Modeling Mott Transition in a Disordered System by Sinc Wavelets and the Minimal Sensitivity Principle

ARMANDO BARRAÑÓN
Department of Basic Sciences
Universidad Autónoma Metropolitana
Av. San Pablo 180
MEXICO
armandobarranon@yahoo.com.mx http://armandobarranon.freewebpages.org

Abstract: - A new method is developed that uses Minimal Sensitivity Principle and Sinc wavelets to obtain the critical impurity concentration in doped semiconductors. Thomas-Fermi theory of metals is employed and results are coincident with those of other methods. Schrödinger equation is solved to obtain the eigenvalue of the ground state for different impurity concentrations until this binding energy is equal to cero signing a Mott transition. Numerical results confirm experimental observations since binding energies are in the experimental range and diminish when impurity concentration is raised. Minimal Sensitivity Principle is used to employ a new invariant in order to obtain the optimal size of the grid used to discretize the eigenvalue problem, significantly reducing space and time complexity. The successful application of this new approach animates us to study more complex systems.

Key-Words: - Minimal Sensitivity Principle, Mott Transition, Sinc Wavelets

1 Introduction

Doped semiconductors with a high concentration of donor centers show a degenerate gas in the conduction band. If this concentration is lowered, an impurity band will split off from the conduction band. When this concentration is still smaller, there will be a gap between the occupied and empty states and a metal-to-nonmetal (MNM) transition will occur. Using a dielectrically screened Coulomb potential and a 1s hydrogenic orbital, Mott obtained a critical density given by:

$$n_c^{1/3} a_H = 0.25 \tag{1}$$

where a_H is the first Bohr radius in the material [1]:

$$a_H = \frac{\hbar^2 \kappa}{me^2} \tag{2}$$

The Mott transition is related to the weakness of an attractive potential to have negative energy eigenstates. Bargmann provided an estimate of this potential weakness[2]:

$$\left(\frac{m}{\hbar^2}\right)\int_0^\infty dr|V(r)| \le \frac{1}{2} \tag{3}$$

For the screened Coulomb potential [3], this relation gives:

$$\left(\frac{m}{\hbar^2}\right)\int_0^\infty dr\left|\frac{Ze^2 e^{-\alpha r}}{\kappa r}\right| \le 0.8399... \tag{4}$$

$$\Rightarrow \alpha^{-1} \le 0.8399\left(\frac{\kappa\hbar^2}{Ze^2 m}\right) \tag{5}$$

Hence if:

$$\alpha^{-1} \le 0.8399\left(\frac{\kappa\hbar^2}{Ze^2 m}\right) = 0.8399a \tag{6}$$

the potential is too weak to have a bound solution of the Schrödinger equation.

Hultén potential is an ansatz potential for doped semiconductors whose exact solution is known:

$$V(r) = \frac{e^2\alpha}{\kappa(e^{\alpha r} - 1)} \tag{7}$$

Clearly, when $\alpha \to 0$, Hultén potential converges to the screened Coulomb potential. Using the exact analytical solution of this potential, the following critical impurity concentration is obtained:

$$n_c^{1/3} a_{Eff} = 0.422 \tag{8}$$

where:

$$a_{Eff} = \left[N^{2/3}\left(\frac{E_c}{E_g}\right)\left(\frac{e^2}{2\kappa E_g}\right)\right] \tag{9}$$

and: $E_g = \frac{me^4}{2\kappa^2\hbar^2}$ is the energy of the center of mass [2].

In this study we use Sinc Collocation and Minimal Sensitivity Principle to obtain a close estimate of the

critical impurity concentration in the range of 0.35 when impurity disorder is considered.

2 Problem Formulation

In order to study the effect of disorder, the impurity potential $v(r)$ is treated as a statistical quantity where $p(t)dt$ is the probability of finding the given value of $v(r)$ within the interval t and $t+dt$, where $t=|v(r)|$.

We take the probability density function as [4]:

$$p(t)=(1/\mu)\exp(-t/\mu) \tag{10}$$

and: $v_d = XP(|X|)$, where $X=v(r)$. Hence:

$$P(|X|)=\int_0^{|X|} p(t)dt \tag{11}$$

and:

$$v_d(r)=v(r)\left[1-|v(r)|/\mu\right] \tag{12}$$

Therefore:

$$v_d(r)=\left(-\frac{2}{r}\right)e^{-r/L}\left[1-\left(\frac{2}{\mu r}\right)e^{-r/L}\right] \tag{13}$$

where:

$$\mu = n\int |v(r)|4\pi r^2 dr \tag{14}$$

$$\mu = n\int \frac{2}{r}\exp\left(-\frac{r}{L}\right)4\pi r^2 dr \tag{15}$$

$$\Rightarrow \mu = 8\pi nL^2\left\{\left[-\exp(-u)\right]_0^{\infty}\right\}=8\pi nL^2 \tag{16}$$

Considering [7]:

$$L^2 = \left(3\pi^2/\nu\right)^{1/3}/\left(12\,\pi a^* n^{1/3}\right) \tag{17}$$

we obtain:

$$\mu=\frac{2\left(c^*\right)^2\left(3\pi^2/\nu\right)^{1/3}}{3\left(a^*\right)^3} \tag{18}$$

where the effective Bohr radius is given by $a^*=207\overset{o}{A}$ and c^* is the impurity concentration.

Finally:

$$v_d(\rho)= \left(-\frac{2}{\rho}\right)e^{-\rho/L}\left[1-\exp\left\{-\left(\frac{3\left(a^*\right)^3}{\rho\left(c^*\right)^2\left(3\pi^2/\nu\right)^{1/3}}\right)e^{-\rho/L}\right\}\right] \tag{19}$$

2.1 Sinc Collocation Method

In Sinc Collocation Method, the following expansions hold [5]:

$$f(x)\approx \sum_{m=-M}^{M} S(m,a)(\phi(x))f(x_m) \tag{20}$$

and:

$$f''(x)\approx \sum_{m=-M}^{M}\left\{\left[(\phi'(x))^2\frac{d^2}{d\phi^2}+\phi''(x)\frac{d}{d\phi}\right]S(m,a)(\phi(x))\right\}f(x_m) \tag{21}$$

where:

$$S(m,a)(x)=\frac{\{\sin[(\frac{\pi}{a})(x-ma)]\}}{[(\frac{\pi}{a})(x-ma)]}=|m,a\rangle \tag{22}$$

Substituting in Schrödinger equation:

$$y''+\left[\lambda-v(\rho)-l(l+1)/\rho^2\right]y=0 \tag{23}$$

leads to:

$$\sum_{m=-M}^{M}\left\{\left[(\phi'(x))^2\frac{d^2S(m,a)(\phi(x))}{d\phi^2}+\phi''(x)\frac{dS(m,a)(\phi(x))}{d\phi}\right]\right\}f(x_m) +\left[\lambda-v_d(\rho)-l(l+1)/\rho^2\right]\sum_{m=-M}^{M}S(m,a)(\phi(x))f(x_m)=0 \tag{24}$$

Since:

$$S(m,a)(x_n)=\delta_{n,m}^{(0)} \tag{25}$$

and:

$$\frac{d}{dx}[S(m,a)(x)]|_{x=x_n}=-(\tfrac{1}{a})\delta_{n,m}^{(1)} \tag{26}$$

where:

$$\delta_{n,m}^{(1)}=\begin{cases}0, m=n\\ \frac{(-1)^{m-n}}{(m-n)}, m\neq n\end{cases} \tag{27}$$

Also:

$$\frac{d^2}{dx^2}[S(m,a)(x)]|_{x=x_n}=(\tfrac{1}{a^2})\delta_{n,m}^{(2)} \tag{28}$$

where:

$$\delta_{n,m}^{(2)}=\begin{cases}-\frac{\pi^2}{3}, m=n\\ 2\frac{(-1)^{m-n+1}}{(m-n)^2}, m\neq n\end{cases} \tag{29}$$

Substituting:

$$\sum_{m=-M}^{m=N}\{I_{n,m}^{(0)}+I_{n,m}^{(1)}+I_{n,m}^{(2)}\}f(\rho_m)=\lambda f(\rho_n) \tag{30}$$

where:

$$I_{n,m}^{(0)}=\delta_{n,m}^{(0)}\left[v_d(\rho)+l(l+1)/\rho^2\right] \tag{31}$$

$$I_{n,m}^{(1)}=\exp(-2na)\frac{\delta_{n,m}^{(1)}}{a} \tag{32}$$

$$I_{n,m}^{(2)}=-(1+\exp(-2na))\frac{\delta_{n,m}^{(2)}}{a^2} \tag{33}$$

where the following conformal mapping has been used:

$$\rho_n = \ln\left[\exp(na) + \sqrt{1+\exp(-2na)}\right] \tag{34}$$

The trace of the system is given by:

$$TrH = \sum_{n=-M}^{N} \left(1+\exp(-2na)\right)\frac{\pi^2}{3a^2} + v_d(\rho_n) + l(l+1)/\rho_n^2 \tag{35}$$

Since it is an invariant, the Minimal Sensitivity Principle may be used to obtain the optimal size of the Sinc expansion series. This is accomplished solving [6]:

$$\frac{d(TrH)}{da} = 0 \tag{36}$$

hence:

$$\begin{aligned}\frac{d(TrH)}{da} &= \sum_{n=-M}^{N} \left(1+\exp(-2na)\right)\left[-\frac{2\pi^2}{3a^3}\right] \\ &- 2n\exp(-2na)\left[\frac{\pi^2}{3a^2}\right] \\ &+ \left[\frac{2}{\rho_n^2}\exp(-\rho_n/L)\right]\left[\frac{n\exp(na)}{\sqrt{1+\exp(2na)}}\right] \\ &+ \left[\frac{2}{L\rho_n}\exp(-\rho_n/L)\right]\left[\frac{n\exp(na)}{\sqrt{1+\exp(2na)}}\right] \\ &- \left[2l(l+1)/\rho_n^3\right]\left[\frac{n\exp(na)}{\sqrt{1+\exp(2na)}}\right] = 0\end{aligned} \tag{37}$$

this gives us the optimal size of the Sinc Collocation Series.

3 Problem Solution

Minimal Sensitivity Principle signed an optimal basis of size N=4 and M=27 and a critical value of a=0.355. Numerical results confirm other experimental observations since binding energies are in the experimental range and diminish when impurity concentration is increased. Fig. 1 shows that binding energy diminishes when impurity concentration is raised and a non metal-metal transition is attained when the impurity concentration is in the range of 0.42.

This critical impurity concentration equal to 0.42 is in the range of other theoretical results, such as the value of the critical impurity concentration equal to 0.43 obtained by Martino et. al. using a Hubbard-Sham dielectric screening function [1]. Also, Green et. al. have obtained a critical impurity concentration equal to 0.398 with a hydrogenic trial function and a Lindhard dielecric screening function [7]. Our critical impurity concentration value is also close to the value of 0.422 as reported in [2] and to the experimental result for doped Germanium in the range of 0.47 [2].

Therefore we may say that results are in the range of other theoretical and experimental results for similar systems. Since computations were carried out in a few minutes using a 3GHz PC, we are motivated to study more complex systems via Sinc Collocation and Minimal Sensitivity Principle.

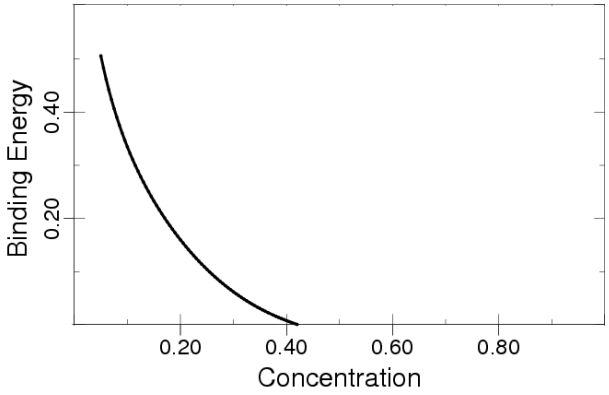

Fig. 1.- shows that binding energy diminishes when impurity concentration is raised and a non metal-metal transition is attained when the impurity concentration is in the range of 0.42 which is between the value reported of 0.398 reported in [7] and the value of 0.422 as reported in [2].

4 Conclusion

We have obtained critical impurity concentrations in the range of experimental and theoretical results by Sinc Collocation Method and Minimal Sensitivity Principle. This animates us to study more complex systems in the future. A.B. acknowledges the support of a Postdoctoral Fellowship at CINVESTAV granted by CONACYT-48795 Fund.

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