Liouville and Boltzmann Equations for mixed States and Oscillation Phenomena

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Introduction: Non-Abelian Liouville Equation

For N_f flavours N_fxN_f density matrices are defined as (Wigner distributions)

$$\varrho_{ij}(\mathbf{r},\mathbf{p}) \equiv \int d^3\mathbf{r}'\, e^{-i\mathbf{p}\cdot\mathbf{r}'} \left\langle a_j^\dagger(\mathbf{r}-\mathbf{r}'/2)a_i(\mathbf{r}+\mathbf{r}'/2)\right\rangle = \int \frac{d^3\mathbf{\Delta}}{(2\pi)^3}\, e^{i\mathbf{\Delta}\cdot\mathbf{r}} \left\langle a_j^\dagger(\mathbf{p}-\mathbf{\Delta}/2)a_i(\mathbf{p}+\mathbf{\Delta}/2)\right\rangle \;,$$

and analogously for anti-neutrinos, with $a_i(\mathbf{p})$ annihilator of neutrino with flavour i and momentum $\mathbf{p}$. Apart from the sources the equations of motion are Liouville equations with vacuum terms and refractive terms from a background medium and from self-interactions,

$$\partial_t\varrho(\mathbf{r},\mathbf{p}) + \mathbf{v}(\mathbf{r},\mathbf{p})\cdot\nabla_{\mathbf{r}}\varrho(\mathbf{r},\mathbf{p}) = -\,i\left[\Omega^0_{\mathbf{p}} + \Omega_m(\mathbf{r}) + \Omega^{\mathrm{S}}(\mathbf{r},\mathbf{p}), \varrho(\mathbf{r},\mathbf{p})\right] \;, \quad (1)$$

where Ω_p^0 is the vacuum term, Ω_m is the matter term, and Ω^S the self-interaction,

$$\Omega^{\mathrm{S}}(\mathbf{r},\mathbf{p}) = \mu(\mathbf{r})\sum_{\mathbf{q}\neq\mathbf{p}}(1-\mathbf{v_p}\cdot\mathbf{v_q})\Big\{G_{\mathrm{S}}[\rho(\mathbf{r},\mathbf{q})-\bar\rho(\mathbf{r},\mathbf{q})]G_{\mathrm{S}} + G_{\mathrm{S}}\mathrm{Tr}\left[(\rho(\mathbf{r},\mathbf{q})-\bar\rho(\mathbf{r},\mathbf{q}))G_{\mathrm{S}}\right]\Big\} \;,$$

where in general G_S=diag(1,…,1) for active neutrinos. For anti-neutrinos only the sign of Ω_p^0 changes in the commutator in Eq.(1).

Generalisation to Non-Abelian Boltzmann Equation

For a Hamiltonian represented by the c-number flavour matrix $\mathsf{H}(t, \mathbf{r}, \mathbf{p})$ the non-Abelian Boltzmann equation for the space-time and momentum dependent c-number flavour density matrix $\varrho(t, \mathbf{r}, \mathbf{p})$ is generally written in the form

$$\partial_t \varrho + \frac{1}{2}\left\{\partial_{\mathbf{r}}\varrho, \partial_{\mathbf{p}}\mathsf{H}\right\} - \frac{1}{2}\left\{\partial_{\mathbf{p}}\varrho, \partial_{\mathbf{r}}\mathsf{H}\right\} = -i\left[\mathsf{H}, \varrho\right] + \mathscr{C}\left[\varrho\right], \quad (2)$$

where the left hand side is known as Liouville term and the right hand side consists of a commutator describing oscillations and the collision term $\mathscr{C}[\varrho]$ describes absorption, emission and scattering between different momentum modes.

If only the kinetic part in H depends on momentum then $\mathbf{V}_{\mathbf{p}} \equiv \partial_{\mathbf{p}}\mathsf{H}$ is a matrix of velocities with eigenvalues in the neutrino mass basis given by $\mathbf{v}_i = \mathbf{p}/(\mathbf{p}^2 + m_i^2)^{1/2}$ and $\frac{1}{2}\{\varrho, \mathbf{V}\}$ becomes a matrix of neutrino fluxes. Note that they contain group velocities, whereas the oscillation term contains phase velocities. The last term in the Liouville term is a force term which is usually neglected. In absence of mixing, forces and collisions the Liouville equation thus just expresses flux conservation. Note that in a stationary situation the flux is conserved, not the neutrino number.

We want to derive the non-Abelian Boltzmann equation from the Heisenberg equation $i\partial_t \hat{A} = [\hat{A}, \hat{H}]$ for operators $\hat{A}$ and Hamilton operator $\hat{H}$. To this end we introduce the annihilation and creation operators of a neutrino or antineutrino of momentum **p** and flavour i, $\hat{a}_i(\mathbf{p}, t), \hat{b}_i(\mathbf{p}, t), \hat{a}_i^\dagger(\mathbf{p}, t), \hat{b}_i^\dagger(\mathbf{p}, t)$ which correspond to the spatial operators

$$\hat{\psi}_i(\mathbf{r}) = \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^{3/2}}\, e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar}\, \hat{a}(\mathbf{p})\,,$$

and satisfy the anti-commutation relations

$$\{\hat{a}_i(\mathbf{p}, t), \hat{a}_j^\dagger(\mathbf{p}', t)\} = (2\pi)^3 \delta^3(\mathbf{p} - \mathbf{p}')\delta_{ij}\,,$$

and analogously for anti-neutrinos.

Derivation through Wigner and Moyal Distributions

We define the operators

$$\hat{\mathsf{D}}_{ij}(\mathbf{p},\mathbf{p}',t) \equiv \hat{a}_j^\dagger(\mathbf{p}',t)\,\hat{a}_i(\mathbf{p},t)\,,$$

and relate them to a space- and momentum dependent density operator through a Wigner transformation,

$$\hat{\varrho}_{ij}(t,\mathbf{r},\mathbf{p}) = \int \frac{d^3\boldsymbol{\Delta}}{(2\pi)^3}\, e^{i\boldsymbol{\Delta}\cdot\mathbf{r}}\, \hat{D}_{ij}\left(\mathbf{p}+\frac{\boldsymbol{\Delta}}{2},\mathbf{p}-\frac{\boldsymbol{\Delta}}{2},t\right)\,.$$

For the Hamilton operator we make the ansatz

$$\hat{H} = \int \frac{d^3\mathbf{p}}{(2\pi)^3}\,\frac{d^3\mathbf{p}'}{(2\pi)^3}\,\hat{a}_i^\dagger(\mathbf{p})\,\mathsf{H}_{ij}(\mathbf{p},\mathbf{p}')\,\hat{a}_j(\mathbf{p}')\,,$$

where H_{ij} is a c-number matrix.

Using Heisenberg's equation and after a few manipulations one arrives at

$$i\hbar\partial_t\hat{\varrho}(\mathbf{r},\mathbf{p}) = \mathsf{H}(\mathbf{r},\mathbf{p})\, e^{\frac{i}{2}\hbar(\overleftarrow{\partial}_{\mathbf{r}}\cdot\overrightarrow{\partial}_{\mathbf{p}}-\overleftarrow{\partial}_{\mathbf{p}}\cdot\overrightarrow{\partial}_{\mathbf{r}})}\,\hat{\varrho}(\mathbf{r},\mathbf{p}) - \hat{\varrho}(\mathbf{r},\mathbf{p})\, e^{\frac{i}{2}\hbar(\overleftarrow{\partial}_{\mathbf{r}}\cdot\overrightarrow{\partial}_{\mathbf{p}}-\overleftarrow{\partial}_{\mathbf{p}}\cdot\overrightarrow{\partial}_{\mathbf{r}})}\,\mathsf{H}(\mathbf{r},\mathbf{p})\,.$$

where the matrix $\mathsf{H}(\mathbf{r},\mathbf{p})$ is related to the matrix $\mathsf{H}_{ij}(\mathbf{p},\mathbf{p}')$ through the same kind of Wigner transformation relating $\hat{\varrho}(\mathbf{r},\mathbf{p})$ to $\hat{D}_{ij}(\mathbf{p},\mathbf{p}')$.

A similar equation for first quantised scalars was first derived by Moyal. This is an operator equation with so far no approximations.

Taking the expectation value $\varrho(\mathbf{r},\mathbf{p}) \equiv \langle\hat{\varrho}(\mathbf{r},\mathbf{p})\rangle$ (mean field theory) and expanding the exponential up to first order then immediately gives the Liouville equation with flavour mixing,

$$\partial_t\varrho + \frac{1}{2}\left\{\partial_{\mathbf{r}}\varrho, \partial_{\mathbf{p}}\mathsf{H}\right\} - \frac{1}{2}\left\{\partial_{\mathbf{p}}\varrho, \partial_{\mathbf{r}}\mathsf{H}\right\} = -\, i\left[\mathsf{H}, \varrho\right]\,. \quad (3)$$

Higher orders would yield the collision terms and other quantum corrections. Planck's constant (here set to unity) appears both on the left hand side and in the exponent of the Moyal equation and thus cancels to lowest order, corresponding to the classicality of Liouville's equation.

Derivation through Husimi Distributions

We here simplify to one flavour $N_f = 1$. Smearing a Wigner distribution $f(\mathbf{x}, \mathbf{p})$ with Gaussians of width η in position and width σ in momentum space gives

$$F(\mathbf{r}, \mathbf{p}) \equiv \frac{1}{(2\pi\eta\sigma)^3} \int d^3\mathbf{r}' d^3\mathbf{p}'\, f(\mathbf{r}', \mathbf{p}') \exp\left[-\frac{(\mathbf{r}-\mathbf{r}')^2}{2\eta^2} - \frac{(\mathbf{p}-\mathbf{p}')^2}{2\sigma^2} \right] .$$

Choosing $\sigma = \hbar/(2\eta)$ the operator version can be put into the form

$$\hat{F}(\mathbf{r}, \mathbf{p}) = \frac{1}{(2\pi\eta^2)^{3/2}} \int \frac{d^3\mathbf{r}_1 d^3\mathbf{r}_2}{(2\pi\hbar)^3} \hat{\psi}^\dagger(\mathbf{r}_1)\hat{\psi}(\mathbf{r}_2) \exp\left[-\frac{(\mathbf{r}-\mathbf{r}_1)^2 + (\mathbf{r}-\mathbf{r}_2)^2}{4\eta^2} + \frac{i\mathbf{p}\cdot(\mathbf{r}_1 - \mathbf{r}_2)}{\hbar} \right] .$$

For the time evolution of the quantum field $\hat{\psi}$ we make the ansatz

$$i\hbar\partial_t \hat{\psi} = \mathbf{v}\cdot\hat{\mathbf{p}}\,\hat{\psi} + V(\mathbf{r})\hat{\psi}\,, \qquad \text{or} \qquad \partial_t\hat{\psi} = -\,\mathbf{v}\cdot\partial_{\mathbf{r}}\hat{\psi} - iV(\mathbf{r})\hat{\psi}/\hbar$$

which for $V(\mathbf{x}) = 0$ gives the relativistic dispersion relation $\hbar\omega = \mathbf{v}\cdot\mathbf{p}$.

A straightforward calculation and taking expectation values gives back the Liouville equation,

$$\partial_t F(\mathbf{r}, \mathbf{p}) = -\mathbf{v} \cdot \partial_{\mathbf{v}} F + \partial_{\mathbf{r}} V \cdot \partial_{\mathbf{p}} F + \mathcal{O}(\hbar)\,,$$

to this order independent of η ! The higher order terms give rise to quantum corrections which become in particular relevant on scales comparable to the de Broglie scale $\hbar/p$.

Solutions of such Liouville/Vlasov equations crucially depend on boundary and initial conditions.

Particle Transport and Wave Equations

Connection between particle transport (Liouville), Schrödinger-type, and wave equations can also be illuminated in a more direct way: Starting from a Klein-Gordon equation

$$(\partial_t^2 - \Delta)\psi = -\,\mathsf{M}^2\psi$$

one can consider plane waves propagating in a direction characterised by unit vector $\mathbf{n}$ with energy E. Then the wave operator becomes

$$(\partial_t^2 - \Delta) \to (\partial_t - \mathbf{n}\cdot\partial_{\mathbf{r}})(\partial_t + \mathbf{n}\cdot\partial_{\mathbf{r}}) \simeq -\,2iE(\partial_t + \mathbf{n}\cdot\partial_{\mathbf{r}})\,,$$

where we have approximated $|\mathbf{p}| \simeq E$. The wave equation then turns into a Liouville equation

$$(\partial_t + \mathbf{n}\cdot\partial_{\mathbf{r}})\psi \simeq -\,i\frac{\mathsf{M}^2}{2E}\psi\,,$$

or for the density matrix $\rho_{ij} \equiv \psi_j^* \psi_i$,

$$(\partial_t + \mathbf{n} \cdot \partial_{\mathbf{r}})\rho = -\,i[\mathsf{H}, \rho]\,, \qquad \text{where} \qquad \mathsf{H} = \frac{\mathsf{M}^2}{2E}\,. \quad (4)$$

In a homogeneous system the above equation simplifies to $\partial_t \rho = -\,i[\mathsf{H}, \rho]$, and in a stationary situation it reads $\partial_x \rho = -\,i[\mathsf{H}, \rho]$ for propagation in x direction.

In general equation (4) has to be solved for each Fourier component $(E, p\mathbf{n})$. Wavepackets can be constructed by superposition; phase relations between different Fourier modes are lost by averaging over many neutrinos. Only kinematic decoherence is possible from above equation; dynamical decoherence requires collision terms.

Phenomenological Consequences

We consider $N_f = 2$ flavours and in the mass basis set

$$\mathbf{V} = \begin{pmatrix} \mathbf{v}_1 & 0 \\ 0 & \mathbf{v}_2 \end{pmatrix} = \mathbf{v}\,\sigma_0 + \frac{\delta\mathbf{v}}{2}\,\sigma_3\,,$$

in terms of Pauli matrices and with $\mathbf{v} = (\mathbf{v}_1 + \mathbf{v}_2)/2$ and $\delta\mathbf{v} = \mathbf{v}_1 - \mathbf{v}_2$. In a stationary situation for propagation in x-direction Eq. (3) for one momentum mode gives

$$\frac{d}{dx}\varrho + \delta_v \left\{ \varrho', \frac{\sigma_3}{2} \right\} = -\,i \left[\frac{\mathsf{H}}{v}, \varrho \right]\,,$$

with $v = (v_1 + v_2)/2$ and $\delta_v = v_1 - v_2$. Expanding into Pauli matrices and polarisation vectors B_j and P_j,

$$\frac{\mathsf{H}}{v} = \sum_{j=1}^{3} B_j \frac{\sigma_j}{2} \qquad \text{and} \qquad \varrho = \sum_{j=0}^{3} P_j \frac{\sigma_j}{2}\,,$$

and defining $\tilde{P}_3 = P_3(1-\delta_v^2)^{1/2}$, $\tilde{P}_{1,2} = P_{1,2}$ and $\tilde{B}_{1,2} = B_{1,2}/(1-\delta_v^2)^{1/2}$, $\tilde{B}_3 = B_3$ one obtains

$$\frac{d}{dx}\tilde{\mathbf{P}} = \tilde{\mathbf{B}} \times \tilde{\mathbf{P}}\,,$$

which gives rise to periodic motion and no decoherence. Note that the length of $\tilde{\mathbf{P}}$ is conserved, but not the one of $\mathbf{P}$.

Collision Terms and Dynamical Decoherence

Assuming molecular chaos for neutral current interactions the collision (Boltzmann) term at a given location $\mathbf{r}$ has the form

$$\partial_t \rho_{\mathbf{p}}\Big|_{\text{coll,NC}} = \frac{1}{2}\int \frac{d^3\mathbf{q}}{(2\pi)^3}\Big[W(q,p)(1-\rho_{\mathbf{p}})G\rho_{\mathbf{q}}G - W(p,q)\rho_{\mathbf{p}}G(1-\rho_{\mathbf{q}})G$$

$$+W(-q,p)(1-\rho_{\mathbf{p}})G(1-\overline{\rho}_{\mathbf{q}})G - W(p,-q)\rho_{\mathbf{p}}G\overline{\rho}_{\mathbf{q}}G + \text{h.c.}\Big],$$

where $W(q,p)$ is the (scalar) scattering rate from state of four-momentum $(E_{\mathbf{q}}, \mathbf{q})$ to a state of four-momentum $(E_{\mathbf{p}}, \mathbf{p})$, with $E_{\mathbf{p}}$ the energy corresponding to three-momentum $\mathbf{p}$, and G a dimensionless flavour matrix characterising the coupling strengths of the different Neutron flavours. The c-number flavour densities $\rho_{\mathbf{p}}$ and $\overline{\rho}_{\mathbf{p}}$ refer to neutrinos and anti-neutrinos, respectively. The first two terms describe scattering and the last two describe pair creation and annihilation. They are related by crossing particles and substituting $p \to -p \quad \rho_{\mathbf{p}} \to 1-\overline{\rho}_{\mathbf{p}}$, which also gives a similar equation for $\partial_t \overline{\rho}_{\mathbf{p}}\Big|_{\text{coll,NC}}$.

Charged current source terms at a given location $\mathbf{r}$ have the form

$$\partial_t \rho_{\mathbf{p}}\Big|_{\text{coll,CC}} = \{\mathscr{P}(p), (1-\rho_{\mathbf{p}})\} - \{\mathscr{A}(p), \rho_{\mathbf{p}}\}\,,$$

with $\mathscr{P}(p)$ and $\mathscr{A}(p)$ flavour-diagonal $N_f \times N_f$ matrices with production and absorption rates of neutrinos of given flavour and four-momentum p on the diagonal. Assuming detailed balance for the background plasma this becomes

$$\partial_t \rho_{\mathbf{p}}\Big|_{\text{coll,CC}} = \left\{\mathscr{P}(\mathbf{p}), \left(1 - \frac{\rho_{\mathbf{p}}}{f_{0\mathbf{p}}}\right)\right\}\,,$$

with $f_{0\mathbf{p}}$ the equilibrium occupation numbers,

$$f_{0\mathbf{p}} \equiv f_{\text{eq}}(E_{\mathbf{p}}) = \frac{1}{e^{(E_{\mathbf{p}}-\mu)/T}+1}\,.$$

Analogous equations for scattering, pair production and annihilation, and production and absorption of single particles for bosons are obtained with the substitution

$$1 - \rho_{\mathbf{p}} \to 1 + \rho_{\mathbf{p}}$$

In words: Pauli blocking turns into stimulated emission.

If the neutrinos are coupled to a medium in thermal equilibrium characterized by a temperature T and a chemical potential μ for the lepton number, then one can show that the neutrino grand canonical potential

$$\Omega_\nu \equiv U_\nu - TS_\nu - \mu L_\nu \,, \quad (5)$$

can never increase, i.e. $\dot{\Omega}_\nu \leq 0$. Here, the internal energy of the neutrino ensemble U_ν, its total lepton number L_ν, and its entropy S_ν are given by

$$U_\nu = \int \frac{d^3\mathbf{p}}{(2\pi)^3} \, |\,\mathbf{p}\,| \, \mathrm{Tr}(\rho_\mathbf{p} + \overline{\rho}_\mathbf{p}) \,,$$

$$L_\nu = \int \frac{d^3\mathbf{p}}{(2\pi)^3} \, \mathrm{Tr}(\rho_\mathbf{p} - \overline{\rho}_\mathbf{p}) \,,$$

$$S_\nu = -\int \frac{d^3\mathbf{p}}{(2\pi)^3} \, \mathrm{Tr}\left[\rho_\mathbf{p} \ln(\rho_\mathbf{p}) + (1 - \rho_\mathbf{p})\ln(1 - \rho_\mathbf{p}) + \overline{\rho}_\mathbf{p} \ln(\overline{\rho}_\mathbf{p}) + (1 - \overline{\rho}_\mathbf{p})\ln(1 - \overline{\rho}_\mathbf{p})\right] .$$

Analogous expressions for bosons are again obtained by substituting $1 - \rho_\mathbf{p} \to 1 + \rho_\mathbf{p}$.

If there are only neutral current interactions, lepton number L_ν will be conserved and Eq. (5) implies that the neutrino free energy $F_\nu \equiv U_\nu - TS_\nu$ can never increase, $\dot{F}_\nu \leq 0$. If neutrinos interact only among themselves, the neutrino energy U_ν will be conserved in addition, and the neutrino entropy S_ν can never decrease, $\dot{S}_\nu \geq 0$. Derivation is similar to Boltzmann's H-theorem, but now with flavour matrices.

Real dynamical decoherence is tied to an increase of entropy, or a decrease of the grand canonical potential or the free energy and thus can only be caused by collision terms.

The entropy does not increase only if the occupation number matrices already equal their equilibrium values, $\partial_t \rho_{\mathbf{p}} = 0\,, \rho_{\mathbf{p}} = f_{0\mathbf{p}}$.

Fluid Equations and Madelung Transformation

Consider a non-relativistic wave function $\psi(t, \mathbf{r})$ of mass m, $|\partial_t \psi|, |\nabla \psi| \ll m|\psi|$, that obeys the nonlinear Gross-Pitaevskii equation

$$i\partial_t \psi = H_\psi \psi \equiv -\frac{\hbar^2}{2m}\Delta\psi + V_{\mathrm{GP}}(t, \mathbf{r})\psi(t, \mathbf{r}),$$

$$V_{\mathrm{GP}}(t, \mathbf{r}) = m\Phi(t, \mathbf{r}) + V_{\mathrm{GP}}^{\mathrm{nl}}(t, \mathbf{r}) \equiv m\Phi(t, \mathbf{r}) + \frac{2\pi\hbar^2}{m} a_{s,0} |\psi(t, \mathbf{r})|^2,$$

with $a_{s,0}$ the self-scattering length and Φ the gravitational potential that in absence of other gravity sources obeys the Poisson equation

$$\Delta\Phi = 4\pi G_{\mathrm{N}} m |\psi|^2 .$$

One can transform this Schrödinger-Poisson equation system into classical fluid equation. This can numerically be advantageous because singularities in the fluid equations are smoothed out by the quantum uncertainty of location.

To this end one can separate $\psi(t, \mathbf{r})$ into an amplitude $A(t, \mathbf{r})$ and a phase $\alpha(t, \mathbf{r})$,

$$\psi(t, \mathbf{r}) = A(t, \mathbf{r}) \exp[i\alpha(t, \mathbf{r})] ,$$

and relate these real valued quantities to energy density $\rho(t, \mathbf{r})$ and velocity field $\mathbf{v}(t, \mathbf{r})$,

$$\mathbf{v}(t, \mathbf{r}) = \frac{\nabla \alpha}{m}, \quad \rho(t, \mathbf{r}) = m \, | \, \psi(t, \mathbf{r}) \, |^2 = m A^2(t, \mathbf{r}) ,$$

which then can be shown to obey the fluid-type equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 , \quad \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = - \nabla \left(\frac{V_{\mathrm{GP}}}{m} - \frac{\Delta \rho^{1/2}}{2 m^2 \rho^{1/2}} \right) ,$$

where the last term in the second (Navier-Stokes type) equation can be interpreted as quantum pressure

$$p \simeq - \left(\frac{\rho^{1/2} \Delta \rho^{1/2}}{2 m^2} \right) = - \left(\frac{A \Delta A}{2m} \right) .$$

Conclusions

1.) There is a deep connection between Schrödinger-like equations for the wave operators and the classical Liouville equation and its generalisation to collisional Vlasov/Boltzmann equations

2.) Classical behaviour emerges on length scales large compared to the de Broglie wavelength $\hbar/p$ to lowest order in an expansion in $\hbar$. To this order one has collisionless particle transport and kinematic decoherence

3.) Higher order terms would describe correlations between momentum modes and collision terms which can also lead to dynamic decoherence

4.) Integrating out momentum modes gives a connection between wave equations and classical fluid equations through the Madelung transformation