При трансформацији старих $(Q_1, Q_2, \ldots, Q_n)$ у нове $(q_1, q_2, \ldots, q_n)$ координате, важи:

$$\frac{\partial}{\partial Q_k} = \sum_{i=1}^{n} \frac{\partial q_i}{\partial Q_k} \frac{\partial}{\partial q_i}, \quad \left(\text{или, идентично}: \frac{\partial}{\partial Q_l} = \sum_{j=1}^{n} \frac{\partial q_j}{\partial Q_l} \frac{\partial}{\partial q_j} \right)$$

Следи,

$$\frac{\partial^2}{\partial Q_k \partial Q_l} = \frac{\partial}{\partial Q_k} \frac{\partial}{\partial Q_l} = \sum_{i=1}^{n} \frac{\partial q_i}{\partial Q_k} \frac{\partial}{\partial q_i} \sum_{j=1}^{n} \frac{\partial q_j}{\partial Q_l} \frac{\partial}{\partial q_j} = \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial q_i}{\partial Q_k} \frac{\partial}{\partial q_i} \left(\frac{\partial q_j}{\partial Q_l} \frac{\partial}{\partial q_j} \right) =$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial q_i}{\partial Q_k} \frac{\partial q_j}{\partial Q_l} \frac{\partial}{\partial q_i} \left(\frac{\partial}{\partial q_j} \right) + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial q_i}{\partial Q_k} \frac{\partial}{\partial q_i} \left(\frac{\partial q_j}{\partial Q_l} \right) \frac{\partial}{\partial q_j} =$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial q_i}{\partial Q_k} \frac{\partial q_j}{\partial Q_l} \frac{\partial^2}{\partial q_i \partial q_j} + \sum_{j=1}^{n} \left(\sum_{i=1}^{n} \frac{\partial q_i}{\partial Q_k} \frac{\partial}{\partial q_i} \right) \left(\frac{\partial q_j}{\partial Q_l} \right) \frac{\partial}{\partial q_j} =$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial q_i}{\partial Q_k} \frac{\partial q_j}{\partial Q_l} \frac{\partial^2}{\partial q_i \partial q_j} + \sum_{j=1}^{n} \frac{\partial}{\partial Q_k} \left(\frac{\partial q_j}{\partial Q_l} \right) \frac{\partial}{\partial q_j} = \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial q_i}{\partial Q_k} \frac{\partial q_j}{\partial Q_l} \frac{\partial^2}{\partial q_i \partial q_j} + \sum_{j=1}^{n} \left(\frac{\partial^2 q_j}{\partial Q_k \partial Q_l} \right) \frac{\partial}{\partial q_j}$$

У једнострукој суми је свеједно како обележавамо индекс по коме сумирамо (i или j), па коначно имамо:

$$\boxed{\frac{\partial^2}{\partial Q_k \partial Q_l} = \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial q_i}{\partial Q_k} \frac{\partial q_j}{\partial Q_l} \frac{\partial^2}{\partial q_i \partial q_j} + \sum_{i=1}^{n} \left(\frac{\partial^2 q_i}{\partial Q_k \partial Q_l} \right) \frac{\partial}{\partial q_i}}$$

Када је $k = l$ претходна формула се своди на

$$\boxed{\frac{\partial^2}{\partial Q_k^2} = \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{\partial q_i}{\partial Q_k} \frac{\partial q_j}{\partial Q_k} \frac{\partial^2}{\partial q_i \partial q_j} + \sum_{i=1}^{n} \left(\frac{\partial^2 q_i}{\partial Q_k^2} \right) \frac{\partial}{\partial q_i}}$$

Подсетимо се елементарних релација:

Дефиниција Кронекеровог симбола: $\delta_{ij} = \begin{Bmatrix} 0, & i \neq j \\ 1, & i = j \end{Bmatrix}$.

$$\sum_{i=1}^{n} \delta_{ik} a_i = \cancel{\delta_{1k}} a_1 + \cancel{\delta_{2k}} a_2 + \ldots + \cancel{\delta_{k-1,k}} a_{k-1} + \delta_{kk} a_k + \cancel{\delta_{k+1,k}} a_{k+1} + \ldots + \cancel{\delta_{n-1,k}} a_{n-1} + \cancel{\delta_{nk}} a_n = a_k$$

$$\sum_{i=1}^{n} 1 = \left(= \sum_{i=1}^{n} (1 + 0 \cdot i) = (1 + 0 \cdot 1) + (1 + 0 \cdot 2) + \ldots + (1 + 0 \cdot n) \right) = \underbrace{(1 + 1 + \ldots 1)}_{n \text{ пута}} = n$$

$$\sum_{i=1}^{N+1} \sum_{j=1}^{N+1} a_i b_j = \sum_{i=1}^{N+1} a_i \sum_{j=1}^{N+1} b_j = \sum_{i=1}^{N+1} a_i \left(b_{N+1} + \sum_{j=1}^{N} b_j \right) = \left(a_{N+1} + \sum_{i=1}^{N} a_i \right) \left(b_{N+1} + \sum_{j=1}^{N} b_j \right) =$$

$$= a_{N+1} b_{N+1} + a_{N+1} \sum_{j=1}^{N} b_j + b_{N+1} \sum_{i=1}^{N} a_i + \sum_{i=1}^{N} a_i \sum_{j=1}^{N} b_j = \sum_{i=1}^{N} \sum_{j=1}^{N} a_i b_j + \sum_{i=1}^{N} \left(b_{N+1} a_i + a_{N+1} b_i \right) + a_{N+1} b_{N+1}$$

$$\sum_{i=1}^{n} \sum_{j \neq i}^{n} a_i a_j = 2 \sum_{i=1}^{n} \sum_{j > i}^{n} a_i a_j$$

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j = \sum_{i=1}^{n} \sum_{j \neq i}^{n} a_i a_j + \sum_{i=1}^{n} a_i^2 = 2 \sum_{i=1}^{n} \sum_{j > i}^{n} a_i a_j + \sum_{i=1}^{n} a_i^2$$

{нпр. за $n = 3$ суме из претходна два израза добијају облик:

$$\sum_{i=1}^{n} \sum_{j \neq i}^{n} a_i a_j = \sum_{i=1}^{n} a_i \sum_{j \neq i}^{n} a_j = a_1 \sum_{j \neq i}^{n} a_j + a_2 \sum_{j \neq i}^{n} a_j + a_3 \sum_{j \neq i}^{n} a_j = a_1 (a_2 + a_3) + a_2 (a_1 + a_3) + a_3 (a_1 + a_2),$$

$$\sum_{i=1}^{n} \sum_{j > i}^{n} a_i a_j = \sum_{i=1}^{n} a_i \sum_{j > i}^{n} a_j = a_1 \sum_{j > i}^{n} a_j + a_2 \sum_{j > i}^{n} a_j + a_3 \cancel{\sum_{j > i}^{n} a_j} = a_1 (a_2 + a_3) + a_2 (a_3) + 0,$$

$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_i a_j = \sum_{i=1}^{n} a_i \sum_{j=1}^{n} a_j = a_1 \sum_{j=1}^{n} a_j + a_2 \sum_{j=1}^{n} a_j + a_3 \sum_{j=1}^{n} a_j = (a_1 + a_2 + a_3)(a_1 + a_2 + a_3),$$

$$\sum_{i=1}^{n} a_i^2 = a_1^2 + a_2^2 + a_3^2 .\}$$

Нека је дата трансформација (M је маса језгра, m маса једног електрона, а N је број електрона):

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \\ X \end{pmatrix} \rightarrow \begin{pmatrix} x_{1r} \\ x_{2r} \\ \vdots \\ x_{Nr} \\ x_0 \end{pmatrix} \quad \text{таква да важи:} \quad \begin{pmatrix} x_{1r} = x_1 - X \\ x_{2r} = x_2 - X \\ \vdots \\ x_{Nr} = x_N - X \\ x_0 (\equiv x_{N+1,r}) = \dfrac{MX + m(x_1 + x_2 + \ldots + x_N)}{M + Nm} \end{pmatrix}$$

(y, z трансформације су потпуно аналогне па их не наводимо). Приметимо да је укупан број старих координата једнак $3(N+1)$, и да је он једнак броју нових координата. Очигледно, $x_k - x_l = x_{kr} + X - (x_{lr} + X) = x_{kr} - x_{lr}$ а уочимо да важи и:

$\dfrac{\partial x_{1r}}{\partial X} = \dfrac{\partial x_{2r}}{\partial X} = \ldots = \dfrac{\partial x_{Nr}}{\partial X} = -1$, или краће $\boxed{\dfrac{\partial x_{ir}}{\partial X} = -1}$, $(i = 1, N)$. Следи да је $\boxed{\dfrac{\partial^2 x_{ir}}{\partial X^2} = 0}$, $(i = 1, N)$. Такође, $\boxed{\dfrac{\partial x_0}{\partial X} = \dfrac{M}{M + Nm}}$ као и $\boxed{\dfrac{\partial^2 x_0}{\partial X^2} = 0}$. Слично, $\boxed{\dfrac{\partial x_{ir}}{\partial x_k} = \delta_{ik}}$, $\boxed{\dfrac{\partial^2 x_{ir}}{\partial x_k^2} = 0}$, $(i = 1, N)$. На крају, $\boxed{\dfrac{\partial x_0}{\partial x_k} = \dfrac{m}{M + Nm}}$, $\boxed{\dfrac{\partial^2 x_0}{\partial x_k^2} = 0}$.

Изразимо сада оператор $\dfrac{\partial^2}{\partial X^2}$ преко нових координата. Применом формуле, имамо:

$$\frac{\partial^2}{\partial X^2} = \sum_{i=1}^{N+1} \sum_{j=1}^{N+1} \frac{\partial x_{ir}}{\partial X} \frac{\partial x_{jr}}{\partial X} \frac{\partial^2}{\partial x_{ir} \partial x_{jr}} + \cancel{\sum_{i=1}^{N+1} \left(\frac{\partial^2 x_{ir}}{\partial X^2} \right) \frac{\partial}{\partial x_{ir}}} = \sum_{i=1}^{N+1} \sum_{j=1}^{N+1} \frac{\partial x_{ir}}{\partial X} \frac{\partial x_{jr}}{\partial X} \frac{\partial}{\partial x_{ir}} \frac{\partial}{\partial x_{jr}} =$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{\partial x_{ir}}{\partial X} \frac{\partial x_{jr}}{\partial X} \frac{\partial^2}{\partial x_{ir} \partial x_{jr}} + \sum_{i=1}^{N} \left[\frac{\partial x_0}{\partial X} \frac{\partial}{\partial x_0} \left(\frac{\partial x_{ir}}{\partial X} \frac{\partial}{\partial x_{ir}} \right) + \frac{\partial x_0}{\partial X} \frac{\partial}{\partial x_0} \left(\frac{\partial x_{ir}}{\partial X} \frac{\partial}{\partial x_{ir}} \right) \right] + \frac{\partial x_0}{\partial X} \frac{\partial}{\partial x_0} \frac{\partial x_0}{\partial X} \frac{\partial}{\partial x_0} =$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} (-1)(-1) \frac{\partial^2}{\partial x_{ir} \partial x_{jr}} + 2 \sum_{i=1}^{N} \frac{\partial x_0}{\partial X} \frac{\partial}{\partial x_0} \left(\frac{\partial x_{ir}}{\partial X} \frac{\partial}{\partial x_{ir}} \right) + \left(\frac{M}{M + Nm} \right)^2 \frac{\partial^2}{\partial x_0^2} =$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{\partial^2}{\partial x_{ir} \partial x_{jr}} + 2 \sum_{i=1}^{N} \left(\frac{M}{M + Nm} \right) \frac{\partial}{\partial x_0} \left((-1) \frac{\partial}{\partial x_{ir}} \right) + \left(\frac{M}{M + Nm} \right)^2 \frac{\partial^2}{\partial x_0^2} =$$

$$\boxed{\frac{\partial^2}{\partial X^2} = \sum_{i=1}^{N} \sum_{j=1}^{N} \frac{\partial^2}{\partial x_{ir} \partial x_{jr}} - 2 \left(\frac{M}{M + Nm} \right) \sum_{i=1}^{N} \frac{\partial^2}{\partial x_0 \partial x_{ir}} + \left(\frac{M}{M + Nm} \right)^2 \frac{\partial^2}{\partial x_0^2}}.$$

Слично,

$$\frac{\partial^2}{\partial x_k^2}=\sum_{i=1}^{N+1}\sum_{j=1}^{N+1}\frac{\partial x_{ir}}{\partial x_k}\frac{\partial x_{jr}}{\partial x_k}\frac{\partial^2}{\partial x_{ir}\partial x_{jr}}+\cancel{\sum_{i=1}^{N+1}\left(\frac{\partial^2 x_{ir}}{\partial x_k^2}\right)\frac{\partial}{\partial x_{ir}}}=$$

$$=\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial x_{ir}}{\partial x_k}\frac{\partial x_{jr}}{\partial x_k}\frac{\partial^2}{\partial x_{ir}\partial x_{jr}}+\sum_{i=1}^{N}\left[\frac{\partial x_0}{\partial x_k}\frac{\partial}{\partial x_0}\left(\frac{\partial x_{ir}}{\partial x_k}\frac{\partial}{\partial x_{ir}}\right)+\frac{\partial x_0}{\partial x_k}\frac{\partial}{\partial x_0}\left(\frac{\partial x_{ir}}{\partial x_k}\frac{\partial}{\partial x_{ir}}\right)\right]+\frac{\partial x_0}{\partial x_k}\frac{\partial}{\partial x_0}\frac{\partial x_0}{\partial x_k}\frac{\partial}{\partial x_0}=$$

$$=\sum_{i=1}^{N}\sum_{j=1}^{N}\delta_{ik}\delta_{jk}\frac{\partial^2}{\partial x_{ir}\partial x_{jr}}+2\sum_{i=1}^{N}\left[\frac{m}{M+Nm}\frac{\partial}{\partial x_0}\left(\delta_{ik}\frac{\partial}{\partial x_{ir}}\right)\right]+\left(\frac{m}{M+Nm}\right)^2\frac{\partial^2}{\partial x_0^2}$$

Како је:

$$\sum_{i=1}^{N}\sum_{j=1}^{N}\delta_{ik}\delta_{jk}\frac{\partial^2}{\partial x_{ir}\partial x_{jr}}=\sum_{i=1}^{N}\delta_{ik}\frac{\partial}{\partial x_{ir}}\left(\sum_{j=1}^{N}\delta_{jk}\frac{\partial}{\partial x_{jr}}\right)=\sum_{i=1}^{N}\delta_{ik}\frac{\partial}{\partial x_{ir}}\left(\frac{\partial}{\partial x_{kr}}\right)=\frac{\partial}{\partial x_{kr}}\left(\sum_{i=1}^{N}\delta_{ik}\frac{\partial}{\partial x_{ir}}\right)=$$

$$=\frac{\partial}{\partial x_{kr}}\left(\sum_{i=1}^{N}\delta_{ik}\frac{\partial}{\partial x_{ir}}\right)=\frac{\partial}{\partial x_{kr}}\left(\frac{\partial}{\partial x_{kr}}\right)=\frac{\partial^2}{\partial x_{kr}^2},$$

као и:

$$2\sum_{i=1}^{N}\left[\frac{m}{M+Nm}\frac{\partial}{\partial x_0}\left(\delta_{ik}\frac{\partial}{\partial x_{ir}}\right)\right]=2\frac{m}{M+Nm}\frac{\partial}{\partial x_0}\sum_{i=1}^{N}\left(\delta_{ik}\frac{\partial}{\partial x_{ir}}\right)=2\frac{m}{M+Nm}\frac{\partial}{\partial x_0}\frac{\partial}{\partial x_{kr}},$$

закључујемо да важи:

$$\boxed{\frac{\partial^2}{\partial x_k^2}=\frac{\partial^2}{\partial x_{kr}^2}+\frac{2m}{M+Nm}\frac{\partial^2}{\partial x_{kr}\partial x_0}+\left(\frac{m}{M+Nm}\right)^2\frac{\partial^2}{\partial x_0^2}}$$

Користећи добијене изразе, целисходно је спровести и следећу трансформацију:

$$-\frac{1}{2M}\frac{\partial^2}{\partial X^2}-\frac{1}{2m}\sum_{k=1}^{N}\frac{\partial^2}{\partial x_k^2}=-\frac{1}{2M}\left[\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial^2}{\partial x_{ir}\partial x_{jr}}-2\left(\frac{M}{M+Nm}\right)\sum_{i=1}^{N}\frac{\partial^2}{\partial x_{ir}\partial x_0}+\left(\frac{M}{M+Nm}\right)^2\frac{\partial^2}{\partial x_0^2}\right]$$
$$-\frac{1}{2m}\sum_{k=1}^{N}\left[\frac{\partial^2}{\partial x_{kr}^2}+\frac{2m}{M+Nm}\frac{\partial^2}{\partial x_{kr}\partial x_0}+\left(\frac{m}{M+Nm}\right)^2\frac{\partial^2}{\partial x_0^2}\right]=$$

$$=-\frac{1}{2M}\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial^2}{\partial x_{ir}\partial x_{jr}}+\left(\frac{1}{M+Nm}\right)\sum_{i=1}^{N}\frac{\partial^2}{\partial x_{ir}\partial x_0}-\frac{1}{2M}\left(\frac{M}{M+Nm}\right)^2\frac{\partial^2}{\partial x_0^2}-\frac{1}{2m}\sum_{k=1}^{N}\frac{\partial^2}{\partial x_{kr}^2}-\frac{1}{M+Nm}\sum_{k=1}^{N}\frac{\partial^2}{\partial x_{kr}\partial x_0}-\frac{1}{2m}\sum_{k=1}^{N}\left(\frac{m}{M+Nm}\right)^2\frac{\partial^2}{\partial x_0^2}=$$

$$=-\frac{1}{2M}\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial^2}{\partial x_{ir}\partial x_{jr}}-\frac{1}{2}\frac{M}{(M+Nm)^2}\frac{\partial^2}{\partial x_0^2}-\frac{1}{2m}\sum_{k=1}^{N}\frac{\partial^2}{\partial x_{kr}^2}-\frac{1}{2m}\left[\left(\frac{m}{M+Nm}\right)^2\frac{\partial^2}{\partial x_0^2}\right]\sum_{k=1}^{N}1=$$

$$=-\frac{1}{2M}\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial^2}{\partial x_{ir}\partial x_{jr}}-\frac{1}{2}\frac{M}{(M+Nm)^2}\frac{\partial^2}{\partial x_0^2}-\frac{1}{2m}\sum_{k=1}^{N}\frac{\partial^2}{\partial x_{kr}^2}-\frac{1}{2}\frac{m}{(M+Nm)^2}\frac{\partial^2}{\partial x_0^2}N$$

Како је $=-\frac{1}{2}\frac{M}{(M+Nm)^2}\frac{\partial^2}{\partial x_0^2}-\frac{1}{2}\frac{m}{(M+Nm)^2}\frac{\partial^2}{\partial x_0^2}N=-\frac{1}{2}\frac{1}{M+Nm}\frac{\partial^2}{\partial x_0^2}$, као и

$$\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial^2}{\partial x_{ir}\partial x_{jr}}=2\sum_{i=1}^{N}\sum_{j>i}^{N}\frac{\partial^2}{\partial x_{ir}\partial x_{jr}}+\sum_{i=1}^{N}\frac{\partial^2}{\partial x_{ir}^2}$$

следи:

$$-\frac{1}{2M}\frac{\partial^2}{\partial X^2}-\frac{1}{2m}\sum_{k=1}^{N}\frac{\partial^2}{\partial x_k^2}=-\frac{1}{2}\frac{1}{M+Nm}\frac{\partial^2}{\partial x_0^2}-\frac{1}{2M}\left(2\sum_{i=1}^{N}\sum_{j>i}^{N}\frac{\partial^2}{\partial x_{ir}\partial x_{jr}}+\sum_{i=1}^{N}\frac{\partial^2}{\partial x_{ir}^2}\right)-\frac{1}{2m}\sum_{k=1}^{N}\frac{\partial^2}{\partial x_{kr}^2}=$$
$$-\frac{1}{2}\frac{1}{M+Nm}\frac{\partial^2}{\partial x_0^2}-\frac{1}{M}\sum_{i=1}^{N}\sum_{j>i}^{N}\frac{\partial^2}{\partial x_{ir}\partial x_{jr}}-\frac{1}{2}\left(\frac{1}{M}+\frac{1}{m}\right)\sum_{k=1}^{N}\frac{\partial^2}{\partial x_{kr}^2}.$$

Коначно:

$$\boxed{-\frac{1}{2M}\frac{\partial^2}{\partial X^2}-\frac{1}{2m}\sum_{k=1}^{N}\frac{\partial^2}{\partial x_k^2}=-\frac{1}{2}\frac{1}{M+Nm}\frac{\partial^2}{\partial x_0^2}-\frac{1}{M}\sum_{k=1}^{N}\sum_{l>k}^{N}\frac{\partial^2}{\partial x_{kr}\partial x_{lr}}-\frac{1}{2}\left(\frac{1}{M}+\frac{1}{m}\right)\sum_{k=1}^{N}\frac{\partial^2}{\partial x_{kr}^2}}$$