# teoria delle perturbazioni statiche

*Fulvio Ciriaco*

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# problema

$$H\Psi_n = E_n\Psi_n$$
$$(H + h)(\Psi_n + \psi_n) = (E_n + e_n)(\Psi_n + \psi_n)$$

# approccio

$$
\begin{aligned}
(H + \lambda h)\psi_n(\lambda) &= E_n(\lambda)\psi_n(\lambda) \\
\psi_n(\lambda) &= |n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle ... \\
E(\lambda) &= E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} ...
\end{aligned}
$$

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\end{aligned}
$$

ricostruendo

$$
(H - E_n^{(0)})|n^{(0)} + \lambda n^{(1)} ...\rangle = (\lambda E_n^{(1)} + \lambda^2 E_n^{(2)} ...)|n^{(0)} + \lambda n^{(1)} + ...\rangle
$$

# soluzione

$$(H - E_n^{(0)})|n^{(0)} + \lambda n^{(1)} ...\rangle = (\lambda E_n^{(1)} + \lambda^2 E_n^{(2)} ...)|n^{(0)} + \lambda n^{(1)} + ...\rangle$$

come esprimere $|n^{(k>0)}\rangle$?

# soluzione

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come esprimere $|n^{(k>0)}\rangle$?

$$|n^{(k)}\rangle = \sum_{m \neq n} |m\rangle\langle m|n^{(k)}\rangle$$

# soluzione

$$(H - E_n^{(0)})|n^{(0)} + \lambda n^{(1)} ...\rangle = (\lambda E_n^{(1)} + \lambda^2 E_n^{(2)} ...)|n^{(0)} + \lambda n^{(1)} + ...\rangle$$

come esprimere $|n^{(k>0)}\rangle$?

$$|n^{(k)}\rangle = \sum_{m \neq n} |m\rangle\langle m|n^{(k)}\rangle$$

chiudo con $\langle n^{(0)}|$ per ottenere:

$$0 = \langle n^{(0)}|H - E_n^{(0)}|n^{(0)} + \lambda n^{(1)} ...\rangle = \langle n^{(0)}|\lambda E_n^{(1)} + \lambda^2 E_n^{(2)} ...|n^{(0)} + \lambda n^{(1)} ..$$

$$E_n^{(k)} = \langle n^{(0)}|h|n^{(k-1)}\rangle$$

# soluzione

$$E_n^{(k)} = \langle n^{(0)}|h|n^{(k-1)}$$

al primo ordine:

$$E_n^{(1)} = \langle n^{(0)}|h|n^{(0)}\rangle$$

per ottenere gli ordini superiori bisogna scalare le relazioni $n^{(k)} \to E_n^{(k+1)} \to n^{(k+1)}$.... Per ottenere le relazioni per $n^{(k)}$ dobbiamo chiudere con $\langle k = k^{(0)}|$.

$$\langle k|H - E_n^{(0)}|n^{(1)}\rangle = -\langle k|h|n^{(0)}\rangle$$

$$\langle k|n^{(1)}\rangle = \frac{\langle k|h|n^{(0)}\rangle}{E_n^{(0)} - E_k^{(0)}} \implies$$

$$|n^{(1)}\rangle = \sum_k |k\rangle \frac{\langle k|h|n\rangle}{E_n^{(0)} - E_k^{(0)}}$$

# soluzione

$$|n^{(1)}\rangle = \sum_k \frac{\langle k|h|n\rangle}{E_n^{(0)} - E_k^{(0)}}$$

$$E_n^{(2)} = \langle n^{(0)}|h|n^{(1)}\rangle = \sum_k \frac{\langle k|h|n\rangle\langle n|h|k\rangle}{E_n^{(0)} - E_k^{(0)}}$$

calcolo perturbativo dell'energia di correlazione

$$F\Psi_n^{\mathrm{monodet}} = E_n^{\mathrm{noncorr}}\Psi_n$$

$$(F + (H - F))\Phi_n \stackrel{?}{=} E_n^{\mathrm{corr}}\Phi_n$$