# Multiple Scattering Theory (MST) and Condensed Matter Nuclear Science —"Super-Absorption" in a Crystal Lattice—

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## Abstract

A simple 1-dimensional model is used to illustrate "super-absorption" in a crystal lattice. The WKB method is applied to calculate the reflection rate and the transmission rate for a single cell. Then matrix algebra is manipulated to give the relation between the single cell and an array of N cells. The selective resonant tunneling in this array of N cells is discussed, and the dependence of the absorption rate on the number of the cells is calculated to show the difference between coherent and non-coherent systems.

## 1. INTRODUCTION

Super radiation was proposed in 1950s by Dick. [1] Super radiation means that the resultant intensity of N coherent optical sources will be proportional to $N^2$ instead of N. One might ask that if light is absorbed by N points of an absorber where the light is coherent in phase; then, what would happen? Would the absorption be enhanced or reduced? The answer is, "the absorption would be enhanced when certain resonant conditions are satisfied". The resonance conditions include not only the ***frequency*** of incident waves, which should be in resonance with the absorbing medium, but also the ***absorption coefficient*** in the medium, which should match with the attenuation of the wave in propagation. We will discuss this matching in the single cell first; then, we will discuss the matching in a crystal lattice. This enhanced absorption might be called as "Super-Absorption" [2,3]. An experiment has been proposed to detect the effect of this "Super-Absorption".

Experiments have showed the wave nature of the deuteron inside the palladium deuteride (hydride) already. [4-7] Hence, the Multiple Scattering Theory (MST) is supposed to show the correlation between the anomalous deuterium flux and heat flow. As a first step, a simplified 1-Dimension model is described to show qualitatively the feature of the Multiple Scattering Theory. Non-coherent diffusion process is quite different from the coherent wave propagating process.

## 2. SELECTIVE RESONANT ABSORPTION IN A SINGLE CELL

Figure 1 shows the single cell of a lattice. The wave function of the incident particle might be reflected by a potential barrier ($U_2$), or trapped by a potential well ($U_1$ or $U_3=U_{3r}+iU_{3i}$), or tunneling through the double barriers. In the plane-wave-representation, a 2×2 matrix *M* may be introduced to describe the relation between the amplitudes of these wave functions. Having assumed that the potential energy in the well and barrier varies so smoothly that the WKB method is valid, we may write the *M* matrix as [2,3,8]:

$$M=\begin{bmatrix} \frac{1}{2}Exp[-i\frac{J_1}{\hbar}][2\sin(\frac{J_2}{2\hbar})+i(4\theta^2+\frac{1}{4\theta^2})\cos(\frac{J_2}{2\hbar})] & -i\frac{1}{2}Exp[-i\frac{J_1}{\hbar}](4\theta^2-\frac{1}{4\theta^2})\cos(\frac{J_2}{2\hbar}) \\ i\frac{1}{2}Exp[i\frac{J_1}{\hbar}](4\theta^2-\frac{1}{4\theta^2})\cos(\frac{J_2}{2\hbar}) & \frac{1}{2}Exp[i\frac{J_1}{\hbar}][2\sin(\frac{J_2}{2\hbar})-i(4\theta^2+\frac{1}{4\theta^2})\cos(\frac{J_2}{2\hbar})] \end{bmatrix} \quad (1)$$

Here,

$$J_1 = \int_1^2 \sqrt{2\mu(E - U_1)}dr; \tag{2}$$

$$\theta = \int_2^3 \sqrt{\frac{2\mu(U_2 - E)}{\hbar^2}}dr \tag{3}$$

$$J_2 = \int_3^4 \sqrt{2\mu(E - U_3)}dr \tag{4}$$

μ is the reduced mass; $U_1$, $U_2$, $U_3$ are the potential in the region 12, 23, and 34 respectively. E is the energy of the incident particle. r is the distance in 1-dimensional space, $\hbar$ is the Planck constant divided by 2π.

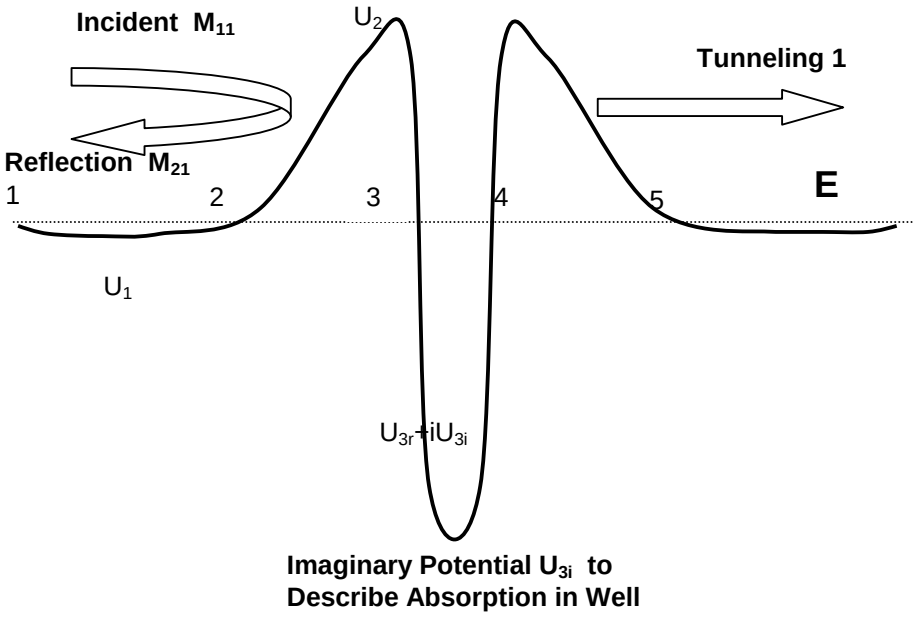


Fig. 1 **M** matrix is used to describe the incident plane wave ($M_{11}$), and the reflecting plane wave ($M_{21}$). The amplitude of the tunneling wave is fixed as 1

In the plane-wave-representation, the tunneling wave is represented by a column vector as:

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{5}$$

On the left side of the single cell, the wave function is represented by

$$\begin{bmatrix} M_{11} \\ M_{21} \end{bmatrix} = M \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{6}$$

Hence, for this single cell, the tunneling rate, $T_1$, is defined as:

$$T_1 = \frac{1}{|M_{11}|^2} \tag{7}$$

The reflection rate, $R_1$, is defined as:

$$R_1 = \frac{|M_{21}|^2}{|M_{11}|^2} \tag{8}$$

When the imaginary part of the potential vanishes, i.e. $U_{3i}$=0; then, the conservation of the probability requires:

$$\left|M_{11}\right|^2 = 1 + \left|M_{21}\right|^2 \tag{9}$$

However, $U_{3i}$ is introduced here to describe the absorption in the region 34. Thus the absorption rate, $A_1$, is defined as :

$$A_1 = 1 - \frac{1 + \left|M_{21}\right|^2}{\left|M_{11}\right|^2} \tag{10}$$

When the wavelength of the incidental particle changes, the phases of the reflecting wave from the first barrier and the second barrier also change. The superposition of these reflecting waves will determine the amplitude of the wave reflected by this single cell (i.e. $M_{21}$). It will show a resonant feature. The resonance happens when

$$\cos(\frac{J_2}{2\hbar}) = 0 \tag{11}$$

In the case of resonance, the perfect tunneling happens and the reflection is zero, i.e. $T_1$=1, and $R_1$=0. However, if there is any absorption in the well region 34; then,

$$\cos(\frac{J_2}{2\hbar}) \neq 0 \tag{12}$$

In other words, the absorption will introduce the reflection ($M_{21}\neq 0$) even if in the case of resonance.

Now one may ask a question: when the module of the imaginary part of the potential, $|U_{3i}|$, is getting greater and greater, will the absorption rate, $R_1$, get larger or smaller? The answer is: "the absorption rate will be get larger first; then it will get smaller". The physical reason is the interference of two reflecting waves. When $|U_{3i}|$ is getting greater, the reflecting wave from the second barrier would be much weaker; then, there is no way to make $M_{21}$=0. Thus, there will be a competition between the absorption and reflection. When the $U_{3i}$ =0, there is no reflection because $M_{21}$ =0 in the case of resonance; however, there is no absorption also in this case also, because $\left|M_{11}\right|^2 = 1 + \left|M_{21}\right|^2$. On the other hand, if $U_{3i} \to$ -∞; then, $\cos(\frac{J_2}{2\hbar}) \to \infty$, and $A_1 \to 0$. Consequently, we may find an intermediate value for $U_{3i}$ which makes $A_1$ maximized. This is a feature of selective resonant absorption [9-14]. Not only the energy, E, has to make the real part of $J_2$ , $J_{2r} = 2n\pi\hbar$ (n=1, 2, 3……), but also the absorption capacity, $U_{3i}$, has to match a specific value. Figure 2 just shows that the absorption rate $A_1$ reaches a peak at the value of $U_{3i}$ between 0 and - ∞.(θ was assumed to be 10 in Fig.2)

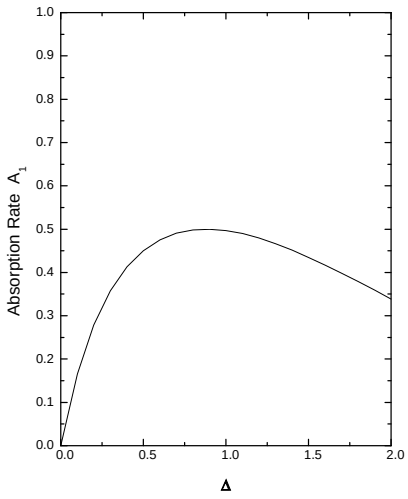


Figure 2 Absorption rate for single cell reaches a peak at selective damping, $U_{3i}$.

Here,

$$\Delta = arc\sinh[(2\theta^2 + \frac{1}{8\theta^2})\sinh(\frac{J_{2i}}{2\hbar})] \tag{13}$$

$$J_{2i} = \mathrm{Im}(\int_3^4 \sqrt{2\mu(E - U_3)}dr \approx \int_3^4 \frac{\mu(-U_{3i})}{\sqrt{2\mu(E - U_{3r})}}dr \tag{14}$$

$$M_{11} = \cos\alpha - i\sqrt{1 - (\frac{\cos\alpha}{Q_p})^2} \tag{15}$$

$$M_{21} = -\frac{Q_m}{Q_p}\cos\alpha \tag{16}$$

$$Q_p = 2\theta^2 + \frac{1}{8\theta^2} \tag{17}$$

$$Q_m = 2\theta^2 - \frac{1}{8\theta^2} \tag{18}$$

$$\alpha = \frac{\pi}{2} + i\Delta \tag{19}$$

We may notice that $J_1$ does not effect the value of tunneling rate or the reflection rate for the single cell. The situation will be quite different when we calculate these rates in the case of multiple cells.

## 3. SELECTIVE RESONANT ABSORPTION IN A CRYSTAL LATTICE

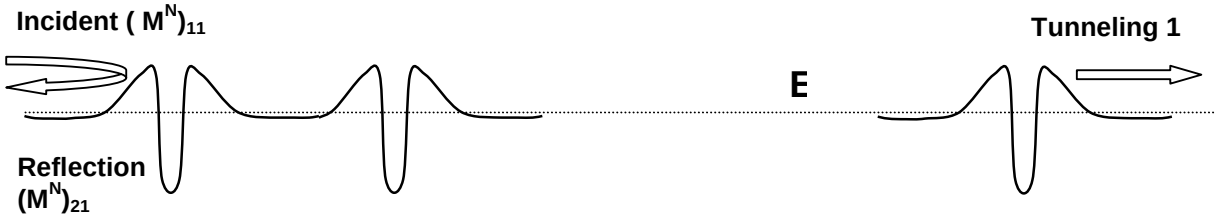


Figure 3. A chain of single cells to represent the potential energy inside a crystal lattice for a charged particle

Figure 3 shows a series of cells, which represent the potential inside a crystal lattice. The reflecting waves from each single cell will affect the total reflection rate, $R_N$.

$$R_N = \frac{\left|M_{21}^N\right|^2}{\left|M_{11}^N\right|^2} \tag{20}$$

The matrix of N cells, $M^N$, may be expressed by the matrix of the single cell, M, in terms of N and $\alpha$:

$$M_{21}^N = \frac{\sin(N\alpha)}{\sin\alpha} M_{21} \tag{21}$$

$$M_{11}^N = \frac{\sin(N\alpha)M_{11} - \sin[(N-1)\alpha]}{\sin\alpha} \tag{22}$$

$$\begin{aligned} \alpha &= arc\cos[\frac{M_{11}+M_{22}}{2}] \\ &= arc\cos[\cos(\frac{J_1}{\hbar})\sin(\frac{J_2}{2\hbar}) + (2\theta^2 + \frac{1}{8\theta^2})\sin(\frac{J_1}{\hbar})\cos(\frac{J_2}{2\hbar})] \end{aligned} \tag{23}$$

The wave propagation in the lattice cell region will affect the phase of the reflecting wave. This effect is represented by $J_1$ in the expression of $\alpha$. When

$$J_1 = \frac{(2n+1)\pi\hbar}{2}, \quad (n=1,2,3\ldots\ldots) \tag{24}$$

$$\alpha = arc\cos[(2\theta^2 + \frac{1}{8\theta^2})\cos(\frac{J_2}{2\hbar})] \tag{25}$$

The resonance condition for a single cell without absorption is:

$$J_2 = m\pi\hbar, \quad (m=1,2,3\ldots\ldots) \tag{26}$$

It gives: $\alpha = m\pi/2$. However, if $U_{3i} \neq 0$; then,

$$J_2 = \pi\hbar + iJ_{2i} \tag{27}$$

$$\alpha = arc\cos[(2\theta^2 + \frac{1}{8\theta^2})(-i\sinh(\frac{J_{2i}}{2\hbar}))] = \frac{\pi}{2} + i\log[y + \sqrt{1+y^2}] = \frac{\pi}{2} + i\Delta \tag{28}$$

$$y \equiv Q_p x \tag{29}$$

$$Q_p \equiv 2\theta^2 + \frac{1}{8\theta^2} \tag{30}$$

$$x \equiv \sinh(\frac{J_{2i}}{2\hbar}) \tag{31}$$

$$\Delta = arc\sinh[(2\theta^2 + \frac{1}{8\theta^2})\sinh(\frac{J_{2i}}{2\hbar})] \tag{32}$$

We may plot the absorption coefficient of N cells, $A_N$, as a function of $\Delta$ in Fig.4. The curves share the same feature that $A_N$ always equals to zero when $\Delta$=0; and there is always a peak of $A_N$ at certain $\Delta_p$. However, when the number of cells, N, increases, this peak value of $A_N$ increases, and the location of this peak, $\Delta_p$ approaches 0. The physical reason for this behavior is just the selectivity of the resonance tunneling [9-14]. When $\Delta$=0, it means $U_{3i}$=0 (i.e. there is no absorption at all); hence, $A_N$=0. However, if the absorption is too strong ($\Delta \to \infty$); then, the reflection from the first cell is inevitable and there is no way to cancel it by any reflection from other cells. As a result, at certain immediate value of $\Delta$, the total absorption coefficient will reach its maximum value. The higher the number of cell is, the higher the chances that reflection wave will be cancelled. It means that more waves will enter the array of the cells and undergo the absorption there. As a result the peak value of absorption, $A_N$ , increases with N. The peak value appears at the lower absorption, $\Delta_p$, for greater N, because the cancellation of the reflecting wave requires less absorption for more cells.

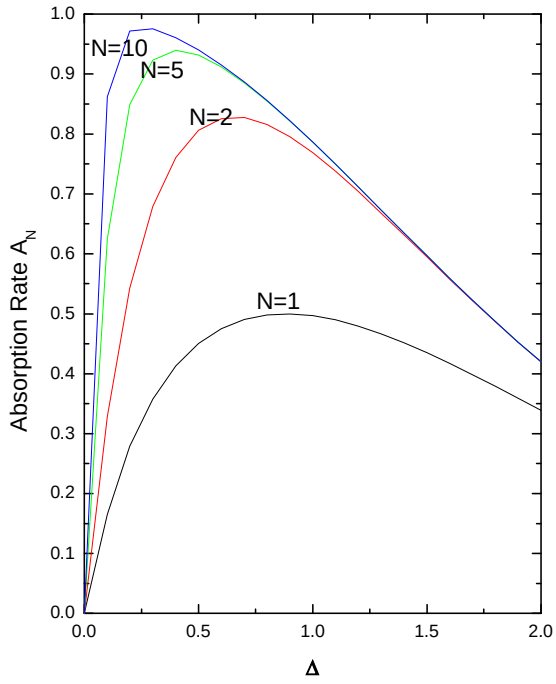


Figure 4 The peak of absorption rate shifts towards smaller $\Delta$, and the peak is getting higher for greater N

## 4. COMPARISON BETWEEN COHERENT AND NON-COHERENT ARRAY OF N CELLS

It is interesting to compare the behavior of coherent cells and the non-coherent cells in order to see the "Super-Absorption". In Fig. 5 the non-coherent beams are plotted for the consequent reflections and penetrations. The phase of the wave disappears in this figure, because only the module of the wave is concerned. We still use the same reflection rate, $R_1$, and the transmission rate, $T_1$, for a single cell, but the phase $J_1$ would not appear any where in the expression of $R_N$(non) , or $T_N$(non). The non-coherent

reflection rate $R_N$(non), and transmission rate $T_N$(non) for N cells may be expressed by recursion formula in terms of $R_1$ and $T_1$ as follows:

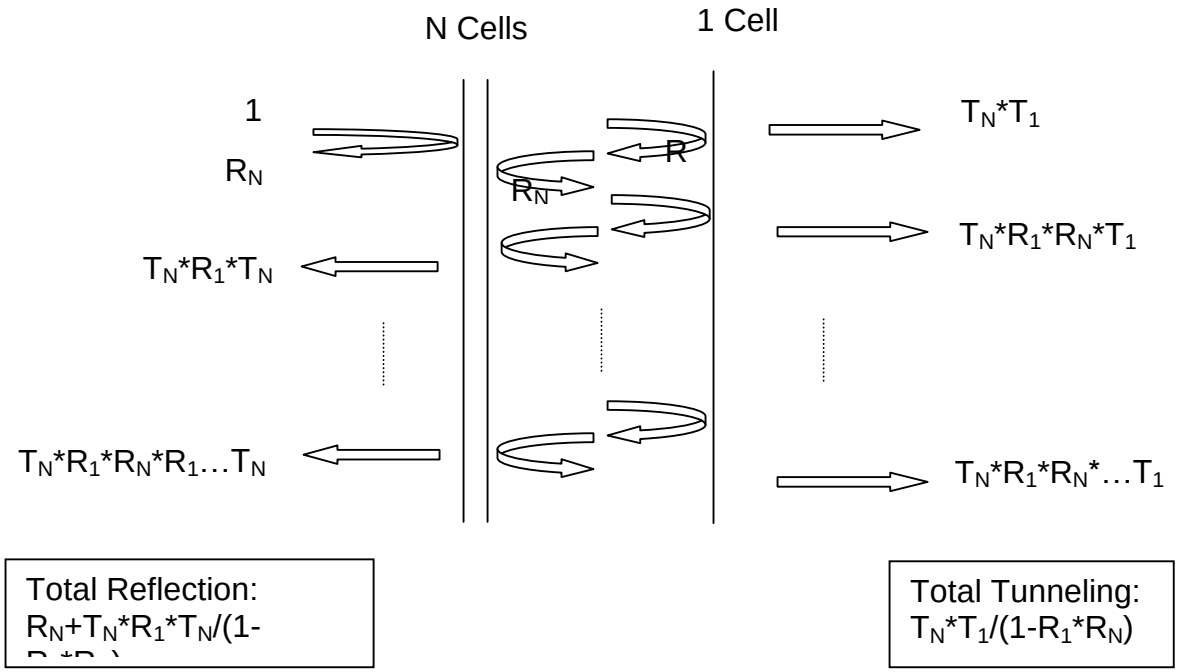


Fig.5 Flux Flow for the Case of Non-Coherent Beam

$$R_{N+1} = R_N + \frac{T_N * R_1 * T_N}{(1 - R_1 * R_N)} \tag{33}$$

$$T_{N+1} = T_N * \frac{T_1}{(1 - R_1 * R_N)} \tag{34}$$

From (33) and (34), it is clear that $R_{N+1} > R_N$, and $T_{N+1} < T_N$. There is no way to make $R_N=0$,if $R_1 \neq 0$. However, in the case of coherent case, $R_N$ may equal to zero even if $R_1 \neq 0$. This is the first distinction between the non-coherent and coherent case. There is another distinction between two cases as follows.

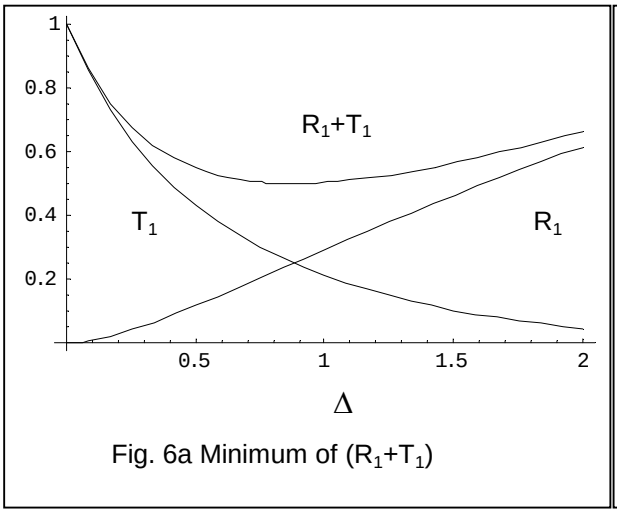


Fig. 6a Minimum of $(R_1+T_1)$

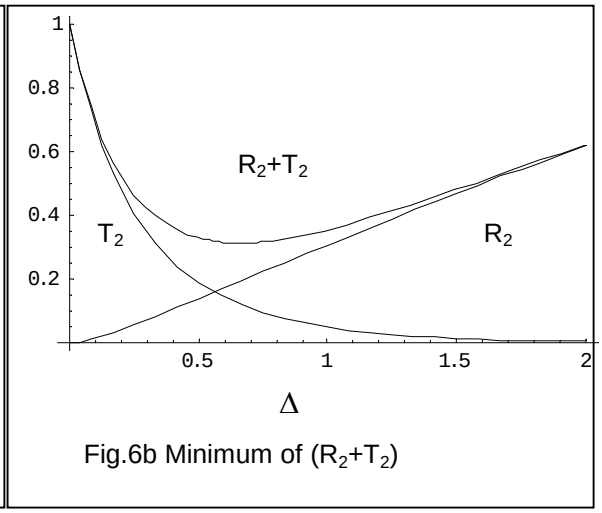


Fig.6b Minimum of $(R_2+T_2)$

For the non-coherent cases, $R_1$ and $T_1$ may be assumed to be same as that for coherent case (Eq. (15)-(19) and Fig. 6a); however, $R_2$ and $T_2$ will be calculated according to formula (33) and (34). In Fig. 6b, we see that $(R_2 + T_2)=1-A_2$ forms a minimum also. Nevertheless, this minimum is different from that of the

coherent case. We may define an escaping rate as (1-$A_N$); then, this escaping rate would reach its minimum value when the absorption rate, $A_N$ , reaches its peak value. In Fig. 7 this minimum escaping rate is plotted as a function the number of the cells. The open circles are for the non-coherent cells (equations (33) and (34)); and the solid circles are for the coherent cells (equations (20), (21), and (22)). Those circles may be fitted by two fitting curves. For non-coherent cells,

$$1 - A_N(\text{non}) \approx \frac{0.5356}{N^{0.82}} \tag{35}$$

For coherent cells,

$$1 - A_N \approx \frac{0.5179}{N^{1.36}} \tag{36}$$

The dependence on N for coherent cells is stronger than that of non-coherent cells. This is the effect of "Super-Absorption". It is not the dependence of $\frac{1}{N^2}$, because in this 1-dimensional case, N cells in an array are not equal. In the slab model, N cells in each slab are equal; then, the result would be different. It would be discussed later in another paper.

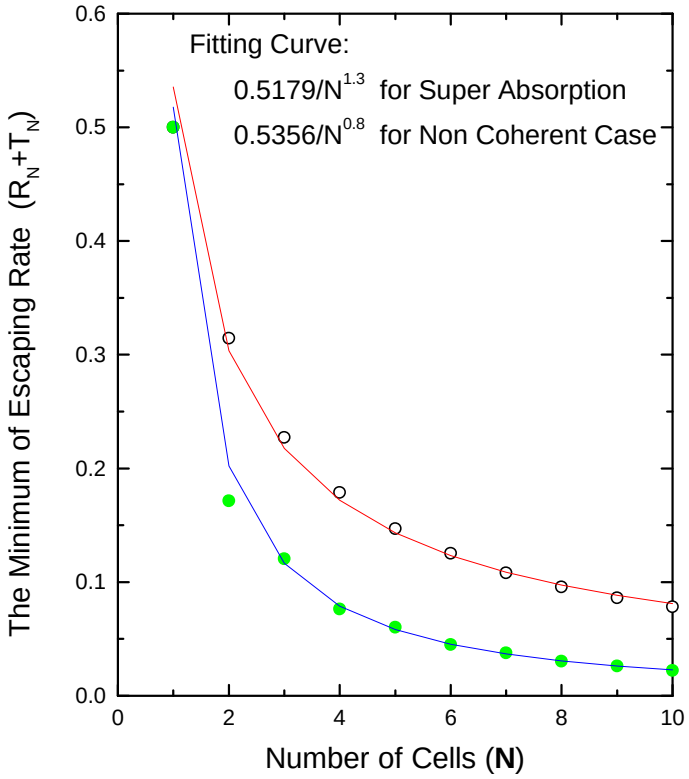


Fig.7 The Minimum of (1-$A_N$) as a Function of Number of Cells

## 5. CONCLUDING REMARKS

Although a special WKB model is used in this illustration, the feature is quite general:

(1) The definition of resonance here is no longer an energy level only. It should include a matching damping, i.e. the absorption capacity $U_{3i}$. This resonance condition varies with the number of the cells. However, it always corresponds to the condition of least reflection; i.e. minimizing the matrix element $(M^N)_{21}$. This concept turns out to be very important when we discuss the correlation between anomalous deuterium flux and the heat flow in a D/Pd system.

(2) The wave of deuterons inside the palladium deuteride is quite different from a non-coherent deuteron beam. Their behavior is very different in propagation (reflection, transmission, and

absorption). Hence, the coherence of the deuterons inside the crystal lattice is essential in explaining the macroscopic behavior of deuterium flux permeating the Pd thin film.

(3) There is no way to have any resonant behavior in a non-coherent deuteron beam, because the reflection rate, $R_N$(non), would never be zero.


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