Past research activity…

Time-Dependent Density Functional Theory For Superfluids

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In collaboration with M. Tosi@SNS

- **Bose-Einstein Condensation in alkali gases has become an ideal laboratory for condensed matter physics, where a inhomogeneous (e.g. trapped) superfluid is made available in the presence of (tunable) interactions and under non-equilibrium conditions**

- **Collective excitations in both the collisional and collisionless regimes, propagation of sound waves, transport behaviour for atom-optical applications have become experimentally available**

- **Need for a theory of inhomogeneous Bose Fluids at finite T, capable of spanning the whole region from the collisionless to the hydrodynamic regimes**

- **Density Functional Theory is a possible approach to inhomogeneous systems. It is based on:**

✓ Hohenberg-Kohn theorem: properties of interacting inhomo system in one-to-one correspondence with the density

✓ Kohn-Sham scheme: density calculated from the Schroedinger eq. for appropriate single-particle fictitious orbitals in external effective potential $V_{eff} = V_e + V_{Hartree} + V_{xc}$

✓ V_{eff} has to be approximated: *e.g* from xc-energy of the homo system at the local density of the inhomo one (Local Density Approx)

- **Time-Dependent Density Functional Theory:**

✓ Hohenberg-Kohn theorem: holds provided n is known at t=0

✓ Kohn-Sham scheme: similarly applies

✓ V_{eff} has to be approximated : LDA fails since the xc-potential is nonlocal! Thus, TD-DFT expressed in terms of current [Vignale&Kohn]

- **Current fluctuation, effective vector potential and KS response**

$$\delta J_i(r,\omega) = \int dr' \, \chi_{ij}^{KS}(r,r',\omega) A_{eff,j}(r',\omega)$$

$$A_{eff} = A_e + A_{Hartree} + A_{xc}$$

$$\chi_{ij}^{KS}(r,r',\omega) = \frac{n_0(r)}{m}\delta(r-r')\delta_{ij} \quad + \quad \chi_{ij}^{RPA}(r,r',\omega)$$

Generalized hydro with complex and freq.-dependent viscosities (collisional) — Landau damping (collisionless)

- **Correlations beyond mean-field are contained into**

$$A_{xc,i}(r,\omega) = \int dr' \, f_{xc,ij}(r,r',\omega) \delta J_j(r',\omega)$$

and the f_{xc} kernels are determined from the homo system through LDA at the local super- and normal-fluid densities

➢ Landau's equations (homo system)

$$\frac{\partial \vec{J}}{\partial t} = -\nabla \cdot \overleftrightarrow{T} = -\vec{\nabla} \cdot \left[p\delta_{ij} - \delta_{ij}\left(\zeta_2 \vec{\nabla} \cdot \vec{v}_n + \zeta_1 \vec{\nabla} \cdot \rho_s(\vec{v}_s - \vec{v}_n)\right) - \eta\left(\nabla_i v_{nj} + \nabla_j v_{ni} - \frac{2}{3}\delta_{ij} \vec{\nabla} \cdot \vec{v}_n\right)\right]$$

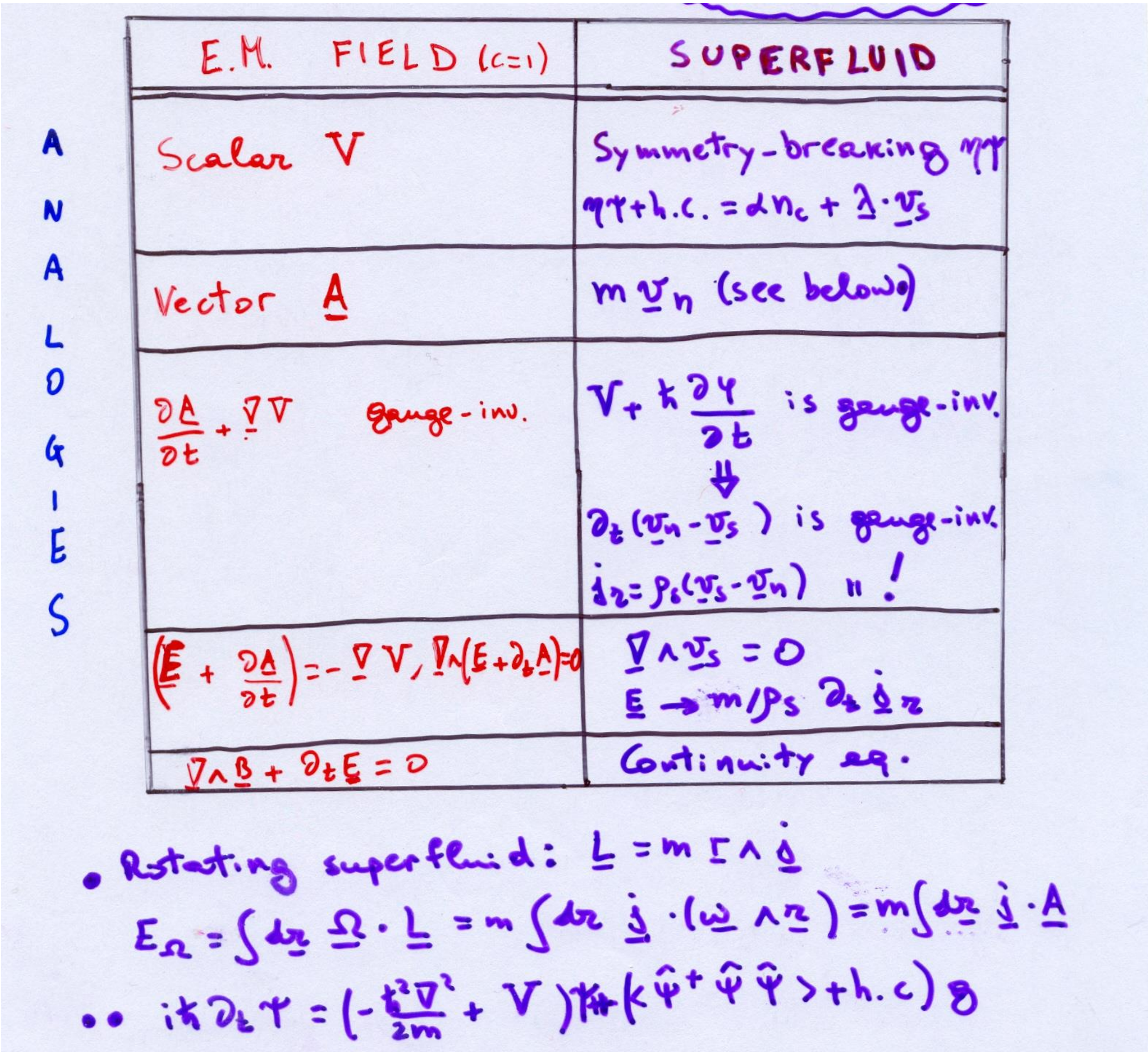
$$\frac{\partial \vec{v}_s}{\partial t} = -\vec{\nabla}\mu^{loc} = -\vec{\nabla}\left[\mu - \zeta_3 \vec{\nabla} \cdot \rho_s(\vec{v}_s - \vec{v}_n) - \zeta_4 \vec{\nabla} \cdot \vec{v}_n\right]$$

- **Galileian invariance holds**
- **The variables are: total current J and superfluid velocity v_s**
- **The 0-force and 0-torque theorems dictate that dJ/dt must be driven by the divergence of a symmetric tensor of 2nd rank**
- **v_s is irrotational in the absence of vortices thus dv_s/dt must be the gradient of a scalar quantity**
- **The internal driving forces are determined by v_n and the interdiffusion current $\rho_s(v_s - v_n)$**

➢ Extension to inhomo system and finite frequency

❖ **First step:**
Identify scalar and vector potentials, currents and driving forces

❖ **Finite frequency:**
Use of memory function formalism



➢ Extension to inhomo system and finite frequency

Use Ward identity to relate the effect of weak inhomo on the xc-kernels to their density dependence: compare the k->0 inhomo response functions to 1st order in the inhomogeneity with those of the homo system after switching on a density modulation

$$\delta\rho_\alpha(\vec{r}) = 2\xi_\alpha\bar{\rho}_\alpha\cos(\vec{q}\cdot\vec{r}), \quad \xi_\alpha = 1$$

$$\lim_{q\to 0}\overleftrightarrow{f}_{\alpha\beta}^{\,in\hom}(\vec{k}+\vec{q},\vec{k},\omega;\{\bar{\rho}_\alpha\}) = \sum_\gamma \xi_\gamma\bar{\rho}_\gamma\frac{\partial}{\partial\bar{\rho}_\gamma}\overleftrightarrow{f}_{\alpha\beta}^{\,\hom}(\vec{k},\omega;\{\bar{\rho}_\alpha\})$$

$$\overleftrightarrow{f}_{\alpha\beta}^{\,in\hom}(\vec{r},\vec{r}\,',\omega) = \overleftrightarrow{f}_{\alpha\beta}^{\,\hom}(\vec{k},\omega;\{\bar{\rho}_\alpha(\vec{r})\})$$

Recipe

- **Ingredients**

❖ **Microscopic expressions for local** $\rho_s^{eq}(r)$ and $\rho_n^{eq}(r)$

❖ **xc Kernels** $f_{\alpha\beta}^{\text{hom}}(k,\omega;\rho_s^{eq}(r),\rho_n^{eq}(r))$

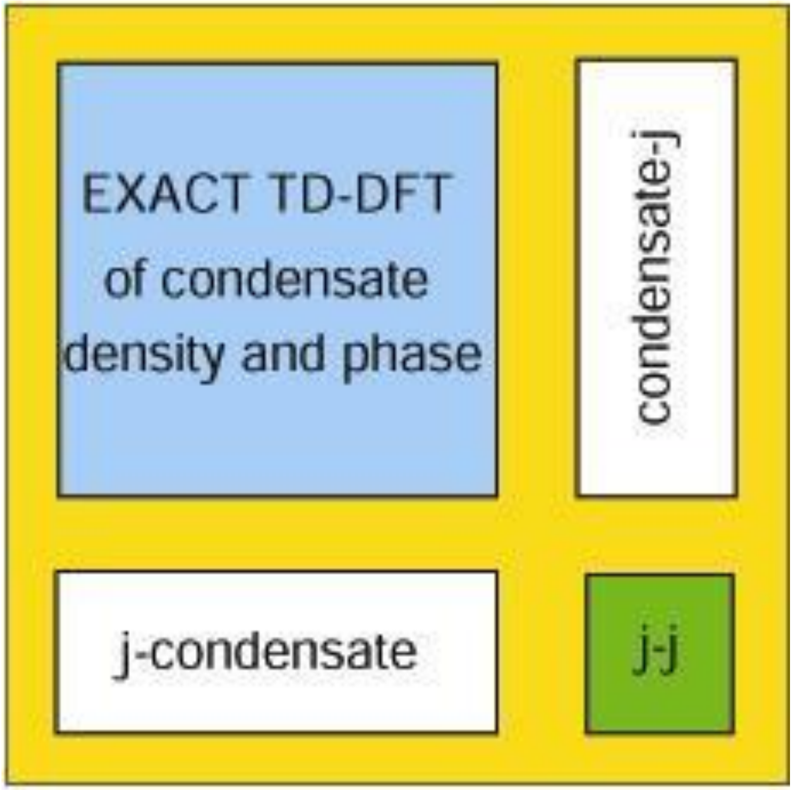
- **Preparation**

❖ **Evaluate** $\rho_s, \rho_n, f_{\alpha\beta}^{\text{hom}}$ **(after QMC or perturbative methods)**

❖ **Relate viscoelastic spectra** $\zeta_i(\omega), \eta(\omega)$ to $f_{\alpha\beta}$

❖ **Put everything into generalized Landau eqs. at finite frequency and solve**

- ➢ **Identification of the ingredients: from the microscopic equations of motion for the currents**



❖ **Super and Normal densities**

$$\lim_{q_{rel}\to 0} \vec{\nabla}_1 \rho_s(1,2) = \vec{\nabla}_2 \frac{\delta \vec{J}(1)}{\delta \vec{\mathrm{v}}_s(2)}\Big|_{\vec{A}} = \vec{\nabla}_R \rho_s(R)$$

$$\rho_n(r) = \rho(r) - \rho_s(r) \qquad\qquad 1 \equiv (r_1, t_1)$$

❖ Relation between the viscoelastic functions and the xc-kernels

$$\overset{t}{f}{}_{\alpha\beta}^{\,hom}(\omega) = \lim_{k\to 0} \frac{\omega^2}{k^2}\rho_\alpha \rho_\beta [\chi_{v_\alpha v_\beta}(k,\omega) - \chi^0_{v_\alpha v_\beta}(k,\omega)] \qquad \alpha,\beta \equiv s,n$$

- **Generalized Kubo formulae:**

$$\mathrm{Re}\left[\zeta_2(\omega) + \frac{4}{3}\eta(\omega)\right] = \lim_{k\to 0} -\frac{\omega m^2}{k^2}\,\mathrm{Im}\,\chi^L_{jj}(k,\omega)$$

$$\mathrm{Re}\left[\eta(\omega)\right] = \lim_{k\to 0} -\frac{\omega m^2}{k^2}\,\mathrm{Im}\,\chi^T_{jj}(k,\omega)$$

$$\mathrm{Re}\left[\zeta_3(\omega)\right] = \lim_{k\to 0} -\frac{\omega}{k^2}\,\mathrm{Im}\,\chi_{v_s v_s}(k,\omega)$$

$$\mathrm{Re}\left[\zeta_1(\omega)\right] = \mathrm{Re}\left[\zeta_4(\omega)\right] = \lim_{k\to 0} -\frac{\omega m}{k^2}\,\mathrm{Im}\,\chi^L_{j v_s}(k,\omega)$$

yielding the frequency-dependent visco-elastic coefficients $\eta(\omega)$, $\zeta_i(\omega)$

❖ And eventually….

$$\zeta_1(\omega; n, T) = -\frac{1}{i\omega}\left[f^{L}_{j\sigma_s}(\omega; \{\rho_\alpha\}) - \frac{\partial P_{ex}(n,T)}{\partial n}\Big|_T \right]$$

$$\zeta_2(\omega; n, T) = -\frac{1}{i\omega}\left[f^{L}_{jj}(\omega; \{\rho_\alpha\}) - \frac{4}{3} f^{T}_{jj}(\omega; \{\rho_\alpha\}) - n\frac{\partial P_{ex}}{\partial n}\Big|_T \right]$$

$$\zeta_3(\omega; n, T) = -\frac{1}{i\omega}\left[f_{\sigma_s\sigma_s}(\omega; \{\rho_\alpha\}) - \frac{\partial \mu_{ex}(n,T)}{\partial n}\Big|_T - \frac{TS}{C_V}\frac{\partial \mu_{ex}(n,T)}{\partial T}\Big|_n \right]$$

$$\zeta_4(\omega; n, T) = -\frac{1}{i\omega}\left[f^{L}_{\sigma_s j}(\omega; \{\rho_\alpha\}) - \frac{\partial P_{ex}(n,T)}{\partial n}\Big|_T \right]$$

$$\eta(\omega; n, T) = -\frac{1}{i\omega} f^{T}_{jj}(\omega; \{\rho_\alpha\})$$