Schrødinger equation in momentspace

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2-particle Scrødinger equation in coordinatespace

$$\left(\frac{\mathbf{p_1}^2}{2m_1} + \frac{\mathbf{p_2}^2}{2m_2} + V(\mathbf{r_1},\mathbf{r_2})\right)\psi(\mathbf{r_1},\mathbf{r_2}) = \mathrm{E}\ \psi(\mathbf{r_1},\mathbf{r_2}) \tag{1}$$

Define relative and center of mass coordinates

$$\mathbf{P} = \mathbf{p_1} + \mathbf{p_2} \tag{2}$$

$$\mathbf{p} = \beta\mathbf{p_1} - \alpha\mathbf{p_2} \tag{3}$$

$$\alpha = \frac{m_1}{M}, \quad \beta = \frac{m_2}{M}, \quad \mathrm{M} = m_1 + m_2 \tag{4}$$

$$\mathbf{r} = \mathbf{r_1} - \mathbf{r_2} \tag{5}$$

$$\mathbf{R} = \frac{1}{2}\left(m_1\mathbf{r_1} + m_2\mathbf{r_2}\right) \tag{6}$$

Assuming central symmetric potential

$$V(\mathbf{r_1},\mathbf{r_2}) = V(|\mathbf{r}|) \tag{7}$$

the wavefunction can be separated in relative and center of mass coordinates. the Schrødinger equation can be written as 2 separate equations relative and center of mass coordinates. Defining reduced mass

$$m = \frac{m_1 m_2}{M}$$

the Schrødinger equation can be written

$$\left(\frac{\mathbf{p}^2}{2m} + \frac{\mathbf{P}^2}{2M} + V(|\mathbf{r}|)\right)\psi(\mathbf{r})\phi(\mathbf{R}) = \mathrm{E}\ \psi(\mathbf{r})\phi(\mathbf{R}) \tag{8}$$

Using standard separation of variables teqniques, this single equation can be written as two separate equations

$$\frac{\mathbf{P}^2}{2M}\phi(\mathbf{R}) = \epsilon_R\ \phi(\mathbf{R}) \tag{9}$$

$$\left(\frac{\mathbf{p}^2}{2m} + V(|\mathbf{r}|)\right)\psi(\mathbf{r}) = \epsilon_r\ \psi(\mathbf{r}) \tag{10}$$

where $E = \epsilon_r + \epsilon_R$.

The second step is to transform these two equations into momentumspace by multiplying from the right with $\frac{1}{(2\pi)^{3/2}}e^{-i\mathbf{k}\cdot\mathbf{r}}$ and integrating over $d\mathbf{r}$ in all space.

$$\frac{\mathbf{P}^2}{2M}\frac{1}{(2\pi)^{3/2}}\int d\mathbf{R}e^{-i\mathbf{P}\cdot\mathbf{R}}\phi(\mathbf{R}) = \frac{\epsilon_R}{(2\pi)^{\frac{3}{2}}}\int d\mathbf{R}\ e^{-i\mathbf{P}\cdot\mathbf{R}}\phi(\mathbf{R})$$

$$\frac{1}{(2\pi)^{\frac{3}{2}}}\left[\frac{\mathbf{p}^2}{2m}\int d\mathbf{r}e^{-i\mathbf{p}\cdot\mathbf{r}}\phi(\mathbf{r}) + \int d\mathbf{r}e^{-i\mathbf{p}\cdot\mathbf{r}}V(|\mathbf{r}|)\psi(\mathbf{r})\right] = \frac{\epsilon_r}{(2\pi)^{\frac{3}{2}}}\int d\mathbf{r}\ e^{-i\mathbf{p}\cdot\mathbf{r}}\phi(\mathbf{r})$$

By using the following Fourier transformations between coordinate and momentum space

$$
\begin{aligned}
\phi(\mathbf{p}) &= \frac{1}{(2\pi)^{3/2}} \int d\mathbf{r} e^{-i\mathbf{p}\cdot\mathbf{r}} \psi(\mathbf{r}) && (11) \\
\psi(\mathbf{r}) &= \frac{1}{(2\pi)^{3/2}} \int d\mathbf{r} e^{i\mathbf{p}\cdot\mathbf{r}} \phi(\mathbf{p}) && (12)
\end{aligned}
$$

the equations can be written

$$
\begin{aligned}
\frac{\mathbf{P}^2}{2M}\phi(\mathbf{P}) &= \epsilon_R \; \phi(\mathbf{P}) && (13) \\
\frac{\mathbf{p}^2}{2m} \; \phi(\mathbf{p}) + \int d\mathbf{p}' V(|\mathbf{p}-\mathbf{p}'|) \; \phi(\mathbf{p}') &= \epsilon_r \; \phi(\mathbf{p}) && (14)
\end{aligned}
$$

where $V(|\mathbf{p}-\mathbf{p}'|)$ has been defined

$$
V(|\mathbf{p}-\mathbf{p}'|) = \frac{1}{(2\pi)^3} \int d\mathbf{r} e^{-i\mathbf{p}\cdot\mathbf{r}} V(|\mathbf{r}|)
$$

The Schrødinger equation in momentumspace and expanded in partial waves reads for relative coordinates

$$
\frac{k^2}{2m}\psi_l(k) + \frac{2}{\pi}\int k'^2 dk' V(|\mathbf{k}-\mathbf{k}'|)\psi_l(k') = \epsilon_l \; \psi_l(k) \qquad (15)
$$

Discretizing this equation by the following substitutions

$$
\begin{aligned}
\psi(k) &\implies (\psi_1 \ldots \psi_n)^T, \qquad \psi_i = \psi(k_i) && (16) \\
k \in [0,\infty) &\implies k_i \in [k_1 \ldots k_n] && (17) \\
V(|\mathbf{k}-\mathbf{k}'|) &\implies V_{i,j} = V(|\mathbf{k_i}-\mathbf{k_j}|) = \langle f|V|i\rangle && (18) \\
\int dk' k'^2 &\implies \sum_{i=1}^{n} k_i^2 w_i && (19)
\end{aligned}
$$

where k_i and w_i are the meshpoints and corresponding weights. This gives a system of n equations in n unknowns

$$
\begin{aligned}
\left(\frac{k_1^2}{2m} + \frac{2}{\pi}k_1^2 w_1 V_{1,1}\right)\psi_1 + \frac{2}{\pi}k_2^2 w_2 V_{1,2}\psi_2 + \ldots + \frac{2}{\pi}k_n^2 w_n V_{1,n}\psi_n &= \epsilon \; \psi_1 \\
\frac{2}{\pi}k_1^2 w_1 V_{2,1}\psi_1 + \left(\frac{k_2^2}{2m} + \frac{2}{\pi}k_2^2 w_2 V_{2,2}\right)\psi_2 + \ldots + \frac{2}{\pi}k_n^2 w_n V_{2,n}\psi_n &= \epsilon \; \psi_2 \\
\vdots &= \vdots \\
\frac{2}{\pi}k_1^2 w_1 V_{n,1}\psi_1 + \frac{2}{\pi}k_2^2 w_2 V_{n,2}\psi_2 + \ldots + \left(\frac{k_n^2}{2m} + \frac{2}{\pi}k_n^2 w_n V_{n,n}\right)\psi_n &= \epsilon \; \psi_n
\end{aligned}
$$

This can be written as an eigenvalue problem

$$
A\psi = \epsilon\psi
$$

where

$$A = \begin{bmatrix} \frac{k_1^2}{2m} + \frac{2}{\pi}k_1^2 w_1 V_{1,1} & \frac{2}{\pi}k_2^2 w_2 V_{1,2} & \dots & \frac{2}{\pi}k_n^2 w_n V_{1,n} \\ \frac{2}{\pi}k_1^2 w_1 V_{2,1} & \frac{k_2^2}{2m} + \frac{2}{\pi}k_2^2 w_2 V_{2,2} & \dots & \frac{2}{\pi}k_n^2 w_n V_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{2}{\pi}k_1^2 w_1 V_{n,1} & \frac{2}{\pi}k_2^2 w_2 V_{n,2} & \dots & \frac{k_n^2}{2m} + \frac{2}{\pi}k_n^2 w_n V_{n,n} \end{bmatrix} \quad (20)$$

$$\psi = [\psi_1 \psi_2 \dots \psi_n]^T \quad (21)$$

$$(22)$$

and ψ, ϵ are the eigenvector/eigenvalue pairs of the matrix A.

This is the correct matrix equation for an uncoupled channel for a block of the total matrix equation. The Hamiltonian is diagonal in total angular momentum J, total isospin T_z, spin S, strange quantum number s. However, for S=1 the criteria for l: $J = l \pm 1$, gives a coupling between different l values if $J > 0$. In addition we have a coupling between particlecombinations (configurations) for a specific channel.

S = 0

T_z	# subchannels	sub 1	sub 2	sub 3	sub 4
-1	1	nn			
0	1	pn			
1	1	pp			

S = -1

T_z	# subchannels	sub 1	sub 2	sub 3	sub 4
$-\frac{3}{2}$	1	$\Sigma^- n$			
$-\frac{1}{2}$	3	Λn	$\Sigma^- p$	$\Sigma^0 n$	
$\frac{1}{2}$	3	Λp	$\Sigma^0 p$	$\Sigma^+ n$	
$\frac{3}{2}$	1	$\Sigma^+ p$			

S = -2

T_z	# subchannels	sub 1	sub 2	sub 3	sub 4
-2	1	$\Sigma^-\Sigma^-$			
-1	2	$\Lambda\Sigma^-$	$\Sigma^0\Sigma^-$		
0	4	$\Lambda\Sigma^0$	$\Lambda\Lambda$	$\Sigma^0\Sigma^0$	$\Sigma^+\Sigma^-$
1	2	$\Lambda\Sigma^+$	$\Sigma^0\Sigma^+$		
2	1	$\Sigma^+\Sigma^+$			

The end result is a block diagonal matrix T, where each block can be diagonalized separately

$$T = \begin{bmatrix} T_1 & 0 & \dots & 0 \\ 0 & T_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & T_n \end{bmatrix} \tag{23}$$

where each of the blocks has a specific set of quantum numbers(J, S, s, T_z) and the form

$$T_\alpha = \begin{bmatrix} K + \langle J-1|S|J-1\rangle & \langle J-1|S|J+1\rangle \\ \langle J+1|S|J-1\rangle & K + \langle J+1|S|J+1\rangle \end{bmatrix} \tag{24}$$

Here α represents the quantum numbers of a specific channel. The submatrix K is defined

$$K = \begin{bmatrix} K_1 & & \\ & \ddots & \\ & & K_i \end{bmatrix} \tag{25}$$

where

$$K_j = \begin{bmatrix} \frac{k_1^2}{2m_j} & & \\ & \ddots & \\ & & \frac{k_n^2}{2m_j} \end{bmatrix} \tag{26}$$

j is identified with the subchannel of channel α and m_j is the reduced mass of the particles in this subchannel. Further

$$\langle L|S|L'\rangle = \begin{bmatrix} \langle L;1|V|L';1\rangle & \dots & \langle L;1|V|L';i\rangle \\ \vdots & \ddots & \vdots \\ \langle L;i|V|L';1\rangle & \dots & \langle L;i|V|L';i\rangle \end{bmatrix} \tag{27}$$

where

$$\langle L;j|V|L';j'\rangle = \begin{bmatrix} \frac{2}{\pi}k_1^2 w_1 V_{11}(j,j',L,L',\alpha) & \dots & \frac{2}{\pi}k_n^2 w_n V_{1n}(j,j',L,L',\alpha) \\ \vdots & \ddots & \vdots \\ \frac{2}{\pi}k_1^2 w_1 V_{n1}(j,j',L,L',\alpha) & \dots & \frac{2}{\pi}k_n^2 w_n V_{nn}(j,j',L,L',\alpha) \end{bmatrix}$$

Again, j identifies the appropriate subchannel of channel α