Absence of Antiferromagnetic Ordering in Hubbard's Simple Decoupling Scheme

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The self-consistency criterion for the antiferromagnetic solution of a single-band Hubbard model in Hubbard's simple decoupling scheme is, here, analyzed in detail as a function of the number n $(0<n<2)$ of electrons per site. It is shown that a self-consistent antiferromagnetic solution exhibiting a first- or a second-order phase transition does not exist for any value of n. For $n=1$ the only possible solution at any temperature is shown to be the one with zero sublattice magnetization. These results are contrary to a claim by Arai.

I. INTRODUCTION

A great deal of effort has been expended in recent years to obtain an antiferromagnetic solution to the Hubbard model in Hubbard's simple decoupling scheme.[1] Penn,[2] Bari and Kaplan,[3] and Hewson and Lindner[4] have shown that for the case of one electron per atomic site, the Hubbard insulator does not exhibit antiferromagnetic order. Recently, Arai[5] has studied the properties of the antiferromagnetic solution in the said decoupling scheme for arbitrary values of electron density. However, Arai failed to investigate the self-consistency criterion for a stable antiferromagnetic state, but simply assumed that one exists, at least, for a certain range of the density. It is the purpose of this article to establish the failure of the simple decoupling scheme of Hubbard to exhibit a stable antiferromagnetic state for any value of the number of electrons per site $(0<n<2)$ and for all values of the parameters involved in the model. This is done by first demonstrating that for $n=1$, the only possible self-consistent solution for the sublattice magnetization χ at an arbitrary T (including $T=0\,^{\circ}\mathrm{K}$) is zero, the trivial one. This result lays to rest possible exceptions taken to the result established in Refs. 2–4. For arbitrary n, the lack of an antiferromagnetic solution is shown as follows: If a nonzero χ existed, we show that the system would not exhibit either a first- or a second-order phase transition. Since χ must drop to zero at high temperatures, we conclude that no self-consistent antiferromagnetic solution leading to a first- or second-order phase transition is possible. In the concluding remarks we point out a possible case that is not covered in our work.

II. CALCULATIONS

The Hubbard-model Hamiltonian is given by

$$H=\sum_{i,j,\sigma} t_{ij}C_{i\sigma}^{\dagger}C_{j\sigma}+U\sum_{i} n_{i\uparrow}n_{i\downarrow}\ . \tag{1}$$

We consider the equations of motion for the double-time Green's functions[6] and follow Hubbard's decoupling scheme.[1] We next break the translational symmetry by considering two interlocking lattices A and B and impose an antiferromagnetic solution by defining

$$\begin{aligned}&\langle n_A^{\uparrow}\rangle=\langle n_B^{\downarrow}\rangle=\tfrac{1}{2}n(1+\chi)\ ,\\ &\langle n_A^{\downarrow}\rangle=\langle n_B^{\uparrow}\rangle=\tfrac{1}{2}n(1-\chi)\quad (0<n<2)\ ,\end{aligned} \tag{2}$$

where n is the number of electrons per site and $n\chi$ is the sublattice magnetization which should be determined self-consistently. We restrict t_{ij}'s to nearest neighbors only and set $t_{ii}=0$ without loss of generality. For a simple cubic lattice we then have

$$\epsilon_k=-2|t|\,(\cos k_x a+\cos k_y a+\cos k_z a)\ , \tag{3}$$

where

$$\begin{aligned}t_{ij}&=-|t| \quad \text{for } i \text{ and } j \text{ nearest neighbors}\\ &=0 \qquad \text{otherwise}\ .\end{aligned} \tag{4}$$

The solution to the Green's functions in this decoupling scheme[5] can then be written in a matrix form as follows:

$$\begin{bmatrix} G_{AA}^{\sigma}(\vec{k},\omega) & G_{AB}^{\sigma}(\vec{k},\omega)\\ G_{BA}^{\sigma}(\vec{k},\omega) & G_{BB}^{\sigma}(\vec{k},\omega)\end{bmatrix}=\frac{1}{[\omega-\xi_1(k)][\omega-\xi_2(k)][\omega-\xi_3(k)][\omega-\xi_4(k)]}$$

$$\times\begin{bmatrix} \omega(\omega-U)[\omega-U(1-\langle n_A^{-\sigma}\rangle)] & \epsilon_k[\omega-U(1-\langle n_A^{-\sigma}\rangle)][\omega-U(1-\langle n_B^{-\sigma}\rangle)]\\ \epsilon_k[\omega-U(1-\langle n_A^{-\sigma}\rangle)][\omega-U(1-\langle n_B^{-\sigma}\rangle)] & \omega(\omega-U)[\omega-U(1-\langle n_B^{-\sigma}\rangle)]\end{bmatrix}, \tag{5}$$

where $\xi_{1,2,3,4}(k)$ are the roots of the quartic equation

$$\omega^2(\omega-U)^2-\epsilon_k^2[\omega-U(1-n_A^{-\sigma})][\omega-U(1-n_B^{-\sigma})]=0\ . \tag{6}$$

From the structure of the Green's functions it appears that the original "two bands" in the Hubbard truncation scheme are split further and one has four bands. This interpretation would be meaningful if a nonvanishing χ exists. It can be noticed that for a tight-binding band given by (3), $\epsilon_k=-\epsilon_{k+Q}$, where $Q=(\pi/a)(1,1,1)$. It is obvious from (6) that at $k=\frac{1}{2}Q$ the solutions to (6) are $\omega=0$ and $\omega=U$, each occurring twice. This suggests that antiferromagnetic ordering does not bring about an additional gap in the excitation spectrum. Thus one could suspect that antiferromagnetic ordering causes no gain in energy and, in fact, we shall see that the paramagnetic state always wins out.

To investigate the stability of the antiferromagnetic solution, we must solve for χ self-consistently and for the chemical potential μ. The two equations are obtained from

$$\tfrac{1}{2}n(1+\chi)=-\frac{2}{N}\sum_{\vec{k}\ (\text{half-zone})}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\,\frac{1}{1+e^{\beta\omega}}\times \mathrm{Im}G^{\sigma}_{AA}(\vec{k},\omega+i0^+) \tag{7}$$

and

$$\tfrac{1}{2}n(1-\chi)=-\frac{2}{N}\sum_{\vec{k}\ (\text{half-zone})}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\,\frac{1}{1+e^{\beta\omega}}\times \mathrm{Im}G^{\sigma}_{BB}(\vec{k},\omega+i0^+)\ . \tag{8}$$

After a straightforward manipulation one obtains the self-consistency criterion in the following form. Assuming that $\chi\neq 0$ is a solution, one must solve the following equation:

$$\frac{1}{U}=-\frac{2}{N}\sum_{\vec{k}\ (\text{half-zone})}\left(\frac{f(\xi_1-\mu)\xi_1(\xi_1-U)}{(\xi_1-\xi_2)(\xi_1-\xi_3)(\xi_1-\xi_4)}+\frac{f(\xi_2-\mu)\xi_2(\xi_2-U)}{(\xi_2-\xi_1)(\xi_2-\xi_3)(\xi_2-\xi_4)}+\frac{f(\xi_3-\mu)\xi_3(\xi_3-U)}{(\xi_3-\xi_1)(\xi_3-\xi_2)(\xi_3-\xi_4)}+\frac{f(\xi_4-\mu)\xi_4(\xi_4-U)}{(\xi_4-\xi_1)(\xi_4-\xi_2)(\xi_4-\xi_3)}\right)\ , \tag{9}$$

where $\xi_{1,2,3,4}$ are defined in (6) and $f(x)=(1+e^{\beta x})^{-1}$. The chemical potential μ is determined from the following equation:

$$n=\frac{2}{N}\sum_{\vec{k}\ (\text{half-zone})}\left(\frac{f(\xi_1-\mu)\xi_1(\xi_1-U)(2\xi_1-2U+Un)}{(\xi_1-\xi_2)(\xi_1-\xi_3)(\xi_1-\xi_4)}+\frac{f(\xi_2-\mu)\xi_2(\xi_2-U)(2\xi_2-2U+Un)}{(\xi_2-\xi_1)(\xi_2-\xi_3)(\xi_2-\xi_4)}+\frac{f(\xi_3-\mu)\xi_3(\xi_3-U)(2\xi_3-2U+Un)}{(\xi_3-\xi_4)(\xi_3-\xi_2)(\xi_3-\xi_1)}+\frac{f(\xi_4-\mu)\xi_4(\xi_4-U)(2\xi_4-2U+Un)}{(\xi_4-\xi_1)(\xi_4-\xi_2)(\xi_4-\xi_3)}\right)\ . \tag{10}$$

III. ANALYSIS OF SELF-CONSISTENCY CRITERION

A. Case 1

The self-consistency criterion can be rigorously analyzed at any arbitrary temperature T for the case of $n=1$. Since the work of Refs. 2–4 is mainly restricted to showing the absence of a second-order transition temperature, it might be argued that a self-consistent antiferromagnetic solution might still exist exhibiting other kinds of phase transitions. We show below that Eq. (9) for $n=1$ has no solution with a finite χ.

First, we observe that for $n=1$, the quartic equation (6) can be solved analytically and that the chemical potential μ, determined from (10), is $\frac{1}{2}U$. Incidentally, this result is exact.[7] The self-consistency equation reduces to the following form:

$$\frac{1}{U}=\frac{2}{N}\sum_{\vec{k}\ (\text{half-zone})}\frac{1}{(\xi_+^2-\xi_-^2)}\left(\frac{\xi_+^2-\frac{1}{4}U^2}{2\xi_+}\tanh\tfrac{1}{2}\beta\xi_+ +\frac{\frac{1}{4}U^2-\xi_-^2}{2\xi_-}\tanh\tfrac{1}{2}\beta\xi_-\right)\ , \tag{11}$$

where

$$\xi_\pm=\tfrac{1}{2}\{[\epsilon_k\pm[\epsilon_k^2+U^2(1-\chi^2)]^{1/2}]^2+U^2\chi^2\}^{1/2}\ . \tag{12}$$

Noting that each term of the integrand and ξ_+ and ξ_- are positive definite, we have

$$\begin{aligned}\frac{2}{N}\sum_{\vec{k}}\frac{1}{\xi_+^2-\xi_-^2}\left(\frac{\xi_+^2-\frac{1}{4}U^2}{2\xi_+}\tanh\tfrac{1}{2}\beta\xi_+ +\frac{\frac{1}{4}U^2-\xi_-^2}{2\xi_-}\tanh\tfrac{1}{2}\beta\xi_-\right)&\\ \leq\frac{2}{N}\sum_{\vec{k}}\frac{1}{2(\xi_++\xi_-)}\left(1+\frac{U}{(U^2+4\epsilon_k^2\chi^2)^{1/2}}\right)&\\ <\frac{2}{N}\sum_{\vec{k}}\frac{1}{\xi_++\xi_-}<\frac{1}{U}\ .&\end{aligned} \tag{13}$$

The last step follows from the fact that the integrand takes its maximum value of $1/U$ for $\epsilon_k=0$. Thus for $0\leq\chi\leq 1$, Eqs. (11) has no nontrivial solution.

B. Case 2

For arbitrary n, Eq. (9) determines χ as a function of the parameters U, T, and $|t|$. Let $\chi \neq 0$ be a solution to (9) at $T=0\,^{\circ}\mathrm{K}$. Then, if χ has a temperature dependence, it must decrease with T, and one can then determine the temperature T_N at which χ goes to zero. If the transition were of second order, then T_N is the Néel temperature, i.e., the temperature at which χ goes to zero continuously. On the other hand, the transition would be of first order if χ decreases with T and drops to zero discontinuously. In this case T_N would not be the transition temperature but would represent the intercept of the analytic continuation of $\chi(T)$ on the temperature axis. In other words, a first-order transition is viewed as an interrupted second-order transition. Existence of a positive real T_N is obviously a necessary condition for the occurrence of even a first-order transition.

The condition (9) then goes into the following condition for determining the Néel temperature:

$$\frac{1}{U}=-\frac{1}{N}\sum_{\substack{\vec{k}\\(\text{half-zone})}}\left(\frac{f_N(\alpha_1-\mu)-f_N(\alpha_2-\mu)}{[(U-\epsilon_k)^2+2Un\epsilon_k]^{1/2}}+\frac{f_N(\alpha_3-\mu)-f_N(\alpha_4-\mu)}{[(U+\epsilon_k)^2-2Un\epsilon_k]^{1/2}}\right) \tag{14}$$

$$=\frac{1}{N}\sum_{\substack{\vec{k}\\(\text{full zone})}}\frac{f_N(\alpha_2-\mu)-f_N(\alpha_1-\mu)}{[(U-\epsilon_k)^2+2Un\epsilon_k]^{1/2}}\ , \tag{15}$$

where

$$\alpha_{1,2}=\tfrac{1}{2}(\epsilon_k+U)\pm\tfrac{1}{2}[(U-\epsilon_k)^2+2Un\epsilon_k]^{1/2}\ ,$$
$$\alpha_{3,4}=\tfrac{1}{2}(-\epsilon_k+U)\pm\tfrac{1}{2}[(U+\epsilon_k)^2-2Un\epsilon_k]^{1/2}\ . \tag{16}$$

The chemical potential at T_N is then determined by the following equation:

$$n=\frac{2}{N}\sum_k\frac{(\alpha_1-U+\frac{1}{2}Un)f_N(\alpha_1-\mu)-(\alpha_2-U+\frac{1}{2}Un)f_N(\alpha_2-\mu)}{[(U-\epsilon_k)^2+2Un\epsilon_k]^{1/2}}\ . \tag{17}$$

Thus, instead of solving (9) for χ at an arbitrary temperature, we analyze the equivalent condition (15) for T_N. The following is a brief outline of the method by which we show that a self-consistent solution to (15) does not exist: First, we establish that there exists no real positive T_N $(0\leq T_N\leq\infty)$ for which (15) has a solution. This then implies that if a nonzero χ satisfied (9) at $T=0\,^{\circ}\mathrm{K}$, it cannot vanish at any T $(0\leq T\leq\infty)$ and, in particular, must remain finite for $T=O(T_F)$, where T_F is the degeneracy temperature. However, for $T=O(T_F)$ all the four Fermi functions tend to one-half, and it can easily be verified in this case that the right-hand side of (9) vanishes identically. Thus the only solution is the trivial one, $\chi=0$, which we canceled out from both sides in the process of deriving (9).

Result 1. We establish that for $1-1/\sqrt{3}\leq n\leq 1+1/\sqrt{3}$, there does not exist a real positive T_N $(0\leq T_N\leq\infty)$ which will satisfy (15) for any value of the parameters U and $|t|$.

Proof. Consider the right-hand side of (15):

$$\frac{1}{N}\sum_{\vec{k}}\frac{f_N(\alpha_2-\mu)-f_N(\alpha_1-\mu)}{[U^2+\epsilon_k^2-2U\epsilon_k(1-n)]^{1/2}}$$
$$\leq\frac{1}{N}\sum_{\vec{k}}\frac{f_N(\alpha_2-\mu)}{[U^2+\epsilon_k^2-2U\epsilon_k(1-n)]^{1/2}} \tag{18a}$$
$$\leq\frac{1}{N}\sum_{\vec{k}}\frac{1}{[U^2+\epsilon_k^2-2U\epsilon_k(1-n)]^{1/2}} \tag{18b}$$
$$=\frac{1}{2N}\sum_{\vec{k}}\left(\frac{1}{[U^2+\epsilon_k^2-2U\epsilon_k(1-n)]^{1/2}}+\frac{1}{[U^2+\epsilon_k^2+2U\epsilon_k(1-n)]^{1/2}}\right) \tag{18c}$$
$$<1/U\ \text{ for } 1-1/\sqrt{3}\leq n\leq 1+1/\sqrt{3}\ . \tag{18d}$$

In going from (18b) to (18c) we have made use of the fact that for every ϵ_k there is a $-\epsilon_k$ in the sum over $\vec{k}$. In arriving at the inequality (18d) we have made use of the fact that the integrand takes its maximum value at $\epsilon_k=0$, if n lies between $1-1/\sqrt{3}$ and $1+1/\sqrt{3}$.

The upper bounds established above are not sufficient to prove similar results for n outside this range. We proceed differently.

Result 2. We now show that for $0<n<1-1/\sqrt{3}$ and $6|t|/U\leq 2/\sqrt{3}$ there is no solution to (15) for a real positive T_N $(0\leq T_N\leq\infty)$.

Proof. We compare Eq. (15) with (17) and show that both equations cannot be satisfied simultaneously. Let us rewrite the equation determining the chemical potential in the following form:

$$\frac{1}{U}=\frac{1}{N}\sum_{\vec{k}}\frac{(2/n-1-2\alpha_2/Un)f_N(\alpha_2-\mu)+(2\alpha_1/Un-2/n+1)f_N(\alpha_1-\mu)}{[U^2+\epsilon_k^2+2U\epsilon_k(n-1)]^{1/2}}\ . \tag{19}$$

It is straightforward to verify that (a) $2\alpha_1/Un-2/n+1>0$ for all U, $|t|$, and n $(0<n<2)$ and (b) $2/n-1-2\alpha_2/Un\geq 1$ for $6|t|/U\leq 2/\sqrt{3}$ and n in the range $0<n<1-1/\sqrt{3}$. Thus each term in (19) is greater than a corresponding term in (15). Thus the right-hand side of (15) is less than $1/U$.

Result 3. The above result can easily be extended to $n > 1+1/\sqrt{3}$. Thus we show, below, that for $2 > n > 1+1\sqrt{3}$ and $6|t|/U \leq 2/\sqrt{3}$ there is no positive real T_N $(0 \leq T_N \leq \infty)$ that satisfies (15).

Define $n' = 2 - n$. The self-consistency equation is written in the form

$$\frac{1}{U} = \frac{1}{N}\sum_{\vec{k}} \frac{[1-f_N(\alpha_1-\mu)]-[1-f_N(\alpha_2-\mu)]}{[U^2+\epsilon_k^2-2U\epsilon_k(n'-1)]^{1/2}} . \tag{20}$$

The equation for μ can be written in the form

$$\frac{1}{U} = \frac{1}{N}\sum_{\vec{k}} \frac{(2\alpha_1/Un-1)[1-f_N(\alpha_1-\mu)]+(1-2\alpha_2/Un')[1-f_N(\alpha_2-\mu)]}{[U^2+\epsilon_k^2-2U\epsilon_k(n'-1)]^{1/2}} . \tag{21}$$

We note that (a) $1-f_N(\alpha-\mu) \geq 0$, (b) $1-2\alpha_2/Un' > 0$ for $0 < n' < 2$, and (c) $2\alpha_1'/Un'-1 \geq 1$ for $n' \leq 1 - 1/\sqrt{3}$ and $6|t|/U \leq 2/\sqrt{3}$. Thus the right-hand side of (21) is greater than the right-hand side of (20).

Thus we have established so far that in the Hubbard truncation scheme there is no antiferromagnetic solution for any value of n $(0 < n < 2)$ as long as $6|t|/U \leq 2/\sqrt{3}$. Furthermore, we extended this result for any value of U and $|t|$ provided that n lies between $1-1/\sqrt{3} \leq n \leq 1+1/\sqrt{3}$. It is worth pointing out that the Hubbard truncation scheme is probably incorrect for $6|t|/U > 2/\sqrt{3}$, as was shown by Hubbard.[8] For $6|t|/U > 2/\sqrt{3}$, Hubbard, in his improved calculations, has shown that the two bands merge into one and that there is no gap in the density of single-particle states. If we accept this conclusion, we can then state that within the range of validity of Hubbard's truncation scheme, no self-consistent antiferromagnetic solution is obtained for any value of n $(0 \leq n \leq 2)$.

In spite of the physical arguments given above to discard the range $6|t|/U > 2/\sqrt{3}$ from our discussion, we can still show that Eq. (18) has no solution for T_N in the range $n < 1-1/\sqrt{3}$ or $n > 1+1/\sqrt{3}$ and $6|t|/U > 2/\sqrt{3}$.

Consider $n < 1-1/\sqrt{3}$. We first show that μ lies in the lower band $\alpha_2(k)$ such that $\mu \leq \alpha_2$ $(\epsilon_k = 0)$. For $n \leq 1$ the total number of states n_{α_2} available in the inner half of the Brillouin zone is given by

$$n_{\alpha_2} = -\frac{2}{N}\sum_{\substack{\vec{k} \\ \text{(inner half-zone)}}} \frac{\alpha_2(k)-U+\frac{1}{2}Un}{[U^2+\epsilon_k^2-2U\epsilon_k(1-n)]^{1/2}}$$
$$= \frac{1}{2}+\frac{1}{N}\sum_{\substack{\vec{k} \\ \text{(inner half-zone)}}} \frac{U(1-n)-\epsilon(k)}{[\epsilon_k^2+U^2-2U\epsilon_k(1-n)]^{1/2}} \geq \frac{1}{2} . \tag{22}$$

The last step follows from the fact that in the inner half-zone $\epsilon_k \leq 0$. Hence for $n \leq 0.5$ the chemical potential $\mu < \alpha_2$ $(\epsilon_k = 0)$. This has the effect of restricting the sum over k in (18) to the inner half-zone at low temperatures. Hence the right-hand side of (18) is now bounded by

$$\frac{1}{N}\sum_k \frac{f(\alpha_2-\mu)-f(\alpha_1-\mu)}{[U^2+\epsilon_k^2+2U\epsilon_k(1-n)]^{1/2}}$$
$$< \frac{1}{N}\sum_{\substack{\vec{k} \\ \text{(inner half-zone } \epsilon_k \leq 0)}} \frac{1}{[U^2+\epsilon_k^2-2U\epsilon_k(1-n)]^{1/2}}$$
$$< \frac{1}{2U} . \tag{23}$$

For finite T_N, one can use the Sommerfeld expansion[9] and the correction terms are $O((1/U)(T_N/U)^2)$ for $6|t|/U > 1$. Thus for $T_N \ll U$ the correction terms are negligible and (15) can still not be satisfied. Also we have seen that for $T_N \geq U$ the Fermi functions $f(\alpha_1-\mu)$ and $f(\alpha_2-\mu)$ can both be replaced by $\frac{1}{2}$, and thus the sum on the right-hand side of (15) vanishes.

Finally, for $n \geq 1+1/\sqrt{3}$ one can give an argument very similar to the above to rule out antiferromagnetism. Here the chemical potential lies in the upper band in such a way that for $n > 1.5$, $\mu > \alpha_1$ $(\epsilon_k = 0)$. Writing Eq. (15) in terms of $1-f(\alpha-\mu)$ instead of $f(\alpha-\mu)$, one can easily verify that the argument given in the preceding paragraph goes through.

IV. SUMMARY

We have shown that Hubbard's simple decoupling scheme fails to show an antiferromagnetic solution for the system with one electron per lattice. For arbitrary electron density, we have established that a stable antiferromagnetic solution that exhibits either a first- or a second-order phase transition does not exist. These results are contrary to the properties of this model in the Hartree–Fock scheme, and it should be emphasized that the Hubbard scheme does not reduce to the Hartree–Fock scheme under any circumstances as was implied by Arai. This point has been already noted in Ref. 3. For $n \neq 1$, it is possible that there may still exist a solution with finite magnetization that tends to zero asymptotically as $T \to \infty$. Our analysis for $n = 1$ shows that this is cleary impossible. Even if such a solution exists, it would clearly give a transition temperature $T_N \simeq O(T_F)$, where T_F is the degeneracy temperature. The properties of such a solution would be essentially those of Slater's split-band model and certainly not the ones envisaged in Ref. 5.

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Irreversibility in Paramagnetic Spin System: Free-Induction Decay and Line Shape In CaF_2

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Complementary data about arguments presented in an earlier paper concerning free-induction decay are discussed. The results of a new scheme of resummation are presented and the line shape is computed.

I. INTRODUCTION

In a previous paper[1] (hereafter I) we obtained a kinetic equation for the free-induction-decay (FID) signal, which was

$$\partial_t \Gamma(t) = \int_0^t G(t-\tau)\,\Gamma(\tau)\,d\tau\,, \tag{1}$$

where

$$\Gamma(t) = \mathrm{Tr}(e^{-iV^0 t/\hbar}\,S^x e^{+iV^0 t/\hbar}\,S^x) \tag{2}$$

and V^0 is the secular part of the dipolar coupling. Since then, a lot of effort has been made by many people in order to obtain a better agreement between theory and experiment. A non-negligible test certainly lies in the fitting of the long-time data of Lowe *et al.* by a theory.[2,3] The situation in the field has recently been reviewed by Lado, Memory, and Parker.[4] The aim of this note is twofold. Firstly, we wish to clarify some arguments presented in I, which it seems to us have

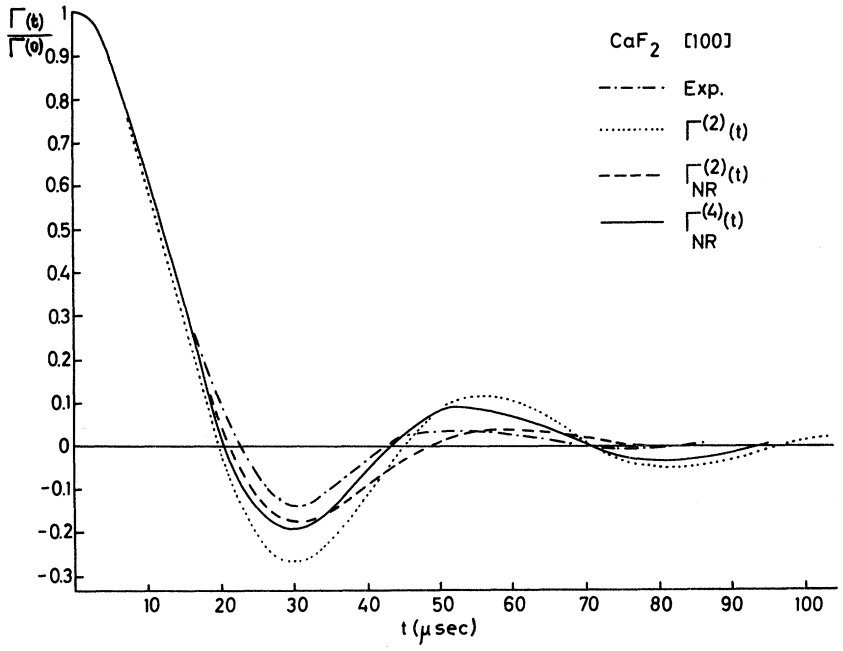

FIG. 1. Free-induction decay for CaF_2 with the field in the [100] direction.