

haviors found here have also their analogs when one studies the effect of a magnetic field.⁷

We would like to thank E. Brezin, B. Duplantier, C. Kipnis, J. L. Lebowitz, and I. Webman for stimulating discussions.

Note added.—After this work was submitted, Professor J. L. Lebowitz and Professor H. Spohn informed us that the same problem has been studied in a different way by mathematicians and similar results can be found in Refs. 8 and 9.

¹J. Bernasconi, S. Alexander, and R. Orbach, Phys.

Rev. Lett. **41**, 185 (1978).

²S. Alexander, J. Bernasconi, W. R. Schneider, and R. Orbach, Rev. Mod. Phys. **53**, 175 (1981).

³T. Odagaki and M. Lax, Phys. Rev. Lett. **45**, 847 (1980).

⁴I. Webman, Phys. Rev. Lett. **47**, 1496 (1981).

⁵Ya. G. Sinai, in Proceedings of the Sixth International Conference on Mathematical Physics, Berlin, August 1981 (to be published), and to be published.

⁶B. Derrida and H. Hilhorst, J. Phys. C **14**, L539 (1981).

⁷B. Derrida and H. Hilhorst, to be published.

⁸H. Kesten, M. V. Kozlov, and F. Spitzer, Compositio Math. **30**, 145 (1975).

⁹F. Solomon, Ann. Prob. **3**, 1 (1975).

Unbiased Estimation of Corrections to Scaling by Partial Differential Approximants

Jing-Huei Chen and Michael E. Fisher

Baker Laboratory, Cornell University, Ithaca, New York 14853

and

Bernie G. Nickel

Physics Department, University of Guelph, Guelph, Ontario, Canada N1G 2W1, and Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138^(a)

(Received 28 October 1981)

High-temperature series for two bcc lattice models which interpolate between the Gaussian (or free-field) model and the $S = \frac{1}{2}$ Ising model are analyzed by partial differential approximants. Series to order 21 in both $x \propto 1/T$ and the interpolation parameter, y , yield unbiased estimates for the correction-to-scaling exponent, $\theta = 0.54 \pm 5$, and the susceptibility exponent, $\gamma = 1.2385 \pm 15$. The results are universal and agree tolerably with field-theoretic estimates and well with biased, one-variable analyses of general spin Ising models.

PACS numbers: 64.60.Fr, 02.60.+y, 05.70.Jk, 75.10.Hk

An important qualitative prediction of the renormalization-group theory of critical phenomena is that the corrections to leading power-law behavior are determined in a universal way through a nontrivial correction-to-scaling exponent θ .¹ Thus a property $f(T, y)$, such as the susceptibility of a ferromagnetic system specified by an "irrelevant" parameter y , e.g., the ambient pressure, should vary as

$$f(T, y) \approx A(y) a_f i^{-\psi} [1 + C(y) c_f i^\theta + \dots], \quad (1)$$

when $i \propto T - T_c(y) - 0+$: The leading exponent ψ and the coefficients a_f and c_f depend on the property studied, but should otherwise be universal, i.e., independent of y ; however, $\theta > 0$ ought to be independent of both y and f ; only $A(y)$ and $C(y)$

should be nonuniversal.¹ Analyses by ratio and Padé-approximant techniques of high-temperature series expansions for lattice spin models have been strikingly successful in estimating leading exponents, such as γ for the susceptibility.² However, convincing, unbiased estimation, or even detection, of the confluent correction exponents and amplitudes has proved an elusive goal in single-variable series expansion studies. In this note we report an attack on the problem for two distinct $d=3$ (d =dimensionality) models which, as y varies from 0 to 1, interpolate smoothly between the exactly solvable Gaussian or free-field model and the standard, discrete spin- $\frac{1}{2}$ Ising model: See Fig. 1 where $x = J/k_B T$ with exchange parameter J . By applying two-

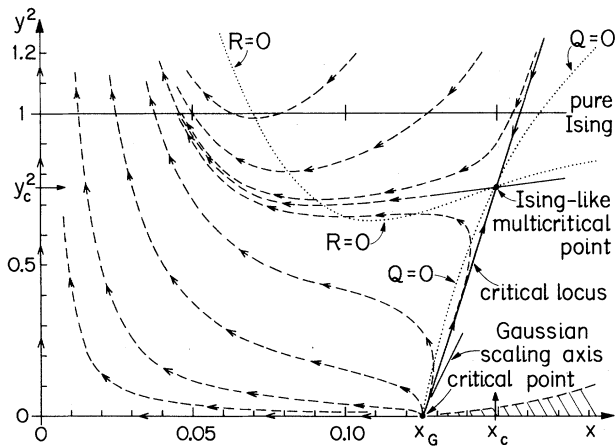


FIG. 1. The $(x = J/k_B T, y)$ plane for the double-Gaussian model showing the critical locus, $x_c(y)$. An analytic continuation of the model exists wherever $|8x(1-y)| < 1$ so that only the small shaded region for $x > x_c$ is unphysical (Ref. 14). The broken curves depict some partial differential flow trajectories (Refs. 3 and 4).

variable series expansion techniques, specifically partial differential approximants^{3,4} (whose power has not previously been demonstrated in this context), to series of order x^{21} recently obtained for the bcc lattice,⁵ we derive unbiased estimates of θ and γ , and verify universality.

To set the scene, recall first that a recent ratio analysis⁶ of the $S = \frac{1}{2}$ Ising-model susceptibility for the fcc, bcc, sc, and diamond lattices (to orders 15, 15, 19, and 22, respectively) reaffirmed the fifteen-year-old estimate⁷ $\gamma = 1.250 \pm 3$ and gave no evidence of significant confluent corrections. Nevertheless, previously observed discrepancies of 0.02 or so in the γ estimates from shorter series for various models expected to be in the same universality class (such as Ising $S = \infty$) have usually been attributed to confluent corrections.⁸

However, a detailed analysis⁹ of the $d = 3$ field-theoretic perturbation expansions¹⁰ leads to $\gamma = 1.241 \pm 2$ and $\theta = 0.498 \pm 20$. This significant disagreement might be attributed merely to the unbounded, continuous spin variables and lack of an explicit momentum cutoff in the underlying field theory; but this intrinsically unpalatable option is effectively foreclosed by the derivation of Ising-model series to order x^{21} for arbitrary spin, S , on the bcc lattice.⁵ Analysis of the series^{5,11} by standard $D \log$ Padé methods² clearly indicates (a) a value $\gamma < 1.243$ for all S , and (b) the presence of significant corrections to scaling for both $S = \frac{1}{2}$ and $S = \infty$.

Now special methods of analysis have been proposed to study expansions when confluent singularities are anticipated.¹² However, the task of finding both ψ and θ in (1) involves intrinsically unstable fitting procedures.¹¹ To circumvent this difficulty *biased* techniques have been invoked. Thus in order to reconcile the $S = \frac{1}{2}$ Ising and field-theoretic results Roskies¹³ assumed $\theta = \frac{1}{2}$ and a critical-point value x_c ; even then, fairly arbitrary "optimal fit" criteria were needed to obtain a preferred γ estimate. To treat the general spin- S model and models with a continuous parameter, y , by second-order differential approximants,¹² Nickel and Rehr^{11,14} varied an assigned θ value and defined the "best" value as that which gave the most nearly universal γ when comparing a finite number of models with S or y fixed. Consistency could be attained¹¹ with $\gamma = 1.239 \pm 2$ and $\theta = 0.53 \pm 15$ but these values are implicitly biased by the subjective choice of models compared. Similarly, a refined ratio analysis of the series by Zinn-Justin¹⁵ convincingly revealed the presence of confluent singularities but his estimates $\gamma = 1.2385 \pm 25$ and $\theta = 0.52 \pm 7$ also depend on the assumption that γ is universal, and on which S values are considered most significant.

Furthermore, (1) represents only the leading effects of the irrelevant variable; higher powers of t^θ must appear and may be important. More explicitly, renormalization-group analysis indicates¹ that on the critical locus, $T_c(y)$, there should be a special point $[y_c, x_c \equiv J/k_B T_c(y_c)]$ (see Fig. 1), and associated nonlinear scaling fields,^{1,3,4} $\Delta\tilde{y}(x, y)$ and $\Delta\tilde{x}(x, y) \sim t^\theta T - T_c(y)$, varying as $(\Delta x - \Delta y/e_2)$ and $(\Delta y - e_1 \Delta x)$ when $\Delta x \equiv x - x_c$, $\Delta y \equiv y - y_c \rightarrow 0$, where e_1 and e_2 specify the scaling axes. Then as $\Delta\tilde{x} \rightarrow 0$ for $\Delta\tilde{y}$ not too large, a better description than (1) should be provided by the multicritical scaling form^{3,4}

$$f(x, y) \approx |\Delta\tilde{x}|^{-\psi} Z(\Delta\tilde{y}/|\Delta\tilde{x}|^\phi) + B_0(x, y), \quad (2)$$

where, up to normalization of amplitude and argument, $Z(z)$ is a universal scaling function while $B_0(x, y)$ is a smooth background. If y is a relevant variable one has $\phi > 0$ and (2) describes *crossover behavior*, e.g., from Heisenberg (for $y = y_c$) to Ising or XY behavior.^{3,4} Here, however, y is irrelevant and $-\phi \equiv \theta$ is positive.

Now the crux of our approach is that the scaling form (2) which implies universality over y is explicitly realizable and *all* the information in the double power series for $f(x, y)$ may be used *without bias* in constructing inhomogeneous par-

tial differential approximants, $F(x, y) \equiv [J/L; M, N | K]_f$, defined by solving the equation^{3,4}

$$U_J + P_L F = Q_M \partial F / \partial x + R_N \partial F / \partial y. \quad (3)$$

Here the polynomials $U_J(x, y) = \sum_{(j, j') \in J} u_{jj'} x^j y^{j'}$, etc. are chosen so that the power series solution of (3) agrees with the known expansion coefficients of $f(x, y)$ for orders $x^k y^{k'}$ with (k, k') in

$$W_{DG}(s; y) \propto b \{ \exp[-b^2(s - \sqrt{y})^2] + \exp[-b^2(s + \sqrt{y})^2] \}, \quad (4)$$

$$W_{KL}(s; y) \propto b |s|^{y/(1-y)} \exp[-b^2(s^2 - 1)], \quad (5)$$

with $b^2(y) = \frac{1}{2}(1 - y)$ so that $\langle s^2 \rangle_{J=0} = 1$. At $y = 1$ both models become the $S = \frac{1}{2}$ Ising model; for $y = 0$ both reduce to the Gaussian or free-field model with $\chi_G = [1 - (x/x_G)]^{-1}$ and $x_G = \frac{1}{8}$.

It proves convenient to analyze the series for $f = x \chi_{DG}(x, y)$ and $f = \chi_{KL}(x, y) - 1$, respectively, both being upper triangular, i.e., with expansion coefficients $f_{ii'} = 0$ for $i' > i$. The exact Gaussian limit form, crossover exponent $\phi_G = \frac{1}{2}$, scaling axes (see Fig. 1), etc., are enforced via suitable constraints on U_J, P_L , etc.^{4,17} Since the arrays $[f_{ii'}]$ are upper triangular it is appropriate to use upper triangular label sets J, L, M, N , and K ; but there remains a vast choice of possible shapes and sizes for the coefficient arrays, many of which, however, yield defective approximants not properly describing the critical locus $T_c(y)$.⁴ Now, for ordinary Padé approximants invariance under the Euler transformation $x \rightarrow \bar{x}/(1 + Ax)$, yields optimal approximants²: invariant and near-invariant approximants prove more reliable, stable, and rapidly convergent. For inhomogeneous partial differential approximants the criteria for Euler invariance in x and, separately, in y have recently been elucidated¹⁸; using these we have computed over 300 unbiased Eulerian or near-Eulerian approximants for the DG model, and over 180 for the Klauder model using coefficients of orders x^{18} to x^{21} . Similar features of reliability, stability, and apparent convergence are observed. *All but a small minority of the approximants specify one and only one Ising-like multicritical point in the range $0 < y < 1.8$. This lies on the critical locus emanating from the Gaussian point, x_G (Fig. 1), and thus the universality of the exponents over the physical range $0 < y \leq 1$ is confirmed, separately, in both models.*

Comparison of the corresponding γ and θ histograms in Fig. 2 provides no reason to doubt that both models have the same Ising-like critical exponents even though the dispersion for the

the label set K . The common zeros of Q_M and R_N yield estimates of x_c and y_c (see Fig. 1) and thence follow unbiased estimates of ψ, ϕ, e_1 , and e_2 .^{3,4} Integration of (3) along trajectories,^{3,4} as illustrated in Fig. 1, to regions where $f(x, y)$ is reliably known yields F for general x and y .

We have studied the bcc scalar *double-Gaussian* (DG) and Klauder¹⁶ (KL) models specified by the single-spin weighting factors

Klauder model is appreciably smaller. These graphs, however, conceal the characteristically strong correlations among the critical parameters evident in Fig. 3, which presents, for the Klauder model, exponent means and standard deviations, σ , grouped by ranges of associated y_c estimates. The outer, dashed deviation lines for θ include the typically erratic^{2,3} extreme

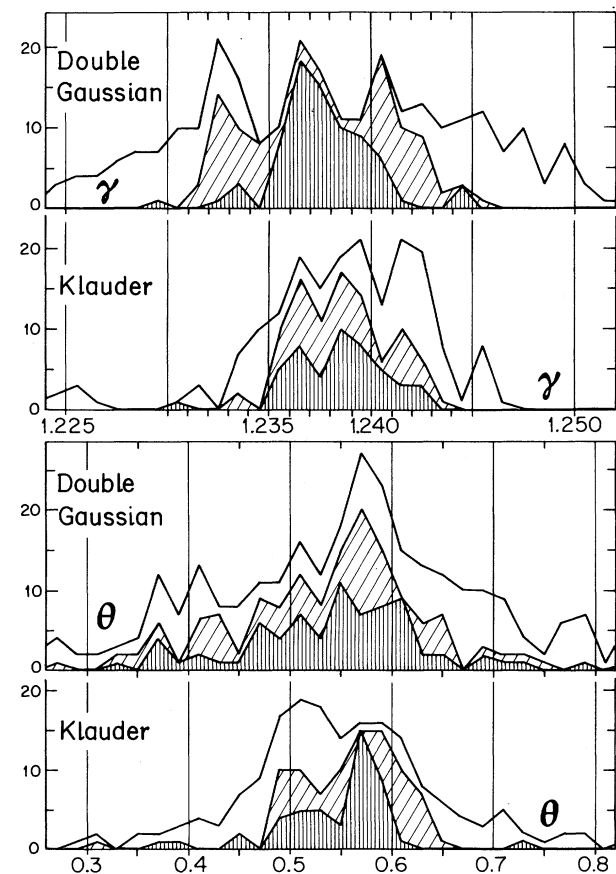


FIG. 2. Histograms of γ and θ estimates for the double-Gaussian and Klauder models (see text).

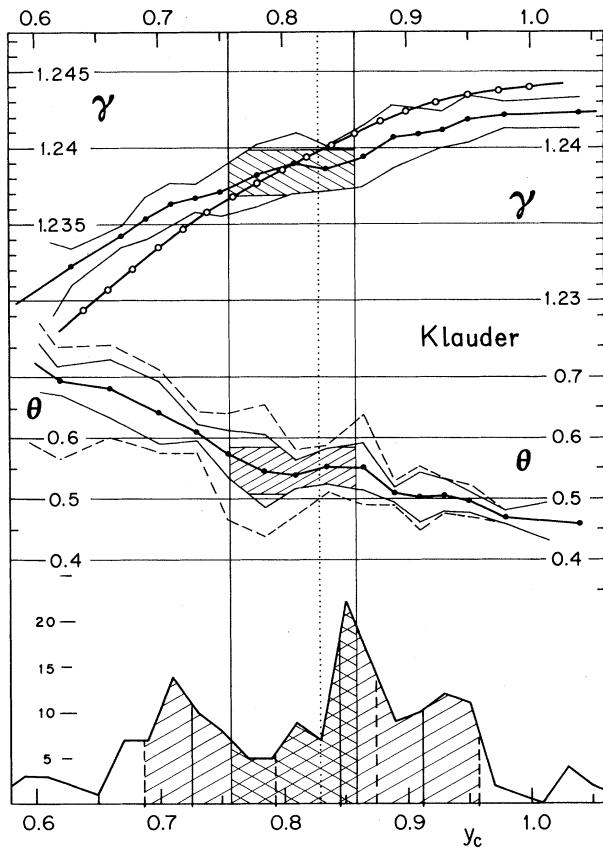


FIG. 3. Histogram of y_c estimates and corresponding exponent means (solid dots) and standard deviation limits for the Klauder model (see text). The open chain curve (circles and dashes) represents single-variable estimates.

estimates. (The corresponding double-Gaussian model figure is similar.¹⁷) The vertical solid and dashed lines on the y_c histogram locate the quartiles and octiles, respectively. Forming the mean, \bar{y}_c [≈ 0.857 (DG), 0.845 (Kl)], of the three central quartiles (shaded in Fig. 3) ameliorates the effects of the sporadic outlying estimates. We will focus attention, for each model, on the quartile centered on \bar{y}_c since we believe the corresponding approximant estimates encompass the true multicritical parameter values. In Fig. 3 the dotted vertical line marks \bar{y}_c and the mean-centered quartile is crosshatched. In Fig. 2 the corresponding estimates are indicated by the heavy shading; they yield $\gamma = 1.2377 \pm 16$ and 1.2384 ± 15 , and $\theta = 0.544 \pm 58$ and 0.546 ± 39 , for DG and Kl, respectively, the uncertainties being $\pm 0.675\sigma$. These estimates are indicated by shading on the γ and θ plots in Fig. 3. The lighter shading in Fig. 2 extends the histograms to two

mean-centered quartiles with insignificant change in mean values.¹⁷

The open chain curve for γ in Fig. 3 represents single-variable estimates from inhomogeneous differential approximants, $[J/L; M]_f$,³ for χ at fixed y . This technique does not allow for strong confluent singularities and, hence, should be most accurate when $y = y_c$. It is thus striking (see Fig. 3) that for both models the single-variable locus intersects the $\bar{\gamma}(y_c)$ plot of two-variable estimates well within the range of the mean-centered quartile.

In conclusion, the unbiased two-variable partial differential approximant technique applied to susceptibility series to order 21 for two distinct models, the double-Gaussian and Klauder models, confirms universality over the parameter y , and between the models with Ising exponents⁷ $\gamma = 1.2385 \pm 15$ and $\theta = 0.54 \pm 5$ (and multicritical values $y_c^{\text{DG}} = 0.87 \pm 4$, $y_c^{\text{Kl}} = 0.81 \pm 6$). The uncertainties quoted are, inevitably, somewhat subjective but the reader may form his own judgment on the evidence presented.¹⁷ The exponent estimates, though more precise, agree very well with biased, single-variable estimates for the Ising model of general spin S ($= \frac{1}{2}$ to ∞).^{11,14,15} In addition, they overlap the field-theoretic estimates^{9,10} although indicating a distinctly higher value of θ and a slightly lower value of γ .

We are indebted to the Natural Sciences and Engineering Research Council of Canada for Grant No. A9348 and grateful for the support of the National Science Foundation through the Applied Mathematics Program, the Condensed Matter Theory Program (including Grant No. DMR-10210), and the Materials Science Center at Cornell University.

^(a)Address for 1981-82.

¹See, e.g., F. J. Wegner, Phys. Rev. B **5**, 4529 (1972).

²See, e.g., *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1974), Vol. 3.

³M. E. Fisher and R. M. Kerr, Phys. Rev. Lett. **39**, 667 (1977); M. E. Fisher and H. Au-Yang, J. Phys. A **12**, 1677 (1979).

⁴M. E. Fisher and J. H. Chen, in *Proceedings of the 1980 Cargèse Summer Institute on Phase Transitions*, edited by M. Levy *et al.* (Plenum, New York, 1981).

⁵B. G. Nickel, in *Proceedings of the Cargèse Summer*

Institute on Phase Transitions, edited by M. Levy *et al.* (Plenum, New York, 1981), and to be published.

⁶D. S. Gaunt and M. F. Sykes, *J. Phys. A* **12**, L25 (1979).

⁷Uncertainties are in units of the last decimal place.

⁸See, e.g., W. J. Camp *et al.*, *Phys. Rev. B* **14**, 3990 (1976).

⁹J. C. Le Guillou and J. Zinn-Justin, *Phys. Rev. B* **21**, 3976 (1980).

¹⁰G. A. Baker, Jr., *et al.*, *Phys. Rev. Lett.* **36**, 1351 (1976).

¹¹B. G. Nickel, *Physica (Utrecht)* **106A**, 48 (1981).

¹²See J. J. Rehr *et al.*, *J. Phys. A* **13**, 1587 (1980).

¹³R. Z. Roskies, *Phys. Rev. B* **24**, 5305 (1981).

¹⁴Also J. J. Rehr and B. G. Nickel, to be published.

¹⁵J. Zinn-Justin, *J. Phys. (Paris)* **42**, 783 (1981).

¹⁶J. R. Klauder, *Ann. Phys. (N.Y.)* **117**, 19 (1979).

¹⁷J.-H. Chen and M. E. Fisher, to be published.

¹⁸M. E. Fisher and D. F. Styer, to be published. The main requirements are met here by J, L, M, and N arrays flush to the right and bottom with $j_{\max} = l_{\max} = n_{\max} = m_{\max} - 2$ while K is flush to left and top.

Dynamic Form Factor, Polarizability, and Intrinsic Conductivity of a Two-Dimensional Dense Electron Gas at Zero Temperature

M. Howard Lee and J. Hong

Department of Physics, University of Georgia, Athens, Georgia 30602

(Received 9 September 1981)

The relaxation function for a two-dimensional dense electron gas is obtained by solving the generalized Langevin equation due to Mori. The dynamic form factor, dynamic polarizability, and conductivity are calculated with use of linear response theory. The conductivity arises from density fluctuations existing at finite wave vectors. The possibility of observing such an effect is considered, especially in the recent work of Allen, Tsui, and DeRossa.

PACS numbers: 72.10.Bg, 72.20.-i, 73.40.Qv

Recent experimental studies of inversion and accumulation layers of the metal-oxide-semiconductor system have stimulated considerable interest in two-dimensional dense-electron-gas models.¹ We report here our solution for the zero-temperature relaxation function for a two-dimensional dense electron gas obtained *exactly* from the generalized Langevin equation (GLE) due to Mori.² Our solution is valid if wave vectors k for density fluctuations ρ_k are small compared with the Fermi wave vector k_F . From this knowledge of the relaxation function, we use linear response theory³ to obtain the dynamic form factor, dynamic polarizability, and conductivity.

Our system is represented by the two-dimensional Sawada Hamiltonian H_0 ,⁴ imposed under an external perturbing potential H_{ext} defined by

$$H_{\text{ext}} = \sum_k \rho_k(t) v_k e^{i\omega t}, \quad (1)$$

where v_k is the Fourier component of the external electric field such as to permit the use of linear response theory, $\rho_k(t) = \exp(iH_0 t) \rho_k \exp(-iH_0 t)$, $\rho_k = \sum_p c_{p+k}^\dagger c_p$, with c_p^\dagger and c_p the fermion creation and annihilation operators, respectively. Mori² has given a formal solution for the relaxation function $\Xi_k(t) = (\rho_k(t), \rho_k) / (\rho_k, \rho_k)$ in a con-

tinued-fraction representation, viz.,

$$\Xi_k(z) = \frac{1}{z + \varphi_k(z)} = \frac{1}{z + \frac{\Delta_1}{z + \frac{\Delta_2}{z + \dots}}}, \quad (2)$$

where $\Xi_k(z)$ is the Laplace transform of $\Xi_k(t)$, φ is the memory function or the kernel of the Langevin equation, $\Delta_1, \Delta_2, \dots$ are static correlation functions² related to moments, not depending on H_{ext} , and finally (A, B) denotes the Kubo scalar product of operators A and B .^{3,5} For small k we find that $\Delta_1 = (\omega_p^{\text{cl}})^2 + 2k^2 \epsilon_F^2$, $\Delta_2 = k^2 \epsilon_F^2 + O(k^4)$, $\Delta_3 = k^2 \epsilon_F^2 + O(k^4)$, \dots , $\Delta_n = k^2 \epsilon_F^2 + O(k^4)$, \dots , where k is expressed in units of k_F , $\hbar = 1$, ϵ_F is the $2d$ Fermi energy, and for the classical plasma frequency⁶ we use $\omega_p^{\text{cl}} = (2\pi n e^2 \hbar / m)^{1/2}$, with n and m the electron number density and mass, respectively. We immediately note that to lowest order in k , $\Delta_n = \Delta$ for $n = 2, 3, \dots$, where we define $\Delta = k^2 \epsilon_F^2$. Recently Lee and Dekeyser⁷ have shown that solutions for the relaxation function can be given for certain forms of $\{\Delta_n\}$, one of which is being realized here in this two-dimensional dense-electron-gas model. Following this work, we obtain the desired solution for the