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Übungen zu Zeitabhängige Phänomene in der Statistischen Physik
Sommer Semester 2006

Übungsblatt 9: Zwanzig-Mori projection operators and Diffusion of transverse momentum

Projection operators In previous exercises we have seen that a useful description of the dynamics of a colloidal particle suspended in a liquid is provided by Langevin stochastic differential equations. Such a description assumes that we can identify the relevant variables in the problem, for example the colloidal particle positions and velocities, and represent the irrelevant variables (positions and velocities of the solvent molecules) by a random noise term. Such an approach is quite general. Given a system of N equations for the N variables $a_i(t)$ we can always choose a subset of the $a_i(t)$ and eliminate the remaining variables to obtain a reduced description. Consider the simplest case of two dynamical variables $\mathbf{a}(t) = (a_1(t), a_2(t))$ whose time evolution is given by the operator $\mathbf{L}$ with components L_{ij}

$$\frac{\partial}{\partial t}\mathbf{a}(t) = \mathbf{L}\cdot\mathbf{a}(t).$$

Let us suppose that the relevant variable is $a_1(t)$. Show that this equation is equivilent to

$$\frac{\partial}{\partial t}a_1(t) = L_{11}a_1(t) + L_{12}\int_0^t ds \exp[L_{22}(t-s)]L_{21}a_1(t) + L_{12}\exp[L_{22}t]a_2(0),$$

interpret the meaning of the three terms on the right hand side. Is this equation for $a_1(t)$ Markovian? This procedure can be formalized using projection operators which project the dynamics of the system onto the subset of relevant variables. If we define the projection operator onto the relevent variable as $\mathbf{P}$ with components $P_{ij} = \delta_{i1}\delta_{j1}$ rewrite the above solution for $a_1(t)$ in terms of $\mathbf{P}$ and it's complement $\mathbf{1}-\mathbf{P}$, which projects onto the irrelevant subspace.
We now consider a large number of variables and seek to derive a Langevin equation starting from the Liouville equation. The projection operator onto the relevent subspace A is given explicitly by $\mathbf{P}B = (B, A)\cdot(A, A)^{-1}\cdot A = \sum_{j,k}(B, A_j)((A, A)^{-1})_{jk}A_k$ where the (B, A) is a vector and (A, A) is a matrix. For convenience we will define the Liouville operator by $L = \partial/\partial t$, additional factors of i can then be replaced at the end. Split the Liouville operator into two parts $L = \mathbf{P}L + (\mathbf{1}-\mathbf{P})L$ and use the operator identity $\exp[Lt] = \exp[(\mathbf{1}-\mathbf{P})Lt] + \int_0^t ds \exp[L(t-s)]\mathbf{P}\exp[(\mathbf{1}-\mathbf{P})Ls]$ to show that

$$\frac{\partial}{\partial t}A(t) = i\Omega\cdot A(t) - \int_0^t ds\mathbf{K}(s)\cdot A(t-s) + F(t),$$

where we have used the anti-Hermitian property of L and have defined $i\Omega = (LA, A)\cdot(A, A)^{-1}$, $\mathbf{K}(t) = -(LF(t), A)\cdot(A, A)^{-1}$ and $F(t) = \exp[(\mathbf{1}-\mathbf{P})Lt](\mathbf{1}-\mathbf{P})LA$. Discuss the origin and meaning of $F(t)$ and $\mathbf{K}(t)$ in our result.

Transverse momentum diffusion

Consider the dynamical variable $A(\mathbf{r},t) = \sum_{i=1}^{N} a_i(t)\delta(\mathbf{r}-\mathbf{r}_i(t))$, where a_i is any physical quantity such as the mass, velocity or angular momentum of particle i. If the variable A ia conserved show that $\dot{A}_{\mathbf{k}}(t) + i\mathbf{k}\cdot\mathbf{j}^A_{\mathbf{k}}(t) = 0$, where $\mathbf{j}^A_{\mathbf{k}}(t)$ is the corresponding current. A particularly important dynamical variable is the density ($a_i = 1$). Express the associated particle current $\mathbf{j}^A_{\mathbf{k}}(t)$ in terms of the velocity of particle i, $\mathbf{u}_i(t)$.

The correlation function of two space ependent dynamical variables is defined as $C_{AB}(\mathbf{r}',\mathbf{r}'';t',t'') = \langle A(\mathbf{r}',t')B(\mathbf{r}'',t'')\rangle$ Show that for homogeneous liquids, translational invariance in space and time $C_{AB}(\mathbf{r}',\mathbf{r}'';t',t'') = C_{AB}(\mathbf{k}',t'-t'')$. What further simplification can we make if the fluid is also isotropic? Thus prove the following sum rule for the ecend frequency moments of the autocorrelation function

$$\langle\omega^2\rangle_{AA} = k^2\langle|\mathbf{j}^A_{\mathbf{k}_l}|^2\rangle,$$

where $\mathbf{j}^A_{\mathbf{k}_l} = \mathbf{k}\cdot\mathbf{j}^A_{\mathbf{k}}$ is the longitudinal current. Show that the auto correlation function of the density current can be written in the form

$$C_{\alpha,\beta}(k,t) = \hat{k}_\alpha\hat{k}_\beta C_l(k,t) + (\delta_{\alpha,\beta} - \hat{k}_\alpha\hat{k}_\beta)C_t(k,t),$$

where $\alpha,\beta = x,y,z$. C_l and C_t are the longitudinal and transverse current correlation functions. Another important example is the momentum $g_i(\mathbf{q}) = \sum_\alpha p_i^\alpha e^{i\mathbf{q}cdot\mathbf{r}_\alpha}$. Write the microscopic conservation law for this quantity in terms of the stress tensor $\sigma_{ij}, i,j = x,y,z$. Use the symmetries of $g_i(\mathbf{q})$ under spatial inversion $\mathbf{r}\to-\mathbf{r}$, $\mathbf{p}\to-\mathbf{p}$ to show that $\langle g_i(\mathbf{q},t)g_z(\mathbf{q})\rangle \propto \delta_{ij}$. Finally show that the Laplace transform of the correlation function of the transverse momentum

$$S^t(z) = \langle g_x^*(\mathbf{q})\frac{1}{L-z}g_x(\mathbf{q})\rangle = -\frac{\langle|g_x(\mathbf{q})|^2\rangle}{z+iq^2\eta_s},$$

where z is the Laplace transform variable and $\eta_s = \int_0^\infty dt\,\frac{\langle\sigma_{xz}(q=0,t)\sigma_{xz}(q=0,0)\rangle}{\langle|g_x(0)|^2\rangle}$ is the shear viscosity.