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Breakdown of the Ginzburg-Landau approximation in superconductor fluctuation theory

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The fluctuation specific heat above transition for a clean superconductor in a uniform magnetic field is calculated microscopically for fixed temperature and varying field. It does not exhibit the premature breakdown of the Ginzburg-Landau approximation, arising from failure of the $(\vec{\nabla}/i)^2 \rightarrow (\vec{\nabla}/i + 2e\vec{A}/\hbar c)^2$ substitution that was found previously for the clean fluctuation diamagnetism.

I. INTRODUCTION

The Ginzburg-Landau (GL) equation governing the order parameter or pair wave function of a superconductor holds for slowly varying wave functions, and is linear in $(\vec{\nabla}/i)^2$. The influence of a magnetic field H on the Cooper pairs in a superconductor is taken into account by the substitution[1] $(\vec{\nabla}/i)^2 \rightarrow \vec{\Pi}^2 \equiv (\vec{\nabla}/i + 2e\vec{A}/\hbar c)^2$. (Here $\vec{A}$ is the vector potential, and the GL approximation keeps only leading-order contributions in $\vec{\Pi}^2$.) The Cooper pair is thus treated by this substitution as a point doubly charged particle. Using this substitution, the fluctuation diamagnetism above transition $M(T)$ was calculated within the GL approximation by Prange[2] who predicted that $M(T_{c0})/H^{1/2} = \text{const}$. Deviations from GL predictions in strong fields were expected only for $H/H_{c2}(0) \sim 1$ as higher powers of $\vec{\Pi}^2$ become important.

Experimentally, however, Gollub, Beasley, and Tinkham[3] found that a plot of $M(T_{c0})/H^{1/2}$ vs field deviated from the GL prediction for unexpectedly low fields, $H/H_{c2}(0) \sim 0.05$, for clean superconductors. For increasingly dirty superconductors, this effect diminished, and in the dirty limit, the deviations occurred at $H/H_{c2}(0) \sim 1$, as expected. Patton, Ambegaokar, and Wilkins[4] (PAW) did an improved calculation that included high-wave-number fluctuations, with the magnetic field included by a $[(\vec{\nabla}/i)^2 \rightarrow \vec{\Pi}^2]$-type substitution. This could not, however, account for the premature breakdown of the GL approximation.

Lee and Payne[5] (LP) and Kurkijarvi, Ambegaokar, and Eilenberger[6] (KAE) showed theoretically that the anomalous results could be accounted for by a consistent inclusion of commutators $[\Pi_x, \Pi_y]$, as well as higher powers of $\vec{\Pi}^2$. This is necessary for consistency, since the field parameter measuring the contribution of both is the same, namely, $h \equiv (2eH/\hbar c)\xi^2(0) = H/H_{c2}(0)$. Here $\xi(0)$ is the GL coherence length and $H_{c2}(0) = \hbar c/2e\xi^2(0)$ is the zero-temperature Ginzburg-Landau critical field. The consistent inclusion of the extra field terms from the commutator was called "nonlocal electrodynamics" (ned) by LP. The calculations[5,6] were done both in the clean and dirty cases, but since the ned effect is largest in the former case, we shall only consider it in this paper. Inclusion of ned resulted in a curve for the diamagnetism[5,6] that deviated from GL predictions for fields about an order of magnitude smaller than the PAW calculation, and so fitted the experimental curve[3] closely.

A question that immediately arises is if nonlocal electrodynamics plays a similiarly essential role in other superconductor fluctuation phenomena in a magnetic field. This is especially important, since the inclusion of ned in theoretical calculations is more involved than the simple substitution.

In this paper we examine the effect of a magnetic field on the fluctuation specific heat for clean superconductors, and show that ned is unimportant. For fixed temperature and varying field, the calculated specific heat that includes both $\vec{\Pi}^2$ and $[\Pi_x, \Pi_y]$ terms consistently (as in LP-KAE), closely matches the calculated curve that includes Π^2 terms alone (as in PAW). This is in contrast to the diamagnetism case, where the two curves are very different, as stated above.

In Sec. II we outline the microscopic calculations, based on the pair propagator,[5] and present our results. In the Appendix we point out that the LP-KAE result for inclusion of ned may be rederived in a simpler manner using properties of special functions instead of operators and coherent states.[5,6]

II. CALCULATIONS AND RESULTS

We follow LP, and outline the calculation of the grand potential from the pair propagator. The grand potential $I = -k_B T \ln \text{Tr} e^{-\beta(H-\mu N)}$ for the superconductor described by a Gorkov[1] Hamiltonian

$$H - \mu N = \int d^3r \sum_\sigma \psi_\sigma^\dagger \left(-\frac{\hbar^2}{2m}\vec{\nabla}^2 - \mu\right)\psi_\sigma - \lambda \int d^3r\, \psi_\uparrow^\dagger(r)\psi_\downarrow^\dagger(r)\psi_\downarrow(r)\psi_\uparrow(r) \quad (1)$$

can be found by differentiating, then integrating I with respect to the coupling constant λ.

Thus[5,6]

$$I(\lambda) - I(0) = -\int_0^\lambda d\lambda \int d^3r\, D(\vec{r},\vec{r};0^-)\,, \quad (2)$$

where

$$D(\vec{r},\vec{r}';\tau) \equiv \langle T[\psi_\downarrow(\vec{r},\tau)\psi_\uparrow(\vec{r},\tau)\psi_\uparrow^\dagger(\vec{r}',0)\psi_\downarrow^\dagger(\vec{r}',0)]\rangle$$

is the finite-temperature pair propagator[5] in the presence of the Gorkov interaction. D satisfies an integral equation that is soluble in the ladder approximation, if D is diagonal in some basis Ψ_α, i.e., if

$$D(\vec{r},\vec{r}';\omega_m) = \sum_\alpha \Psi_\alpha(\vec{r})\Psi_\alpha^*(\vec{r}')D_\alpha(\omega_m).$$

Here $\omega_m = 2\pi m k_B T$, m is an integer, and is henceforth set equal to zero and suppressed, since for the clean case it is $D_\alpha(0)$ that diverges at transition and dominates the $\omega_m \neq 0$ contribution.[5-7] Therefore, we have with $D_\alpha = \Pi_\alpha/(1-\lambda\Pi_\alpha)$ that

$$I(\lambda) - I(0) = k_B T \sum_\alpha \ln(1 - \lambda\Pi_\alpha)\,, \quad (3)$$

where

$$\Pi_\alpha \equiv \int d^3r_1\, d^3r_2\, \Psi_\alpha^*(\vec{r}_1)\Pi(\vec{r}_1,\vec{r}_2)\Psi_\alpha(\vec{r}_2) \quad (4)$$

and $\Pi(\vec{r}_1,\vec{r}_2)$ is the polarization part,

$$\Pi(\vec{r}_1,\vec{r}_2) = k_B T \sum_\nu G_0(r_1,r_2;\nu)G_0(r_1,r_2;-\nu).$$

In zero magnetic field, $\Pi(\vec{r}_1\vec{r}_2)$ at $H=0$ is $\equiv \Pi_0(|\vec{r}_1 - \vec{r}_2|)$ and the propagator is diagonal in plane waves, $\Pi_\alpha \rightarrow \Pi(\vec{q}) = \Pi_0(|\vec{q}|)$ with

$$1 - \lambda\Pi_0(|\vec{q}|) = N(0)\lambda[\epsilon_0 + K(|\vec{q}|)] \approx N(0)\lambda[\epsilon_0 + \xi^2(0)\vec{q}^2].$$

Here $N(0)$ is the single-spin electron density of states at the Fermi surface, $\epsilon_0 \equiv \ln(T/T_{c0})$ and the zero-field kernel $K(|\vec{q}|) \equiv [\Pi_0(0) - \Pi_0(|\vec{q}|)]/N(0)$.

This is in the GL approximation, where $K(|\vec{q}|)$ has been expanded up to order $\vec{q}^2$. In order to include the effect of high-wave-number fluctuations, PAW essentially put

$$1 - \lambda\Pi_0(|\vec{q}|) = 1 - \exp\{-N(0)\lambda[\epsilon_0 + \xi^2(0)\vec{q}^2]\},$$

and included the effect of a magnetic field by the simple substitution on the pair momentum, $\xi^2(0)\vec{q}^2 \rightarrow \xi^2(0)k^2 + 2h(n+\frac{1}{2})$. Here k is the pair wave number parallel to the field, and $n = 0,1,2,\ldots$.

LP-KAE showed that the simple substitution above, equivalent to $(\vec{\nabla}/i)^2 \rightarrow \vec{\Pi}^2$, failed for the fluctuation diamagnetism, especially for the clean case. With the pair propagator diagonal in pair Landau states, their result[5,6] rederived in the Appendix, for $1-\lambda\Pi_\alpha \rightarrow (1-\lambda\Pi_{nk})$ was

$$1 - \lambda\Pi_{nk} = N(0)\lambda\left(\epsilon_0 + \frac{(-1)^n}{2}\int_0^\infty dx\, e^{-x/2}L_n(x) \times K((k^2+\beta x)^{1/2})\right). \quad (5)$$

Here $\beta \equiv eH/\hbar c$. The effect of the extra commutator terms, or ned, is to cause the folding of the zero-field kernel $K(|\vec{q}|)$ with a Laguerre polynomial $L_n(x)$.

LP showed[5] that for $h < 0.28$ the contribution of the exact kernel K under the Laguerre folding of Eq. (5) could be simulated by a PAW form

$$K(|\vec{q}|) = 1 - \exp[-\xi^2(0)\vec{q}^2(T_{c0}/T)^2]\,. \quad (6)$$

Using this simulation and Eqs. (5) and (6) in Eq. (3) they found, after expanding the logarithm and integrating, that

$$I(\lambda) - I(0) = -[Vk_B T(T/T_{c0})h/4\pi^{3/2}\xi^3(0)]\sum_{r=1}^\infty F_r^{-1}. \quad (7)$$

Here $F_r \equiv (1-A^r)(QA_+)^r$, $A_\pm \equiv 1 \pm h$, $A \equiv A_-/A_+$, $Q \equiv 1+\epsilon_0$, and h is a dimensionless but temperature-dependent field variable $h \equiv h(T_{c0}/T)^2$. [Terms such as $\sim \ln(1+\epsilon_0)$ not leading to a divergent specific heat at transition have been extracted and neglected.]

From Eq. (7) we find the specific heat per unit volume, $C = -V^{-1}T\,\partial^2[I(\lambda) - I(0)]\partial T^2$, including ned effects, to be given by

$$C_{\text{ned}}(T) = \kappa \sum_{r=1}^\infty F_r^{-1}\left[r\frac{(r+1)}{Q^2} + 4 - \frac{3r}{Q} - \frac{4hr^2(1+A^{r-1})}{QA_+(1-A^r)} + 8\left(\frac{hr(1+A^{r-1})}{A_+(1-A^r)}\right)^2 - 4\frac{h^2r(r-1)(1-A^{r-2})}{A_+^2(1-A^r)}\right] - 2\frac{H}{T}M_{\text{ned}}(T)\,, \quad (8)$$

where

$$M_{\text{ned}}(T) = \frac{\kappa T}{H}\sum_{r=3}^\infty F_r^{-1}\left[1 - \frac{rh(1+A^{r-1})}{A_+}\right] \quad (9)$$

and

$$\kappa \equiv hk_B T/[4\pi^{3/2}T_{c0}\xi^3(0)].$$

Here the last term in Eq. (8) is in terms of the diamagnetism $M_{\rm ned}$ calculated by LP-KAE, and found by them to be sensitive to the magnetic field. Note that the sum for $M_{\rm ned}$ begins at the $r=3$ term, since the $r=1,2$ terms are zero, as may be easily checked. Such cancellation does not occur in the other terms of $C_{\rm ned}$ in Eq. (8). Both series of Eqs. (8) and (9) diverge at a $T_{c2}(H)$ defined by $QA_+=1$ with $\ln[T/T_{c2}(H)]=\epsilon_0+h/(1+h)$. Equation (8) has previously been plotted[8] for fixed field and varying temperature. Here we will consider fixed temperature and varying field.

In order to compare with $C_{\rm ned}$, we also determine the specific heat $C_{\rm PAW}$ with higher orders in $\vec{\Pi}^2$ included, but with the commutators $[\Pi_x, \Pi_y]$ neglected. The Laguerre folding in Eq. (5) is omitted and the $\xi^2(0)\vec{q}^{\,2} \to \xi^2(0)k^2 + 2h(n+\frac{1}{2})$ substitution into Eq. (6) is used.[4-6] This gives us a $C_{\rm PAW}$ expression as in Eq. (8) but with the substitution $A_\pm \to A'_\pm \equiv e^{\pm h}$. The $M_{\rm PAW}$ term does not exhibit a cancellation of the $r=1,2$ terms.[9]

From Eq. (8) $C(T)\xi^3(0)h^{1/2}$ is a function of dimensionless scaled variables ϵ_0 and h only. Thus, plots versus these variables will be universal in the sense that all clean superconductors with fluctuations above $T_{c2}(H)$, i.e., intrinsic type-II materials and supercooled type-I materials, will give the same curve.

In Fig. 1, we plot $C(T)\xi^3(0)h^{1/2}$ vs h, for various fixed values of $\epsilon_0(=0, \pm 0.003)$. For $\epsilon_0=0$ and $h \ll 1$, $C(T)\xi^3(0)h^{1/2} \sim {\rm const} + h$, where, in the GL approximation, the constant is[8]

$$(k_B/8\pi)\sum_{n=0}^{\infty}(2n+1)^{-3/2} \approx 0.91\times 10^{-17}({\rm erg}/{}^\circ{\rm K}).$$

The solid curves are the $C_{\rm ned}$ curves of Eq. (8). The $\epsilon_0=\pm 0.003$ curves merge with the $\epsilon_0=0$ curve for $h \gg \epsilon_0$, fitting it to within 1% for $h>0.1$. For clarity, they are terminated at $h=0.05$. The $\epsilon_0=0.003$ curve goes to zero like $h^{1/2}$ for $h\ll 1$, and the $\epsilon_0=0.003$ curve diverges at $T_{c2}(H)$.

In order to judge the importance of ned, we plot, for $\epsilon_0=0$ only, the corresponding $C(T)\xi^3(0)h^{1/2}$ curve using the $C_{\rm PAW}$, neglecting ned (dashed line). The PAW curve, coming from the simple $(\vec{\nabla}/i)^2 \to \vec{\Pi}^2$ substitution, matches the ned curve to within 7% or less, with both changing by one-half the GL value (horizontal line), by about $h=0.3$. This is to be compared to the diamagnetism, where the ned curve changes by one-half the GL value at $h=0.05$, with the corresponding change in the PAW curve occurring only for fields about a factor of 10 larger. Thus for the fluctuation specific heat, the extra commutator terms do not cause anomalous behavior and the deviations from the GL prediction are mainly due to higher order $\vec{\Pi}^2$ terms.

This behavior is better understood if we also

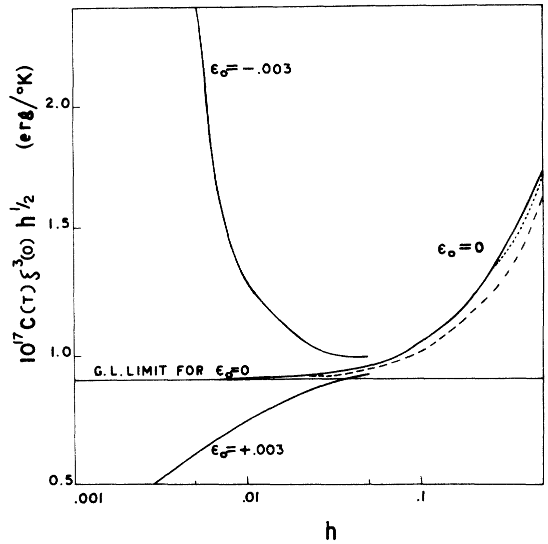

FIG. 1. $C(T)\xi^3(0)h^{1/2}$ is plotted vs h on a semilog scale for fixed $\epsilon_0(=0, \pm 0.003)$, where the variables are defined in the text. The solid lines are predicted specific heats, including ned effects. The $\epsilon_0=\pm 0.003$ curves merge with the $\epsilon_0=0$ curve, but are terminated at $h=0.05$ for clarity. The dashed and dotted lines are the PAW specific-heat and dominant-term contributions, respectively, for $\epsilon_0=0$. (The corresponding curves for $\epsilon_0=\pm 0.003$ are not shown.) The horizontal line is the GL limit.

plot (dotted line) the contribution to $C_{\rm ned}$ from terms excluding the $M_{\rm ned}$ term in Eq. (8). In the field range shown these terms alone match the ned curve to better than 2%. The $M_{\rm ned}$ term, which is known to be sensitive to ned effects, is thus small compared to these dominant terms.

III. CONCLUSION AND COMMENTS

In conclusion, for the fluctuation specific heat, the corrections to the $(\vec{\nabla}/i)^2 \to \vec{\Pi}^2$ substitution are small, in contrast to the fluctuation diamagnetism[5,6] where such corrections lead to a premature breakdown of the GL approximation. Measurement of the universal curves predicted in Fig. 1 would confirm this.

In clean superconductors, fluctuations are much harder to measure than in the dirty case, owing to the smallness of the critical region. However, the application of a magnetic field widens the critical region and enhances the fluctuation specific heat.[8] Previous measurements in a magnetic field[10] were done only for very dirty superconductors, for which ned effects were found to be unimportant for the diamagnetism.[5-7] Therefore, these results[10] cannot be directly compared with the theory presented here.

Finally, in view of recent theoretical[11] and experimental[12] work on fluctuations inside the critical region, we must emphasize that our calculations are valid only outside the critical region in a magnetic field[8] since we assumed only bare electron Green's functions G_0, in the polarization part Π_0 above. The question of the role of ned in fluctuation effects inside the critical region is, however, worth examining.

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APPENDIX

The result of Eq. (5) for the inclusion of ned in the pair propagator has been obtained previously by LP-KAE. However, the methods they use are somewhat involved,[5,6] using operator algebra and coherent states. Here we outline an alternative and somewhat simpler derivation using properties of special functions.

We want to determine $\Pi_\alpha \to \Pi_{nkq}$ of Eq. (4) where $\Psi_\alpha \to \Psi_{nkq}$, which are pair Landau states, and eigenfunctions of $\vec{\Pi}^2$, i.e.,

$$\xi^2(0)\vec{\Pi}^2\Psi_{nkq} = [\xi^2(0)k^2 + 2h(n+\tfrac{1}{2})]\Psi_{nkq}.$$

In the gauge $\vec{A} = (0, Hx, 0)$ and with volume $V \equiv L_x L_y L_Z$ and $\beta \equiv eH/\hbar c$, the pair Landau state is

$$\Psi_{nkq}(\vec{r}) = \frac{(2\beta)^{1/4} e^{i(kz+qy-\beta(x-x_0)^2}}{(2^n n!\, \pi^{1/2} L_y L_z)^{1/2}} H_n((2\beta)^{1/2}(x-x_0)). \tag{A1}$$

Here q is the degeneracy label, $x_0 = -q/2\beta$, and $H_n(x)$ is a Hermite polynomial. Making the eikonal approximation on the Green's function (valid for $k_B T/\hbar \gg \omega_c$, the electronic cyclotron frequency) and writing it as a zero-field Green's function times a phase factor, we get

$$\Pi_{nkq} = \int d^3r_1\, d^3r_2\, \Psi_{nkq}(\vec{r}_1)\Pi_0(|\vec{r}_1 - \vec{r}_2|) \times e^{-i\phi(r_1 r_2)}\Psi_{nkq}(\vec{r}_2), \tag{A2}$$

where Π_0 is the zero-field polarization, and

$$\phi(12) = (2e/\hbar c)\int_2^1 \vec{A}(\vec{s})\, d\vec{s}$$

integrated along a straight line path.

Invoking Werthamer's trick[5,13] we obtain with $\vec{R} \equiv \vec{r}_2 - \vec{r}_1$

$$\Pi_{nkq} = \int d^3r_1\, \Psi^*_{nkq}(\vec{r}_1)\Big[\int d^3R\, \Pi_0(|\vec{R}|)e^{i\vec{R}\cdot\vec{\Pi}}\Big]\Psi_{nkq}(\vec{r}_1). \tag{A3}$$

LP evaluate Eq. (A3) by converting the differential operator $\vec{\Pi}$ to creation and annihilation operators, expanding in coherent states, and performing some integrals over special functions. It is here that we diverge from previous treatments.[5,6] Note that in Eq. (A3) odd powers of $\vec{R}\cdot\vec{\Pi}$ vanish by symmetry, leaving a series[14] in $\vec{\Pi}^2 \sim h$ and $[\Pi_x, \Pi_y] \sim ih$. This series is independent of the degeneracy label q, and so actually Π_{nkq} is Π_{nk}. Thus in Eq. (A1) we may sum both sides over q and divide by the degeneracy factor $(2eHL_xL_y | 2\pi\hbar c)$ leaving Π_{nk} unchanged, but resulting in an S_{nk} term on the right, with $Z = z_2 - z_1$ and

$$S_{nk} = \sum_q \frac{\Psi_{nkq}{}^*(\vec{r}_1)\Psi_{nkq}(\vec{r}_1)}{2eHL_xL_y/2\pi\hbar c} = \frac{e^{ikZ}I_n}{V}. \tag{A4}$$

The sum over the degeneracy label of a product of electron Landau states is known, and has been used in a different context.[15] For completeness, we outline the steps for pair Landau states.

By invoking the Hermite polynomial generating function[16]

$$\sum_{n=0}^{\infty} z^n \frac{H_n(x)H_n(y)}{2^n n!} = (1-z^2)^{-1/2} \times \exp\{[2xyz - (x^2+y^2)z^2]/(1-z^2)\}, \tag{A5}$$

we get a generating function for I_n,

$$\sum_{n=0}^{\infty} z^n I_n = e^{i\phi(r_1 r_2)}(1-z)^{-1}\exp[(1+z)\beta\rho^2/2(1-z)]. \tag{A6}$$

Here $\rho^2 \equiv (x_2 - x_1)^2 + (y_2 - y_1)^2$ and the phase integral, in our gauge is $\phi(12) = \beta(x_2 + x_1)(y_1 - y_2)$. Comparing this with the standard Laguerre generating function $\sum z^n L_n(x) = (1-z)^{-1}\exp[-xz/(1-z)]$ we obtain from Eq. (A4)

$$S_{nk} = V^{-1}e^{ikZ}e^{i\phi(r_1 r_2)}e^{-\beta\rho^2/2}L_n(\beta\rho^2). \tag{A7}$$

Inserting this into the equation for Π_{nk}, the phase factors cancel, giving, with d^3R in cylindrical coordinates,

$$\Pi_{nk} = \int \rho\, d\rho\, d\theta\, dz\, \Pi_0(|\vec{R}|)e^{ikz-\beta\rho^2/2}L_n(\beta\rho^2). \tag{A8}$$

Fourier transforming $\Pi_0(|\vec{R}|)$ and doing the θ integration in Eq. (A8) gives a zero order Bessel function. Doing the ρ integration[17] and adding and subtracting $\Pi_0(|\vec{q}| = 0)$, with a Debye cutoff,[5] gives the LP-KAE result.

$$1-\lambda\Pi_{nk}=N(0)\lambda\left(\epsilon_0+\frac{(-1)^n}{2}\int_0^\infty dx\, e^{-x/2}L_n(x)\times K\big((k^2+\beta x)^{1/2}\big)\right). \tag{A9}$$

The Laguerre polynomial appears because its generating function is related to that of the generating function for a product of Hermite polynomials. We see that the infinite degeneracy of the Landau states states with respect to q plays an essential role in obtaining the final result.

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[9]The cancellation may be traced back to different behavior under differentiation, $\partial A_\pm/\partial h=\pm 1$, but $\partial A'_\pm/\partial h = A'_\pm$. The author is indebted to Dr. M. G. Payne for pointing out the importance of this cancellation for the ned in the diamagnetism calculation of Ref. 5.

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[14]Even if we had not assumed the pair propagator to be diagonal in pair Landau states, the $\vec{r}_1$ integral in Eq. (A3) would be essentially an orthonormality integral, enforcing such diagonality.

[15]See, for example, A. K. Rajagopal, Phys. Lett. A 5, 40 (1963); R. R. Gerhardt and D. T. Lee, Z. Phys. 252, 162 (1972).

[16]*Higher Transcendental Functions*, edited by A. Erdelyi (McGraw Hill, New York, 1973), Vol. II, p.194, Eq. (22).

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