dt\, e^{(i\omega-\varepsilon)t} \int_0^\beta \left\langle J_\beta(-i\hbar\lambda)\, J_\alpha(t) \right\rangle d\lambda$$

Zero frequency limit: Ziman-Faber formula, Spitzer result
High frequency limit: Bremsstrahlung, Kramers formula

More explicit: Kubo-Greenwood formula

$$\sigma_{\alpha\beta}(\omega) = \frac{\pi e^2}{m^2 \omega V} \sum_{k_1 k_2} \left\langle k_1 \middle| p_\alpha \middle| k_2 \right\rangle \left\langle k_2 \middle| p_\beta \middle| k_1 \right\rangle \left(f_{k_1} - f_{k_2} \right) \delta\left[\hbar\omega + \left(\varepsilon_{k_1} - \varepsilon_{k_2} \right) \right]$$

(perturbation expansion at zero frequency is diverging, partial summations)

Classical ED: radiation reaction

- Lorentz-Abraham-Dirac (LAD) equation

$$m\frac{d}{dt}\vec{v} = e\vec{E}_{ext} + \frac{e}{c}\left[\vec{v}\times\vec{H}_{ext}\right] + \frac{2}{3}\frac{e^2}{c^3}\frac{d^2}{dt^2}\vec{v}$$

- self-acceleration

$$\frac{d}{dt}\vec{v}(t) = \frac{d}{dt}\vec{v}(0)e^{\frac{3mc^3}{2e^2}t}$$

- non-relativistic motion, weak reaction fields

Quantum Statistical Approach to Nonequilibrium

System Hamiltonian (electron - impurity scattering)

$$H_s = \sum_p E_p a_p^+ a_p + \sum_{pq} V(q)\, a_{p+q}^+ a_p$$

External time dependent field

$$H_f^t = -e\vec{E}(t)\sum_i \vec{r}_i$$

Equation of motion for the statistical operator (v. Neumann)

$$\frac{\partial}{\partial t}\rho(t) + \frac{i}{\hbar}\left[H_s + H_f^t, \rho(t)\right] = 0$$

Initial conditions? Entropy? Equilibrium: Gibbs ensemble

Kinetic equations

Selection of the set of relevant observables $\{B_n\}$

Single-particle distribution function $f_1(\mathbf{r}, \mathbf{p}, t)$

$$\mathrm{Tr}\{\rho_{\mathrm{rel}}(t) B_n\} \equiv \langle B_n \rangle^t_{\mathrm{rel}} = \langle B_n \rangle^t$$

Boltzmann equation

$$\frac{\partial}{\partial t} f_1 + \mathbf{v} \frac{\partial}{\partial \mathbf{r}} f_1 + \mathbf{F}^{\mathrm{external}} \frac{\partial}{\partial \mathbf{p}} f_1 = \left(\frac{\partial}{\partial t} f_1 \right)_{\mathrm{St}}$$

Collision integral

$$\left(\frac{\partial}{\partial t} f_1 \right)_{\mathrm{St}} = \int d^3\mathbf{v}_2 \int d\Omega \frac{d\sigma}{d\Omega} |\mathbf{v}_1 - \mathbf{v}_2| \{ f_1(\mathbf{r}, \mathbf{p}'_1, t) f_1(\mathbf{r}, \mathbf{p}'_2, t) - f_1(\mathbf{r}, \mathbf{p}_1, t) f_1(\mathbf{r}, \mathbf{p}_2, t)$$

Formation of clusters: Coalescence model

$$\frac{\partial}{\partial t}\rho(t) + \frac{\mathrm{i}}{\hbar}\left[\mathrm{H}^t, \rho(t)\right] = 0.$$

Fluctuation - Dissipation Theorem

Relation between the dielectric function, the polarization function,
and the dynamical conductivity

response of homogeneous plasma to external fields, local thermal equilibrium

$$\epsilon(\mathbf{k},\omega) = 1 + \frac{i}{\epsilon_0\omega}\sigma(\mathbf{k},\omega) = 1 - \frac{\omega_{\rm pl}^2}{\omega(\omega - i\nu(\mathbf{k},\omega))} \qquad \omega_{\rm pl}^2 = \frac{e^2 n_{\rm e}}{\epsilon_0 m_{\rm e}}$$

calculation of dynamical conductivity and dynamical collision frequency within linear response theory (going beyond RPA)

- current-current correlation function [1] $\qquad \sigma(\omega) = \beta\Omega\langle\vec{j};\vec{j}\rangle_{\omega+i\eta}$

  molecular dynamics simulation [2,3]

- force-force correlation functions [4]

$$\nu(\omega) = \frac{\beta}{n_e\Omega}\left\langle\dot{\vec{P}};\dot{\vec{P}}\right\rangle_{\omega+i\eta} \qquad \dot{\vec{P}} = \vec{F} = \vec{F}_{ei} + \vec{F}_{ee} + \vec{F}_{ea}$$

perturbation theory, MD

[1] Kubo, J. Phys. Soc. Jpn. **120** *570 (1957); [2] Reinholz et al., PRE* **69** *(2004), Morozov et al. PRE* **71** *(2005);*
[3] Belkacem et al. Eur. Phys. J. D **40** *(2006); [4] Reinholz Ann. de Phys.* **30** *(2005)*

Quantum Statistical Approach to Nonequilibrium

- statistical operator for generalized grand canonical ensemble by introducing set of relevant observables $\{B_n\}$

β

Fluctuation - Dissipation Theorem for Absorption

equilibrium correlation functions

$$\langle A; B\rangle_z = \int_0^\infty dt\, e^{izt}\,(A(t);B) = -\frac{i}{\beta}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\,\frac{1}{z-\omega}\,\frac{1}{\omega}\,\mathrm{Im}\,G_{AB^+}(\omega - i0)$$

$$(A(t);B) = \frac{1}{\beta}\int_0^\infty d\tau\ \mathrm{Tr}\left[A(t-i\hbar\tau)\ B^+\rho_0\right]$$

- application to electrical current density using set $\{B_n\} = \vec{P} = m_e\dot{\vec{R}}$

$$\vec{J} = \left\langle \vec{j}\right\rangle = \mathrm{Tr}\left\{\rho\vec{j}\right\} = \frac{e}{\Omega}\mathrm{Tr}\left\{\rho\dot{\vec{R}}\right\} = \frac{e}{\Omega\, m_e}\mathrm{Tr}\left\{\rho_{\mathrm{rel}}\vec{P}\right\} = \sigma\vec{E}$$

- solution for electrical conductivity

$$\sigma = \beta\Omega\langle j;j\rangle = \frac{\beta e^2}{\Omega\, m_e}\,\frac{(P;P)^2}{\langle\dot{P};\dot{P}\rangle}$$

Kubo-Greenwood formula $\Longleftrightarrow$ force force correlation functions

$(\dot{P} = F_{ei} + F_{ee} + F_{ea})$

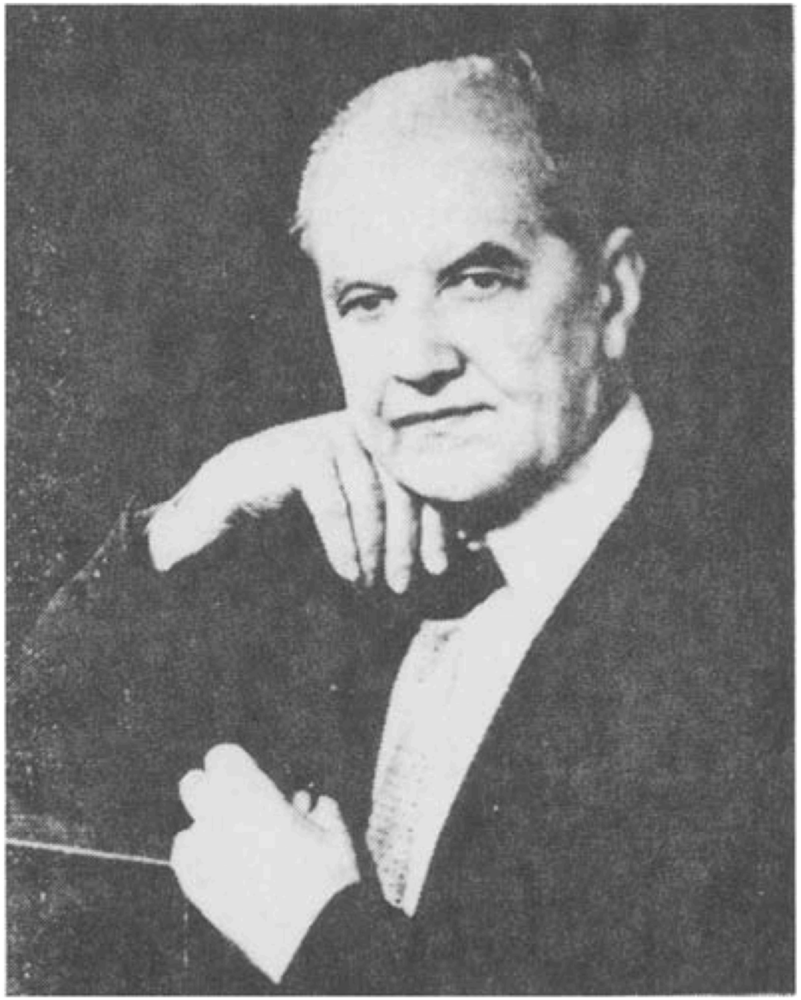
*Röpke, Meister, Ann. Phys. **36** (1979) 377; Röpke, PRA **38** (1988) 3001; Reinholz et al. , PRE 52 (1995) 6368*

Dubna, 18.4.2018

Laudatio D.N. Zubarev

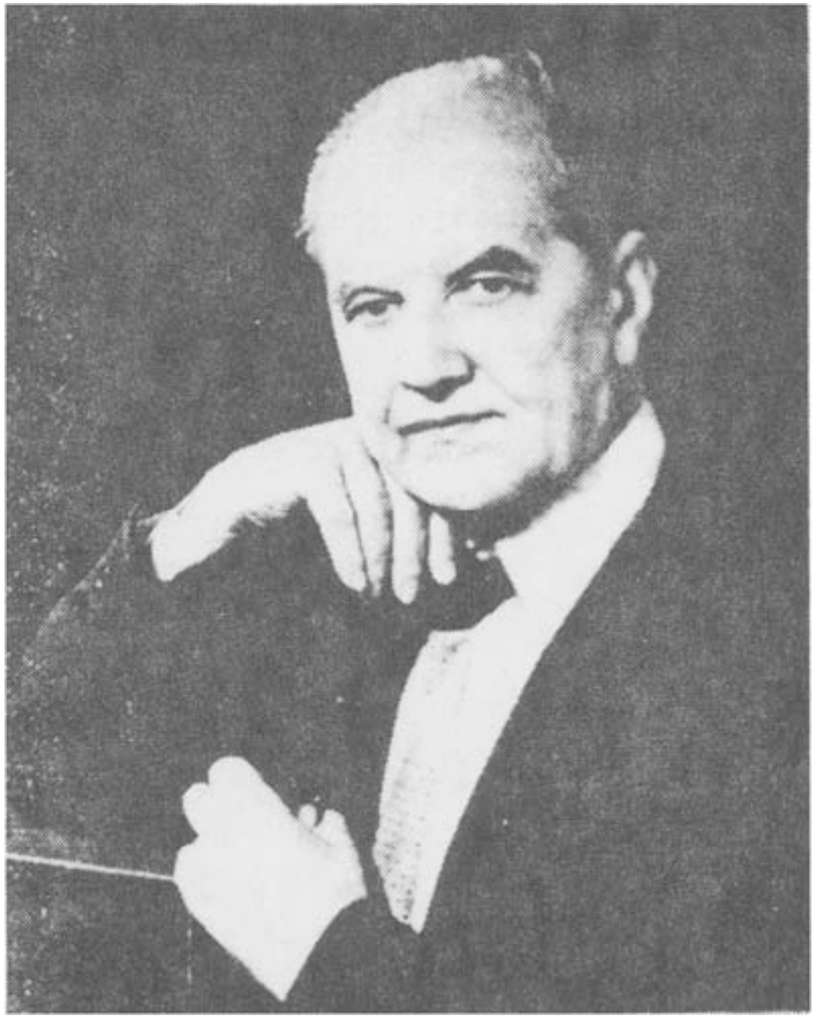
The NSO method

Gerd Röpke
Universitaet Rostock



BIOGRAPHY OF D. N. ZUBAREV (1917 - 1992)

born Nov. 27, 1917, Moscow , Russia.
died July 29, 1992, Moscow , Russia.



Nonequilibrium statistical operator (NSO)

- D. N. Zubarev, *Nonequilibrium Statistical Thermodynamics* [in Russian], Nauka, Moscow (1971); English transl., Consultants Bureau, New York (1974)*; "The statistical operator for nonequilibrium systems,"* Sov. Phys. Dokl., 6, 776–778 (1962).
- D. Zubarev, V. Morozov, and G. Ropke, *Statistical Mechanics of Nonequilibrium Processes, Vol. 1, Basic Concepts, Kinetic Theory,* Akademie-Verlag, Berlin (1996).
- D. Zubarev, V. Morozov, and G. Ropke, *Statistical Mechanics of Nonequilibrium Processes, Vol. 2, Relaxation and Hydrodynamic Processes*, Akademie-Verlag, Berlin (1997).
- N. N. Bogoliubov, *Problems of Dynamical Theory in Statistical Physics* [in Russian], Gostekhteorizdat, Moscow (1946).
- L. Boltzmann, *Vorlesungen ueber Gastheorie*, Vol. 2, J. A. Barth, Leipzig (1912).
- DeGroot-Mazur, Gibbs, Shannon, etc.

Father of methods

principle of weakening of initial correlations (Bogoliubov)

$$\rho_\epsilon(t) = \epsilon \int_{-\infty}^{t} e^{\epsilon(t_1 - t)} U(t, t_1) \rho_{\rm rel}(t_1) U^\dagger(t, t_1) \, dt_1$$

time evolution operator $U(t, t_0)$

relevant statistical operator: maximum of information entropy

Selection of the set of relevant observables $\{B_n\}$

self-consistency relations $\mathrm{Tr}\{\rho_{\rm rel}(t) B_n\} \equiv \langle B_n \rangle^t_{\rm rel} = \langle B_n \rangle^t$

Extended von Neumann equation

$$\frac{\partial}{\partial t} \varrho_\varepsilon(t) + \frac{i}{\hbar} [H, \varrho_\varepsilon(t)] = -\varepsilon \left(\varrho_\varepsilon(t) - \varrho_{\rm rel}(t) \right)$$

$\varrho(t) = \lim_{\varepsilon \to 0} \varrho_\varepsilon(t)$ after thermodynamic limit

The freeze-out approach

Selection of the set of relevant observables $\{B_n\}$ H, N_n, N_p

maximum of information entropy $\mathrm{Tr}\{\rho_{\mathrm{rel}}(t) B_n\} \equiv \langle B_n \rangle_{\mathrm{rel}}^t = \langle B_n \rangle^t$

Gibbs ensembles

Lagrange parameters T, μ_n, μ_p elimination: EoS

$$\rho_\epsilon(t) = \epsilon \int_{-\infty}^{t} e^{\epsilon(t_1 - t)} U(t, t_1) \rho_{\mathrm{rel}}(t_1) U^\dagger(t, t_1) \, dt_1$$

Markov approximation

Expanding fireball: dependence on time t

Composition (formation of bound states) Relaxation time

L. P. Csernai and J. I. Kapusta, Phys. Rep. **131**, 223 (1986)

Kinetic equations

Selection of the set of relevant observables $\{B_n\}$

Single-particle distribution function $f_1(\mathbf{r}, \mathbf{p}, t)$

$$\mathrm{Tr}\{\rho_{\mathrm{rel}}(t) B_n\} \equiv \langle B_n \rangle^t_{\mathrm{rel}} = \langle B_n \rangle^t$$

Boltzmann equation $$\frac{\partial}{\partial t} f_1 + \mathbf{v} \frac{\partial}{\partial \mathbf{r}} f_1 + \mathbf{F}^{\mathrm{external}} \frac{\partial}{\partial \mathbf{p}} f_1 = \left(\frac{\partial}{\partial t} f_1 \right)_{\mathrm{St}}$$

Collision integral

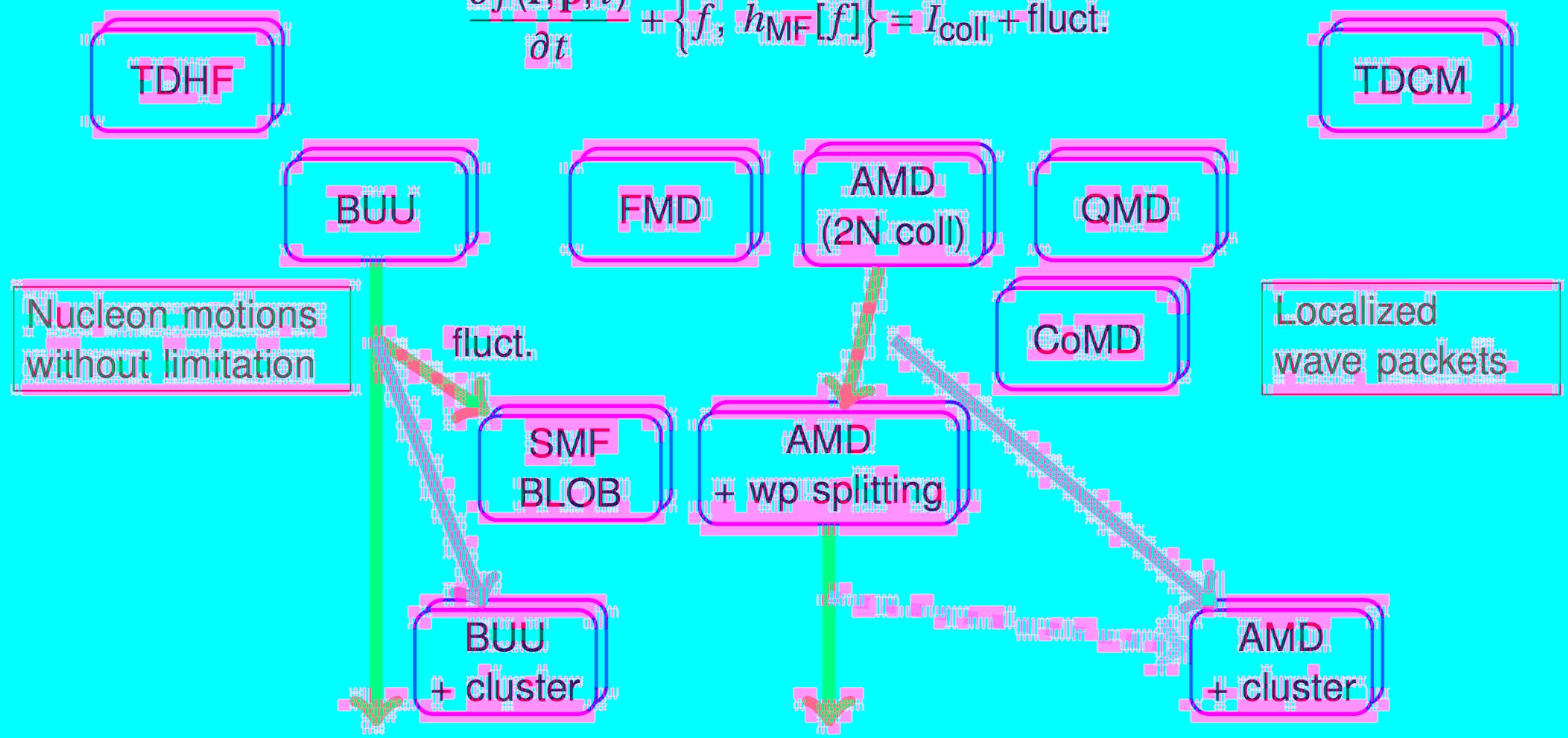
$$\left(\frac{\partial}{\partial t} f_1 \right)_{\mathrm{St}} = \int d^3\mathbf{v}_2 \int d\Omega \frac{d\sigma}{d\Omega} |\mathbf{v}_1 - \mathbf{v}_2| \{ f_1(\mathbf{r}, \mathbf{p}'_1, t) f_1(\mathbf{r}, \mathbf{p}'_2, t) - f_1(\mathbf{r}, \mathbf{p}_1, t) f_1(\mathbf{r}, \mathbf{p}_2, t)$$

Formation of clusters: Coalescence model

Various transport theories

Based on the one-body distribution function $f(\mathbf{r}, \mathbf{p}, t)$ ⇔ One-body density matrix $\rho(\mathbf{r}, \mathbf{r}')$

$$\frac{\partial f(\mathbf{r},\mathbf{p},t)}{\partial t} + \left\{f,\ h_{\text{MF}}[f]\right\} = I_{\text{coll}} + \text{fluct.}$$



- Fluctuation/branching is a way to handle many-body correlations.
- Not many models treat cluster correlations explicitly.

Cluster formation

Selection of the set of relevant observables $\{B_n\}$

Single-particle distribution function

quasi-particle distribution function of bound states

$$T(\mathbf{r},t), \mu_n(\mathbf{r},t), \mu_p(\mathbf{r},t)$$

$$f_{A\nu}^{\mathrm{Wigner}}(\mathbf{p},\mathbf{r},t)$$

D. N. Zubarev, V. G. Morozov, I. P. Omelyan, and M. V. Tokarchuk, Theoret. Math. Phys. **96**, 997 (1993)

G. Ropke and H. Schulz, Nucl. Phys. A **477**, 472 (1988)

Formation of light clusters in heavy ion reactions, transport codes

PHYSICAL REVIEW C, VOLUME 63, 034605

Medium corrections in the formation of light charged particles in heavy ion reactions

C. Kuhrts,[1] M. Beyer,[1,*] P. Danielewicz,[2] and G. Röpke[1]
[1] *FB Physik, Universität Rostock, Universitätsplatz 3, D-18051 Rostock, Germany*
[2] *NSCL, Michigan State University, East Lansing, Michigan 48824*
(Received 13 September 2000; published 12 February 2001)

Wigner distribution

cluster mean-field potential

$$\partial_t f_X + \{\mathcal{U}_X, f_X\} = \mathcal{K}_X^{\text{gain}}\{f_N, f_d, f_t, \ldots\}(1 \pm f_X) - \mathcal{K}_X^{\text{loss}}\{f_N, f_d, f_t, \ldots\} f_X,$$

$$X = N, d, t, \ldots .$$

loss rate

in-medium
breakup transition operator

$$\mathcal{K}_d^{\text{loss}}(P,t) = \int d^3k \int d^3k_1\, d^3k_2\, d^3k_3 |\langle k_1 k_2 k_3 | U_0 | kP\rangle|^2_{dN\to pnN} \times f_N(k_1,t) f_N(k_2,t) f_N(k_3,t) f_N(k,t) + \cdots . \qquad (3)$$

breakup cross section

$$\sigma_{\text{bu}}^0(E) = \frac{1}{|v_d - v_N|} \frac{1}{3!} \int d^3k_1\, d^3k_2\, d^3k_3 |\langle kP | U_0 | k_1 k_2 k_3\rangle|^2 \times 2\pi\delta(E' - E)(2\pi)^3 \delta^{(3)}(k_1 + k_2 + k_3), \qquad (4)$$

P. Danielewicz and Q. Pan, Phys. Rev. C 46, 2002 (1992)

Mott effect, in-medium cross section

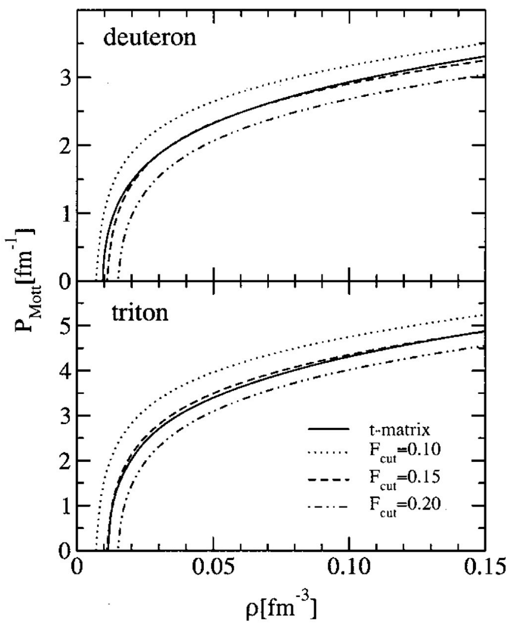


FIG. 1. Deuteron and triton Mott momenta P_{Mott} shown as a function of density ρ at fixed temperature of $T=10$ MeV. The solid line represents results of the t matrix approach. The dashed, dotted, and dashed-dotted lines represent the deuteron Mott momenta from the parametrization given in Eq. (24) for three different cutoff values F_{cut}.

$$\int d^3 q \; f\left(\mathbf{q}+\frac{\mathbf{P}_{\mathrm{c.m.}}}{2}\right) \; |\phi(\mathbf{q})|^2 \leqslant F_{\mathrm{cut}}$$

C. Kuhrts, PRC **63**,034605 (2001)

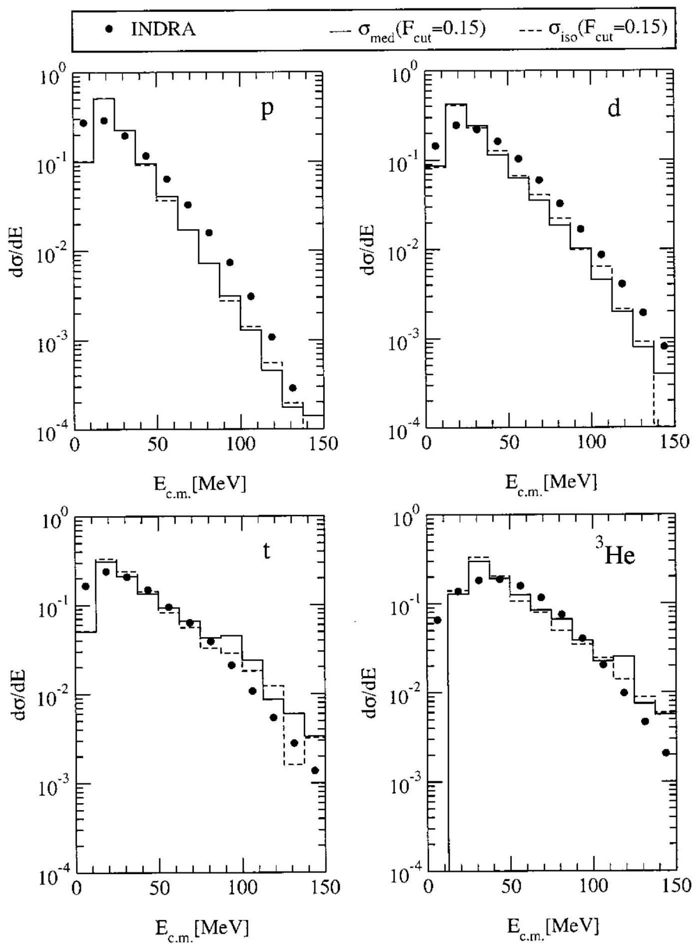
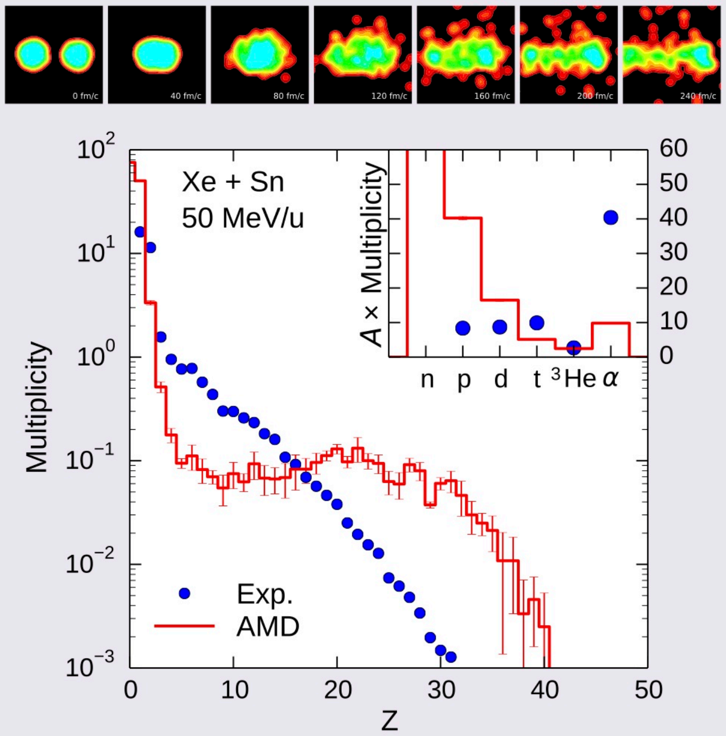


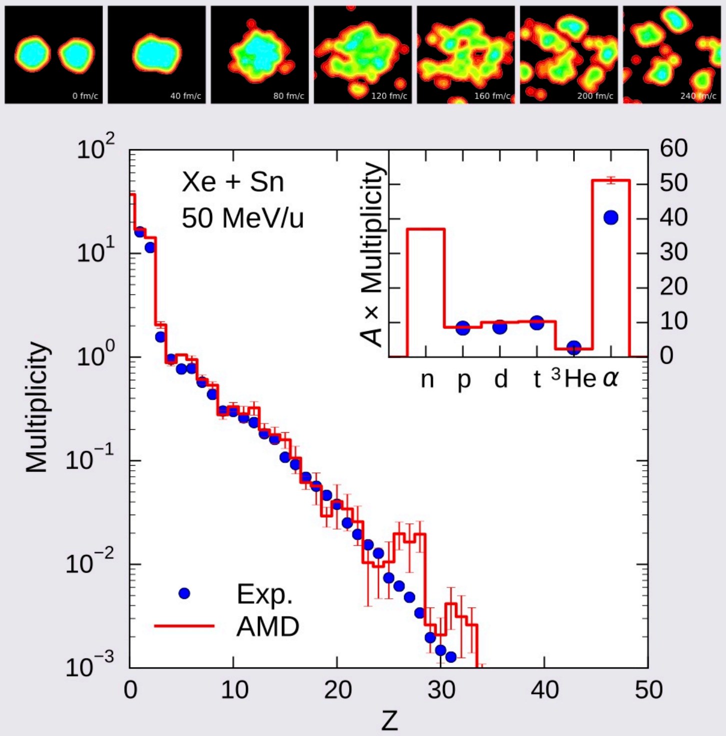
FIG. 5. Renormalized light charged light particle spectra in the center of mass system for the reaction ^{129}Xe+^{119}Sn at 50 MeV/nucleon. The filled circles represent the data of the INDRA Collaboration [21]. The solid line shows the calculations with the in-medium Nd reaction rates, while the dashed line shows a calculation using the isolated Nd breakup cross section; both with $F_{\mathrm{cut}}=0.15$.

Effect of cluster correlations: central Xe + Sn at 50 MeV/u

Without clusters



With clusters



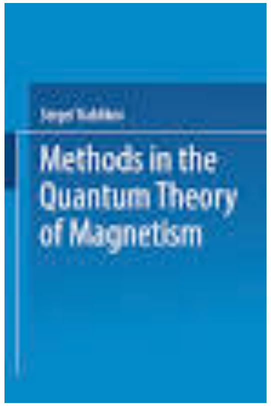
My stay at MIAN 1968 - 69

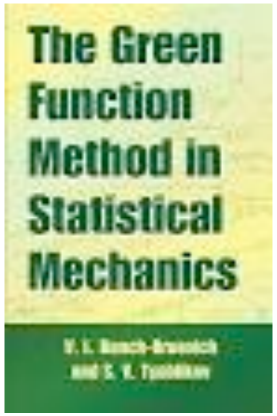
Spin waves
in magnetism

- S. V. Tyablikov
- Born: September 7, 1921, Klin
- Died: March 17, 1968, Moscow

Y.G. Rudoy, Theor. Math. Phys. **168**, 1318 (2011)

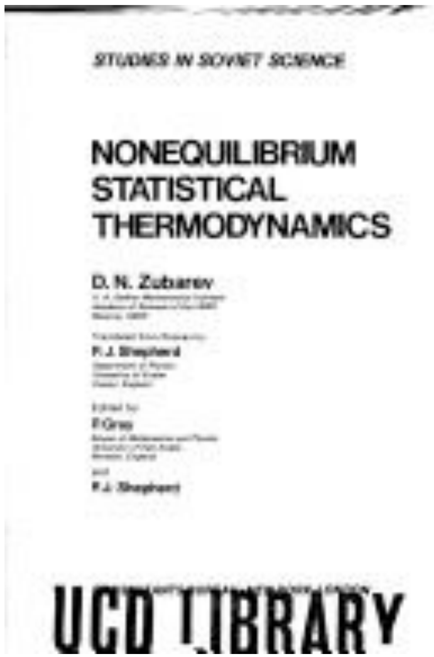
The Bogoliubov-Tyablikov Green's function method in the quantum theory of magnetism





Zubarev's Book on NSO

D. N. Zubarev, *Nonequilibrium Statistical Thermodynamics* [in Russian], Nauka, Moscow (1971)



- Nonequilibrium Statistical Thermodynamics, Consult Bureau, New York, 1974,
- (Dmitrii Nikolaevich Zubarev. Nonequilibrium Statistical Thermodynamics. Studies in Soviet Science. Consultants Bureau, New York, 1974.
- Translated from Russian by P. J. Shepherd. Edited by P. J. Shepherd and P. Gray. 243)
- where he presented the method of the Nonequilibrium Statistical Operator.

German translation:
Statistische Thermodynamik fuer das Nichtgleichgewicht


Гостиница
„Владимир"

P. J. Shepherd

johnshepherd1943@hotmail.co.uk

08.02.2013

Our books, and Russia in 1969

Герд, привет!

I remember you well from the days when we both worked with Dmitrii Nikolaevich Zubarev at the Steklov Institute in 1969. (I subsequently translated his Nonequilibrium Statistical Mechanics for Plenum.)

I attach a photo taken when we visited Vladimir in June 1969. I hope you like it. I like it very much, not least because we all look so young!

Best wishes,

John

Some personal retrospections

- 25 years after 2nd world war
- participated in the Battle of Moscow and met the end of the war in Berlin (de-miner).
- With G. Hertz who was made head of Institute G, in Agudzery, about 10 km southeast of Sukhumi and a suburb of Gulrip'shi. Separation of isotopes by diffusion in a flow of inert gases.
- Participation in Soviet Nuclear Project
- Wife: Galina Rudolfovna, Leningrad
- Overnight at a railway station: main idea
- accommodation: book1, book 2 for a car.
- Accurate and “European” style
- Contacts to many people, Nikolay Nikolayevich
- visits to Germany/Rostock

Publication output

citations

Total Publications

53

***h*-index**

17

Average citations per item

42.09

Sum of Times Cited

2,231

Without self citations

2,181

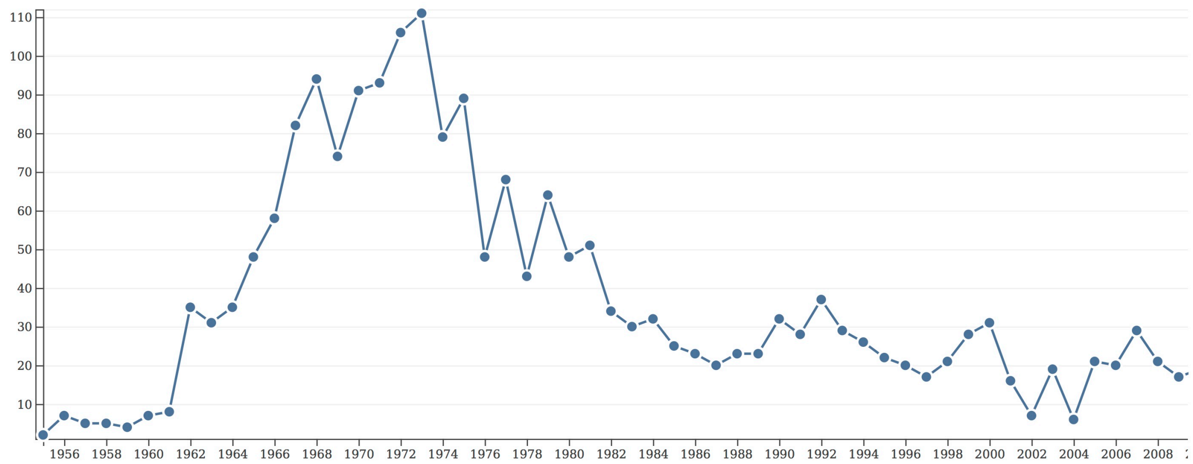
Citing articles

1,989

Without self citations

1,964

Sum of Times Cited per Year



The mostly cited papers

2-TIME GREEN FUNCTIONS IN STATISTICAL PHYSICS

By: ZUBAREV, DN
USPEKHI FIZICHESKIKH NAUK Volume: 71 Issue: 1 Pages: 71-116 Published: 1960

THE WAVE FUNCTION OF THE LOWEST STATE OF A SYSTEM OF INTERACTING BOSE PARTICLES

By: BOGOLIUBOV, NN; ZUBAREV, DN
SOVIET PHYSICS JETP-USSR Volume: 1 Issue: 1 Pages: 83-90 Published: 1955

STATISTICAL OPERATOR FOR NO-EQUILIBRIUM SYSTEMS

By: ZUBAREV, DN
DOKLADY AKADEMII NAUK SSSR Volume: 140 Issue: 1 Pages: 92-& Published: 1961

METHOD OF NON-EQUILIBRIUM STATISTICAL OPERATOR AND ITS APPLICATIONS .1.

By: ZUBAREV, DN
FORTSCHRITTE DER PHYSIK-PROGRESS OF PHYSICS Volume: 18 Issue: 3 Pages: 125-& Published: 1970

THE PHASE TRANSITION THEORY

By: BOGOLUBOV, NN; ZUBAREV, DN; TSERKOVNIKOV, YA
DOKLADY AKADEMII NAUK SSSR Volume: 117 Issue: 5 Pages: 788-791 Published: 1957

STATISTICAL-MECHANICS OF NON-LINEAR HYDRODYNAMIC FLUCTUATIONS

By: ZUBAREV, DN; MOROZOV, VG
PHYSICA A Volume: 120 Issue: 3 Pages: 411-467 Published: 1983

GIBBSS LOCAL EQUILIBRIUM ENSEMBLE AND ITS RELATION TO THEORY OF FLUCTUATIONS AND TRANSFER PHENOMENA

By: ZUBAREV, DN
DOKLADY AKADEMII NAUK SSSR Volume: 162 Issue: 3 Pages: 532-& Published: 1965

AN ASYMPTOTICALLY EXACT SOLUTION FOR THE MODEL HAMILTONIAN OF THE THEORY OF SUPERCONDUCTIVITY

By: BOGOLYUBOV, NN; ZUBAREV, DN; TSERKOVNIKOV, YA
SOVIET PHYSICS JETP-USSR Volume: 12 Issue: 1 Pages: 88-93 Published: 1961

DERIVATION OF NONEQUILIBRIUM STATISTICAL OPERATOR FROM EXTREMUM OF INFORMATION ENTROPY

By: ZUBAREV, DN; KALASHNIKOV, VP
PHYSICA Volume: 46 Issue: 4 Pages: 550-+ Published: 1970

TRANSFER PROCESSES IN SYSTEMS OF PARTICLES WITH INTERNAL DEGREES OF FREEDOM

By: ZUBAREV, DN
DOKLADY AKADEMII NAUK SSSR Volume: 162 Issue: 4 Pages: 794-& Published: 1965

NSO: progress and challenges

- General method, unifying different approaches
- Very powerful, various problems
- Discussion of entropy, irreversibility,
- Open questions: selection of relevant observables, limit eps to 0, really increase of entropy?
- turbulence