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Asymptotics of Zener double-well splittings and magnetic gaps

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Abstract. We consider a Zener double-well problem related to the magnetic bands in a superlattice Bloch operator. We give the precise asymptotic behaviour of the level splittings. This way we extend the Peierls substitution rule to an exponentially small term and furthermore, for the first time, we rigorously compute an exponentially small term in a Zener problem.

In this paper we consider the Schrödinger equation of an electron in a superlattice under a uniform magnetic field $B \parallel z$ perpendicular to the growth direction x of the superlattice (see, for a review, Altarelli 1988). By choosing the Landau gauge $A = (0, Bx, 0)$ one has that the electron wavefunction associated to the energy λ can be written as $\phi(x) \exp[ik_y y + ik_z z]$, where the function $\phi(x)$ is a solution of the one-dimensional effective mass Schrödinger equation,

$$[H_{x_0} - E] \phi = 0 \quad H_{x_0} = [p_x^2 + \omega^2(x - x_0)^2] + V(x) \quad E = \left[\lambda - \frac{\hbar^2 k_z^2}{2m^*} \right]. \quad (1)$$

Here, $V(x)$ is the periodic potential of the superlattice with period L ,

$$p_x = -i\hbar \frac{d}{dx} \quad \hbar = \frac{\hbar}{\sqrt{2m^*}} \quad \omega = \hbar m^* \omega_c \quad \text{and} \quad x_0 = -k_y l^2 \quad (2)$$

where $\omega_c = eB/m^*c\hbar$ is the cyclotronic frequency, m^* is the effective mass and $l = \sqrt{\hbar c/eB}$ is the magnetic length (for sake of simplicity we shall assume $h = 1$).

It is well known that for fixed weak magnetic field and relatively bounded $V \neq 0$ the Landau levels are changed into magnetic bands which show different behaviours depending on whether they are in the superlattice band or in the superlattice gap (Altarelli 1988 and the references therein). At low energy the x_0 -depending dispersion law is nearly flat. The width of the magnetic bands becomes appreciable near the top of the superlattice band and, furthermore, in the superlattice gap the dispersion law is locally quadratic with respect to x_0 and the gaps between the magnetic bands are very narrow.

This picture can be easily understood by means of the crystal momentum representation (CMR) and the single-band approximation where H_{x_0} becomes a *dual* Bloch operator and x_0

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acts as a crystal momentum (Grecchi and Sacchetti 1989). More precisely, in the CMR H_{x_0} is formally defined on $\mathcal{H} = \bigoplus_{n=1}^{\infty} L^2(\mathcal{B}, dk)$ as

$$H_{x_0} = (i\omega D + \omega X)^2 + \mathcal{E} \quad (3)$$

where a vector ψ of the domain can be written as $e^{ikx_0} u(k)$ with $u \in C^1(\mathcal{B})$ and \mathcal{B} is the Brillouin zone, i.e. the torus $R/(2\pi/L)$ with representatives in $(-\pi/L, \pi/L]$. Here, $D = \text{diag}(dk)$, $\mathcal{E} = \text{diag}(\mathcal{E}_n(k))$, where $\mathcal{E}_n(k)$ is the n th superlattice band function of the Bloch operator $p^2 + V$, and X is the term which couples the bands:

$$(Xa)_n(k) = \sum_{m=1}^{\infty} X_{n,m}(k) a_m(k) \quad a = (a_n)_n \in \mathcal{H} \quad (4)$$

where $X_{n,m}(k) = \overline{X_{m,n}(k)}$ and each $X_{n,n}(k)$ can be made constant by means of a suitable gauge choice of the n th Bloch function $\varphi_n(x, k)$.

The single band approximation of H_{x_0} acts on $\mathcal{H}_1 = L^2(\mathcal{B}, dk)$ and it is given by

$$H_1 = -\omega^2 \frac{d^2}{dk^2} + \mathcal{E}_1(k) + \omega^2 \sum_{n=1}^{\infty} X_{1,n}(k) X_{n,1}(k). \quad (5)$$

Therefore, it is a *dual* Bloch operator with x_0 -quasi-periodic boundary conditions and the results quoted above on the magnetic bands follow from the asymptotic analysis for the Bloch problem with periodic potential \mathcal{E}_1 (see, for instance, Weinstein and Keller 1985 and 1987 where they give the semi-classical behaviour of band and gap width). Furthermore, in such an approximation and for symmetric superlattices, i.e. $V(x) = V(-x)$, a new phenomenon is exhibited for energy levels in the first gap of the superlattice: the gap between the magnetic bands has exponentially small width for weak magnetic field. This result is not surprising because of the symmetry property (see, for instance, §50 in Landau and Lifshitz 1959) and one can perform a heuristic estimate of the gap width by means of a semi-classical double-well argument. For the energy in the superlattice gap, the Zener barrier simulates a barrier-tunnelling effect (see Buslaev 1987) so that the magnetic gap width is of the order of the square of the Zener transmission amplitude through half a barrier:

$$\Delta E \sim \exp \left[-\frac{2}{\omega} \int_{E_1^{\dagger}}^E \frac{\chi(\nu)}{2\sqrt{\nu - E_1^{\dagger}}} d\nu \right] \quad \text{as } \omega \rightarrow 0 \quad (6)$$

where $E_1^{\dagger} = \max_{k \in \mathcal{B}} \mathcal{E}_1(k)$ is the top of the first superlattice band, $\chi(\nu) = |\text{Im} k(\nu)|$ and $k(\nu)$ is the crystal momentum in the first gap.

Let us stress that the barrier-tunnelling effect works for *high* fixed energy levels while for energy levels close to the ground state (i.e. close to the bottom of the first superlattice band) the width of the magnetic gaps is of the order of the magnetic field. This is the opposite of what happens for usual semi-classical double-well models where the tunnelling effect appears for lower energy. Because of these reasons, and since the semi-classical double-well problem has received much attention recently for the presence of exponentially small terms in the eigenvalues behaviour (see, for instance, Helffer and Sjöstrand 1984 and Caliceti *et al* 1993 where the Borel summability of the perturbation series is discussed), we think that our model itself is of interest.

Our aim is to give the precise exponentially small gap width for weak magnetic field in the first superlattice gap.

Proposition. Let E be in the interval $[E_1^t + \delta, E_2^b - \delta]$, for any fixed $\delta > 0$, and $E \neq \mathcal{E}_1(z_n)$, $n \in \mathbf{N}$, where $z_n = \pi/L + ih_n$ is a branch point of the n th band function. The width of the magnetic gap is given by

$$\Delta E = \frac{2}{T(\omega)} \exp\left[-\frac{2}{\omega} \rho(E)\right] (1 + O(\omega^{3/4})) \quad \text{as } \omega \rightarrow 0$$

where

$$T(\omega) = \frac{1}{\omega} \int_{\mathcal{B}} \frac{dk}{2\sqrt{E - \mathcal{E}_1(k)}}$$

is the period of the classical motion on the torus \mathcal{B} with potential \mathcal{E}_1 and mass $1/2\omega^2$, $\rho(E)$ is defined by

$$\rho(E) = \int_0^{\chi(E)} \sqrt{E - \mathcal{E}_1(\pi/L + ih)} dh$$

for $E < \mathcal{E}_1(z_1)$ and

$$\rho(E) = \int_0^{h_1} \sqrt{E - \mathcal{E}_1(\pi/L + ih)} dh + \int_{\chi(E)}^{h_1} \sqrt{E - \mathcal{E}_2(\pi/L + ih)} dh$$

for $\mathcal{E}_1(z_1) < E$.

Remark. Let us stress that this exponentially small behaviour coincides with the one given in (6). Indeed, assuming $E < \mathcal{E}_1(z_1)$ for simplicity, we have

$$\begin{aligned} \int_0^{\chi(E)} \sqrt{E - \mathcal{E}_1(\pi/L + ih)} dh &= \int_0^{\chi(E)} \frac{h}{2\sqrt{E - \mathcal{E}_1(\pi/L + ih)}} \left(-\frac{d\mathcal{E}_1(\pi/L + ih)}{dh}\right) dh \\ &= \int_{E_1^t}^E \frac{\chi(\lambda)}{2\sqrt{E - \lambda}} d\lambda \\ &= \int_{E_1^t}^E \frac{\chi(v)}{2\sqrt{v - E_1^t}} dv \end{aligned}$$

integrating by parts and taking $\lambda = \mathcal{E}_1(\pi/L + ih)$ and $v = E + E_1^t - \lambda$.

This result extends a previous one (Grecchi and Sacchetti 1989) where the gap width was rigorously estimated only by $O(\omega^2)$.

By comparing our result for the complete operator H_{x_0} with the one obtained (in a different way) by Weinstein and Keller 1987 and März 1992 for the *dual* Bloch operator H_1 we stress that the two results coincide even if the coupling term between the bands in not exponentially small is ω but it is $O(\omega^2)$.

Here we give the proof of the above Proposition where we use the single band approximation, the Feshbach partition method and the stationary phase method.

Let $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$, $\mathcal{H}_2 = \bigoplus_{n=2}^{\infty} L^2(\mathcal{B}, dk)$, and let us consider H_{x_0} on \mathcal{H} as

$$H_{x_0} = \text{diag}(H_1, H_2) + \omega T \quad T = \begin{pmatrix} 0 & T_{1,2} \\ T_{2,1} & 0 \end{pmatrix} \quad T_{1,2} = T_{2,1}^*. \quad (7)$$

H_1 is the single band approximation (5),

$$H_2 = (i\omega D + \omega \tilde{X})^2 + \omega^2 W W^* + \mathcal{E} \quad \text{and} \quad T = [i\omega D + \omega \tilde{X}, W + W^*]_+ \quad (8)$$

where $X = \tilde{X} + W + W^*$, and W is the bounded coupling term defined as

$$a \in \mathcal{H}_1 \rightarrow Wa \in \mathcal{H}_2, (Wa)_n(k) = X_{n,1}(k)a(k) \quad (9)$$

and W^* denotes the adjoint of W . Being \mathcal{E} bounded below one then immediately obtains that T is infinitesimally relatively bounded with respect to $\text{diag}(H_1, H_2)$. We study the spectral problem for H_{x_0} in the interval $(-\infty, E_2^b)$, where E_2^b is the bottom of the second superlattice band, via the Feshbach operator on \mathcal{H}_1 given by

$$H_F(E) = H_1 - \omega^2 F(E) \quad F(E) = T_{1,2}[H_2 - E]^{-1}T_{2,1}. \quad (10)$$

That is $E < E_2^b$ is an eigenvalue of H_{x_0} if and only if $\Lambda(E)$ is an eigenvalue of $H_F(E)$ such that $\Lambda(E) = E$ (Combes *et al* 1981). Since T is infinitesimally relatively bounded with respect to $\text{diag}(H_1, H_2)$, $F(E)$ is a relatively bounded operator with respect to H_1 . Thus it is natural to consider the spectral problem for the Feshbach operator (10) in the framework of the regular perturbation theory (Kato 1984) setting $H_F(E, \beta) = H_1 - \beta F(E)$ where β is an auxiliary perturbative parameter. The unperturbed problem $H_F(E, 0) = H_1$ is the single-band approximation and, of course, $H_F(E, \omega^2) = H_F(E)$. Now, by arranging the x_0 -quasi-periodic conditions for the semi-classical solutions of the unperturbed problem and by using the regular perturbation theory one obtains the Onsager-type relation for the eigenvalues of the Feshbach operator $H_F(E)$:

$$A_C(\Lambda) = 2(n \pm x_0/L)\pi\omega + O(\omega^2) \quad \text{as } \omega \rightarrow 0 \quad (11)$$

for energy levels Λ in the superlattice gap; A_C is the classical action area. In (11) we consider the usual semi-classical limit: $\omega \rightarrow 0$ and $n \rightarrow \infty$ such that $2n\pi\omega \rightarrow A$ where $A_C(E_2^b - \delta) > A > A_C(E_1^i + \delta)$ for some $\delta > 0$. From the analytic dependence on E in the Feshbach term $F(E)$ there exists at least one $E_0 < E_2^b$ in a ω -neighbourhood of $A_C^{-1}(A \pm 2x_0\pi\omega/L)$ such that $\Lambda(E_0) = E_0$ and it is an eigenvalue of H_{x_0} . Since $\Lambda(E)$ is a monotonically decreasing function there exists exactly one eigenvalue of H_{x_0} close to the value defined by (11). Let us stress that from (11) one immediately obtains a draft estimate of the magnetic gap width for energy in the superlattice gap (Grecchi and Sacchetti 1989). Indeed, by taking $x_0 = 0$ (or $x_0 = L/2$) the two eigenvalues coincide up to $O(\omega^2)$.

Fixing $x_0 = 0$ for sake of definiteness and since the operators H_0 and $H_F(E)$ are invariant under the inversion $k \rightarrow -k$ (indeed for symmetric superlattice potentials $X_{n,m}(k) = -X_{n,m}(-k)$) they can be restricted to

$$L_D^2(\mathcal{B}, dk) \quad (\text{or } L_N^2(\mathcal{B}, dk)) \quad (12)$$

where D (N) denotes Dirichlet (Neumann) condition at the origin. In order to obtain the exponentially small behaviour of the gap width we go back to the x -representation where the splitting of the two eigenvalues $E_{D,N}$ of H_0 is given by the Herring formula (Wilkinson and Hannay 1987):

$$\Delta E = E_D - E_N = \frac{\phi_N(x)\overline{\phi_D}'(x) - \phi_N'(x)\overline{\phi_D}(x)}{\int_x^\infty \phi_N(t)\overline{\phi_D}(t)dt} \quad \text{for any } x. \quad (13)$$

Here $\phi_{D,N}$ denote the eigenvectors in the x -representation associated to the eigenvectors $\Psi_{D,N} \in \mathcal{H}$ in the CMR representation via the formula (theorem XIII.98 in Reed and Simon 1978)

$$\phi_{D,N} = \frac{1}{\sqrt{2\pi}} \langle \bar{\varphi}, \Psi_{D,N} \rangle_{\mathcal{H}} \tag{14}$$

$\varphi = (\varphi_n)_n$ and φ_n is the n th Bloch function normalized on $L^2([0, L], dx/L)$. Now we compute the eigenvectors $\Psi_{D,N}$ by means of the regular perturbation theory and after we evaluate (14) using the saddle-point method.

The Dirichlet–Neumann unperturbed eigenvectors associated to the unperturbed Dirichlet–Neumann eigenvalues are given by $\psi_{D,N}^0 = C_1(\mathbf{1} \pm \mathbf{U})\psi$ where $(\mathbf{U}a)(k) = a(-k)$ and $\psi(k)$ is a solution of the unperturbed equation $[H_1 - E]\psi = 0$ which is given by the usual WKB approximation (where it works):

$$\psi(k) = \frac{1}{\sqrt{u(k)}} \exp \left[-\frac{i}{\omega} \int^k u dt \right] \quad u(k) = \sqrt{E - \mathcal{E}_1(k)} + O(\omega^2). \tag{15}$$

The eigenvalues $E = E_{D,N}$ of H_0 coincide, up to $O(\omega^2)$, with the unperturbed ones and

$$C_1 = \left[2 \int_B [E - \mathcal{E}_1(k)]^{-1/2} dk \right]^{-1/2} (1 + O(\omega)) \tag{16}$$

is a normalization constant. Now, for small ω , from the regular perturbation theory on $L^2_{D,N}$, the eigenvectors of the full operator $H_F(E)$ are given by

$$\Psi_{D,N} = \frac{P \psi_{D,N}^0}{\|P \psi_{D,N}^0\|} \quad P = -\frac{1}{2\pi i} \oint_{\Gamma} [H_F(E) - z]^{-1} dz \tag{17}$$

where P is the eigenprojection and Γ is a clockwise circle surrounding E with radius $c\omega$, $c > 0$ suitable. The eigenvectors $\Psi_{D,N}$ of H_0 associated to $E = E_{D,N}$ are given by

$$\Psi_{D,N} = (\psi_{D,N}, \omega[H_2 - E]^{-1} T_{2,1} \psi_{D,N}). \tag{18}$$

Since $[P, (\mathbf{1} \pm \mathbf{U})_-] = 0$ and $\|P \psi_{D,N}^0\| = 1 + O(\omega)$, from (14) we have that

$$\begin{aligned} \phi_{D,N}(x) &= \frac{1}{\sqrt{2\pi}} \left\langle Q\bar{\varphi}, \frac{P \psi_{D,N}^0}{\|P \psi_{D,N}^0\|} \right\rangle_{\mathcal{H}_1} \\ &= \frac{1}{\sqrt{2\pi}} \left\langle Q\bar{\varphi}, \frac{\psi_{D,N}^0}{\|P \psi_{D,N}^0\|} - \frac{\omega^2}{2\pi i} \oint_{\Gamma} [H_F(E) - z]^{-1} F(E) \frac{dz}{E - z} \frac{\psi_{D,N}^0}{\|P \psi_{D,N}^0\|} \right\rangle_{\mathcal{H}_1} \\ &= \frac{1}{\sqrt{2\pi}} \langle \bar{f}, \psi \rangle_{\mathcal{H}_1} \end{aligned} \tag{19}$$

where we have used the first resolvent identity for $[H_F(E) - z]^{-1} = [H_1 - \omega^2 F(E) - z]^{-1}$ and the eigenvalue equation $H_1 \psi_{D,N}^0 = E \psi_{D,N}^0$. Q is defined as

$$Q = \mathcal{P}_{\mathcal{H}_1} + \omega T_{1,2} [H_2 - E]^{-1} \mathcal{P}_{\mathcal{H}_2} \tag{20}$$

where $\mathcal{P}_{\mathcal{H}_i}$ are the projectors on the subspace \mathcal{H}_i , $i = 1, 2$, and

$$f = \frac{C_1}{\|P\psi_{D,N}^0\|} \left(\mathbf{1} - \frac{\omega^2}{2\pi i} \oint [H_F(E) - z]^{-1} F(E) \frac{dz}{E - z} \right) (\mathbf{1} \pm \mathbf{U}) Q\varphi$$

$$= C_1[\varphi_1(x, k) \pm \varphi_1(x, -k)] + O(\omega). \tag{21}$$

From (19) one immediately obtains $\phi_{D,N}(0) = O(\omega^\infty)$ by integrating by parts infinitely many times. Indeed, one has that

$$\phi_{D,N}(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathcal{B}} f(k, x)\psi(k)dk \tag{22}$$

where

$$\psi(k) \sim [E - \mathcal{E}_1(k)]^{-1/4} \exp \left[-\frac{i}{\omega} \int^k \sqrt{E - \mathcal{E}_1(t)} dt \right]. \tag{23}$$

Furthermore, from the saddle-point method the exponential behaviour follows. Let us consider the complex quasi-momentum plane with cuts directly linking the Kohn branch points of the first band z_1 and \bar{z}_1 . Let \mathbb{k} be the saddle point: $\mathbb{k} = \pi/L - 0 + i\chi(E)$, $0 < \chi(E) < h_1$, and $\mathcal{E}_1(\mathbb{k}) = E$ if $\mathcal{E}_1(z_1) < E$, or $\mathbb{k} = \pi/L + 0 + i\chi(E)$, $0 < \chi(E) < h_1$, and $\mathcal{E}_2(\mathbb{k}) = E$ if $\mathcal{E}_1(z_1) = \mathcal{E}_2(z_1) > E$ (see Firsova 1979). We deform in the complex plane the interval of integration $(-\pi/L, \pi/L]$, representing the torus \mathcal{B} , of (22) to a path γ passing through \mathbb{k} . There are two possible kinds of paths γ depending on whether $E < \mathcal{E}_1(z_1)$ or not. In fact, if $E > \mathcal{E}_1(z_1)$ the path γ should turn around z_1 in both directions in order to have $\mathcal{E}_2(z) = E$ in the second sheet of \mathcal{E}_1 . While γ should directly link \mathbb{k} with the endpoints of $(-\pi/L, \pi/L]$ without turning around z_1 if $E < \mathcal{E}_1(z_1)$; for sake of definiteness we discuss this case, the case $E > \mathcal{E}_1(z_1)$ follows in a similar way. A further complication is given by the fact that, generically, there are infinitely many other Kohn branch points $z_n = \pi/L + ih_n$, for the band functions, with $\lim_n h_n = 0$ (Kohn 1959). However, if we avoid the energy values $\mathcal{E}_1(z_n)$, $n = 1, 2, \dots, N$, the saddle point does not coincide with a Kohn branch point and the asymptotic expansion (21) holds for any $k \in \gamma$; N is such that $\mathcal{E}_1(z_{N+1}) < E_1^* + \delta$. Therefore, the domain enclosed by γ and $(-\pi/L, \pi/L]$ is free from singularities of $f(x, k)$ and the Cauchy theorem and the saddle point method give

$$\phi_{D,N}(x) = \frac{1}{\sqrt{2\pi}} \int_{\gamma} f(x, k)\psi(k)dk = \frac{1}{\sqrt{2\pi}} \int_{\bar{\gamma}} f(x, k)\psi(k)dk (1 + O(\omega^{3/4})) \tag{24}$$

where $\bar{\gamma} = \gamma \cap B_{\mathbb{k}}(\omega)$, $B_{\mathbb{k}}(\omega)$ is a ball of centre \mathbb{k} and radius ω ; endpoints of γ do not give contributions in the saddle-point method because the function $f(k, x)\psi(k)$ in (22) is periodic for k in the torus \mathcal{B} . Since \mathbb{k} is a complex turning point for $[H_1 - E]\psi = 0$ the WKB approximation (23) fails for k in $B_{\mathbb{k}}(\omega)$ and one has

$$\psi(k) \sim C_2 \text{Ai} \left[i|\dot{\mathcal{E}}_1(\mathbb{k})|^{1/3} \omega^{-2/3} (k - \mathbb{k}) \right] \tag{25}$$

where Ai is the Airy function (Abramowitz and Stegun 1972) and

$$C_2 = 2\sqrt{\pi} [-\omega|\dot{\mathcal{E}}_1(\mathbb{k})|]^{-1/6} \exp \left[\frac{i}{\omega} \int_0^{\mathbb{k}} \sqrt{E - \mathcal{E}_1(k)} dk \right] \tag{26}$$

is obtained by matching the two asymptotic expansion (23) and (25) on the vertical direction passing through \mathbb{k} . Therefore, one obtains

$$\phi_{D,N}(x) = \frac{\sqrt{2\omega}C_1[\varphi_1(x, \mathbb{k}) \pm \varphi_1(x, -\mathbb{k})]}{\sqrt{|\dot{\mathcal{E}}_1(\mathbb{k})|}} \exp\left[\frac{i}{\omega} \int_0^{\mathbb{k}} \sqrt{E - \mathcal{E}_1(k)} dk\right] (1 + O(\omega^{3/4})) \quad (27)$$

since $\int_{-R}^R \text{Ai}(t)dt = 1 + O(R^{-3/4})$. Finally, one has

$$\Delta E = K(\mathbb{k})\omega \exp\left[-\frac{2}{\omega} \int_0^{x(E)} \sqrt{E - \mathcal{E}_1\left(\frac{x}{L} + i\hbar\right)} dh\right] (1 + O(\omega^{3/4})) \quad \text{as } \omega \rightarrow 0 \quad (28)$$

since $\int_x^{\infty} \phi_N(t)\bar{\phi}_D(t)dt = \frac{1}{2}(1 + O(\omega))$ for $x \in [-L/2, +L/2]$. Here,

$$K(k) = \frac{\mathcal{W}(k)}{|\dot{\mathcal{E}}_1(k)| \int_B dk / \sqrt{E - \mathcal{E}_1(k)}} \quad (29)$$

where $\mathcal{W} = \varphi_1\bar{\varphi}'_1 - \bar{\varphi}_1\varphi'_1$ is the constant Wronskian of φ_1 and $\bar{\varphi}_1$; therefore

$$\mathcal{W}(k) = \int_{-L/2}^{+L/2} \mathcal{W}(k) \frac{dx}{L} = 2 \int_{-L/2}^{+L/2} \varphi_1(x, k)\bar{\varphi}'_1(x, k) \frac{dx}{L} = -i\dot{\mathcal{E}}_1(k) \quad (30)$$

from the group velocity formula (see, for instance, formula A1.5.1 in Jones 1973). Hence, $K(\mathbb{k}) = 4 \left[\int_B dk / \sqrt{E - \mathcal{E}_1(k)}\right]^{-1}$ and so we have obtained the exponential behaviour for weak magnetic field and proved the proposition.

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