Chapter 3

Quantum orbital motion of a charged particle on a discrete triangular ring linking an A-B flux: decoherence of the diamagnetic moment through Lindblads(phenomenological approach)

3.1 Abstract

Following the finding of Chapter **2,** namely, that the Lindblad operators, despite their infinite heating effects, do provide a physically reasonable description of the quantum motion on a discrete bandwidth-limited lattice coupled to the dissipative environment, we now study in this Chapter yet another quantum phenomenon that has no classical analogue–the orbital diamagnetic moment of a charged particle moving on a discrete

ring linking an A-B flux and presumably 'decohered' through the Lindblad operators. For this, we consider a tight-binding 1-band Hamiltonian for a finite three-center-system (an idealized annulene), where the A-B flux enters through the Peierls phase factors multiplying the tunneling matrix elements. Time(t) evolutions of several physical physical quantities are derived, in particular, those of the orbital magnetization (M) and the diagonal elements ρ_{ii} of the reduced density matrix. By eliminating the time (t) in favour of a functional relation between $M(t)$ and a certain ratio(to be identified with the instantaneous Boltzmann factor) of the diagonal elements$\rho_{ii}(t)$ of the reduced density matrix defining the instantanious temperature $T(t)$, we obtain the temperature (T) dependance of the magnetization M(T) despite the fact that the Lindblads heat up the system to infinite temperature as t $\rightarrow \infty$. Thusly calculated M-T plot is found to be consistent with the equilibrium statistical-mechanical results for the system giving a non-zero magnetization. We do, however, demand that the heating time be reasonably long as compared to the internal dynamic time-scale of the system, namely, $\hbar/Band$ Width.

3.2 The isolated system(no coupling to the bath):

The system Hamiltonian H is

$$H = -Ve^{i\theta}[|a\rangle\langle b| + |b\rangle\langle c| + |c\rangle\langle a|] + h.c. \tag{3.1}$$

where $-V$(taken to be negative real) is the transfer matrix element in the absence of the flux ϕ, and $\theta = \frac{A}{3\phi_0}B$ is the Peierls phase.(Here A is the area of the three-center plaquette and ϕ_0 is the flux quantum $= hc/|e|$). The energy eigenvalues of the above elementary Hamiltonian are readily found to be

$$\lambda_0 = -2V\cos\theta \ ,$$
$$\lambda_1 = V[\cos\theta + \sqrt{3}\sin\theta] \ ,$$
$$\lambda_2 = V[\cos\theta - \sqrt{3}\sin\theta]. \tag{3.2}$$

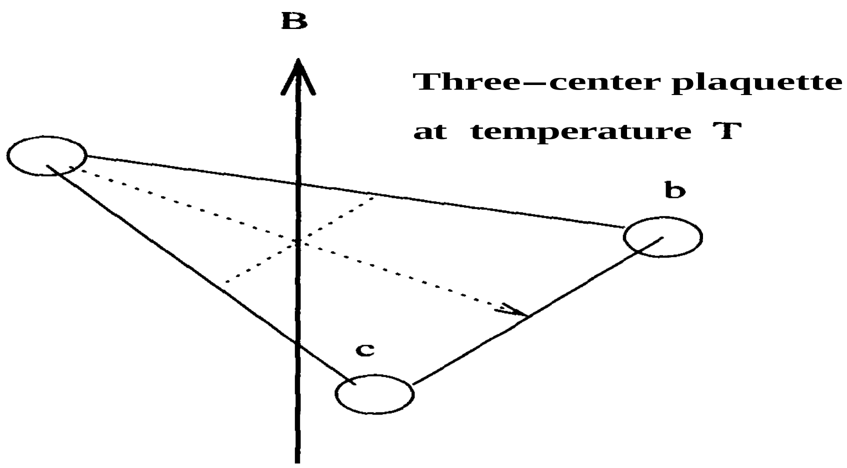

Figure 3.1: The three-center plaquette at temperature T with A-B flux.

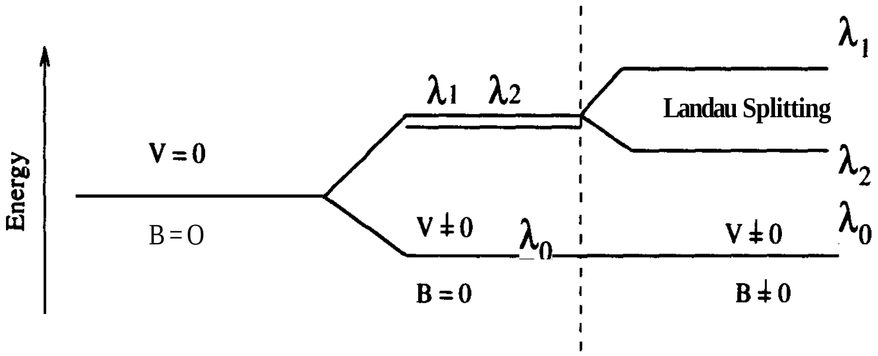

Figure 3.2: Energy level diagram.

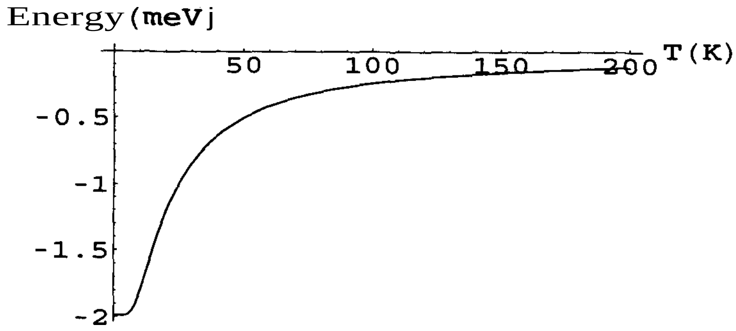

Figure 3.3: An illustrative plot of system's mean energy(in meV)as a function of temperature@ K) at magnetic field B $= 1/2\pi$ tesla. Here the matrix element V $= 1meV$, and inter-site distance = 40nm

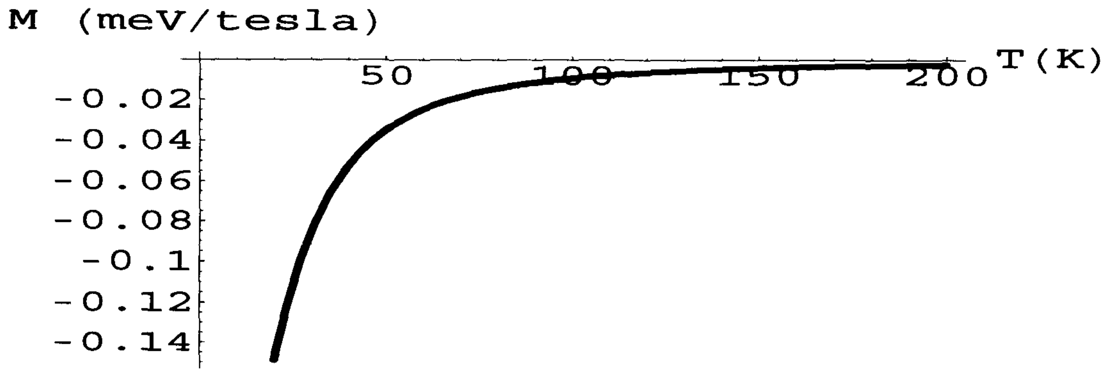

Figure 3.4: Magnetization$M(eV/tesla)$ as a function of temperature $T(K)$ at B $= 1/2\pi$ tesla.

For this elementary model, all physical quantities are readily calculable. Thus, from the mean energy (Figure 3.3) of the particle

$$\langle E\rangle = \frac{\sum_i \lambda_i e^{-\frac{\lambda_i}{K_B T}}}{\sum_i e^{-\frac{\lambda_i}{K_B T}}}, \tag{3.3}$$

the system magnetization is calculated by taking the B-field derivative of the mean energy, i.e., M $= -\frac{\partial\langle E\rangle}{\partial B}$. These are plotted in Figure 3.4 and Figure 3.5.

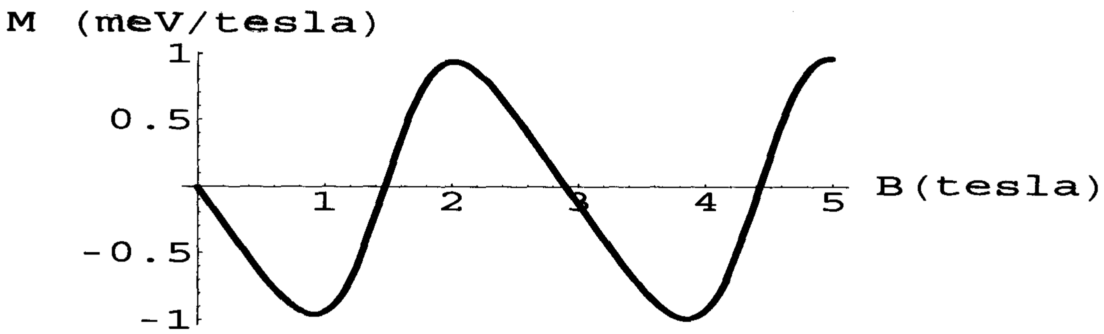

Figure **3.5:** Orbital magnetization vs. magnetic field at temperature $T = 10K$.

3.3 Suppression of orbital diamagnetic moment due to coupling to the dissipative environment: Lindblad operators.

Next, we couple our three-center system to the dissipative environment through the Lindblad operators projecting on to the sites, and investigate the effect of the induced decoherence on the mean energy and the magnetization, i.e., how these quantities evolve as function of time when the system is prepared in a chosen initial state. In order to solve this problem, we (1)derive the time evolution for the reduced density matrix using the Lindblad master equation, **(2)**then from the reduced density matrix and the system Hamiltonian, we calculate the mean energy, and finally **(3)** by differentiating it w. r. t. the magnetic field, we get the magnetization. As noted above, the effect of the magnetic field is taken into account through the Peierls phase factors in the Harniltonian, and the effect of the dissipative environment through the Lindblad operators. The latter are chosen so as to project on to the sites ($\eta = a, b, c$), i.e.,$L_\eta = \sqrt{C}|\eta\rangle\langle\eta|$, with C = coupling constant. The time evolution given by the Master equation –the Liouville equation– for the reduced density matrix (in the Lindblad form) is then

$$\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}[H,\rho] + \sum_{\eta}\{2L_\eta \rho L_\eta - L_\eta L_\eta \rho - \rho L_\eta L_\eta\}. \tag{3.4}$$

Equation (3.4) in the site representation becomes

$$\begin{aligned}
\frac{\partial \rho_{\alpha,\beta}}{\partial t} &= -\frac{i}{\hbar} V e^{i\phi}[\langle\alpha|a\rangle\langle b|\rho|\beta\rangle + \langle\alpha|b\rangle\langle c|\rho|\beta\rangle + \langle\alpha|c\rangle\langle a|\rho|\beta\rangle] \\
&-\frac{i}{\hbar} V e^{-i\phi}[\langle\alpha|b\rangle\langle a|\rho|\beta\rangle + \langle\alpha|c\rangle\langle b|\rho|\beta\rangle + \langle\alpha|a\rangle\langle c|\rho|\beta\rangle] \\
&+\frac{i}{\hbar} V e^{i\phi}[\langle\alpha|\rho|a\rangle\langle b|\beta\rangle + \langle\alpha|\rho|b\rangle\langle c|\beta\rangle + \langle\alpha|\rho|c\rangle\langle a|\beta\rangle] \\
&+\frac{i}{\hbar} V e^{-i\phi}[\langle\alpha|\rho|b\rangle\langle a|\beta\rangle + \langle\alpha|\rho|c\rangle\langle b|\beta\rangle + \langle\alpha|\rho|a\rangle\langle c|\beta\rangle] \\
&+C\sum_{\eta}[2\langle\alpha|\eta\rangle\langle\eta|\rho|\eta\rangle\langle\eta|\beta\rangle - \langle\alpha|\eta\rangle\langle\eta|\rho|\beta\rangle - \langle\alpha|\rho|\eta\rangle\langle\eta|\beta\rangle].
\end{aligned} \tag{3.5}$$

We now introduce the dimensionless time and coupling parameters, $\tau = tV/\hbar$, $\gamma = C\hbar/V$. With these, the reduced density matrix elements evolve as

$$\begin{aligned}
\dot{\rho}_{aa} &= i[e^{-i\phi}\rho_{ab} - e^{i\phi}\rho_{ba} + e^{i\phi}\rho_{ac} - e^{-i\phi}\rho_{ca}] \\
\dot{\rho}_{bb} &= i[e^{-i\phi}\rho_{bc} + e^{i\phi}\rho_{ba} - e^{i\phi}\rho_{cb} - e^{-i\phi}\rho_{ab}] \\
\dot{\rho}_{ab} &= ie^{i\phi}[\rho_{aa} - \rho_{bb}] + ie^{-i\phi}[\rho_{ac} - \rho_{cb}] - 2\gamma\rho_{ab} \\
\dot{\rho}_{ac} &= ie^{i\phi}[\rho_{ab} - \rho_{bc}] + ie^{-i\phi}[\rho_{aa} - \rho_{cc}] - 2\gamma\rho_{ac} \\
\dot{\rho}_{bc} &= ie^{i\phi}[\rho_{bb} - \rho_{cc}] + ie^{-i\phi}[\rho_{ba} - \rho_{ac}] - 2\gamma\rho_{bc} \\
&with\ \ \dot{\rho} = \frac{d\rho}{d\tau}\ and\ \ \rho_{aa} + \rho_{bb} + \rho_{cc} = 1,
\end{aligned} \tag{3.6}$$

This system of coupled linear differential equations is solved numerically using the runge-kutta method (4th order) under the initial condition that the particle is prepared in the unperturbed ground state ($|\lambda_0\rangle$) at time $t = 0$. The unperturbed eigenstates for the system Hamiltonian in Eq.(3.1) are

$$|\lambda_0\rangle = \frac{1}{\sqrt{3}}\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, |\lambda_1\rangle = \begin{bmatrix} \frac{3i\cos\theta + \sqrt{3}\cos\theta + \sin\theta + i\sqrt{3}\sin\theta}{-3i\cos\theta + \sqrt{3}\cos\theta + \sin\theta - i\sqrt{3}\sin\theta} \\ \frac{-2(\sqrt{3}\cos\theta + \sin\theta)}{-3i\cos\theta + \sqrt{3}\cos\theta + \sin\theta - i\sqrt{3}\sin\theta} \\ 1 \end{bmatrix}, \tag{3.7}$$

$$|\lambda_2\rangle = \begin{bmatrix} -\frac{3i\cos\theta - \sqrt{3}\cos\theta + \sin\theta - i\sqrt{3}\sin\theta}{3i\cos\theta + \sqrt{3}\cos\theta - \sin\theta - i\sqrt{3}\sin\theta} \\ \frac{-2(\sqrt{3}\cos 8 - \sin\theta)}{3i\cos\theta + \sqrt{3}\cos e - sin\theta - i\sqrt{3}\sin e} \\ 1 \end{bmatrix}, \tag{3.8}$$

In the site space then, the density matrix elements have the initial values

$$\begin{aligned}
\rho_{aa}(t=0) &= \langle a|\lambda_0\rangle\langle\lambda_0|a\rangle = 1/3 \\
\rho_{bb}(t=0) &= \langle b|\lambda_0\rangle\langle\lambda_0|b\rangle = 1/3 \\
\rho_{cc}(t=0) &= \langle c|\lambda_0\rangle\langle\lambda_0|c\rangle = 1/3 \\
\rho_{ab}(t=0) &= \langle a|\lambda_0\rangle\langle\lambda_0|b\rangle = 1/3 \\
\rho_{ac}(t=0) &= \langle a|\lambda_0\rangle\langle\lambda_0|c\rangle = 1/3 \\
\rho_{bc}(t=0) &= \langle b|\lambda_0\rangle\langle\lambda_0|c\rangle = 1/3
\end{aligned} \tag{3.9}$$

The system's mean energy $\langle E(t)\rangle$ is calculated by taking the trace of Hp, and the magnetization $M(t)$ is calculated by taking the B-field derivative of the mean mean energy $\langle E(t)\rangle$ i.e., $M(t) = -\frac{\partial\langle E(t)\rangle}{\partial B}$. These are plotted in Figures (3.6) and (3.7).

We now ask the question if and how it may be possible to connect this time-dependent solution for the open system (evolving under heating by the Lindblads towards infinite temperature) with a finite-temperature equilibrium system. We find that this can indeed be realized under the condition that the Lindblad heating is slow enough as compared to the internal dynamical time scale of the system, i.e., $\frac{1}{C} \gg \frac{\hbar}{Band\ Width}$ Under this condition the system temperature $T(t)$ can be 'monitored' by the relative population of the two sublevels 1 and 2(identified with the Blotzmann factor), and is given by

$$T(t) = \frac{\lambda_2 - \lambda_1}{k_B ln[\rho_1(t)/\rho_2(t)]}. \tag{3.10}$$

Figure (3.8) illustrates this point. Now, we eliminate the time t between the temperature $T(t)$ and the magnetization $M(t)$, and thus obtain magnetization as a function of temperature which is plotted in Figure (3.9). Clearly, this graph for an open system is equivalent to the graph (Figure 3.4) for a closed system. Thus, we recover the classical equilibrium statistical mechanical result(Figure 3.4) from lindblad theory (Figure 3.9) provided that the system-bath coupling is weak and therefore the Lindblad heating time scales are much larger than the internal dynamical time-scales of the system.

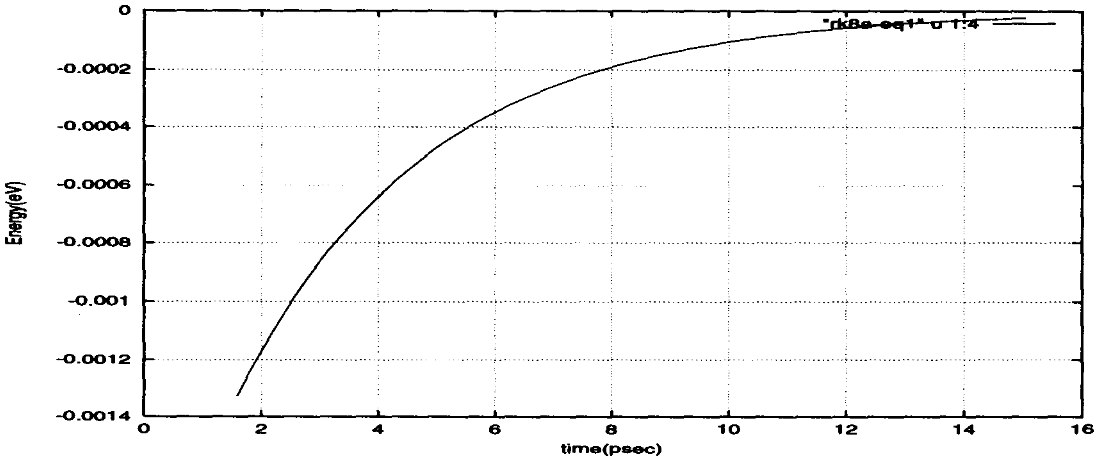

Figure 3.6: Mean energy $\langle E\rangle(in\ \ eV)$ vs time(in peco-seconds), $\gamma = 0.1$, B $= 0.16$.

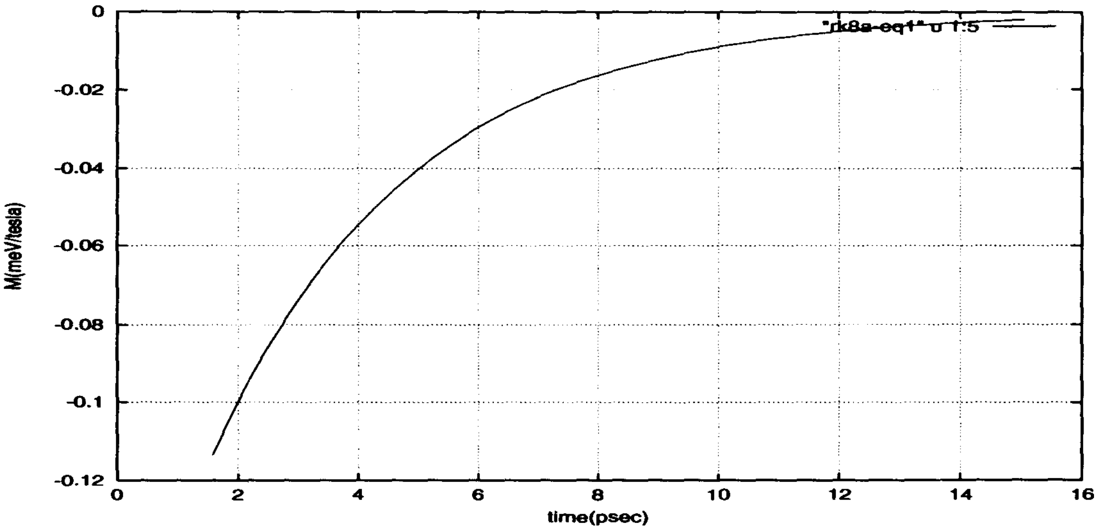

Figure **3.7:** The magnetization M in $meV/tesla$ vs time in pico-seconds, $\gamma = 0.1$, B $=$ 0.16. Magnetization goes to zero in about 20 pico-seconds as it should. This clearly shows the decohering role of Lindblad operators and in this sense system makes a quantum to classical transition.

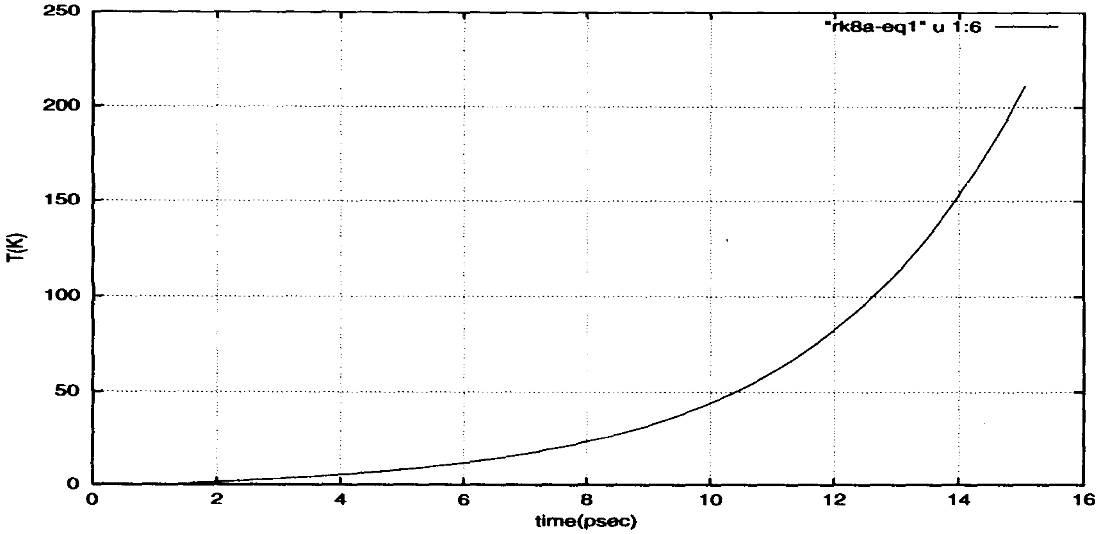

Figure **3.8:** The rise of system temperature T in K with time (in peco-seconds) with y = 0.1 , B = 0.16 *tesla.*

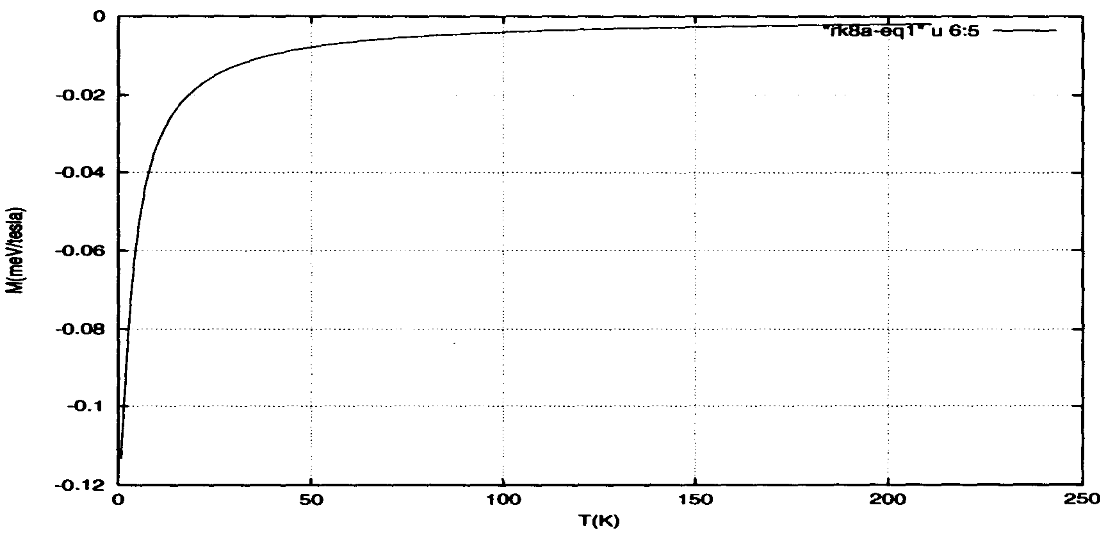

Figure **3.9:** Plot shows magnetization M in $meV/tesla$ as a function of system temperature for $\gamma = 0.1$ and $B = 0.16$ *tesla.* This graph for an open system is equivalent to the graph (Fig. **3.4)** for a closed system. Thus we obtain classical statistical mechanical results with Lindblad theory when the system-bath coupling is weak and external heating time scales are much larger than internal dynamical time-scales of the system.

3.4 Discussion

In this Chapter we have shown how under certain quasistatic condition the finite-temperature equilibrium statistical mechanical results can be recovered from the time-dependent reduced density matrix evolving through the Liouville equation, under constant heating by the lindblad coupling to the environment. The condition required is that the internal dynamical time-scales of the system be much less than the heating time scale. We have illustrated this for the simple case of a triatomic annulene threaded by an A-B flux. Here the instantaneous temperature $T(t)$ could be introduced through the relative population of any two energy levels(1 and 2 in the present case) identifies with the Boltzmann weight factor. Under the above condition, one can eliminate time (t) between the two time-dependent physical quantities, e.g., $M(t)$ and $T(t)$, in favour of a functional relation between the two, obtaining in this case a magnetization versus temperature plot which is found to be consistent with the canonical equilibrium statistical mechanical M-T plot, with finite M for a finite T.