Irreversibility from a Reversible Equation

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After a discussion on the state of local equilibrium with temperature inhomogeneity, comparing mixture state representation in statistical mechanics and pure state representation in thermo field dynamics, a simple model is solved to show that a reversible equation of motion with the initial condition having inhomogeneous temperature can lead to irreversible, viz. diffusive, behaviour. Yet, the solution is time symmetric exhibiting diffusion both towards future and past.

I. INTRODUCTION

The irreversible processes remain to be understood despite the long history and many attempts \[1,2\]. In particular, those processes caused by temperature gradient, say, heat conduction and thermal diffusion, have no approaches from the first principles that are commonly accepted, while those driven mechanically, say, electric conduction, has been handled by the perturbation theory in Hamiltonian dynamics, at least for the purpose of computing the transport coefficients \[3\].

We have been trying to obtain a microscopic picture for the heat conduction \[4\] and thermal diffusion \[5\] by using the thermo field dynamics \[6\]. However, the calculations got so involved as to obscure the picture. We are led to try a simple model, if not quite realistic, to see in a mathematically transparent way that an irreversibility can result from a reversible equation when the initial condition involves temperature inhomogeneity. In this calculation, we use the standard machinery of statistical mechanics.

After a brief introduction to the thermo field dynamics in Sec.2, we shall relate in Sec.3 the formulations of the state of local equilibrium under temperature gradient in the thermo field dynamics and in the more usual statistical mechanics. It is interesting that the thermo field dynamics exhibits a non-local feature, though microscopic, of the local equilibrium states; statistical mechanics gives an equivalent description but in a more indirect way. Then in Sec. 4, we employ a simple model to show in a mathematically transparent way that a reversible equation of motion with the initial condition having inhomogeneous temperature can lead to irreversibility. Our result is irreversible in that it shows a diffusive behaviour among other features, and yet symmetric with respect to the direction of time in that the diffusion towards future/past comes out when the equation is solved towards future/past, respectively.

II. THERMO FIELD DYNAMICS

The basic idea of the thermo field dynamics is to represent the thermal state not by the mixture state with the density matrix $\rho(\beta)$ but by a pure state $|\beta\rangle$ which can be obtained from $\rho(\beta)$ by the GNS construction. Thus, the thermal average of an observable $A$ reads

$$\text{Tr}[\rho(\beta) A] = \langle \beta | A | \beta \rangle,$$

the left-hand side belonging to the usual statistical mechanics and the right to the thermo field dynamics.

With any complete set $\{|n\rangle\}$ of orthonormal states, one can write

$$|\beta\rangle := \sum_n \rho(\beta)^{1/2} |n\rangle \otimes \langle n|.$$

In fact

$$\langle \beta | A | \beta \rangle = \sum_m \sum_n \langle m | \rho(\beta)^{1/2} A \rho(\beta)^{1/2} | n \rangle \langle n | m \rangle = \sum_n \langle n | A | n \rangle = \text{Tr} [\rho(\beta) A].$$

The thermo field dynamics further introduces operators that act on the bra part as

$$(I \otimes A) |\psi\rangle \otimes |\chi\rangle := |\psi\rangle \otimes \left( A^\dagger |\chi\rangle \right)^t,$$

thus doubling the number of operators to be considered. One uses shorthand notations,

$$\tilde{A}^\dagger := I \otimes A, \quad |\psi\rangle |\chi\rangle := |\psi\rangle \otimes |\chi\rangle.$$

Then, one finds: $\tilde{cA} = c^* A$, and...
\[ [\alpha, \alpha^\dagger] = 1 \implies [\tilde{\alpha}, \tilde{\alpha}^\dagger] = 1, \text{ etc.} \quad (5) \]

Suppose \( \alpha \) acts on \(|n\rangle \) as an annihilation operator,
\[
\alpha|n\rangle = \sqrt{n}|n-1\rangle
\]
and \( \rho = Z^{-1}_1 e^{-\beta H} \) with \( H = \omega \alpha^\dagger \alpha \), so that
\[
|\beta\rangle = Z_1(\beta)^{-1/2} \sum_n e^{-\beta \omega/2} |n\rangle \langle n|,
\]
then
\[
\begin{align*}
\alpha|\beta\rangle &= \frac{1}{Z_1(\beta)^{1/2}} \sum_{n=1}^{\infty} e^{-\beta \omega/2} \sqrt{n}|n-1\rangle \langle n| \\
&= \frac{e^{-\beta \omega/2}}{Z_1(\beta)^{1/2}} \sum_{n=0}^{\infty} e^{-\beta \omega/2} \sqrt{n+1}|n+1\rangle \langle n+1|,
\end{align*}
\]
\[
\tilde{\alpha}^\dagger |\beta\rangle = \frac{1}{Z_1(\beta)^{1/2}} \sum_{n=0}^{\infty} e^{-\beta \omega/2} \sqrt{n+1}|n+1\rangle \langle n+1|,
\]
implying
\[
\left( \alpha - e^{-\beta \omega/2} \tilde{\alpha}^\dagger \right) |\beta\rangle = 0,
\]
which is the thermal state condition. In terms of \( \theta \) as defined for the \( \beta \) by \( \tanh \theta = e^{-\beta \omega/2} \),
\[
\left( \alpha \cosh \theta - \tilde{\alpha}^\dagger \sinh \theta \right) |\beta\rangle = 0,
\]
which reminds us of the Bogoliubov transformation \( [7] \):
\[
U(\beta)\alpha U(\beta)^{-1} = \alpha \cosh \theta - \tilde{\alpha}^\dagger \sinh \theta,
\]
with
\[
U(\beta) = \exp \left[ \left( \alpha^\dagger \tilde{\alpha} - \alpha \tilde{\alpha}^\dagger \right) \theta \right].
\]
This operator generates the state \(|\beta\rangle \) from the "no particle state" \(|\Omega\rangle := |0\rangle \langle 0| \) of \( \alpha \),
\[
U(\beta)|\Omega\rangle = |\beta\rangle
\]
as one sees from the operator \( [8] \) annihilating \( [\tilde{\alpha}] \), or from
\[
U(\beta)|\Omega\rangle = \frac{1}{Z_1(\beta)^{1/2}} \exp [\alpha^\dagger \tilde{\alpha} - \tilde{\alpha}^\dagger \alpha] \tanh \theta |\Omega\rangle
\]
\[
= \frac{1}{Z_1(\beta)^{1/2}} \sum_{n=0}^{\infty} e^{-\beta \omega/2} |n\rangle \langle n| = |\beta\rangle.
\]

We have so far considered only a single mode. In general, however, the object has many modes, and often infinitely many, to which a tensor product of the states considered above corresponds.

### III. NONUNIFORM TEMPERATURE

Suppose we change the temperature a bit uniformly all over the system. Then,
\[
|\beta + \Delta \beta\rangle = U(\beta + \Delta \beta)|\Omega\rangle
\]
\[
= \frac{1}{Z_1(\beta + \Delta \beta)^{1/2}} \exp \left[ \alpha^\dagger \tilde{\alpha} - \tilde{\alpha}^\dagger \alpha \right] e^{-\beta \omega/2} |\Omega\rangle,
\]
which can be approximated as
\[
|\beta + \Delta \beta\rangle = N_1 \left( 1 - \frac{\omega \Delta \beta}{2} e^{-\beta \omega/2} \alpha^\dagger \tilde{\alpha} \right) |\beta\rangle
\]
with \( N_1 = Z_1(\beta)^{1/2} / Z_1(\beta + \Delta \beta)^{1/2} \), the normalization factor.

For a system with many modes labelled by \( k \), \( Z_1 \) is replaced by \( Z \), and
\[
|\beta + \Delta \beta\rangle = N(1 - i \Gamma)|\beta\rangle
\]
with
\[
\Gamma = -\frac{1}{2} \sum_k \frac{\omega_k \Delta \beta}{2} e^{-\beta \omega_k/2} \alpha_k^\dagger \tilde{\alpha}_k^\dagger.
\]

Define:
\[
\phi(x) := \frac{1}{\sqrt{V}} \sum_k \alpha_k e^{ikx}, \quad \tilde{\phi}(x) := \frac{1}{\sqrt{V}} \sum_k \tilde{\alpha}_k e^{ikx},
\]
then
\[
G = -i \Delta \beta \int \phi^\dagger \left( x + \frac{\xi}{2} \right) g(\xi) \tilde{\phi}^\dagger \left( x - \frac{\xi}{2} \right) d^3xd^3\xi.
\]

For a gas of free particles (or quasi-particles), for which
\[
\omega_k = \frac{k^2}{2m},
\]
one has, in high temperature approximation,
\[
g(\xi) = \left( \frac{m^3}{\pi^3 \beta^3 h^3} \right)^{1/2} \left( 3 - \frac{2m}{\beta \hbar^2 \xi^2} \right) \exp \left[ -\frac{m}{\beta \hbar^2 \xi^2} \right],
\]
which is short-ranged as shown in Table 1.

| Table 1 | The range of \( g \) |
|---------|----------------------|
| \( m \) | nucleon | electron |
| \( \sqrt{\frac{\beta \hbar^2}{m}} = T(K)^{-1/2} \times \) | \( 7 \times 10^{-10} \) | \( 3 \times 10^{-8} \) |
Since \( g(\xi) \) is short-ranged, the operator \([13]\) can be regarded as a sum of local operators. Therefore, the state with nonuniform temperature \( \beta + \beta_a(x) \) may be represented as
\[
|\beta + \beta_a(x)\rangle = N \left( 1 - i \Gamma[\beta_a(x)] \right) |\beta\rangle
\]
with the temperature inhomogeneity \( \beta_a(x) \) being pushed into the integrand of \([13]\):
\[
\Gamma[\beta_a(x)] = -i \int \phi^\dagger \left( x + \frac{\xi}{2} \right) \phi \left( x - \frac{\xi}{2} \right) g(\xi) \beta_a(x) d^3x d^3\xi,
\]
(17)
since the temperature inhomogeneity \( \beta_a(x) \) we are concerned with in studying thermal processes varies only slowly on a macroscopic scale.

We add that \([13]\) is often written as
\[
\Gamma[\beta_a(x)] = \int \Phi^\dagger \left( x + \frac{\xi}{2} \right) e^{-V} \Phi \left( x - \frac{\xi}{2} \right) g(\xi) \beta_a(x) d^3x d^3\xi.
\]
(18)
in terms of the thermal doublet,
\[
\Phi(x) := \begin{pmatrix} \phi_1(x) \\ \phi_2(x) \end{pmatrix} = \frac{1}{\sqrt{N}} \begin{pmatrix} a_k \\ \bar{a}_k \end{pmatrix} e^{ikx}.
\]

This is the representation we have been using for the state with nonuniform temperature in our studies of heat conduction and thermal diffusion \([1] [10]\).

As is clear from its derivation, this representation is equivalent to the one by the density matrix,
\[
\rho[\beta + \beta_a(x)] := \frac{1}{N} \exp \left[ -\beta \mathcal{H} - \int \beta_a(x) \mathcal{H}(x) d^3x \right],
\]
(20)
or, more precisely, to its expansion to the first order in \( \beta_a \),
\[
\rho[\beta + \beta_a(x)] = N^{-1} e^{-\beta \mathcal{H}} \times \left( 1 - \int_0^1 d\lambda e^{\lambda \beta \mathcal{H}} \int d^3x \beta_a(x) \mathcal{H}(x)e^{-\lambda \beta \mathcal{H}} \right),
\]
(21)
provided that \( \beta_a(x) \) is slowly varying.

It is interesting to compare \([21]\) and \([16]+[17]\) observing that the effect of the temperature inhomogeneity \( \beta_a(x) \) appears not to be strictly local in thermo field dynamics but has a small extension as represented by \( g(\xi) \).

We repeat that the two representations are equivalent, and the effect of \( g(x) \) is also there in \([21]\) as a little analysis shows. It is only that the effect can be seen more easily in the thermo field dynamics.

Another remark concerns Zubarev’s assertion \([8]\) that no irreversible processes can follow from the density matrix \([21]\). Our model calculation in the next section will provide a counterexample to his assertion. Further discussion will be given in Sec. V.

IV. A MODEL EXHIBITING IRREVERSIBILITY

To see that irreversibility can result from the interaction of particles even when their equation of motion is reversible, we consider a simple model \([9] [10]\) of a Bose gas (particle mass: \(1/2\)) with a quadratic Hamiltonian,
\[
\mathcal{H}(x) = \frac{1}{2} \sum_p p^2 a_p^+ a_p + \frac{\nu_0}{2} \sum_{p \leq K} v_0 (a_p^+ a_{-p} + 2a_p a_{p})
\]
(22)
This Hamiltonian is time-reversible, as one sees by applying time reversal \( p \to -p \) to the momenta that label the operators \( a_p \). The price we have to pay for the simplicity of its analysis is the non-conservation of the particle number; this is serious because we are going to look at the particle diffusion as a sign of irreversibility. Nevertheless, we shall be able to see this sign \([11]\), though superposed with an unwanted decay of the particle number.

We use the representation \([20]\) of the temperature inhomogeneity in terms of the density matrix, for which we need the Hamiltonian density,
\[
\mathcal{H}(x) = \frac{\partial \phi^\dagger(x)}{\partial x_i} \frac{\partial \phi(x)}{\partial x_i} + \frac{\nu_0}{2} \int v(r) \left[ \phi^\dagger(x + \frac{1}{2}r) \phi^\dagger(x - \frac{1}{2}r) \right. \\
\left. + \phi^\dagger(x + \frac{1}{2}r) \phi(x - \frac{1}{2}r) + \phi^\dagger(x - \frac{1}{2}r) \phi(x + \frac{1}{2}r) + \phi(x + \frac{1}{2}r) \phi(x - \frac{1}{2}r) \right] d^3r.
\]
(23)
where \( v(r) \) is such that
\[
\hat{v}(k) = \int v(r) e^{-ik\cdot r} d^3r = \begin{cases} v_0 & \text{for } k \leq K \\ 0 & \text{for } k > K, \end{cases}
\]
or
\[
v(r) = 4\pi^2 v_0 K^2 j_1(Kr)/r.
\]
In terms of the Fourier transform, we find
\[
\int v(r) \phi^\dagger(x + \frac{1}{2}r) \phi(x - \frac{1}{2}r) d^3r = \frac{1}{V} \sum_{p'p} \hat{v}(\frac{p' + p}{2}) a_{p'}^+ a_p e^{ip'\cdot x}
\]
and similarly for their Hermitian relatives. We assume for simplicity that \( K \) is sufficiently large to make all the \( \hat{v}(k) \)'s for thermally agitated particles to have the constant value \( v_0 \): we shall hereafter suppress the proviso \( p \leq K \).

For the particle number density,
\[
j_0(x) = \phi^\dagger(x) \phi(x) = \frac{1}{V} \sum_{p'p} a_{p'}^+ a_p e^{ip\cdot x},
\]
(24)
we wish to find out the long-time behaviour of the deviation,
\[
\langle \hat{j}_0(x, t) \rangle ^{(1)} = -\frac{1}{Z(0)} \text{Tr} \left[ e^{-\beta \mathcal{H}} \int_0^1 d\lambda \int d^3x' \beta_a(x') \mathcal{H}(x') \times e^{i\mathcal{H}\tau} j_0(x) e^{-i\mathcal{H}\tau} \right],
\]
from the average,
\[
\langle \hat{j}_0(x, t) \rangle ^{(0)} = \frac{1}{Z(0)} \text{Tr} [e^{-\beta \mathcal{H}} j_0(x)]
\]
where
\[
\tau = t + i\lambda\beta
\]
and we have assumed that
\[
\int \beta_a(x) d^3x = 0.
\]

The Hamiltonian \((\mathcal{H})\) can be diagonalized as
\[
\mathcal{H} = \sum_p \omega_p \alpha_p^\dagger \alpha_p \quad (\omega_p := p\sqrt{p^2 + 2c^2}, \quad c^2 := \rho_0 v_0),
\]
where the zero-point energy has been dropped, by a Bogoliubov transformation
\[
a_p = \alpha_p \cosh \theta_p - \alpha_p^\dagger \sinh \theta_p,
\]
with
\[
\sinh^2 \theta_p = \frac{p^2 + c^2}{2p\sqrt{p^2 + 2c^2}} - \frac{1}{2}, \quad \cosh \theta_p \sinh \theta_p = \frac{2p\sqrt{p^2 + 2c^2}}{c^2}.
\]

The thermal average\((25)\) turns out to be given by the sum:
\[
\langle j_0(x, t) \rangle ^{(1)} = \langle j_0(x, t) \rangle ^{(s, -)} + \langle j_0(x, t) \rangle ^{(s, +)} + \langle j_0(x, t) \rangle ^{(c, -)} + \langle j_0(x, t) \rangle ^{(c, +)},
\]
where
\[
\langle j_0(x, t) \rangle ^{(s, \pm)} = -\frac{1}{2(2\pi)^3} \int d^3k \beta_a(k) e^{ik\cdot x} \int_0^1 F^{(s, \pm)}(k, \lambda) d\lambda,
\]
with
\[
F^{(s, \pm)}(k, \tau) = \int d^3P \ g(p', p) \sinh (\theta_{p'} + \theta_p) \times \left\{ f(\omega_{p'}) f(\omega_p) e^{-(\omega_{p'} + \omega_p)\tau} + \{ f(\omega_{p'}) + 1 \} \{ f(\omega_p) + 1 \} e^{(\omega_{p'} + \omega_p)\tau} \right\}
\]
and
\[
F^{(c, \pm)}(k, \tau) = \int d^3P \ h(p', p) \cosh(\theta_{p'} + \theta_p) \times \left\{ f(\omega_{p'}) f(\omega_p) e^{-(\omega_{p'} - \omega_p)\tau} + \{ f(\omega_{p'}) + 1 \} \{ f(\omega_p) + 1 \} e^{(\omega_{p'} - \omega_p)\tau} \right\},
\]

Here, \( p' = P + k/2, \ p = P - k/2, \) and
\[
g(p', p) = \begin{cases} \sinh (\theta_{p'} - \theta_p) (\cosh \theta_{p'} - \sinh \theta_{p'}) (\cosh \theta_p - \sinh \theta_p), & \text{if } \theta_{p'} - \theta_p < 0, \\ 1, & \text{otherwise}. \end{cases}
\]

A. Evaluation of the integral \( F^{(s, \pm)} \)

As a key for the following calculations, the temperature inhomogeneity \( \beta_a(x) \) is assumed to be varying on a macroscopic scale, so that the support of its Fourier transform is very small in comparison with the scales on which \( \omega_p \) and the coefficients of the Bogoliubov transformation vary.

We begin the evaluation of \((29)\) from the \( P \)-integration,
\[
F^{(s, +)}(k, \tau) = \int_0^\infty P^2 dP \sinh(2\theta_P) \left( f(\omega_P) \right)^2 \times \int d\Omega_{P} g(p', p) e^{-(\omega_{p'} + \omega_p)\tau},
\]
where, in \( \sinh \) and \( f \), we have put \( p = p' = P \) taking advantage of the small support of \( \beta(k) \). However, we cannot do so in \( g \) and the exponent, because \( g \) would vanish if we did and the exponent is proportional to \( \tau \) that involves the macroscopically large variable \( t \). Instead, we expand to order \( k^2 \),
\[
\omega_{p'} + \omega_p = 2\omega_p + \frac{P^2 + c^2}{2\omega_p} k^2 - \frac{c^4}{\omega_p^2} (P \cdot k)^2
\]
and put
\[
g(p', p) = g_0(P) + g_1(P)(P \cdot k) + g_2(P)k \cdot k + \frac{g_3(P)(P \cdot k)^2}{c^2};
\]
finding, however, that \( g_0 = g(P, P) = 0 \) by the Bogoliubov transformation diagonalizing \( \mathcal{H} \) \((cf. \ the \ remark \ after \ (22))\), \( g_1 = 0 \) by the symmetry \( g(p', p) = g(p, p') \)
from (32); we take in advance the later result into account that
\[ g_3(P) = \cosh 2\theta_P \sinh^2 2\theta_P \]
vanishes at the value of \( P \) that concerns us. Thus,
\[ g(p', p) = g_2(P) \quad \text{with} \quad g_2(P) = -\frac{1}{2} \sinh 2\theta_P. \quad (36) \]
The integration over the angles in (34),
\[ I_0 = \int_0^\pi e^{\imath \alpha \cos^2 \gamma \sin \gamma d\gamma} = \frac{2}{\sigma} \int_0^\pi e^{-y^2} dy, \]
is carried out by adding and subtracting \( \frac{2}{\sigma} \int_\sigma^\infty e^{-y^2} dy \) taking advantage of \( \text{Im} \alpha = \lambda \beta > 0 \), where \( \gamma \) is the angle between \( P \) and \( k \),
\[ \alpha = \frac{c^4 P^2}{\omega_P^3} k^2 \tau, \quad \sigma := (-\imath \alpha)^{1/2}, \quad \text{and} \quad y = \sigma x. \quad (37) \]
We note \( -\pi/2 < \arg \sigma < 0 \) and \( |\sigma| \to \infty \) as \( t \to \infty \). Then, asymptotically
\[ I_0 \sim \frac{\sqrt{\pi}}{\sigma} - \frac{1}{\sigma^2} e^{-\sigma^2}. \quad (38) \]
Thus,
\[ F^{(s,+)}(k, \tau) \]
\[ \sim 2\pi \int_0^\infty P^2 dP \sinh[2\theta_P] \left( f(\omega_P) + 1 \right)^2 g_2(P) k^2 \]
\[ \times \left\{ \frac{\sqrt{\pi}}{\sigma} - \frac{1}{\sigma^2} \exp \left[ \frac{c^4 P^2}{\omega_P^3} k^2 \tau \right] \right\} \]
\[ \times \exp \left[ -i \left( 2\omega_P + \frac{P^2 + c^2}{2\omega_P} k^2 \right) \tau \right]. \quad (39) \]

Similar calculations give
\[ F^{(s,-)}(k, \tau) \]
\[ \sim 2\pi \int_0^\infty P^2 dP \sinh[2\theta_P] \left( f(\omega_P) + 1 \right)^2 g_2(P) k^2 \]
\[ \times \left\{ \frac{i}{\sqrt{\pi}} + \frac{1}{\sigma^2} \exp \left[ -\frac{c^4 P^2}{\omega_P^3} k^2 \tau \right] \right\} \]
\[ \times \exp \left[ i \left( 2\omega_P + \frac{P^2 + c^2}{2\omega_P} k^2 \right) \tau \right]. \quad (40) \]
If we change the variable of integration \( P \) to \( -P \) in (41) after analytically continuing the integrand to the complex \( P \)-plane with two cuts to cope with the singularity of \( (P^2 + 2c^2)^{1/2} \); one extending along the imaginary axis from \( i\sqrt{2c} \) to \( i\infty \), and the other from \( -i\sqrt{2c} \) to \( -i\infty \), then \( \omega_+ = -\omega_P \), and consequently
\[ f(\omega_P) + 1 = \frac{e^{-\beta k\omega_P}}{e^{-\beta k\omega_P} - 1} = -f(\omega_P), \]
\[ \sinh \theta_P = -\sinh \theta_P \quad (41) \]
so that for \( F^{(s)} := F^{(s,+)} + F^{(s,-)} \),
\[ F^{(s)}(k, \tau) \]
\[ \sim \int_{-\infty}^\infty dP G(P) \left\{ \frac{\sqrt{\pi}}{\sigma} - \frac{1}{\sigma^2} \exp \left[ \frac{c^4 P^2}{\omega_P^3} k^2 \tau \right] \right\} \]
\[ \times \exp \left[ -i \left( 2\omega_P + \frac{P^2 + c^2}{2\omega_P} k^2 \right) \tau \right], \quad (42) \]
where
\[ G(P) := 2\pi P^2 \sinh[2\theta_P] \left( f(\omega_P) \right)^2 g_2(P) k^2. \]

1. Long-time behavior of \( F^{(s)}_1 \)

The time scale we are interested in is macroscopic. To evaluate the integral (42) asymptotically for \( t \to \infty \), we use the saddle-point method. Candidates for the saddle point \( P_{s,1} \) for the part of the integral (43),
\[ J_1 := -\frac{1}{\sigma^2} \int_{-\infty}^\infty dP G(P) \]
\[ \times \exp \left[ -i \left( 2\omega_P + \left( \frac{P^2 + c^2}{2\omega_P} - \frac{c^4 P^2}{\omega_P^3} \right) k^2 \right) \tau \right], \quad (43) \]
are determined by the condition of vanishing derivative of the exponent.
\[ 2 \frac{d\omega_P}{dP} - \left\{ \left( \frac{P^2 + c^2}{2\omega_P} - \frac{3c^4 P^2}{\omega_P^3} \right) \frac{d\omega_P}{dP} \right\} k^2 = 0, \]
where
\[ \frac{d\omega_P}{dP} = \frac{2(P^2 + c^2)}{\sqrt{P^2 + 2c^2}}. \]
For small \( k \), the main part of the root is given by \( P = \pm ic \). Then, we put \( P^2 = -c^2 + \xi \), finding \( \xi = -(3/4)k^2 \) up to order \( k^2 \), and hence \( P_{s,1} = \pm ic \{ 1 + (3/8)(k^2/c^2) \} \) as candidates for the saddle points. Since
\[ \frac{d^2\omega_P}{dP^2} = \frac{2(P^2 + 3c^2)}{(P^2 + 2c^2)^{3/2}} \]
takes the value \( \pm 4i + O(k^2/c^2) \) at the saddle points, the exponent behaves like
\[ 2\omega_P + \left( \frac{P^2 + c^2}{2\omega_P} - \frac{c^4 P^2}{\omega_P^3} \right) k^2 \]
\[ = \pm i \left\{ (2c^2 + k^2) + 4(P - P_{s,1})^2 \right\} \]
in the neighborhood of \( P_{s,1} \), so that
\[ J_1 \sim -\frac{1}{\sigma^2} e^{\pm (2c^2 + k^2)^2} \int_{-\infty}^\infty G(P)e^{\pm 4(P - P_{s,1})^2} dP. \quad (44) \]
For $\tau \sim t \to +\infty$, therefore, we should take the lower sign here

$$P_{s,1} = -ic \left(1 + \frac{1}{8} \frac{k^2}{\sigma^2} \right)$$

(45)

for the saddle point which the path of integration should pass. Thus,

$$F^{(s)} \sim -\frac{1}{\sigma(P)^2} G(P_{s,1}) e^{-\left(2c^2+k^2\right)\tau} \int_{-\infty}^{\infty} e^{-4\tau^2} ds,$$  

(46)

and we have only to carry out the expansion (36) around $P = P_{s,1}$, obtaining

$$F^{(s)}(k, \tau) \sim -\frac{1}{2} \left( \frac{\pi}{\tau} \right)^{3/2} f(\omega_{P_{s,1}})^2 e^{-(2c^2+k^2)\tau}.$$  

(47)

Note that the small factor $k^2$ of $G$ has been cancelled by $1/\sigma^2$. The factor $e^{-k^2\tau}$ is a welcome sign of the diffusive behavior. However, it is accompanied by $e^{-2c^2\tau}$, a damping, which is an unexpected feature.

2. Long-time behavior of $F^{(s)}$

We still have to evaluate the other part of the integral (42).

$$J_2 := \frac{\sqrt{\pi}}{\sigma} \int_{-\infty}^{\infty} dP G(P)$$

$$\times \exp \left[ -i \left( 2\omega_P + \frac{P^2 + c^2}{2\omega_P} \right) k^2 \right].$$  

(48)

Candidates for the saddle point $P_{s,2}$ for this integral are given by the roots of

$$2\frac{d\omega_P}{dP} - \left( \frac{P^2 + c^2}{2\omega_P} \right) \frac{dP}{\omega_P} k^2 = 0,$$

and hence

$$P_{s,2} = \pm ic \left(1 + \frac{1}{8} \frac{k^2}{\sigma^2} \right)$$

(49)

up to order $k^2$. Since

$$\omega_{P_{s,2}} = \pm ic \left(1 + \frac{k^2}{8\sigma^2} \right) \left(c^2 - \frac{k^2}{4} \right)^{1/2} = \pm ic + O(k^4),$$

we see the exponent in (48) behaves as

$$-i \left( 2\omega_P + \frac{P^2 + c^2}{2\omega_P} k^2 \right) \tau = \pm 2 \left( c^2 + 2\left(P - P_{s,2}\right)^2 \right) \tau$$

in a neighborhood of $P_{s,2}$. Therefore, we choose the saddle point $P_{s,2} = -ic \left(1 + \frac{k^2}{8\sigma^2} \right)$ to let the path of integration (48) pass, obtaining

$$F^{(s)}(k, \tau) \sim \frac{1}{2} k \left( \frac{\pi}{\tau} \right) f(\omega_{P_{s,1}})^2 e^{-2c^2\tau},$$

(50)

which implies a simple damping without any diffusive character.

3. Integration over $\lambda$

It remains to integrate (47) and (54) over $\lambda$. We may consider only the part,

$$f(\omega_P)^2 \int_0^1 e^{-2ic^2\beta\lambda} d\lambda = -\frac{1}{2\beta c^2} \cot \frac{\beta c^2}{2}.$$  

(51)

Thus, summarizing

$$\langle j_0(\mathbf{x}, t) \rangle^{(s)} = -\frac{1}{2(2\pi)^6} \frac{1}{\beta c^2} \cot \frac{\beta c^2}{2}$$

$$\times \left( \frac{\pi}{\tau} \right)^{3/2} e^{-2c^2\tau} \int \left( e^{-k^2t} - \sqrt{\pi k^2 t} \right) \beta_4(k) d^3k.$$  

(52)

Two remarks are in order. (1) $e^{-k^2t}$ leads to a diffusion. This does not contradict the basic reversibility of our model. If we reversed the time to look at the evolution towards the past, $t < 0$, then we must take the path of integration crossing the other saddle point as given by (48) with the upper sign, obtaining the diffusion towards the past. Our result is time symmetric in this sense, yet exhibiting the irreversible features. The same circumstance (but no damping) was found in our previous approach (4) with the thermo field dynamics using a more realistic model.

(2) The simple damping implied by (47) should call for an interpretation if it could be taken as an irreversible behavior. Its amplitude has a factor $k\sqrt{t}$ extra to (47), $k$ being small but $t$ large. The damping might be an artifact due to our model Hamiltonian not conserving the particle number.

B. Evaluation of the integral (31)

Since

$$h(P, P) = \omega_P, \quad \cosh[2\theta_P] = \frac{P^2 + c^2}{\omega_P},$$

$$\omega_{P+k^2/2} - \omega_{P+k/2} = \frac{2P^2 + c^2}{\omega_P} \left(P \cdot k \right)$$

(54)

turns out to be

$$F^{(c, \pm)} = \int_0^{\infty} P^2 dP \left(P^2 + c^2 \right) f(\omega_P) \left\{ f(\omega_P) + 1 \right\}$$

$$\times \int d\Omega_P \exp \left[ \mp 2ic\left( P^2 + c^2 \right) k^2 \cos \gamma \right].$$

The integration over angles gives the same result $F^{(c)}/2$ for both $F^{(c, \pm)}$.

$$\frac{1}{2} F^{(c)}$$

$$= \pi \int_0^{\infty} P^2 dP \sqrt{P^2 + 2c^2 \omega_P} \left\{ f(\omega_P) + 1 \right\}$$

$$\times \sum_{\pm} \exp \left[ \pm 2ic\sqrt{P^2 + 2c^2} k^2 \right].$$  

(55)
We use the saddle-point method after analytically continuing the integrand on the complex $P$-plane with two cuts, $[i\sqrt{2}\epsilon, \infty)$ and $(-\infty, -i\sqrt{2}\epsilon]$ as before. The saddle points are determined from the exponent by
\[
\frac{d}{dP} \left( \frac{P^2 + c^2}{(P^2 + 2c^2)^{3/2}} \right) = 0 \tag{56}
\]
as $P_s = \pm i\sqrt{3}\epsilon + \epsilon$, two twins, each of which, being separated by one of the cuts, consists of the right and the left cut with an infinitesimal $\epsilon = +0$ and $\epsilon = -0$, respectively. The other root $P = 0$ of the saddle point equation (59) is discarded because the prefactor vanishes there. In the neighborhood of the saddle points $P_s$, the exponent behaves like
\[
\frac{P^2 + c^2}{(P^2 + 2c^2)^{3/2}} \bigg|_{P = \pm i\sqrt{3}\epsilon + \epsilon} = \frac{3c^4}{(P^2 + 2c^2)^{3/2}} \bigg|_{P = \pm i\sqrt{3}\epsilon + \epsilon} (P - P_s)^2
\]
times $\pm 2ik\tau$. We note
\[
(P^2 + 2c^2)^{1/2} \bigg|_{P = \pm i\sqrt{3}\epsilon + \epsilon} = \begin{cases} 
\pm ic & (\epsilon = +0) \\
\mp ic & (\epsilon = -0).
\end{cases}
\]
Let us try the right members of the two twins, $P_{s+} = \pm i\sqrt{3}\epsilon + 0$. Then,
\[
\pm 2ik\tau \frac{P^2 + c^2}{(P^2 + 2c^2)^{1/2}} = \mp 4ck\tau \frac{6c}{c} (P - P_s)^2, \tag{57}
\]
which requires that the path of integration be deformed along the imaginary axis and the quadrant of a large circle to come back to the real axis. But, on the circle, the exponential behaves like
\[
\exp \left[ \pm 2ik\tau \frac{P^2 + c^2}{(P^2 + 2c^2)^{1/2}} \right] \sim \exp [\mp 2k\tau R \sin \phi] \tag{58}
\]
($P := Re^{i\phi}$ requiring that $0 \leq \phi \leq \pi/2$ for $t > 0$). We remark that \(|f(\omega_p)\{f(\omega_p) + 1\}|\) behaves on the circle as $e^{-R^2 \cos 2\phi}$, not decreasing as $R \rightarrow \infty$ when $\phi = \pm \pi/4$, while helping suppress (58) when $\phi = 0, \pi$.

Thus, we take the path of integration passing the saddle $[\beta, i\epsilon + 0]$, \{iy : y runs from 0 to $\pm R\} \cup \{Re^{i\phi} : \phi \text{ runs from } \pm \pi/2 \text{ to } 0\}$, with $R \rightarrow \infty$, obtaining the same results for the two terms $\pm$ in (55):
\[
F(c) = -\sqrt{\frac{3}{2}} e^{\frac{7}{2}} \left( \frac{\pi}{k\epsilon} \right)^{3/2} f(\omega_p) \{f(\omega_p) + 1\} e^{-4ck\tau}. \tag{59}
\]

We remark that the double poles $P = \pm i\sqrt{2}c$ due to \(f(\omega_p)\{f(\omega_p) + 1\}$ have the residues killed by the exponential.

In (59), $\lambda$ appears only in $e^{-4ck(\pm i\lambda \beta)}$ and may be neglected because of the small factor $c$. Then,
\[
\langle j_0(x, t) \rangle(t) = \frac{1}{2(2\pi)^6} \int_0^\infty \frac{e^{\frac{7}{2}}}{\sin^2 \sqrt{\frac{3}{2}c^2}} \left( \frac{\pi}{k\epsilon} \right)^{3/2} 4\pi^{5/2} \sin \phi(|x|, t) d|k|
\]
\[
= \sqrt{\pi} \delta(|x|, t) \left( |x| = \frac{1}{2} \tan^{-1} \frac{|x|}{4\epsilon t} \right), \tag{60}
\]
which is to be added on (52).

Note that this result implies a kind of slow oscillatory diffusion as illustrated by
\[
\left( \frac{\pi}{k\epsilon} \right)^{3/2} \int e^{4ckx - 4ckt} d^3k = \sqrt{\pi} \delta(|x|, t) \sin \phi(|x|, t) \{x^2 + (4\epsilon t)^2\}^{1/4}, \tag{61}
\]
where the sin of
\[
\phi(|x|, t) := \frac{1}{2} \tan^{-1} \frac{|x|}{4\epsilon t}
\]
is responsible for the oscillation mentioned.

Thus, we have seen that an irreversible behaviour can arise from the Hamiltonian dynamics with the initial condition having the temperature inhomogeneity represented by the density matrix (20) and with the model Hamiltonian (22) which is time-reversal invariant.

### V. Discussion

In this paper, we have first pointed out that the thermo field dynamics reveals a nonlocal structure hidden behind the local-equilibrium density matrix with temperature inhomogeneity in the standard statistical mechanics. We have then shown with a simple model that, in a system of interacting particles, diffusive behaviour can arise from the Hamiltonian dynamics with an initial condition having temperature varying slowly in space even when the Hamiltonian is time-reversal invariant. The diffusive behaviour is seen when we look at the system in macroscopic scales both in time and space. The macroscopic scale is incorporated in our calculation by expansion in powers of the wave numbers, and the macroscopic time scale by applying the saddle point method to the integration over angular frequency.

It has to be remarked, however, that the diffusive behaviour (22) we have obtained has in $x$-space the form
\[
\int t^{-3/2} e^{-m(x-y)^2/(4\epsilon t)} f(y) d^3y, \tag{62}
\]
multiplied by a damping factor $e^{-2mc^2t/\hbar}$, if written fully with the particle mass $m$, the strength of the interaction $c$ and $\hbar$ restored.

The damping just mentioned and the slow oscillatory diffusion we saw in (61) are interesting new features. The latter may be a sound wave associated with the diffusion,
which could have been smeared out to become invisible in macroscopic treatments, while the former could probably be an artifact due to our model Hamiltonian not conserving the particle number.

We notice further that the diffusion constant in (62) is independent of the strength $c$ of the interaction against our expectation. This is a result of using expansions of different quantities in powers of the wave number $k$ and that, as is seen in (45), for example, many of the expansion coefficients have the interaction strength $c$ in their denominators, limiting the validity of our results, say (62), to $k < c$ or $|x - x'| > 1/c$. Therefore, we cannot let $c \to 0$ without losing the space region of validity of our results. If $c$ was 0, in fact, we would lose the diffusive behaviour because $\theta_0$ should vanish and consequently $F(s, \pm \xi) = 0$ in (39) and (40).

After seeing all these features, we stress once again that we have shown by a simple example that the Hamiltonian dynamics with an initial condition having temperature inhomogeneity can lead to an irreversible behaviour even when the Hamiltonian is time-reversal invariant. This is a fact we have established mathematically, though our model and some of its consequences are not quite physical.

The irreversibility so derived stands against Zubarev’s assertion quoted at the end of Sec. III, but not entirely against his arguments because he argues simply that the results from Hamiltonian dynamics with a time-reversible Hamiltonian should be time-reversal symmetric. Our result is in fact symmetric under time reversal $t \to - t$ as remarked earlier. It is of course not symmetric under time reversal with respect to any instant of time other than $t = 0$. The instant $t = 0$ is special because the initial condition, which itself is time-symmetric, is given at this instant of time.

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