# The magnetic field Influence on the absorption threshold of $\mathrm{VO}_{2}$ 

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## ABSTRACT

The vanadium dioxide $\mathrm{VO}_{2}$ is a material described as being intelligent because it can transit [1,2] from a reversible way of the semiconductor state to the metal state at a temperature $\theta_{\mathrm{t}}=68^{\circ} \mathrm{C}$. When we are at a temperature $\theta_{\mathrm{t}}<68^{\circ} \mathrm{C}$, this material is in the semiconductor state with a gap [3,4] approximately 0.7 ev . When $\theta_{\mathrm{t}}>68^{\circ} \mathrm{C}$, the vanadium dioxide becomes metal [14], there is an abrupt change of its structure and its optical properties [14,15] and electronic. We are interested in this study in the $\mathrm{VO}_{2}$ semiconductor state [15] and, especially, in widening its gap by the application of a magnetic field $\overrightarrow{\mathrm{B}}=\mathrm{B} \overrightarrow{\mathrm{z}}$. By taking into account the spin of the electron of the band of conduction after having neglected the term of Coulomb interaction, we solved the Schrödinger's equation in an exact way. Obtaining the levels of Landau [5,6,7] enables us to conclude the variation of the gap of $\Delta \mathrm{E}_{\mathrm{g}}=\frac{1}{2} \hbar \omega_{c}$, where $\omega_{\mathrm{c}}$ is the frequency cyclotron $\omega_{c}=\frac{\mathrm{eB}}{\mu}$, with e: the electron charge; $\mu$ : the reduced mass of the quasi particle (electron-hole); $\hbar$ : the Planck's constant reduced, and B is the intensity of the applied magnetic field. We will simulate by Maple this variation according to B for fixed $\mu$ on the one hand, and $\Delta \mathrm{E}_{\mathrm{g}}$ according to $\mu$ for fixed B on the other hand.



Simulated curves of the variation $\Delta \mathrm{E}_{\mathrm{g}}$ of the vanadium dioxide according to the magnetic field $B$ for the fixed reduced mass $\mu$ on the one hand, and on the other hand according to $\mu$ for fixed $B$.

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## Academic Discipline And Sub-Disciplines

Science; Quatum Physics; materials optics

## SUBJECT CLASSIFICATION

Materials Physics.

## TYPE (METHOD/APPROACH)

Calculation by exactly solving the Schrödinger's equation, based on simulation and modeling.

## INTRODUCTION

The semiconductor gap depends on several physical parameters. We quote, for example, the temperature, the pressure, the containment effect of the exciton or the size quantum effect and the magnetic field effect. We will apply a magnetic field $\vec{B}$ according to the direction (OZ) in the massive vanadium dioxide whose energy of gap is about 0.7 ev . After the exact resolution of the Schrödinger's equation of an electron in the band of conduction, we obtain the levels of Landau's energy $[5,8,9]$ by taking into account the spin $[10,11]$ of the electron after having neglected the term of the Coulomb's interaction. This technique involves a growth of the gap of $\mathrm{VO}_{2}$ which is considered as a weak gap [12].

## Methods

We solve the Schrödinger's equation $[10,11]$ in an exact method: $\mathrm{H} \psi=\mathrm{E} \psi$
H : The Hamiltonian of the system ( the electron of the conduction band).
$\Psi$ : The wave function of the electron.

$$
\mathrm{H}=\frac{1}{2 \mathrm{~m}^{*}}\left(-\mathrm{i} \hbar \vec{\nabla}+\frac{\mathrm{e}}{\mathrm{c}} \overrightarrow{\mathrm{~A}}_{0}\right)^{2}+\frac{1}{2} \mathrm{~g}_{0} \mu_{\mathrm{B}} \overrightarrow{\mathrm{~B}}_{0} \cdot \vec{\sigma}
$$

$\mu_{B}$ : the magneton of Bohr. $\mu_{B}=\frac{e \hbar}{2 \mathrm{~m}^{*}}$ Where $\mathrm{m}^{*}$ : the electron effective mass.
$\mathrm{g}_{0}$ : the factor of Lande
e : the elementary charge
$\hbar=\frac{\mathrm{h}}{2 \pi}$; h: Planck's constant
$\overrightarrow{\mathrm{M}}$ : the electron magnetic moment linked to its spin existence, $\overrightarrow{\mathrm{M}}=-\gamma \overrightarrow{\mathrm{S}}$.
$\vec{S}$ : the spin operator.
$\gamma$ : the gyromagnetic report.
$\vec{\sigma}$ : the vector whose components are the Pauli matrices $\sigma_{x}, \sigma_{y}, \sigma_{z}$.

$$
\begin{array}{ccc}
\vec{\sigma}=\left\lvert\, \begin{array}{l}
\sigma_{\mathrm{x}} \\
\sigma_{\mathrm{y}} \\
\sigma_{\mathrm{z}}
\end{array} \quad\right. ; \quad \gamma=\frac{2}{\hbar} \mu_{\mathrm{B}} \quad ; \quad \overrightarrow{\mathrm{S}}=\frac{\hbar}{2} \vec{\sigma} \\
{\left[\sigma_{\mathrm{x}}, \sigma_{\mathrm{y}}\right]=2 \mathrm{i} \sigma_{\mathrm{z}} ;} & {\left[\sigma_{\mathrm{y}}, \sigma_{\mathrm{z}}\right]=2 \mathrm{i} \sigma_{\mathrm{x}} \quad ; \quad\left[\sigma_{\mathrm{z}}, \sigma_{\mathrm{x}}\right]=2 \mathrm{i} \sigma_{\mathrm{y}}}
\end{array}
$$


$\mathrm{S}_{\mathrm{z}}=\frac{\hbar}{2} \sigma_{\mathrm{z}}=\frac{\hbar}{2}\left(\begin{array}{cc}1 & 0 \\ 0 & -1\end{array}\right) ; \quad \mathrm{S}_{\mathrm{z}}|+\rangle=\frac{\hbar}{2}|+\rangle \quad ; \quad \mathrm{S}_{\mathrm{z}}|-\rangle=-\frac{\hbar}{2}|-\rangle \quad ; \quad \sigma_{\mathrm{z}}=\left(\begin{array}{cc}1 & 0 \\ 0 & -1\end{array}\right)$

## 1 Coulomb's Gauge

The following gauge is chosen : div $\overrightarrow{\mathrm{A}}_{0}=0$ (Coulomb's gauge). We have $\vec{\nabla} \wedge \overrightarrow{\mathrm{A}}_{0}=\overrightarrow{\mathrm{B}}_{0} ; \overrightarrow{\mathrm{B}}_{0}=\overrightarrow{\mathrm{B}}_{0} \overrightarrow{\mathrm{Z}}$

$$
\begin{gathered}
\overrightarrow{\mathrm{A}}_{0}=\left|\begin{array}{l}
\mathrm{A}_{0 \mathrm{x}} \\
\mathrm{~A}_{0 \mathrm{y}} \\
\mathrm{~A}_{0 \mathrm{z}}
\end{array} ; \quad ; \vec{\nabla} \wedge \overrightarrow{\mathrm{A}}_{0}=\left|\begin{array}{l}
\frac{\partial}{\partial \mathrm{x}} \\
\frac{\partial}{\partial \mathrm{y}} \\
\frac{\partial}{\frac{\partial}{\partial}}
\end{array} \wedge\right| \begin{array}{l}
\mathrm{A}_{0 \mathrm{x}} \\
\mathrm{~A}_{0 \mathrm{y}} \\
\mathrm{~A}_{0 \mathrm{z}}
\end{array}\right| \begin{array}{l}
\frac{\partial \mathrm{A}_{0 \mathrm{z}}}{\partial \mathrm{y}}-\frac{\partial \mathrm{A}_{0 \mathrm{y}}}{\partial \mathrm{z}} \\
\frac{\partial \mathrm{~A}_{0 \mathrm{x}}}{\partial \mathrm{z}}-\frac{\partial \mathrm{A}_{0 \mathrm{z}}}{\partial \mathrm{x}} \\
\frac{\partial \mathrm{~A}_{0 \mathrm{y}}}{\partial \mathrm{x}}-\frac{\partial \mathrm{A}_{0 \mathrm{x}}}{\partial \mathrm{y}}
\end{array} \\
\operatorname{div} \overrightarrow{\mathrm{~A}}_{0}=\vec{\nabla} \wedge \overrightarrow{\mathrm{A}}_{0}=0 \Rightarrow \frac{\partial \mathrm{~A}_{0 \mathrm{x}}}{\partial \mathrm{x}}+\frac{\partial \mathrm{A}_{0 \mathrm{y}}}{\partial \mathrm{y}}+\frac{\partial \mathrm{A}_{0 \mathrm{z}}}{\partial \mathrm{z}}=0 \Rightarrow \mathrm{~A}_{0 \mathrm{z}}=\mathrm{A}_{0 \mathrm{y}}=\text { cste }=0 \\
\mathrm{~A}_{0 \mathrm{x}} \text { does not depend on } \mathrm{x} ; \quad-\frac{\partial \mathrm{A}_{0 \mathrm{x}}}{\partial \mathrm{y}}=\overrightarrow{\mathrm{B}}_{0} \Rightarrow \mathrm{~A}_{0 \mathrm{x}}=-\mathrm{B}_{0 \mathrm{y}}
\end{gathered}
$$

Where: $\quad \vec{A}_{0}=\left\lvert\, \begin{aligned} & A_{0 x}=B_{0} \\ & A_{0 y}=0 \\ & A_{0 \mathrm{z}}=0\end{aligned} \quad \Rightarrow \vec{A}_{0}=-B_{0 y} \overrightarrow{\mathrm{X}}\right.$
The gauge enables us to choose $\vec{A}_{0}=-B_{0 y} \overrightarrow{\mathrm{x}}$ since $\overrightarrow{\mathrm{A}}_{0}$ is not unique:

$$
\overrightarrow{\mathrm{A}}_{0}^{\prime}=\overrightarrow{\mathrm{A}}_{0}+\vec{\nabla} \mathrm{g}(\mathrm{r}) \text { where } \mathrm{g}(\mathrm{r}) \text { is a scalar function, } \vec{\nabla} \wedge \overrightarrow{\mathrm{A}}_{0}^{\prime}=\vec{\nabla} \wedge \overrightarrow{\mathrm{A}}_{0} \operatorname{car} \vec{\nabla}(\vec{\nabla} \mathrm{~g}(\mathrm{r}))=0
$$

## 2 Eigenvalues and eigenvectors of the Hamiltonian H.

In the representation $|\mathrm{r}\rangle$, we have $\overrightarrow{\mathrm{p}} \rightarrow-i \hbar \vec{\nabla}$, where:

$$
\begin{gathered}
\mathrm{H}=\frac{1}{2 \mathrm{~m}^{*}}\left(\overrightarrow{\mathrm{p}}+\frac{\mathrm{e}}{\mathrm{c}} \overrightarrow{\mathrm{~A}}_{0}\right)^{2}+\frac{1}{2} \mathrm{~g}_{0} \mu_{\mathrm{B}} \overrightarrow{\mathrm{~B}}_{0} \cdot \vec{\sigma} \\
\mathrm{H}=\mathrm{H}_{1}+\mathrm{H}_{2} \text { où } \mathrm{H}_{1}=\frac{1}{2 \mathrm{~m}^{*}}\left(\overrightarrow{\mathrm{p}}+\frac{\mathrm{e}}{\mathrm{c}} \overrightarrow{\mathrm{~A}}_{0}\right)^{2} ; \mathrm{H}_{2}=\frac{1}{2} \mathrm{~g}_{0} \mu_{\mathrm{B}} \overrightarrow{\mathrm{~B}}_{0} \cdot \vec{\sigma}
\end{gathered}
$$

We have:

$$
\begin{align*}
& \mathrm{H}_{1}=\frac{1}{2 \mathrm{~m}^{*}}\left(\mathrm{p}_{\mathrm{x}}^{2}+\mathrm{p}_{\mathrm{y}}^{2}+\mathrm{p}_{\mathrm{z}}^{2}\right)+\frac{1}{2 \mathrm{~m}^{*}} \cdot \frac{\mathrm{e}^{2}}{\mathrm{c}^{2}} \overrightarrow{\mathrm{~A}}_{0}^{2}+\frac{1}{2 \mathrm{~m}^{*}} \cdot \frac{\mathrm{e}}{\mathrm{c}} \overrightarrow{\mathrm{p}} \cdot \overrightarrow{\mathrm{~A}}_{0}+\frac{1}{2 \mathrm{~m}^{*}} \cdot \frac{\mathrm{e}}{\mathrm{c}} \overrightarrow{\mathrm{p}} \cdot \overrightarrow{\mathrm{~A}_{0}} \\
& H_{1}=\frac{1}{2 m^{*}}\left(p_{x}^{2}+p_{y}^{2}+p_{z}^{2}\right)+\frac{e^{2} B_{0}^{2}}{2 m^{*} c^{2}} y^{2}+\frac{e}{2 m^{*} c}\left(2 p_{x} \cdot A_{0 x}\right) \\
& H_{1}=\frac{1}{2 m^{*}}\left(p_{x}^{2}+p_{y}^{2}+p_{z}^{2}\right)+\frac{e^{2} B_{0}^{2}}{2 m^{*} c^{2}} y^{2}-\frac{e B_{0}}{m^{*} c} y p_{x} \\
& H_{1}=\frac{1}{2 m^{*}}\left[p_{x}^{2}-\frac{2 e B_{0}}{c} y p_{x}+\left(\frac{e B_{0}}{c} y\right)^{2}\right]+\frac{1}{2 m^{*}}\left(p_{y}^{2}+p_{z}^{2}\right) \\
& H_{1}=\frac{1}{2 m^{*}}\left(p_{x}-\frac{e B_{0}}{c} y\right)^{2}+\frac{1}{2 m^{*}}\left(p_{y}^{2}+p_{z}^{2}\right) \\
& \mathrm{H}_{1}=\frac{1}{2 \mathrm{~m}^{*}}\left[\left(\mathrm{p}_{\mathrm{x}}-\frac{\mathrm{e} \mathrm{~B}_{0}}{\mathrm{c}} \mathrm{y}\right)^{2}+\mathrm{p}_{\mathrm{y}}^{2}\right]+\frac{1}{2 \mathrm{~m}^{*}} \mathrm{p}_{\mathrm{z}}^{2} \quad ; \quad \mathrm{H}_{1}=\mathrm{H}_{1 \perp}+\mathrm{H}_{1 \|} \\
& \mathrm{H}_{1 \perp}=\frac{1}{2 \mathrm{~m}^{*}}\left[\left(\mathrm{p}_{\mathrm{x}}-\frac{\mathrm{eB}}{\mathrm{c}} \mathrm{y}\right)^{2}+\mathrm{p}_{\mathrm{y}}^{2}\right] \quad ; \quad \mathrm{H}_{1 \|}=\frac{1}{2 \mathrm{~m}^{*}} \mathrm{p}_{\mathrm{z}}^{2} \tag{1}
\end{align*}
$$

We consider $\varphi(x, y, z)$ solution of the equation $\mathrm{H}_{1} \varphi=\mathrm{E}_{1} \varphi$ :

$$
\begin{aligned}
& \varphi(x, y, z)=e^{i\left(k_{x} x+k_{z} z\right)} f(y) \\
& \left\{\frac{1}{2 m^{*}}\left(p_{x}-\frac{e B_{0}}{c} y\right)^{2}+\frac{1}{2 m^{*}}\left(p_{y}^{2}+p_{z}^{2}\right)\right\} e^{i\left(k_{x} x+k_{z} z\right)} f(y)=E_{1} e^{i\left(k_{x} x+k_{z} z\right)} f(y)
\end{aligned}
$$

In the representation $|\mathrm{r}\rangle$, we have :

$$
\mathrm{p}_{\mathrm{x}} \rightarrow-\mathrm{i} \hbar \frac{\partial}{\partial \mathrm{x}} ; \mathrm{p}_{\mathrm{y}} \rightarrow-\mathrm{i} \hbar \frac{\partial}{\partial \mathrm{y}} ; \mathrm{p}_{\mathrm{z}} \rightarrow-\mathrm{i} \hbar \frac{\partial}{\partial \mathrm{z}}
$$

We calculate:

$$
\begin{gathered}
\frac{1}{2 m^{*}}\left(p_{x}-\frac{e B_{0}}{c} y\right)^{2} e^{i\left(k_{x} x+k_{z} z\right)} f(y)=\frac{1}{2 m^{*}}\left(p_{x}-\frac{e B_{0}}{c} y\right)\left(-i \hbar \frac{\partial}{\partial x}-\frac{e B_{0}}{c} y\right) e^{i\left(k_{x} x+k_{z} z\right)} f(y) \\
\quad=\frac{1}{2 m^{*}}\left(-i \hbar \frac{\partial}{\partial x}-\frac{e B_{0}}{c} y\right)\left(\hbar k_{x}-\frac{e B_{0}}{c} y\right) e^{i\left(k_{x} x+k_{z} z\right)} f(y) \\
\quad=\frac{1}{2 m^{*}}\left(\hbar k_{x}-\frac{e B_{0}}{c} y\right)^{2} e^{i\left(k_{x} x+k_{z} z\right)} f(y)
\end{gathered}
$$

$\frac{1}{2 m^{*}} p_{y}^{2} e^{i\left(k_{x} x+k_{z} z\right)} f(y)=-\frac{1}{2 m^{*}} \hbar^{2} e^{i\left(k_{x} x+k_{z} z\right)} \frac{\partial^{2} f(y)}{\partial y^{2}}=-\frac{1}{2 m^{*}} \hbar^{2} e^{i\left(k_{x} x+k_{z} z\right)} f^{\prime \prime}(y)$
$\frac{1}{2 m^{*}} p_{z}^{2} e^{i\left(k_{x} x+k_{z} z\right)} f(y)=\frac{1}{2 m^{*}} \hbar^{2} k_{z}^{2} e^{i\left(k_{x} x+k_{z} z\right)} f(y)$
Where :

$$
\begin{align*}
& \frac{1}{2 m^{*}}\left\{\left(\hbar k_{x}-\frac{e B_{0}}{c} y\right)^{2} f(y)-\hbar^{2} f^{\prime \prime}(y)+\hbar^{2} k_{z}^{2} f(y)\right\}=E_{1} f(y)  \tag{4}\\
& \Rightarrow \frac{1}{2 m^{*}}\left\{-\hbar^{2} f^{\prime \prime}(y)+\left(\hbar k_{x}-\frac{e B_{0}}{c} y\right)^{2} f(y)\right\}=\left(E_{1}-\frac{\hbar^{2} k_{z}^{2}}{2 m^{*}}\right) f(y) \\
& \Rightarrow \frac{1}{2 m^{*}}\left\{\left(-i \hbar \frac{\partial}{\partial y}\right)^{2} f(y)+\left(y-y_{0}\right)^{2}\left(\frac{e B_{0}}{c}\right)^{2} f(y)\right\}=\left(E_{1}-\frac{\hbar^{2} k_{z}^{2}}{2 m^{*}}\right) f(y) \tag{5}
\end{align*}
$$

We pose:

$$
\mathrm{y}_{0}=\frac{\hbar c \mathrm{k}_{\mathrm{x}}}{\mathrm{eB}_{0}} ; \quad \omega_{0}=\frac{\mathrm{eB}_{0}}{\mathrm{~m}^{*} \mathrm{c}} ; \quad \varepsilon^{\prime}=\mathrm{E}_{1}-\frac{\hbar^{2} \mathrm{k}_{z}^{2}}{2 \mathrm{~m}^{*}}
$$

$$
\begin{align*}
\Rightarrow \frac{1}{2 m^{*}}\left\{p_{y}^{2}+\right. & \left.\left(y-y_{0}\right)^{2}\left(\frac{e B_{0}}{c}\right)^{2}\right\} f(y)=\varepsilon^{\prime} f(y) \\
& \Rightarrow\left\{\frac{p_{y}^{2}}{2 m^{*}}+\frac{1}{2} m^{*} \omega_{0}^{2}\left(y-y_{0}\right)^{2}\right\} f(y)=\varepsilon^{\prime} f(y) \tag{6}
\end{align*}
$$

Thus, $f(y)$ respects the harmonic oscillator's equation [10,11] of the energy $\varepsilon^{\prime}=E_{1}-\frac{\hbar^{2} k_{2}^{2}}{2 \mathrm{~m}^{*}}$ We know that $\varepsilon^{\prime}$ is quantified: $\varepsilon^{\prime}=\hbar \omega_{0}\left(\mathrm{n}+\frac{1}{2}\right)$ where $\mathrm{n}=0 ; 1 ; 2 ; 3 ; \ldots$,
Where :

$$
\begin{equation*}
\mathrm{E}_{1}=\varepsilon^{\prime}+\frac{\hbar^{2} \mathrm{k}_{z}^{2}}{2 \mathrm{~m}^{*}} ; \quad \mathrm{E}_{1}=\hbar \omega_{0}\left(\mathrm{n}+\frac{1}{2}\right)+\frac{\hbar^{2} \mathrm{k}_{z}^{2}}{2 \mathrm{~m}^{*}} \tag{7}
\end{equation*}
$$

$\mathrm{E}_{1}$ is eigenenergy of the Hamiltonien H .
We search for the eigenvalues and the eigenvectors associated with $\mathrm{H}_{2}$

$$
\mathrm{H}_{2}=\frac{1}{2} \mathrm{~g}_{0} \mu_{\mathrm{B}} \overrightarrow{\mathrm{~B}}_{0} \cdot \vec{\sigma}=\frac{1}{2} \mathrm{~g}_{0} \mu_{\mathrm{B}} \mathrm{~B}_{0} \cdot \sigma_{\mathrm{z}}
$$

We know that $\sigma_{z}=\left(\begin{array}{cc}1 & 0 \\ 0 & -1\end{array}\right)$ in the base $\{|+\rangle,|-\rangle\}$ space $\mathrm{E}_{\mathrm{s}}$ the spin's states of the electron.

$$
\begin{aligned}
\mathrm{H}_{2}|+\rangle= & \frac{1}{2} \mathrm{~g}_{0} \mu_{\mathrm{B}} \mathrm{~B}_{0} \cdot \sigma_{\mathrm{z}}|+\rangle=\frac{1}{2} \mathrm{~g}_{0} \mu_{\mathrm{B}} \mathrm{~B}_{0}|+\rangle=\mathrm{E}_{2+}|+\rangle \\
& \Rightarrow \mathrm{E}_{2+}=\frac{1}{2} \mathrm{~g}_{0} \mu_{\mathrm{B}} \mathrm{~B}_{0} \xrightarrow{\text { eigenvector }}|+\rangle
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{H}_{2}|-\rangle= & \frac{1}{2} \mathrm{~g}_{0} \mu_{\mathrm{B}} \mathrm{~B}_{0} \cdot \sigma_{\mathrm{z}}|-\rangle=-\frac{1}{2} \mathrm{~g}_{0} \mu_{\mathrm{B}} \mathrm{~B}_{0}|-\rangle=\mathrm{E}_{2-}|-\rangle \\
& \Rightarrow \mathrm{E}_{2-}=-\frac{1}{2} \mathrm{~g}_{0} \mu_{\mathrm{B}} \mathrm{~B}_{0} \xrightarrow{\text { eigenvect or }}|-\rangle
\end{aligned}
$$

Where the total energy of the system is:

$$
\begin{align*}
& \mathrm{E}_{+}=\mathrm{E}_{1}+\mathrm{E}_{2+}=\hbar \omega_{0}\left(\mathrm{n}+\frac{1}{2}\right)+\frac{\hbar^{2} \mathrm{k}_{z}^{2}}{2 \mathrm{~m}^{*}}+\frac{1}{2} \mathrm{~g}_{0} \mu_{\mathrm{B}} \mathrm{~B}_{0}  \tag{8}\\
& \mathrm{E}_{-}=\mathrm{E}_{1}+\mathrm{E}_{2-}=\hbar \omega_{0}\left(\mathrm{n}+\frac{1}{2}\right)+\frac{\hbar^{2} \mathrm{k}_{z}^{2}}{2 \mathrm{~m}^{*}}-\frac{1}{2} \mathrm{~g}_{0} \mu_{\mathrm{B}} \mathrm{~B}_{0} \tag{9}
\end{align*}
$$

These are the energy levels of Landau by taking into consideration the spin of the electron in a magnetic field $\overrightarrow{\mathrm{B}}_{0}=\mathrm{B}_{0} \overrightarrow{\mathrm{z}}$.

## 3 The eigenstate of $\mathrm{H}_{1}$

The eigenfunction is: $\varphi(\mathrm{x}, \mathrm{y}, \mathrm{z})=\mathrm{e}^{\mathrm{i}\left(\mathrm{k}_{\mathrm{x}} \mathrm{x}+\mathrm{k}_{z} z\right)} \mathrm{f}(\mathrm{y})$
$\varepsilon^{\prime}=\hbar \omega_{0}\left(n+\frac{1}{2}\right)$ is the eigenenergy with the eigenfunction $f(y) \Rightarrow f(y)=C_{n} e^{-\frac{a^{2}}{2} y^{2}} H_{n}(y \alpha)$

$$
\text { with } \alpha^{2}=\frac{\mathrm{m}^{*} \omega_{0}}{\hbar} ; \mathrm{H}_{\mathrm{n}} \text { is the Hermit polynomial; } \mathrm{C}_{\mathrm{n}}=\left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}}\left(2^{\mathrm{n}} \cdot \mathrm{n}!\right)^{-\frac{1}{2}} \text { is the standardization constant }
$$

$$
\Rightarrow f(y)=\left(\frac{m^{*} \omega_{0}}{\pi^{2} \hbar}\right)^{\frac{1}{8}}\left(2^{n} \cdot n!\right)^{-\frac{1}{2}} e^{-\frac{m^{*} \omega_{0}}{2 \hbar} y^{2}} H_{n}(y \alpha)
$$

$$
H_{n}(y \alpha)=(-1)^{n} e^{\alpha^{2} y^{2}} \frac{d^{n}}{(d(\alpha y))^{n}} \exp \left(-\alpha^{2} y^{2}\right)
$$

$$
\begin{equation*}
\Rightarrow \varphi(x, y, z)=\left(\frac{m^{*} \omega_{0}}{\pi^{2} \hbar}\right)^{\frac{1}{8}}\left(2^{n} \cdot n!\right)^{-\frac{1}{2}} e^{i\left(k_{x} x+k_{z} z\right)} e^{-\frac{m^{*} \omega_{0}}{2 \hbar} y^{2}} H_{n}(y \alpha) \tag{10}
\end{equation*}
$$

$\varphi(\mathrm{x}, \mathrm{y}, \mathrm{z})$ is the eigenfunction associated with $\mathrm{H}_{1}$
$S_{z}$ has the eigenvector $|+\rangle$ et $|-\rangle$ as it is the case with $\sigma_{z}$.
We associate the energy $\mathrm{E}_{+}$to the eigenstate $\varphi(\mathrm{x}, \mathrm{y}, \mathrm{z}) \otimes|+\rangle=\varphi(\mathrm{x}, \mathrm{y}, \mathrm{z})|+\rangle$ noted $\left|\psi_{+}\right\rangle$
$\left|\Psi_{+}\right\rangle=\left(\frac{m^{*} \omega_{0}}{\pi^{2} \hbar}\right)^{\frac{1}{8}}\left(2^{n} \cdot n!\right)^{-\frac{1}{2}} e^{i\left(k_{x} x+k_{z} z\right)} e^{-\frac{m^{*} \omega_{0}}{2 \hbar} y^{2}} H_{n}(y \alpha)|+\rangle$
We associate the energy $\mathrm{E}_{-}$to the eigenstate $\varphi(\mathrm{x}, \mathrm{y}, \mathrm{z}) \otimes|-\rangle=\varphi(\mathrm{x}, \mathrm{y}, \mathrm{z})|-\rangle$ noted $\left|\psi_{-}\right\rangle$
$\left|\psi_{-}\right\rangle=\left(\frac{m^{*} \omega_{0}}{\pi^{2} \hbar}\right)^{\frac{1}{8}}\left(2^{n} \cdot n!\right)^{-\frac{1}{2}} e^{i\left(k_{x} x+k_{z} z\right)} e^{-\frac{m^{*} \omega_{0}}{2 \hbar} y^{2}} H_{n}(y \alpha)|-\rangle$
Thus, $\left|\psi_{+}\right\rangle$and $\left|\psi_{-}\right\rangle$are the eigenvectors of the Hamiltonian $H$ of the respective eigenenergies $E_{+}$and $E_{-}$, such as :

$$
\begin{align*}
& \mathrm{E}_{+}=\mathrm{E}_{1}+\mathrm{E}_{2+}=\hbar \omega_{0}\left(\mathrm{n}+\frac{1}{2}\right)+\frac{\hbar^{2} \mathrm{k}_{\mathrm{z}}^{2}}{2 \mathrm{~m}^{*}}+\frac{1}{2} \mathrm{~g}_{0} \mu_{\mathrm{B}} \mathrm{~B}_{0}  \tag{13}\\
& \mathrm{E}_{-}=\mathrm{E}_{1}+\mathrm{E}_{2-}=\hbar \omega_{0}\left(\mathrm{n}+\frac{1}{2}\right)+\frac{\hbar^{2} \mathrm{k}_{\mathrm{z}}^{2}}{2 \mathrm{~m}^{*}}-\frac{1}{2} \mathrm{~g}_{0} \mu_{\mathrm{B}} \mathrm{~B}_{0} \tag{14}
\end{align*}
$$



Figure 1: Landau's Levels associated with the conduction band and the valence band of a direct gap semiconductor.

We note that in the presence of a magnetic field $\overrightarrow{\mathrm{B}}_{0}$, the gap energy [12] undergoes an increase in this variation :

$$
\begin{equation*}
\Delta \mathrm{E}_{\mathrm{g}}=\frac{1}{2}\left(\frac{1}{\mathrm{~m}_{\mathrm{c}}}+\frac{1}{\mathrm{~m}_{\mathrm{v}}}\right) \frac{\mathrm{e} \hbar \mathrm{~B}_{0}}{\mathrm{c}} \quad \text { unit (C.G.S) } \tag{15}
\end{equation*}
$$

$\frac{1}{\mathrm{~m}_{\mathrm{c}}}+\frac{1}{\mathrm{~m}_{\mathrm{v}}}=\frac{1}{\mu} ; \quad$ where $\mu$ is the reduced mass of the particle (electron - hole)
We see that $\Delta \mathrm{E}_{\mathrm{g}}$ is proportional to $\frac{1}{\mu}$ and to $\mathrm{B}_{0}$; and we write :

$$
\begin{equation*}
\Delta \mathrm{E}_{\mathrm{g}}=\frac{\mathrm{e} \hbar}{\mathrm{c}} \cdot \frac{1}{2 \mu} \mathrm{~B}_{0} \tag{16}
\end{equation*}
$$

## Results

By using the following data in the system (S.I):

$$
4 \mathrm{~m}_{0} \leq \mu \leq 14 \mathrm{~m}_{0}
$$

We vary the reduced mass [13] by fixing the magnetic field $B=B_{0}$ in intensity as follows:

$$
\text { for } B=10 \mathrm{~T} ; B=45 \mathrm{~T} ; B=2000 \mathrm{~T}
$$

We obtain the following results:




Figure 2: (a), (b) and (c) variation of the $\mathrm{VO}_{2}$ gap according to the reduced mass $\mu$ for a magnetic field $B=10 \mathrm{~T}, \mathrm{~B}=45 \mathrm{~T}, \mathrm{~B}=2000 \mathrm{~T}$.

By using the following data in the system (S.I):

$$
0 \mathrm{~T} \leq \mathrm{B} \leq 2000 \mathrm{~T}
$$

$$
\mathrm{m}_{0}=9.1 \cdot 10^{-31} ; \hbar=1.05457 \cdot 10^{-34} ; \mathrm{e}=1.6 \cdot 10^{-19} ;
$$

We vary the magnetic field $B$ in intensity by fixing the reduced mass as follows:

$$
\text { for } \mu=4 \cdot \mathbf{m}_{0} ; \mu=14 \cdot \mathbf{m}_{0}
$$

We make the simulation of the variation $\Delta \mathrm{E}_{\mathrm{g}}$ gap of the massive vanadium dioxide, our results are as follows:



Figure 3: (d) and (h) variation of the massive $\mathrm{VO}_{2}$ gap according to the magnetic field B for the reduced mass $\mu=4 \mathrm{~m}_{0}$ and $\mu=14 \mathrm{~m}_{0}$

## Discussion :

For $\mathrm{B}=0 \mathrm{~T}$, the energy of the vanadium dioxide gap is $\mathrm{E}_{\mathrm{g}}=0.7 \mathrm{ev}$. During the application of the magnetic field of intensity $B=10 \mathrm{~T}$, we clearly notice a variation $\Delta \mathrm{E}_{\mathrm{g}}$ from 0.00018 ev to 0.00006 ev in the interval $4 \mathrm{~m}_{0} \leq \mu \leq 14 \mathrm{~m}_{0}$, which corresponds obviously to a decrease in $\Delta \mathrm{E}_{\mathrm{g}}$, but the gap widens and becomes $\mathrm{E}=\Delta \mathrm{E}_{\mathrm{g}}+\mathrm{E}_{\mathrm{g}}$. The absorption threshold is :

$$
\lambda_{1}=\lambda_{\mathrm{c}}(\mathrm{~nm})=\frac{\mathrm{hc}(\mathrm{ev} \cdot \mathrm{~nm})}{\mathrm{E}_{\mathrm{g}}(\mathrm{ev})}
$$

For the vanadium dioxide $\mathrm{VO}_{2}$ semiconductor:

$$
\lambda_{1}=\lambda_{\mathrm{c}}(\mathrm{~nm})=\frac{1242,4125(\mathrm{ev} \cdot \mathrm{~nm})}{\mathrm{E}_{\mathrm{g}}(\mathrm{ev})}=1774,875 \mathrm{~nm}
$$

This threshold is located in the average infra-red.
When $\lambda<\lambda_{1}$, the absorption becomes fast since the broad absorption coefficient $\alpha$ is very big. But when the gap is widened of $\Delta \mathrm{E}_{\mathrm{g}}$, we have a new absorption threshold:

$$
\lambda_{2}=\lambda_{\mathrm{c}}(\mathrm{~nm})=\frac{1242,4125(\mathrm{ev} \cdot \mathrm{~nm})}{\mathrm{E}_{\mathrm{g}}+\Delta \mathrm{E}_{\mathrm{g}}}
$$

When the threshold of absorption becomes: $\lambda<\lambda_{2}$, we have a widening in the spectral band of the $\mathrm{VO}_{2}$ absorption.
For $B=45 T$, the gap variation becomes : $0.0008 \leq \Delta \mathrm{E}_{\mathrm{g}}(\mathrm{ev}) \leq 0.0002$ in the interval of the reduced mass $4 \mathrm{~m}_{0} \leq \mu \leq 14 \mathrm{~m}_{0}$. We note an important increase in the gap even if $\Delta \mathrm{E}_{\mathrm{g}}(\mathrm{ev})$ according to $\mu$ decreases when $\mu$ increases.

The absorption threshold becomes:

$$
\lambda_{3}=\frac{1242,4125(\mathrm{ev} \cdot \mathrm{~nm})}{\mathrm{E}_{\mathrm{g}}+\Delta \mathrm{E}_{\mathrm{g}}}
$$

The absorption of the incidental photons is fast for $\lambda<\lambda_{3}$.
For $B=2000 \mathrm{~T}$, the variation of the gap becomes: $0.035 \leq \Delta \mathrm{E}_{\mathrm{g}}(\mathrm{ev}) \leq 0.010$ in the interval of the reduced mass [13], $4 \mathrm{~m}_{0} \leq \mu \leq 14 \mathrm{~m}_{0}$. We see that $\Delta \mathrm{E}_{\mathrm{g}}(\mathrm{ev})$ decreases when $\mu$ increases, but the gap variation $\mathrm{E}=\mathrm{E}_{\mathrm{g}}+\Delta \mathrm{E}_{\mathrm{g}}$ becomes important. The absorption threshold is in this case:

$$
\lambda_{4}=\frac{1242,4125(\mathrm{ev} \cdot \mathrm{~nm})}{\mathrm{E}_{\mathrm{g}}+\Delta \mathrm{E}_{\mathrm{g}}}
$$

The absorption of the incidental photons is fast for $\lambda<\lambda_{4} ; \lambda=\lambda_{\text {photon }}$.
Tables. Calculation of the absorption threshold and $\mathrm{VO}_{2}$ gap during the application of the magnetic field $B$ for $\mu=4 m_{0}$ and $\mu=14 m_{0}$.

| $\lambda_{\mathrm{c}}(\mathrm{nm})$ | $\mu=4 \mathrm{~m}_{0}$ | $\mathrm{~B}(\mathrm{~T})$ | Condition of <br> absorption | $\mathrm{E}(\mathrm{ev})=\mathrm{E}_{\mathrm{g}}+\Delta \mathrm{E}_{\mathrm{g}}$ |
| :---: | :---: | :---: | :---: | :---: |
| $\lambda_{1}$ | 1774,8750 | 0 | $\lambda_{\mathrm{ph}}<\lambda_{1}$ | 0,7 |
| $\lambda_{2}$ | 1774,4187 | 10 | $\lambda_{\mathrm{ph}}<\lambda_{2}$ | 0,70015 |
| $\lambda_{3}$ | 1772,8488 | 45 | $\lambda_{\mathrm{ph}}<\lambda_{3}$ | 0,7006 |
| $\lambda_{4}$ | 1690,3571 | 2000 | $\lambda_{\mathrm{ph}}<\lambda_{4}$ | 0,732 |


| $\lambda_{\mathrm{c}}(\mathrm{nm})$ | $\mu=14 \mathrm{~m}_{0}$ | $\mathrm{~B}(\mathrm{~T})$ | Condition of <br> absorption | $\mathrm{E}(\mathrm{ev})=\mathrm{E}_{\mathrm{g}}+\Delta \mathrm{E}_{\mathrm{g}}$ |
| :---: | :---: | :---: | :---: | :---: |
| $\lambda_{1}$ | 1774,8750 | 0 | $\lambda_{\mathrm{ph}}<\lambda_{1}$ | 0.7 |
| $\lambda_{2}$ | 1774,7228 | 10 | $\lambda_{\mathrm{ph}}<\lambda_{2}$ | 0,70004 |
| $\lambda_{3}$ | 1774,3680 | 45 | $\lambda_{\mathrm{ph}}<\lambda_{3}$ | 0,70015 |
| $\lambda_{4}$ | 1749,8767 | 2000 | $\lambda_{\mathrm{ph}}<\lambda_{4}$ | 0,7083 |

## Conclusion

According to this study, we retain a good result by obtaining a broad absorption threshold for $\mu=4 \mathrm{~m}_{0}$ while comparing it with $\mu=14 \mathrm{~m}_{0}$. Indeed, we need a very intense field for $\mu=14 \mathrm{~m}_{0}$ so as to widen this gap.
As a result, we have the increase in the absorption coefficient $\alpha$ in the average I.R. This can be of a good practical utility in the industry, particularly the scanners, the microwaves, telecommunication means, and the photovoltaics.
Perspectives: to perform the same study for the thin layers of $\mathrm{VO}_{2}$ where the potential of containment $\mathrm{V}_{\text {conf }}$ is added in the Hamiltonian, in order to solve the Schrödinger's equation and to study the variation of the absorption coefficient a of these layers [16] in the I.R, the U.V and the visible specters.

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