N-body Microscopic Heat Current Expression

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Suppose the Hamiltonian of a collection of particles is written as

$$\mathcal{H} = \sum_i K_i + \sum_{i<j} V_2(\mathbf{r}_i, \mathbf{r}_j) + \sum_{i<j<k} V_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + .. + \sum_{i_1<i_2<..<i_n} V_n(\mathbf{r}_{i_1}, \mathbf{r}_{i_2}, .., \mathbf{r}_{i_n}) + .., \tag{1}$$

where K_i is the kinetic energy of each particle:

$$K_i = \frac{1}{2} m_i |\mathbf{v}_i|^2, \tag{2}$$

and the n-body potential $V_n(\mathbf{r}_{i_1}, \mathbf{r}_{i_2}, .., \mathbf{r}_{i_n})$ is invariant with respect to any permutation of particles,

$$\mathbf{r}_{i_\alpha} \rightleftharpoons \mathbf{r}_{i_\beta}, \quad 1 \leq \alpha, \beta \leq n, \tag{3}$$

i.e., the functional form puts no extra emphasis on any specific particle, then the division of $\mathcal{H}$

$$\mathcal{H} = \sum_i E_i \tag{4}$$

into "single particle energies" E_i is intuitively clear:

$$E_i = K_i + \sum_{pairs} V_2(\mathbf{r}_i, \mathbf{r}_j)/2 + \sum_{triplets} V_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k)/3 + .. + \sum_{n-lets} V_n(\mathbf{r}_i, \mathbf{r}_{i_2}, .., \mathbf{r}_{i_n})/n + .. \tag{5}$$

where "pairs", "triplets" etc. refer to all interactions that this ith particle participates in, and it is reasonable to say that it "owns" $1/n$ of all the V_n interactions that it took parts in.

The net heat current of the system, $\mathbf{J}$, is defined as

$$\begin{aligned}\mathbf{J} = & \quad \frac{d}{dt}\left(\sum_i E_i \mathbf{r}_i\right) \\ = & \quad \sum_i E_i \mathbf{v}_i + \dot{E}_i \mathbf{r}_i \\ = & \quad \sum_i E_i \mathbf{v}_i + \tilde{\mathbf{J}}. \end{aligned} \tag{6}$$

It is easy to show that $\tilde{\mathbf{J}}$ is *linearly superpositionable*, in the sense that the influence of any n-let interaction (via V_n) *directly adds* onto $\tilde{\mathbf{J}}$,

$$\tilde{\mathbf{J}} = \sum_{i<j} \tilde{\mathbf{J}}^2_{ij} + \sum_{i<j<k} \tilde{\mathbf{J}}^3_{ijk} + .. + \sum_{i_1<i_2<..<i_n} \tilde{\mathbf{J}}^n_{i_1 i_2 .. i_n} + .. \tag{7}$$

which is true even if V_n does not have permutation symmetry. One underlying reason is that

$$\dot{K}_i = \mathbf{F}_i \cdot \mathbf{v}_i, \tag{8}$$

but $\mathbf{F}_i$ is the linear sum of all interactions,

$$\mathbf{F}_i = \sum_{pairs} \mathbf{F}^i_{ij} + \sum_{triplets} \mathbf{F}^i_{ijk} + .. + \sum_{n-lets} F^i_{ii_2 i_2 i_n} + .. \tag{9}$$

in which, for instance, $\mathbf{F}^i_{ijk}$ is the force contribution of any ijk-triplet interaction to particle i.

So now we can focus on a specific n-let interaction, and simply add everything together in the end onto $\tilde{\mathbf{J}}$. Let me denote the particles involved $\mathbf{r}_1, \mathbf{r}_2, .., \mathbf{r}_n$, and the part that this n-let interaction contributes to by Δ. Because of Eqn. (5), $\Delta\dot{E}_i$ contains two parts: a kinetic energy part and a potential energy part. With $\Delta\dot{K}_i = \Delta\mathbf{F}_i \cdot \mathbf{v}_i$ and

$$\Delta V = \Delta V(\mathbf{r}_1, \mathbf{r}_2, .., \mathbf{r}_n), \tag{10}$$

there is

$$\Delta\left(\frac{\dot{V}}{n}\right) = \quad \frac{1}{n}\sum_{j=1}^{n} \frac{\partial \Delta V}{\partial \mathbf{r}_j} \cdot \mathbf{v}_j$$

$$= \quad -\frac{1}{n}\sum_{j=1}^{n} \Delta\mathbf{F}_j \cdot \mathbf{v}_j, \tag{11}$$

as by definition,

$$\Delta\mathbf{F}_j = -\frac{\partial \Delta V}{\partial \mathbf{r}_j}. \tag{12}$$

So, there is

$$\begin{aligned}
\Delta\tilde{\mathbf{J}} &= \sum_{i=1}^{n} (\Delta\dot{E}_i)\mathbf{r}_i \\
&= \sum_{i=1}^{n} \left(\Delta\mathbf{F}_i \cdot \mathbf{v}_i - \frac{1}{n}\sum_{j=1}^{n} \mathbf{F}_j \cdot \mathbf{v}_j \right) \mathbf{r}_i.
\end{aligned} \tag{13}$$

One can see from Eqn. (13) that $\Delta\tilde{\mathbf{J}}$ depends only on the relative separations of $\mathbf{r}_1, \mathbf{r}_2, .., \mathbf{r}_n$ and not on the origin of the coordinate frame, i.e., it is *frame-independent*, because for any uniform shift: $\mathbf{r}_i \to \mathbf{r}_i + \mathbf{a}$, where $\mathbf{a}$ is a constant,

$$\begin{aligned}
\Delta(\Delta\tilde{\mathbf{J}}) &= \sum_{i=1}^{n} \left(\Delta\mathbf{F}_i \cdot \mathbf{v}_i - \frac{1}{n}\sum_{j=1}^{n} \mathbf{F}_j \cdot \mathbf{v}_j \right) \mathbf{a} \\
&= \left(\sum_{i=1}^{n} \Delta\mathbf{F}_i \cdot \mathbf{v}_i - \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{n} \Delta\mathbf{F}_j \cdot \mathbf{v}_j \right) \mathbf{a} \\
&= 0.
\end{aligned} \tag{14}$$

Thus, in evaluating Eqn. (13), we are free to pick any coordinate origin that we like.

One further simplification is

$$\sum_{i=1}^{n} (\Delta\mathbf{F}_i) = 0, \tag{15}$$

which can be derived from the translational invariance of V_n.

- **Two-body interaction:**

For any particle pair $(i,\, j)$ that falls into the interaction range,

$$\Delta V = V_2(\mathbf{r}_i, \mathbf{r}_j), \tag{16}$$

and there is

$$\Delta\mathbf{F}_i = -\Delta\mathbf{F}_j. \tag{17}$$

Because I am free to choose any coordinate frame origin, I can let $\mathbf{r}_i = 0$, and so only one term in Eqn. (13) (the $n = j$ term) contributes,

$$\begin{aligned} \Delta\tilde{\mathbf{J}}_2 = & \left(\Delta\mathbf{F}_j \cdot \mathbf{v}_j - \frac{1}{2}(\Delta\mathbf{F}_i \cdot \mathbf{v}_i + \Delta\mathbf{F}_j \cdot \mathbf{v}_j)\right)\mathbf{r}_j \\ = & \frac{1}{2}\left(\Delta\mathbf{F}_j \cdot (\mathbf{v}_j + \mathbf{v}_i)\right)\mathbf{r}_j, \end{aligned} \tag{18}$$

where we have made use of Eqn. (17). If one remembers that the present frame origin is on particle i, the expression must be

$$\Delta\tilde{\mathbf{J}} = \frac{1}{2}\left(\Delta\mathbf{F}_j \cdot (\mathbf{v}_j + \mathbf{v}_i)\right)(\mathbf{r}_j - \mathbf{r}_i) \tag{19}$$

in other frames.

- **Three-body interaction:**

Now,

$$\Delta V = V_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k), \tag{20}$$

and

$$\Delta\mathbf{F}_i = -\Delta\mathbf{F}_j - \Delta\mathbf{F}_k. \tag{21}$$

I still can choose $\mathbf{r}_i = 0$, then

$$\begin{aligned} & \Delta\tilde{\mathbf{J}}_3 \\ = & \left(\Delta\mathbf{F}_j \cdot \mathbf{v}_j - \frac{1}{3}(\Delta\mathbf{F}_i \cdot \mathbf{v}_i + \Delta\mathbf{F}_j \cdot \mathbf{v}_j + \Delta\mathbf{F}_k \cdot \mathbf{v}_k)\right)\mathbf{r}_{ji} + \\ & \left(\Delta\mathbf{F}_k \cdot \mathbf{v}_k - \frac{1}{3}(\Delta\mathbf{F}_i \cdot \mathbf{v}_i + \Delta\mathbf{F}_j \cdot \mathbf{v}_j + \Delta\mathbf{F}_k \cdot \mathbf{v}_k)\right)\mathbf{r}_{ki} \\ = & \frac{1}{3}\left\{\left(\Delta\mathbf{F}_j \cdot (2\mathbf{v}_j + \mathbf{v}_i) + \Delta\mathbf{F}_k \cdot (\mathbf{v}_i - \mathbf{v}_k)\right)\mathbf{r}_{ji} + \left(\Delta\mathbf{F}_k \cdot (2\mathbf{v}_k + \mathbf{v}_i) + \Delta\mathbf{F}_j \cdot (\mathbf{v}_i - \mathbf{v}_j)\right)\mathbf{r}_{ki}\right\}, \end{aligned} \tag{22}$$

where

$$\mathbf{r}_{ji} = \mathbf{r}_j - \mathbf{r}_i, \quad \mathbf{r}_{ki} = \mathbf{r}_k - \mathbf{r}_i. \tag{23}$$