On the periodicity of superconducting shape resonances in thin films

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The pairing temperature of superconducting thin films is expected to display, within the Bardeen–Cooper–Schrieffer theory, oscillations as a function of the film thickness. We show that the pattern of these oscillations switches between two different periodicities at a density-dependent value of the superconducting coupling. The transition is most abrupt in the anti-adiabatic regime, where the Fermi energy is less than the Debye energy. To support our numerical data, we provide new analytical expressions for the chemical potential and the pairing temperature as a function of thickness, which only differ from the exact solution at weak coupling by exponentially-small corrections.

I. INTRODUCTION

Since the pioneering study of Thompson and Blatt raised hopes to observe improved critical temperature in thin films made of superconducting materials [1], a large number of experimental [2–17] and theoretical [18–30] works have followed up on this idea. Thanks to the quantum confinement along one direction, the thin-film geometry splits the three-dimensional dispersion law of the superconductor into a set of two-dimensional subbands. The energy separation between the subbands varies with changing film thickness such that the Fermi level, which is fixed by the bulk electron density, must adjust as well. In the Thompson–Blatt model (a free-electron like metal confined in the film by hard walls), the critical temperature varies with reducing film thickness, drawing a sawtooth-like increase (Fig. 1), where jumps occur each time the Fermi level crosses the bottom of a subband. These quantum oscillations have become known as superconducting shape resonances. The resulting “period” (actually a wavelength) of critical-temperature oscillations is

$$\Lambda_0 = \frac{\pi}{k_F} \approx n^{-1/3},$$  \hspace{1cm} (1)

where $k_F$ and $n$ are the bulk Fermi wave vector and electron density, respectively. For typical metallic densities of order 10$^{22}$ cm$^{-3}$, the expected oscillations period is a few Angström. The period $\Lambda_0$ obtained by Thompson and Blatt tracks discontinuities of the critical temperature $T_c$ versus film thickness $L$. These discontinuities arise due to a simplification adopted when solving the Bardeen–Cooper–Schrieffer (BCS) gap equation, while the exact dependence when the Fermi energy is sufficiently close to the bottom of a band

$$\frac{\partial}{\partial L} T_c = \frac{\pi}{\sqrt{k_F^2 + 2m\omega_D^2}} \approx \frac{1}{\sqrt{E_p + \hbar\omega_D}},$$ \hspace{1cm} (2)

where jumps occur each time the Fermi level crosses the bottom of a subband coincides with the upper edge of the interaction window, i.e., rather than triggering a discontinuity of $T_c$ when it crosses the subband edge, the Fermi level triggers a discontinuity of $dT_c/dL$ when it reaches $\hbar\omega_D$ below the subband edge. This leads to a corrected period $\Lambda_0$ which tracks the discontinuities of $dT_c/dL$. The exact period (2) is shorter than the Thompson–Blatt result (1), although both coincide in the adiabatic limit $E_p \gg \hbar\omega_D$. Equations (1) and (2) are asymptotic results obtained in the weak-coupling regime $\lambda \ll 1$, where $\lambda$ is the dimensionless coupling constant for pairing. In this limit, $T_c$ approaches zero and the chemical potential at $T_c$ is close to the zero-temperature Fermi energy. Furthermore, these expressions are valid for large $L$, where the period becomes well defined and the Fermi energy approaches the bulk value.

Simulations performed at intermediate to strong coupling show that Eq. (2) works in this regime as well [32]. The discontinuities of $dT_c/dL$ are large in that case (in a sense to be made precise below) and the $T_c(L)$ curve has cusps pointing downward at the discontinuities, separated by maxima in-between each cusp (Fig. 2). Since the optimal condition to observe the difference between Eqs. (1) and (2) is the anti-adiabatic regime $E_p \ll \hbar\omega_D$, which is often associated with strong coupling [33–35], it is interesting that Eq. (2) is valid beyond weak coupling. Of course, the applicability of the static BCS approach is not guaranteed for these cases. Luckily, there exists low-density systems such as $n$-doped SrTiO$_3$ which, albeit falling into the class of anti-adiabatic superconductors [36], have low values of the coupling constants [37–41]. Simulations of the $T_c(L)$ curves performed at low values of $\lambda$ show, however, that the oscillation pattern changes as $\lambda \to 0$. The size of the discontinuities in $dT_c/dL$ decreases and the relative amplitude of the oscillations in $T_c(L)$ increases. While the separation between discontinuities continues to be described by Eq. (2), the new oscillation pattern is not controlled by these discontinuities any more and approaches a period given, somewhat surprisingly, by Eq. (1). Thus, in the anti-adiabatic regime, where Eq. (2) would suggest that the period of $T_c$ oscillations becomes independent of the density, this is true only for moderate to strong coupling, while the density dependence given by Eq. (1) reappears at weak coupling. This is the main message of the present report, which we elaborate in the following.
We consider a simple BCS superconductor with parabolic dispersion and a local electron-electron attraction, that is, confined by two parallel hard walls. The more realistic case of a finite-depth potential well can be treated similarly at the cost of introducing one additional parameter, but this plays a marginal role in the question of the periodicity discussed here. The value of the critical temperature $T_c$ is found by solving the following set of coupled equations:

\[
\begin{aligned}
 n &= \frac{m k_B T_c}{\pi \hbar^2 L} \sum_q \ln \left( 1 + e^{\frac{-E}{\hbar c T_c}} \right) \\
 \Delta_p &= \sum_q V_{pq} \Delta_q \frac{m}{2 \pi \hbar^2} \int_{-\hbar \omega_0}^{\hbar \omega_0} dE \frac{\theta(\mu + E - E_q) \tanh \left( \frac{E}{2 T_c} \right)}{2E}.
\end{aligned}
\]  

Equation (3a) sets the chemical potential $\mu(n, L, T_c)$, such as to keep the electron density fixed when $L$ and $T_c$ vary. The $q$ sum runs over all nonzero positive integers, with $E_q = \frac{m}{2 \pi \hbar^2} \left( \frac{q}{L} \right)^2$, giving the minima of the subbands in the quantum well. The simple form of the density equation with a logarithm results after summing the Fermi occupation factors for the momenta parallel to the confinement walls. Equation (3b) is the linearized gap equation at $T_c$, where the pairing order parameters $\Delta_q$ in all subbands vanish. The 3D electron-electron attraction has the same matrix element $V$ between all states having energy within the range $[-\hbar \omega_0, +\hbar \omega_0]$ from the chemical potential. Equation (3b) is however written in the basis of the quantum-well eigenstates, where the matrix elements are no longer all identical, but are larger for the intra-subband processes than for the inter-subband ones: $V_{pq} = \frac{V}{1 + \delta_{pq}/2} [1, 31]$. The integration variable $E$ spans the dynamical range of the interaction and accounts for the energy gained by pairing states of subband $q$ in that range, weighted by $m/(2 \pi \hbar^2)$, which is the density of states of the subband. When $\mu + E < E_q$, the energy $E$ falls below the subband, where there are no states to pair, hence the Heaviside function for removing that energy window.

The model has five parameters ($m, V, \hbar \omega_0, n, L$), which can be reduced to four by using $\hbar \omega_0$ as the unit of energy. Following Ref. 42, we define a dimensionless density parameter

\[
\tilde{n} = \frac{n}{2 \left( m \omega_0 / (2 \pi \hbar^2) \right)^{3/2}} = \frac{4}{3 \sqrt{\pi}} \left( \frac{E_F}{\hbar \omega_0} \right)^{3/2}.
\]  

It is seen that $\tilde{n}$ is not, strictly speaking, a measure of the density—for instance, at fixed physical density, $\tilde{n}$ changes if the mass of the particles changes—but rather a measure of the adiabatic ratio $E_F / \hbar \omega_0$. The value $\tilde{n} \approx 0.75$ marks the transition between the anti-adiabatic regime $E_F < \hbar \omega_0$ and the adiabatic regime $E_F > \hbar \omega_0$. The dimensionless pairing strength is usually measured by the product of the interaction with the 3D density of states at the chemical potential, $\lambda = VN(\mu)$. This definition is impractical when $\mu$ is adjusted self-consistently and Ref. 42 used instead $\lambda = VN(\hbar \omega_0)$. With the latter convention, the values of the coupling constant are not easily compared with experimentally-determined values. In the present study, we use the more conventional definition $\lambda = VN(E_F)$, where $E_F$ is computed from $n$ using non-interacting-electron expressions, like in Eq. (4). In terms of the model parameters, the coupling constant is

\[
\lambda = \frac{m V}{2 \pi \hbar^2 \left( \frac{3n}{\pi} \right)^{1/3}}.
\]  

With the definitions (4) and (5), the coupled equations (3) only involve the four parameters $m, \lambda, \tilde{n}$, and $L$.

Two simplifications are often made to Eqs. (3): the density equation is replaced by its zero-temperature limit and in Eq. (3b), $\theta(\mu + E - E_q)$ is replaced by $\tilde{\theta}(\mu - E_q)$. The resulting simplified equations are:

\[
\begin{aligned}
 n &= \frac{m}{\pi \hbar^2 L} \sum_q \max(0, \mu - E_q) \\
 \Delta_p &= \sum_q V_{pq} \Delta_q \frac{m}{2 \pi \hbar^2} \frac{\theta(\mu - E_q) \tanh \left( \frac{E}{2 T_c} \right)}{2E}.
\end{aligned}
\]  

By solving Eqs. (6) numerically, we obtain the discontinuous variations of $T_c$ shown in Fig. 1 as black lines. This is reminiscent of the Thompson–Blatt results who, rather than solving Eqs. (6) at $T_c$, computed the order parameters at $T = 0$ using equivalent simplifications. The system of equations (6) admits a closed solution that reproduces accurately the data shown in the figure (see Appendix A). Figure 1 also shows the solution of Eqs. (3) in red for comparison. There are significant differences, but the red lines seem to approach the approximate result at weak coupling.
this measure is somewhat noisy, it shows well the transition from the period (2) to the period (1) as the coupling is reduced. The transition is sharp in the anti-adiabatic regime and becomes more and more gradual as one enters the adiabatic regime. At large $\tilde{n}$, both periods become similar and their difference reaches the resolution limit of our Fourier transform.

The change of period is associated with a suppression of the discontinuities in $dT_c/dL$. In order to quantify the strength of the discontinuities, we consider the dimensionless quantity

$$A = \frac{(dT_c/dL)_+ - (dT_c/dL)_-}{T_c/L},$$

which can be evaluated at each singularity of the $T_c(L)$ curve. Figure 3 shows this quantity calculated with the data plotted in Figs. 2(a) and 2(b) at the first discontinuity following $L = 10\Lambda_0$. It is seen that $A$ is approximately constant across the transition between the two periods. This means that the size of the discontinuity scales like $T_c$ and therefore drops exponentially at weak coupling. The evolution of $T_c$ is also shown in Fig. 3 for comparison.

When the singularities become subdominant on the $T_c(L)$ curve and the periodicity turns to Eq. (1), it is tempting to attribute each $T_c$ maximum to a coincidence between the chemical potential and the edge of a subband. This is not the case, as Fig. 4 shows for the data of Fig. 2(a). To describe this figure, we start at $L/\Lambda_0 = 12$ with $\lambda = 0.26$ (red curves). The chemical potential lies inside the 11th subband. Upon reducing $L$, everything else held fixed, the electron density would increase like $1/L$ due to compression, such that a lowering of the chemical potential would be needed to compensate. However, all subbands move upward in energy like $1/L^2$ with reducing thickness: the ensuing loss of states overweights the compression such that the chemical potential must follow the trend of the bands and increase like $1/L$. The critical temperature also has an increasing trend because the pairing matrix elements vary like $1/L$ [1]. Below

Figures 2(a) and 2(b) show some more results from Eqs. (3), with $T_c(L)$ displaying quantum oscillations on top of a background that increases with decreasing $L$. At sufficiently large coupling (red curves), the oscillation period is set by the discontinuities of $dT_c/dL$, which correspond to downward-pointing cusps, leading to Eq. (2). In the adiabatic regime [Fig. 2(b)], additional discontinuities appear in-between, that occur when the Fermi level is $\hbar \omega_D$ above the bottom of a subband [31]. As the coupling is reduced, the discontinuities of $dT_c/dL$ are suppressed and the quantum oscillations display the period $\Lambda_0$ (blue curves). In order to measure the evolution of the period as a function of coupling, we calculate the dependence $T_c(L)$ for $10\Lambda_0 < L < 100\Lambda_0$, we remove the background by fitting it to the form $T_c(\infty) + 1/(a + bL)$, and we compute the cosine transform of the remaining function. The ratio of the Fourier coefficients at $2\pi/\Lambda$ and $2\pi/\Lambda_0$ indicates the dominant period. Repeating this calculation at each density and coupling, we obtain the data shown in Fig. 2(c). Although

![Figure 2](image.png)

**FIG. 2.** (a), (b) Evolution of $T_c$ with film thickness in the anti-adiabatic (a) and adiabatic (b) regimes. $T_c(L)$ is normalized to its value at $L = 10\Lambda_0$. Different curves correspond to different coupling constants, as indicated by the dots in (c). The horizontal red and blue bars show $\Lambda$ and $\Lambda_0$, respectively. The dotted lines show the fitted background. (c) Illustration of the crossover from Eq. (2) (bright) to Eq. (1) (dark) with decreasing $\lambda$ across the anti-adiabatic and adiabatic regimes. The gray scale shows the ratio of Fourier components at $2\pi/\lambda$ and $2\pi/\Lambda_0$ (see text). $T_c$ is smaller than machine precision in the yellow region. The green curve (right scale) shows that $\Lambda$ and $\Lambda_0$ become difficult to distinguish in the adiabatic regime. All calculations are done for a mass equal to the bare electron mass.

![Figure 3](image.png)

**FIG. 3.** Evolution of the discontinuity measure (left scales) and critical temperature at the discontinuity (right scales) across the transition from $\Lambda$ to $\Lambda_0$ periodicity in the anti-adiabatic (a) and adiabatic (b) regimes.
The thick green lines show the minima of subbands 10 and 11 as they vary with $L$ and the lines labeled 22 to 25 indicate an energy lying $\hbar \omega_D$ below the corresponding subbands.

$L/\Lambda_0 = 11.8$, the 25th subband at energy $\mu + \hbar \omega_D$ ceases contributing to pairing and this induces a cusp in $T_c$ and the discontinuity in $dT_c/dL$. Accidentally, this is also the point where the chemical potential leaves the 11th subband, but this crossing imprints no signature in $T_c$, as can be seen when $\mu$ crosses the 10th subband at lower thickness. For $\lambda = 0.19$ (blue curves), the critical temperature is lower and the chemical potential is correspondingly higher. For the rest, a precise interpretation seems difficult. Starting from $L/\Lambda_0 = 12$, both $T_c$ and $\mu$ show an increasing trend like for stronger coupling. However, near $L/\Lambda_0 = 11.9$, $T_c$ starts to decrease before the chemical potential leaves the 11th subband and then goes through a minimum at a thickness where $\mu$ has no obvious coincidence with the subband energies. The feature in $T_c(L)$ which seems to correlate best with $\mu$ crossing a subband is a zero of the second derivative, where the curvature change from negative to positive with decreasing $L$. The same conclusion is reached in the adiabatic regime with the data of Fig. 2(b).

Figure 1 suggests that the exact $T_c$ at weak coupling interpolates smoothly across the discontinuities of the approximate result. These discontinuities occur when $\mu_0$ crosses a subband edge, where $\mu_0$ is the chemical potential given by Eq. (6a). Provided that the difference between the exact $\mu$ and $\mu_0$ becomes negligible at weak coupling, this would explain the coincidence between the curvature changes of $T_c(L)$ and $\mu$ crossing a subband edge. In Appendix B, we show that the exact chemical potential from Eqs. (3) indeed approaches the value $\mu_0$ given by Eq. (6a) when $T_c \to 0$, unless the vanishing of $T_c$ is driven by taking another limit, either $L \to 0$ or $n \to 0$. In the latter cases, $\mu(T_c = 0) \neq \mu_0$ [31, 42]. But for any finite $L$ and $n$, we find that the deviation of $\mu(T_c = 0)$ from $\mu_0$ is exponentially small in $k_B T_c/\mu_0$. Furthermore, we also show based on a closed solution that the $T_c$ resulting from Eqs. (3) approaches the one from Eqs. (6) with corrections that are exponentially small for $\lambda \to 0$ (except in the two limits mentioned above). This allows us to conclude that in the regime where the solution of Eqs. (3) oscillates with the period $\Lambda_0$, the inflection points where the curvature changes from positive to negative with increasing $L$ signal the population of a new subband.

The boundary between the two periodicities in Fig. 2(c) depends on the carrier mass. In Fig. 5, we show the boundary extracted from Fig. 2(c), together with boundaries obtained with other values of the mass. In order to compare different masses, we normalize the density on the horizontal axis using the bare electron mass $m_e$ in all cases. As the mass increases, the domain of Thompson–Blatt periodicity shrinks and moves to higher densities. We also show in Fig. 5 the density-dependent coupling constants $\lambda_1$ and $\lambda_3$ for SrTiO$_3$, as determined in Ref. 40 for the light ($l$) and heavy ($h$) bands with masses $m_l = m_e$ and $m_h = 4m_e$, respectively. As it turns out, in the whole range of densities, SrTiO$_3$ falls in the regime of the Thompson–Blatt periodicity Eq. (1). Therefore, in spite of the fact that this low-density material lies well within the anti-adiabatic regime, thin films of doped SrTiO$_3$ are expected to display oscillations of $T_c$ with the period (1), because of the low coupling [11, 43]. Specifically, for bulk densities $n = 10^{17}$–$10^{21}$ cm$^{-3}$, Eq. (1) gives $\Lambda_0 = 22$–1 nm.

III. CONCLUSION

A clearcut experimental demonstration of critical-temperature shape resonances in superconducting thin films has proven difficult. A mere increase or decrease of $T_c$ with changing thickness, as routinely observed, is not a proof of quantum-size effects, as these variations can be attributed to other causes [15, 16]. Oscillations of $T_c$ with varying the film thickness must be demonstrated. For simple band structures, the oscillation pattern is linked with microscopic parameters of the bulk material, allowing for an unambigu
ous demonstration that the variations of $T_c$ are controlled by the confinement. We have shown that this link changes between weak coupling, where the oscillation period is ruled solely by the electron density, and intermediate to strong coupling, where it also depends on the pairing interaction.

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Appendix A: Shape resonances in the Thompson–Blatt model

The enhancement of $T_c$, relative to the bulk value shown in Fig. 1 with the black lines was computed by solving numerically Eqs. (6). These equations can also be solved (almost) exactly. We give here a closed formula that produces curves undistinguishable from the numerical data shown in Fig. 1. The relation becomes exact only in the limit $k_B T_c \ll \hbar \omega_D$. If Eq. (A1) is also used for the calculation of $T_c^\text{3D}$, a similar error is made and both errors can be expected to cancel in the ratio $T_c / T_c^\text{3D}$. This cancellation works as long as the difference between $T_c$ and $T_c^\text{3D}$ is small compared to $\hbar \omega_D$. It therefore breaks down in the limit $L \to 0$, where $T_c$ diverges. The numerics shows that all subband gaps approach zero with the same slope at $T_c$, such that we have

$$\sum_q V_{1q}^2 \Delta_q^2 \frac{m}{2\pi \hbar^2} \theta(\mu - E_q) = \frac{mV}{2\pi \hbar^2} \left( \frac{1}{2} + N_{sb} \right),$$

where $N_{sb}$ is the number of occupied subbands. Equation (6b) is then readily solved to yield

$$T_c \approx \frac{k_B T_c}{T_c^\text{3D}} \approx \exp \left( \frac{1}{\lambda} \left[ 1 - \left( \frac{3nL^3}{\pi} \right)^{1/3} \right] \right).$$

Discontinuities occur because $N_{sb}$ is a discontinuous function of $n$ and $L$. This function follows by solving Eq. (6a). The latter equation can be satisfied as long as the chemical potential is in the range $E_{N_{sb}} < \mu < E_{N_{sb} + 1}$, such that one can set $\mu = E_{N_{sb}}$ and solve for $N_{sb}$. The result is

$$N_{sb} = \text{floor} \left[ \frac{1}{4} \left( 1 + C^{1/3} + \frac{7}{3} C^{-1/3} \right) \right],$$

$$C = 3 + 2^2 \frac{3nL^3}{\pi} + \sqrt{(3 + 2^2 \frac{3nL^3}{\pi})^2 - \left( \frac{7}{3} \right)^3},$$

where the function floor$(\cdot)$ returns the largest integer smaller than its argument. Equation (A3a) coincides with the black lines in Fig. 1 up to several decimal figures. Deviations are visible only for $L \to 0$ (not shown in Fig. 1), where $T_c$ diverges while Eqs. (A3) approaches the finite value $T_c / T_c^\text{3D} = \exp(1/\lambda)$.

Appendix B: Weak-coupling limit of Eqs. (3)

The BCS equations (3) present non-analyticities that are not captured by the approximate Eqs. (6). As a manifestation of these non-analyticities, the three limits $\lambda \to 0$, $L \to 0$, and $n \to 0$ do not commute. Specifically, if the limit $\lambda \to 0$ is taken first, Eqs. (3) reduce to Eqs. (6) as will be shown below. If the limit $L \to 0$ is then taken in Eqs. (6), the resulting chemical potential approaches the bottom of the lowest subband and the resulting $T_c$ diverges. On the contrary, if the limit $L \to 0$ is taken first in Eqs. (3), $\mu$ approaches $E_1 - \hbar \omega_D$ irrespective of the value of $\lambda$ and $T_c$ vanishes as a non-analytic function of both $L$ and $\lambda$ [31]. On the other hand, if the limit $n \to 0$ is taken after the limit $\lambda \to 0$, $\mu$ again approaches the bottom of the lowest subband and $T_c$ approaches a finite value, while if the limit $n \to 0$ is taken first, $\mu$ approaches a value below the lowest subband and $T_c$ approaches zero as a non-analytic function of $n$ and $\lambda$ [42].

Here, we study the limit $\lambda \to 0$ of Eqs. (3) at finite $L$ and $n$. In such conditions, $\mu$ takes at $T_c = 0$ the value given by Eq. (6a), but the relation $\mu(T_c)$ is non-analytic at $T_c = 0$. A Sommerfeld-type expansion in powers of $T_c$ is therefore not possible. In order to study the behavior of $\mu(T_c \to 0)$, we split the sum in Eq. (3a) and we use the relation $\ln(1 + e^{\lambda}) = x + \ln(1 + e^{-x})$ for the terms $q \ll N_{sb}$:

$$n = \frac{m k_B T_c}{\pi \hbar^2 L} \left[ \sum_{q=1}^{N_{sb}} \left( \frac{\mu - E_q}{k_B T_c} + \ln \left( 1 + e^{\frac{-|\mu - E_q|}{k_B T_c}} \right) \right) \right]$$

$$+ \sum_{q=N_{sb}+1}^{\infty} \ln \left( 1 + e^{\frac{-|\mu - E_q|}{k_B T_c}} \right), \quad \text{(B1)}$$

where we have taken into account that $E_{N_{sb}} < \mu < E_{N_{sb}+1}$. We define $\mu = \mu_0 + \delta \mu$, where $\mu_0$ is the solution of Eq. (6a), which we write down for completeness:

$$\mu_0 = \frac{\pi^2 \hbar^2}{3 m L^2 N_{sb}} \left[ \frac{3 n L^3}{\pi} + \frac{N_{sb}(N_{sb} + 1)(2N_{sb} + 1)}{4} \right].$$

Equation (B1) becomes

$$n = n + \frac{m k_B T_c}{\pi \hbar^2 L} \sum_q \ln \left( 1 + e^{\frac{-|\mu_0 - E_q|}{k_B T_c}} \right). \quad \text{(B2)}$$

Since for all values of $q$ the exponential approaches zero for $T_c \to 0$, we can use the expansion $\ln(1 + x) = x$. Furthermore, except at isolated points where $\mu_0 = E_q$, the correction $\delta \mu$ is negligible compared to $\mu_0 - E_q$ and Eq. (B3) can be solved to yield

$$\delta \mu \approx - \frac{k_B T_c}{N_{sb}} \sum_q e^{\frac{-|\mu_0 - E_q|}{k_B T_c}}. \quad \text{(B4)}$$
We have confirmed numerically the accuracy of this expression. It shows that the deviation of the chemical potential from \( \mu_0 \) is exponentially small for \( T_c \to 0 \) (or equivalently for \( \lambda \to 0 \)).

We now derive a closed expression for \( T_c \), which matches the solution of Eqs. (3) at weak coupling and converges to Eqs. (A3) for \( \lambda \to 0 \). If one starts from Eq. (6b), there are two types of corrections needed in order to reproduce Eq. (3b). The first corrections arise from subbands such that \( \mu - \hbar \omega_D < E_q < \mu \). For these subbands, Eq. (6b) counts the pairing of inexistent states between \( \mu - \hbar \omega_D \) and \( E_q \). To remove this contribution, we need the integral

\[
- \int_{\mu - \hbar \omega_D}^{E_q - \mu} \frac{dE}{\omega_D} \tanh \left( \frac{E}{2\omega_D} \right) = \frac{1}{2} \ln \left( \frac{|\mu - E_q|}{\hbar \omega_D} \right). \tag{B5}
\]

The relation (B5) is exact for \( T_c \to 0 \), because \( E \) is negative in the whole integration range and the hyperbolic tangent can be replaced by \(-1\). The subbands that bring this correction have indices \( q = N_{sb}^+, \ldots, N_{sb} \) with \( E_{N_{sb}^+ - 1} - \mu < \hbar \omega_D < E_{N_{sb}^+} \), therefore

\[
N_{sb}^+ = 1 + \text{floor} \left[ \sqrt{\frac{2mL^2}{\pi^2 \hbar^2} (\mu - \hbar \omega_D)} \right]. \tag{B6}
\]

The corrections of the second kind arise from subbands with \( \mu < E_q < \mu + \hbar \omega_D \) that are excluded from Eq. (6b), which therefore fails to account for the pairing of unoccupied states between \( E_q \) and \( \mu + \hbar \omega_D \). Adding this contribution requires the integral

\[
+ \int_{E_q - \mu}^{\hbar \omega_D} \frac{dE}{2E} \tanh \left( \frac{E}{\omega_D} \right) = -\frac{1}{2} \ln \left( \frac{|\mu - E_q|}{\hbar \omega_D} \right). \tag{B7}
\]

These subbands have indices \( q = N_{sb} + 1, \ldots, N_{sb}^+ \) with \( E_{N_{sb}^+} < \mu + \hbar \omega_D < E_{N_{sb}^+ + 1} \), which implies

\[
N_{sb}^+ = \text{floor} \left[ \sqrt{\frac{2mL^2}{\pi^2 \hbar^2} (\mu + \hbar \omega_D)} \right]. \tag{B8}
\]

Proceeding like in Appendix A and adding the corrections, we arrive at

\[
\frac{k_B T_c}{\hbar \omega_D} = \frac{2e^\gamma}{\pi} \times \exp \left[ -\frac{\left( 3mL^2/\pi \right)^{1/3} - \frac{1}{2} \sum_{q=N_{sb}}^{N_{sb}^+} \text{sign}(\mu - E_q) \ln \left( \frac{|\mu - E_q|}{\hbar \omega_D} \right) }{1/2 + N_{sb}} \right]. \tag{B9}
\]

As the deviation of \( \mu \) from \( \mu_0 \) is exponentially small in the weak-coupling regime, we can replace \( \mu \) by \( \mu_0 \) in Eqs. (B6), (B8), and (B9), which together with Eqs. (A3b) and (B2) provide a closed expression for \( T_c \). This expression compares favorably with the numerical result as seen in Fig. 6. Remarkably, the discontinuities contained in \( N_{sb} \) are precisely cancelled by the correction term in Eq. (B9) for the lowest values of \( \lambda \) and the resulting \( T_c(L) \) curve is smooth. At larger \( \lambda \), the cancellation is imperfect and spikes appear at the thicknesses where \( N_{sb} \) is discontinuous. Being independent of \( \lambda \), the correction term in Eq. (B9) becomes irrelevant for \( \lambda \to 0 \) and the expression (A3) is therefore recovered in this limit.

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