Mott problem

Consider the emission of an α particle in a cloud chamber. The quantum mechanical model of an α particle is a spherical wave emanating from the origin. A spherical wave should ionize atoms throughout the cloud chamber. However, only straight tracks are observed. Nevill Mott showed that straight tracks are consistent with the Schrodinger equation.

Let $\mathbf{R}$ be the position of the α particle, let $\mathbf{a}_1$ and $\mathbf{a}_2$ be the positions of two atoms ionized by the α particle, and let $\mathbf{r}_1$ and $\mathbf{r}_2$ be the positions of the free electrons. The Hamiltonian for the system is

$$\hat{H} = \hat{K}_\alpha + \hat{K}_1 + \hat{K}_2 + U_1 + U_2 + V_1 + V_2$$

where

$$\hat{K}_\alpha = -\frac{\hbar^2}{2M}\nabla_\alpha^2 \qquad \text{kinetic energy of } \alpha \text{ particle}$$

$$\hat{K}_1 = -\frac{\hbar^2}{2m}\nabla_1^2 \qquad \text{kinetic energy of 1st electron}$$

$$\hat{K}_2 = -\frac{\hbar^2}{2m}\nabla_2^2 \qquad \text{kinetic energy of 2nd electron}$$

$$U_1 = -\frac{e^2}{|\mathbf{r}_1 - \mathbf{a}_1|} \qquad \text{potential energy of 1st electron}$$

$$U_2 = -\frac{e^2}{|\mathbf{r}_2 - \mathbf{a}_2|} \qquad \text{potential energy of 2nd electron}$$

$$V_1 = -\frac{2e^2}{|\mathbf{R} - \mathbf{r}_1|} \qquad \text{potential energy of } \alpha \text{ and 1st electron}$$

$$V_2 = -\frac{2e^2}{|\mathbf{R} - \mathbf{r}_2|} \qquad \text{potential energy of } \alpha \text{ and 2nd electron}$$

Let ψ_1 and ψ_2 be atomic wavefunctions such that

$$\left(\hat{K}_1 + U_1\right)\psi_1 = E_1\psi_1, \quad \left(\hat{K}_2 + U_2\right)\psi_2 = E_2\psi_2$$

We want to find a wavefunction $F(\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2)$ such that

$$\hat{H}F = EF$$

Let

$$F = F_0 + F_1 + F_2 + \cdots$$

and let

$$\hat{H}_0 = \hat{K}_\alpha + E_1 + E_2$$

Start by finding an F_0 such that

$$\hat{H}_0 F_0 = EF_0$$

The solution is

$$F_0(\mathbf{R},\mathbf{r}_1,\mathbf{r}_2) = f_0(\mathbf{R})\psi_1(\mathbf{r}_1-\mathbf{a}_1)\psi_2(\mathbf{r}_2-\mathbf{a}_2) \tag{1}$$

where

$$f_0(\mathbf{R}) = \frac{1}{|\mathbf{R}|}\exp\left(\frac{ik|\mathbf{R}|}{\hbar}\right), \quad k=\sqrt{2M(E-E_1-E_2)}$$

It follows that for the full Hamiltonian $\hat{H}$ we have

$$\hat{H}F_0 = EF_0 + (V_1+V_2)F_0$$

To cancel $(V_1+V_2)F_0$ from the full Hamiltonian, find an F_1 such that

$$\hat{H}_0F_1 = EF_1 - (V_1+V_2)F_0$$

Rewrite as

$$\left(\hat{H}_0 - E\right)F_1 = -(V_1+V_2)F_0$$

Expand F_1 and F_0.

$$\left(\hat{H}_0 - E\right)f_1(\mathbf{R})\psi_1(\mathbf{r}_1-\mathbf{a}_1)\psi_2(\mathbf{r}_2-\mathbf{a}_2) = -(V_1+V_2)f_0(\mathbf{R})\psi_1(\mathbf{r}_1-\mathbf{a}_1)\psi_2(\mathbf{r}_2-\mathbf{a}_2)$$

To solve for $f_1(\mathbf{R})$ multiply both sides by

$$\psi_1^*(\mathbf{r}_1-\mathbf{a}_1)\psi_2^*(\mathbf{r}_2-\mathbf{a}_2)$$

and integrate over $\mathbf{r}_1$ and $\mathbf{r}_2$ to obtain

$$\left(\hat{H}_0 - E\right)f_1(\mathbf{R}) = V_1(\mathbf{R})f_0(\mathbf{R}) + V_2(\mathbf{R})f_0(\mathbf{R}) \tag{2}$$

where

$$V_1(\mathbf{R}) = 2e^2\int\frac{|\psi_1(\mathbf{r})|^2}{|\mathbf{R}-\mathbf{a}_1-\mathbf{r}|}\,d\mathbf{r}, \quad V_2(\mathbf{R}) = 2e^2\int\frac{|\psi_2(\mathbf{r})|^2}{|\mathbf{R}-\mathbf{a}_2-\mathbf{r}|}\,d\mathbf{r}$$

Per Mott the solution to (2) is

$$f_1(\mathbf{R}) = \frac{M}{2\pi\hbar^2}\int\frac{V_1(\mathbf{r})f_0(\mathbf{r})}{|\mathbf{R}-\mathbf{r}|}\exp\left(\frac{ik|\mathbf{R}-\mathbf{r}|}{\hbar}\right)d\mathbf{r} + \frac{M}{2\pi\hbar^2}\int\frac{V_2(\mathbf{r})f_0(\mathbf{r})}{|\mathbf{R}-\mathbf{r}|}\exp\left(\frac{ik|\mathbf{R}-\mathbf{r}|}{\hbar}\right)d\mathbf{r}$$

Let I_1 be the first integral. Substitute for f_0 in I_1 to obtain

$$I_1(\mathbf{R}) = \frac{M}{2\pi\hbar^2}\int\frac{V_1(\mathbf{r})}{|\mathbf{R}-\mathbf{r}||\mathbf{r}|}\exp\left(\frac{ik|\mathbf{R}-\mathbf{r}|}{\hbar}+\frac{ik|\mathbf{r}|}{\hbar}\right)d\mathbf{r}$$

Change of variable $\mathbf{r}\to\mathbf{r}+\mathbf{a}_1$

$$I_1(\mathbf{R}) = \frac{M}{2\pi\hbar^2}\int\frac{V_1(\mathbf{r}+\mathbf{a}_1)}{|\mathbf{R}-\mathbf{r}-\mathbf{a}_1||\mathbf{r}+\mathbf{a}_1|}\exp\left(\frac{ik|\mathbf{R}-\mathbf{r}-\mathbf{a}_1|}{\hbar}+\frac{ik|\mathbf{r}+\mathbf{a}_1|}{\hbar}\right)d\mathbf{r}$$

Per Mott (see also Figari and Teta)

$$I_1(\mathbf{R}) \approx \frac{1}{|\mathbf{R}-\mathbf{a}_1|} \exp\left(\frac{ik|\mathbf{R}-\mathbf{a}_1|}{\hbar}\right) \\ \times \frac{M}{2\pi\hbar^2} \int \frac{V_1(\mathbf{r}+\mathbf{a}_1)}{|\mathbf{r}+\mathbf{a}_1|} \exp\left(-\frac{ik\mathbf{u}_1(\mathbf{R})\cdot\mathbf{r}}{\hbar} + \frac{ik|\mathbf{r}+\mathbf{a}_1|}{\hbar}\right) d\mathbf{r}$$

where

$$\mathbf{u}_1(\mathbf{R}) = \frac{\mathbf{R}-\mathbf{a}_1}{|\mathbf{R}-\mathbf{a}_1|}$$

The condition for stationary phase is

$$g' = \frac{d}{d\mathbf{r}}\left(-\mathbf{u}_1(\mathbf{R})\cdot\mathbf{r} + |\mathbf{r}+\mathbf{a}_1|\right) = -\mathbf{u}_1(\mathbf{R}) + \frac{\mathbf{r}+\mathbf{a}_1}{|\mathbf{r}+\mathbf{a}_1|} = 0$$

Note that $V_1(\mathbf{r}+\mathbf{a}_1)$ is small except for $\mathbf{r} \approx 0$ so we only require stationarity at the origin. Hence for $\mathbf{r} = 0$ the integral is stationary ($g' = 0$) when $\mathbf{R}$ satisfies the condition

$$\mathbf{u}_1(\mathbf{R}) = \frac{\mathbf{a}_1}{|\mathbf{a}_1|}$$

By symmetry of the integrals, I_2 is stationary when $\mathbf{R}$ satisfies the condition

$$\mathbf{u}_2(\mathbf{R}) = \frac{\mathbf{a}_2}{|\mathbf{a}_2|}$$

Because nonstationary integrals vanish we have

$$f_1(\mathbf{R}) = \begin{cases} I_1(\mathbf{R}), & \mathbf{u}_1(\mathbf{R}) = \frac{\mathbf{a}_1}{|\mathbf{a}_1|} \quad \text{and} \quad \mathbf{u}_2(\mathbf{R}) \neq \frac{\mathbf{a}_2}{|\mathbf{a}_2|} \\ I_2(\mathbf{R}), & \mathbf{u}_1(\mathbf{R}) \neq \frac{\mathbf{a}_1}{|\mathbf{a}_1|} \quad \text{and} \quad \mathbf{u}_2(\mathbf{R}) = \frac{\mathbf{a}_2}{|\mathbf{a}_2|} \\ I_1(\mathbf{R}) + I_2(\mathbf{R}), & \mathbf{u}_1(\mathbf{R}) = \frac{\mathbf{a}_1}{|\mathbf{a}_1|} \quad \text{and} \quad \mathbf{u}_2(\mathbf{R}) = \frac{\mathbf{a}_2}{|\mathbf{a}_2|} \\ 0, & \text{otherwise} \end{cases}$$

The first two cases represent states in which just one atom is ionized. The third case has both V_1 and V_2 contributing to f_1. Hence when both atoms are ionized we have

$$f_1(\mathbf{R}) = \begin{cases} I_1(\mathbf{R}) + I_2(\mathbf{R}), & \frac{\mathbf{a}_1}{|\mathbf{a}_1|} = \frac{\mathbf{a}_2}{|\mathbf{a}_2|} \\ 0, & \text{otherwise} \end{cases}$$

To satisfy the condition, $\mathbf{a}_1$ and $\mathbf{a}_2$ must be on the same ray emanating from the origin. Hence straight tracks are consistent with the Schrodinger equation.

Note

The condition for stationarity

$$\mathbf{u}_1(\mathbf{R}) = \frac{\mathbf{R} - \mathbf{a}_1}{|\mathbf{R} - \mathbf{a}_1|} = \frac{\mathbf{a}_1}{|\mathbf{a}_1|}$$

is satisfied by all $\mathbf{R}$ and constant $c > 1$ such that

$$\mathbf{R} = c\mathbf{a}_1$$

Condition $c > 1$ implies that $|\mathbf{R}| > |\mathbf{a}_1|$ so technically the condition

$$\frac{\mathbf{a}_1}{|\mathbf{a}_1|} = \frac{\mathbf{a}_2}{|\mathbf{a}_2|}$$

is less stringent than

$$\mathbf{u}_1(\mathbf{R}) = \frac{\mathbf{a}_1}{|\mathbf{a}_1|} \quad \text{and} \quad \mathbf{u}_2(\mathbf{R}) = \frac{\mathbf{a}_2}{|\mathbf{a}_2|}$$

The exact condition for stationarity of both I_1 and I_2 is

$$\frac{\mathbf{a}_1}{|\mathbf{a}_1|} = \frac{\mathbf{a}_2}{|\mathbf{a}_2|} \quad \text{and} \quad |\mathbf{R}| > \max(|\mathbf{a}_1|, |\mathbf{a}_2|)$$