

SOTTRATTO IL SOLVENTE

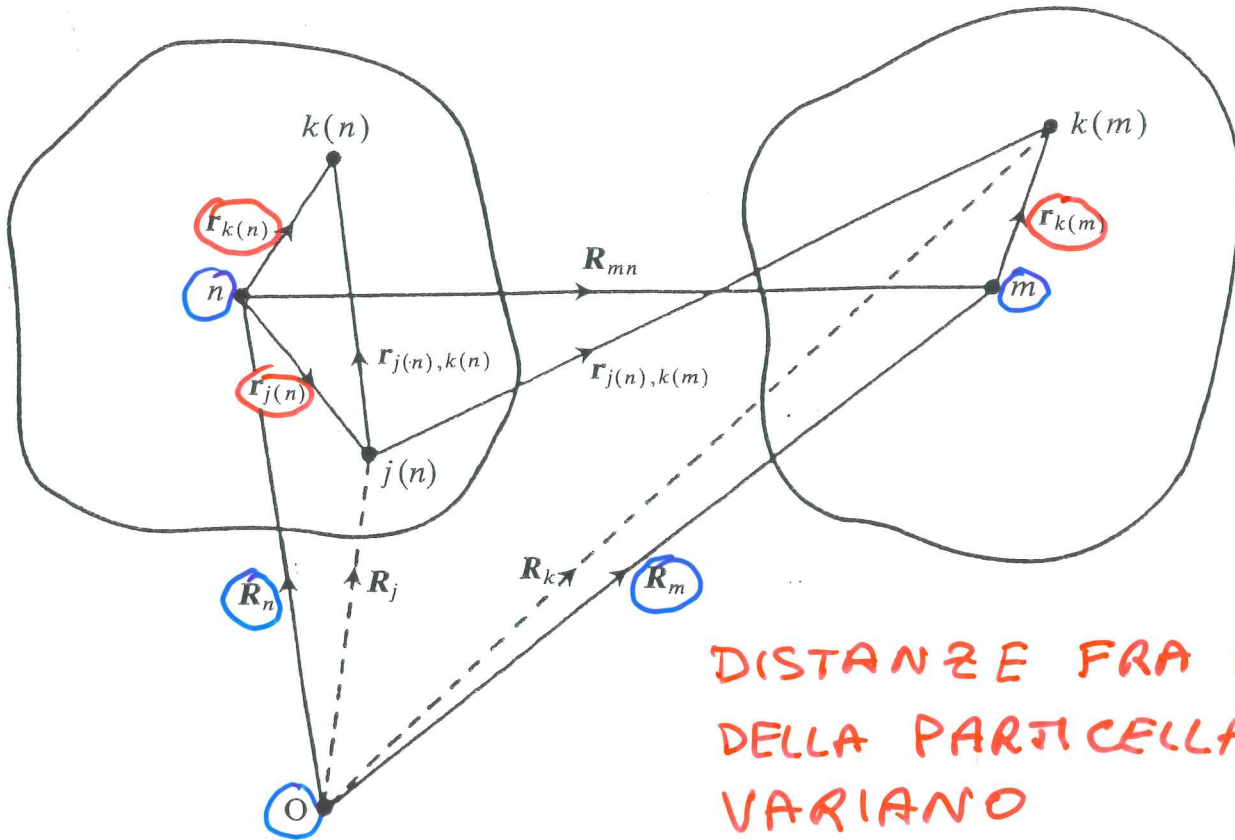


FIG. 14.3.3. Relationships between interparticle and intraparticle vectors used in the text.

\bar{n}, \bar{m} CENTRO DI MASSA (C.D.M.) DELLE DUE PARTICELLE

$\underline{R}_n, \underline{R}_m$ DISTANZA DA O DEL C.D.M. DELLE PARTICELLE

$\underline{R}_{j(n)}, \underline{R}_{k(n)}, \underline{R}_{k(m)}$ DISTANZA DA O DEGLI ATOMI DELLE PARTICELLE

$\underline{r}_{j(n)}, \underline{r}_{k(n)}, \underline{r}_{k(m)}$ DISTANZA DEGLI ATOMI DELLE PARTICELLE DAL C.D.M. DELLA PARTICELLA

CONTRIBUTO DI 2 ATOMI DI UNA PARTICELLA

$$\begin{aligned} \underline{R}_{j(m)} &= \underline{R}_m + \underline{r}_{j(m)} \\ \underline{R}_{k(m)} &= \underline{R}_m + \underline{r}_{k(m)} \end{aligned} \Rightarrow \underline{R}_{j(m)} - \underline{R}_{k(m)} = \underline{r}_{j(m)} - \underline{r}_{k(m)}$$

CONTRIBUTO DI 2 ATOMI DI 2 PARTICELLE

$$\underline{R}_{j(m)} = \underline{R}_m + \underline{r}_{j(m)} ; \underline{R}_{k(m)} = \underline{R}_m + \underline{r}_{k(m)}$$

$$\begin{aligned} \underline{R}_{j(m)} - \underline{R}_{k(m)} &= \underbrace{\underline{R}_m - \underline{R}_m}_{=0} + \underline{r}_{j(m)} - \underline{r}_{k(m)} = \\ &= \underline{R}_{mm} + \underline{r}_{j(m)} - \underline{r}_{k(m)} \end{aligned}$$

INTENSITA' DI SCATTERING

$$I(\underline{Q}) = \left\langle \left| \sum_j b_j e^{i\underline{Q} \cdot \underline{R}_j} \right|^2 \right\rangle$$

$\langle \rangle$ E' LA MEDIA CONFIGURAZIONALE O DI INSIEME, OSSIA LA MEDIA SU TUTTE LE POSSIBILI CONFIGURAZIONI ATOMICHE

$$I(\underline{Q}) = \left\langle \sum_j \sum_k b_j b_k e^{i\underline{Q} \cdot (\underline{R}_j - \underline{R}_k)} \right\rangle$$

$$z = r e^{i\phi} \quad z^* = r e^{-i\phi} ; |z| = z \cdot z^*$$

$$I(\underline{Q}) = \sum_m \left[\sum_{j(m)} \sum_{k(m)} b_{j(m)} b_{k(m)} e^{i\underline{Q} \cdot (\underline{R}_{j(m)} - \underline{R}_{k(m)})} \right] +$$

↑
TERMINE INTRA-PARTICELLA

$$+ \left(\sum_{m \neq m'} \sum_{j(m)} \sum_{k(m')} e^{i\underline{Q} \cdot (\underline{R}_{j(m)} - \underline{R}_{k(m')})} \right)$$

↑
TERMINE INTER-PARTICELLE

LA DIFFERENZA FRA VETTORI POSIZIONE DEGLI ATOMI NELLE DIVERSE PARTICELLE PUO' ESSERE SCRITTA COME DIFFERENZA FRA I CENTRI DELLE DUE PARTICELLE, \underline{R}_{mm} , E DELLE POSIZIONI DEGLI ATOMI, $\underline{r}_{j(m)}$ O $\underline{r}_{k(m')}$, RELATIVE AD OGNI CENTRO

$$\underline{R}_{j(m)} - \underline{R}_{k(m')} = \underline{R}_{mm} + \underline{r}_{k(m')} - \underline{r}_{j(m)}$$

QUINDI

$$I(\underline{Q}) = \sum_m \left[\sum_{j(m)} \sum_{k(m)} b_{j(m)} b_{k(m)} e^{i\underline{Q} \cdot (\underline{r}_{j(m)} - \underline{r}_{k(m)})} \right] +$$

INTRA-PARTICELLA

$$+ \left(\sum_{m \neq m'} e^{i\underline{Q} \cdot \underline{R}_{mm}} \sum_{j(m)} \sum_{k(m')} b_{j(m)} b_{k(m')} e^{i\underline{Q} \cdot (\underline{r}_{j(m)} - \underline{r}_{k(m')})} \right)$$

INTER-PARTICELLE