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Dynamic and statistical thermodynamic properties of electrons in a thin quantum well in a parallel magnetic field

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Abstract
We carry out a theoretical analysis of quantum well electron dynamics in a parallel magnetic field of arbitrary strength, for a narrow quantum well. An explicit analytical closed-form solution is obtained for the retarded Green's function for Landau-quantized electrons in skipping states of motion between the narrow well walls, effectively involving in-plane translational motion, and hybridized with the zero-field lowest subband energy eigenstate. The dispersion relation for electron eigenstates is examined, and we find a plethora of such discrete Landau-quantized modes coupled to the subband state. In the weak field limit, we determine low magnetic field corrections to the lowest subband state energy associated with close-packing (phase averaging) of the Landau levels in the skipping states. At higher fields the discrete energy levels of the well lie between adjacent Landau levels, but they are not equally spaced, albeit undamped. Furthermore, we also examine the associated thermodynamic Green's function for Landau-quantized electrons in a thin quantum well in a parallel magnetic field and construct the (grand) thermodynamic potential (logarithm of the grand partition function) determining the statistical thermodynamics of the system.

1. Introduction

The frontier of semiconductor device technology research is focused on the nanostructure length scale, including quantum wells, wires and dots. On this scale, quantum dynamics yields a host of fascinating and technologically significant new physical phenomena and the field is further enriched by the application of a magnetic field. In particular, recent experiments by Peralta and Allen [1] on the photoconductivity of a double-quantum-well field-effect transistor subject to terahertz irradiation in a parallel magnetic field have shown that the response is strongly dependent on the strength of the magnetic field. The role of a normal magnetic field in quantum well electron dynamics has been explored exhaustively [2]. Substantial work has also been done on the case of a parallel magnetic field [2–11] and the present paper is intended to provide further theoretical insight into the problem as there is a resurgence of experimental interest [1, 12]. To examine this matter more fully, we carry out in this paper a theoretical analysis of electron dynamics in a thin quantum well modelled by a delta function potential profile, $U(z) = U_0\delta(z)$, in a parallel magnetic field, taking full account of Landau quantization of orbits. In this, we obtain a closed form analytical solution for the appropriate retarded Green's function $G(\mathbf{r}, \mathbf{r}'; t - t')$ for the parallel field case, both within the quantum well as well as outside the quantum well, along with useful analytic representations. Furthermore, we construct the associated single-particle thermodynamic Green's function and derive the (grand) thermodynamic potential (logarithm of the grand partition function), determining the statistical thermodynamics of the thin quantum well in a parallel magnetic field.

2. Green's functions in a magnetic field for bulk and with a thin (parallel) quantum well

In the absence of a quantum well the bulk *infinite-space* retarded Green's function in a magnetic field $\mathbf{H} = H\hat{y}$ has the form [13, 14],

$$G_\infty(\mathbf{r}, \mathbf{r}'; t - t') = C(\mathbf{r}, \mathbf{r}')\mathcal{G}_\infty(|\mathbf{r} - \mathbf{r}'|; t - t'; H), \tag{1}$$

where the Peierls phase factor (dropping extraneous gauge phase factors)

$$C(\mathbf{r}, \mathbf{r}') = \exp[\mathrm{i}(e/2)\mathbf{r} \cdot \mathbf{H} \times \mathbf{r}'] \tag{2}$$

is not translationally invariant due to nonconservation of the momentum direction in a magnetic field. The detailed structure of $\mathcal{G}_\infty$ (for infinite space) was long ago determined explicitly in closed form in direct-time representation in terms of elementary functions which generate the Landau eigenfunction series when Fourier transformed to an energy–frequency representation. The retarded bulk function $\mathcal{G}_\infty(|\mathbf{r} - \mathbf{r}'|; t - t'; H)$ is translationally invariant and can be Fourier transformed in all coordinate-difference variables to single momenta $x - x' \to p_x$, $y - y' \to p_y$ (we leave $z - z'$ in position representation). The spectral weight function for $\mathcal{G}_\infty(p_x, p_y, |z - z'|; T)$ $(T = t - t')$ is defined as

$$A_\infty(p_x, p_y, |z - z'|; T) = \mathrm{i}[G^{\xi,\tau}_{\infty>}(p_x, p_y, |z - z'|; T) - G^{\xi,\tau}_{\infty<}(p_x, p_y, |z - z'|; T)]$$

$(G^{\xi,\tau}_{\infty\{\lessgtr\}}$ refer to the bulk thermodynamic Green's function at chemical potential ξ and temperature τ; greater, $>$, and lesser, $<$, parts), and it is given in direct time representation by [13, 14]

$$A_\infty(p_x, p_y, |z - z'|; T) = \mathrm{e}^{-\mathrm{i}\mu_0 H\sigma_3 T} \int_{-\infty}^{\infty} \frac{\mathrm{d}p_z}{2\pi} \mathrm{e}^{\mathrm{i}p_z(z-z')} \times \frac{\mathrm{e}^{-\mathrm{i}p_y^2 T/2m}}{\cos(\omega_\mathrm{c}T/2)} \exp\left[-\mathrm{i}\frac{p_x^2 + p_z^2}{m\omega_\mathrm{c}} \tan(\omega_\mathrm{c}T/2)\right], \tag{3}$$

(suppressing $C(\mathbf{r}, \mathbf{r}')$; σ_3 is the Pauli spin matrix, μ_0 is the Bohr magneton and ω_c is the Landau level separation ($\hbar \to 1$)). For the energy spectrum of the narrow quantum well, we will need the retarded infinite-space $\mathcal{G}_\infty$-function with $z = z' = 0$, given by ($\Theta_+(T)$ is the Heaviside unit step function)

$$\mathcal{G}_\infty(p_x, p_y, |0 - 0|; T) = -\mathrm{i}\Theta_+(T)A_\infty(p_x, p_y, |0 - 0|; T). \tag{4}$$

Carrying out the p_z-integral of equation (3) and Fourier transforming to frequency representation, $T \to \omega$, we obtain

$$\mathcal{G}_\infty(p_x, p_y, |0 - 0|; \omega) = -\frac{1 + i}{2}\sqrt{\frac{m\omega_\mathrm{c}}{2\pi}} \int_0^\infty \mathrm{d}T\, \mathrm{e}^{\mathrm{i}T(\omega - p_y^2)/2m} \sqrt{\cot(\omega_\mathrm{c}T/2)} \frac{\mathrm{e}^{-\mathrm{i}\mu_0 H\sigma_3 T}}{\cos(\omega_\mathrm{c}T/2)} \times \exp\left[-\frac{\mathrm{i}p_x^2}{m\omega_\mathrm{c}} \tan\left(\frac{\omega_\mathrm{c}T}{2}\right)\right]. \tag{5}$$

The Dyson integral equation for the Green's function in the presence of a quantum well, $U(\mathbf{r})$ ($1 = \mathbf{r}_1, t_1$, etc),

$$G(1,2) = G_\infty(1,2) + \int \mathrm{d}3\, G_\infty(1,3)U(3)G(3,2), \tag{6}$$

is complicated by the Peierls phase factor $C(\mathbf{r},\mathbf{r}')$ in $G_\infty(1,3)$. Nevertheless, holding $C(\mathbf{r},\mathbf{r}')$ intact, we have solved this integral equation exactly analytically in closed form for a thin one-dimensional $\delta(z)$-function potential profile for a quantum well, $U(z) = U_0\delta(z)$, centred at $z = 0$ in frequency–energy representation. As the magnetic field is taken to be in the $\hat{y}$-direction, equation (6) takes the form ($\alpha \equiv e/2$, and we Fourier transform $y - y' \to p_y$ and $t - t' \to \omega$)

$$G(x,z;\,p_y;\,x',z';\,\omega) = \mathrm{e}^{\mathrm{i}\alpha H(xz'-x'z)}\mathcal{G}_\infty(|x-x'|;\,p_y;\,|z-z'|;\,\omega) + U_0\int \mathrm{d}\tilde{x}\,\mathrm{e}^{-\mathrm{i}\alpha Hz\tilde{x}}$$
$$\times\,\mathcal{G}_\infty(|x-\tilde{x}|;\,p_y;\,|z-0|;\,\omega)G(\tilde{x},0;\,p_y;\,x',z';\,\omega).$$

The solution of this integral equation requires knowledge of $G(\tilde{x},0;\,p_y;\,x',z';\,\omega)$ on the right-hand side, so we set $z \to 0$ on the left:

$$G(x,0;\,p_y;\,x',z';\,\omega) = \mathrm{e}^{\mathrm{i}\alpha Hxz'}\mathcal{G}_\infty(|x-x'|;\,p_y;\,|0-z'|;\,\omega)$$
$$+\,U_0\int \mathrm{d}\tilde{x}\,\mathcal{G}_\infty(|x-\tilde{x}|;\,p_y;\,|0-0|;\,\omega)G(\tilde{x},0;\,p_y;\,x',z';\,\omega),$$

and can now solve algebraically by Fourier transforming $x \to p_x$, obtaining

$$G(p_x,0;\,x',z';\,p_y;\,\omega) = \mathrm{e}^{\mathrm{i}\alpha Hx'z'}\mathrm{e}^{-\mathrm{i}p_x x'}\mathcal{G}_\infty(p_x-\alpha Hz',\,p_y;\,|0-z'|;\,\omega)$$
$$\times\,\left[1-U_0\mathcal{G}_\infty(p_x,\,p_y;\,|0-0|;\,\omega)\right]^{-1}.$$

Substituting this result on the right-hand side of the integral equation above, we obtain an explicit closed-form solution for the Green's function for electrons in a thin quantum well with a parallel magnetic field as

$$G(\mathbf{r},\mathbf{r}';\,\omega) = G_\infty(\mathbf{r},\mathbf{r}';\,\omega) + U_0\mathrm{e}^{\mathrm{i}(eH/2)(x'z'-xz)}\int_{-\infty}^{\infty}\frac{\mathrm{d}p_x}{2\pi}\int_{-\infty}^{\infty}\frac{\mathrm{d}p_y}{2\pi}\mathrm{e}^{\mathrm{i}p_x(x-x')}\mathrm{e}^{\mathrm{i}p_y(y-y')}$$
$$\times\,\mathcal{G}_\infty(p_x-eHz/2,\,p_y;\,|z-0|;\,\omega)\mathcal{G}_\infty\left(p_x-eHz'/2,\,p_y;\,|0-z'|;\,\omega\right)$$
$$\times\,[1-U_0\mathcal{G}_\infty(p_x,\,p_y;\,|0-0|;\,\omega)]^{-1}. \tag{7}$$

Our retention of the Peierls phase factor $C(\mathbf{r},\mathbf{r}')$ (equation (2)) in this analysis is responsible for the shifting of the p_x-variable ($p_x \to p_x - eHz/2$; $p_x \to p_x - eHz'/2$) in equation (7). Of course, equation (7) also bears the full complement of Landau quantization effects in $\mathcal{G}_\infty$. It should be noted that the Green's function of equation (7) and associated eigenfunctions extend off the plane $z = 0$, notwithstanding the δ-function confinement potential of the well.

3. Eigenenergy dispersion relation

The dispersion relation for the electron energy eigenstates of the narrow quantum well in a parallel magnetic field is given by the vanishing of the denominator term on the right of equation (7) (in examining the energy spectrum, we execute the spin trace taking Zeeman splitting equal to Landau level separation for illustrative purposes; in this case spin shifts the energy levels by $\hbar\omega_c/2$):

$$\frac{1}{U_0} = \mathcal{G}_\infty\left(p_x,\,p_y;\,|0-0|;\,\omega\right), \tag{8}$$

in which we can employ $\mathcal{G}_\infty$ given by equation (5) modified by the spin trace. In the absence of a magnetic field, equation (5) yields

$$\mathcal{G}_\infty\left(p_x, p_y; |0-0|; \omega\right) = -\sqrt{2m}\left[\frac{\theta(\varepsilon-\omega)}{\sqrt{\varepsilon-\omega}} + \mathrm{i}\frac{\theta(\omega-\varepsilon)}{\sqrt{\omega-\varepsilon}}\right],$$

where $\varepsilon = (p_x^2 + p_y^2)/2m$ and m is effective mass, and $\hbar \to 1$. Consequently, there is just one stable subband state for electron motion across the quantum well given by

$$\omega \to E_0 = \frac{p_x^2 + p_y^2}{2m} - 2mU_0^2, \tag{9}$$

provided that $U_0 < 0$ and $2m\omega < (p_x^2 + p_y^2)$ (including in-plane translational energy and, of course, there is a continuum of states for motion above the barriers confining the well).

To examine the effects of a low magnetic field we expand the right-hand side of equation (5) in powers of the field to order ω_c^2, obtaining

$$\mathcal{G}_\infty\left(p_x, p_y; |0-0|; \omega\right) = -\sqrt{\frac{\mathrm{i}2m}{\pi}}\int_0^\infty \mathrm{d}T\, \frac{\mathrm{e}^{\mathrm{i}(\omega-\varepsilon)T}}{\sqrt{T}} \times \left[1 - \frac{\omega_c^2 T^2}{24} + \cdots\right]\left[1 - \frac{\mathrm{i}\omega_c^2 p_x^2 T^3}{24m} + \cdots\right],$$

whence we find

$$\mathcal{G}_\infty\left(p_x, p_y; |0-0|; \omega\right) = -\frac{\sqrt{2m}}{|\varepsilon-\omega|^{7/2}}\left\{\Theta(\varepsilon-\omega)\left[(\varepsilon-\omega)^3 + \frac{\omega_c^2}{32}\left(\varepsilon-\omega+5\frac{p_x^2}{2m}\right)\right] + \mathrm{i}\Theta(\omega-\varepsilon)\left[(\omega-\varepsilon)^3 + \frac{\omega_c^2}{32}\left(\omega-\varepsilon-5\frac{p_x^2}{2m}\right)\right]\right\}. \tag{10}$$

Correspondingly, the dispersion relation of equation (8) results in the seventh-order algebraic equation,

$$\eta^7 - \eta^6 - a\eta^2 - b = 0, \tag{11}$$

with

$$\eta = \sqrt{\frac{\varepsilon-\omega}{2mU_0^2}}, \qquad a = \frac{\omega_c^2}{128m^2U_0^4}, \qquad b = \frac{5\omega_c^2 p_x^2}{512m^4U_0^6}.$$

This equation has a unique real positive root provided that $\varepsilon > \omega$ with $U_0 < 0$. The mode is given to order ω_c^2 by

$$\omega = \left[1 - \frac{5}{64}\frac{\omega_c^2}{m^2U_0^4}\right]\frac{p_x^2}{2m} + \frac{p_y^2}{2m} - \frac{\omega_c^2}{32mU_0^2} - 2mU_0^2. \tag{12}$$

This single real eigenenergy root corresponds to the phase averaging/mixing of the closely packed Landau eigenstates for 'skipping' electron motion between the narrow quantum well walls admixed with the zero-field lowest subband state of the quantum well. The coefficient of $p_x^2/2m$ includes a shift of order ω_c^2 which may be interpreted as a mass shift [8], and there is also shift of order ω_c^2 in the subband level $2mU_0^2$. The absence of a subband level shift of order ω_c seems to be due to the symmetry of our $\delta(z)$-potential confining the quantum well [10].

In analysing the full effects of Landau quantization using equations (5) and (8), one must proceed with caution in addressing subtleties associated with the imaginary behaviour of $\sqrt{\cot(\omega_c T/2)}$ over half the fundamental interval. To deal with this matter we decompose the T-integration range of equation (5) into segments $[\frac{2\pi}{\omega_c}n, \frac{2\pi}{\omega_c}(n+1)]$ $(n = 0, 1, 2, \ldots)$, and translate all of them to the fundamental interval, which we then further subdivide into

$[0, \frac{\pi}{\omega_c}] \cup [\frac{\pi}{\omega_c}, \frac{2\pi}{\omega_c}]$. To avoid ambiguity of branch choice of $\sqrt{\cot(\omega_c T/2)}$, we also transform $[\frac{\pi}{\omega_c}, \frac{2\pi}{\omega_c}]$ to $[0, \frac{\pi}{\omega_c}]$ using $T \to \frac{2\pi}{\omega_c} - T$. This procedure yields

$$\mathcal{G}_\infty\left(p_x, p_y; |0-0|; \omega\right) = -\sqrt{\frac{2m}{\pi\omega_c}}(1+\mathrm{i})f(\Omega,\lambda)\sum_{n=0}^{\infty}\mathrm{e}^{\mathrm{i}n\Omega\pi}, \tag{13}$$

with

$$f(\Omega,\lambda) = \int_0^\pi \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(\Omega t - \lambda\tan t)}\sqrt{\cot t} \tag{14}$$

and

$$f(\Omega,\lambda) = \int_0^{\pi/2} \frac{\mathrm{d}t}{\sqrt{\tan t}}\left[\mathrm{e}^{\mathrm{i}(\Omega t-\lambda\tan t)} + \mathrm{i}\mathrm{e}^{\mathrm{i}\Omega\pi}\mathrm{e}^{-\mathrm{i}(\Omega t - \lambda\tan t)}\right], \tag{15}$$

where we have set $t = \omega_c T/2$, $\lambda = p_x^2/m\omega_c$ and $\Omega = 2(\omega - p_y^2/2m)\omega_c^{-1}$. Furthermore, we employ an identity that can be derived from Mehler's formula [15] (see appendix A)

$$\sqrt{\cot t}\,\mathrm{e}^{-\mathrm{i}\lambda\tan t} = \mathrm{e}^{\mathrm{i}\pi/4}\mathrm{e}^{-\lambda}\sum_{n=0}^{\infty}C_n\mathrm{e}^{-2n\mathrm{i}t}, \tag{16}$$

where ($H_n(x)$ are Hermite polynomials)

$$C_0 = 1, \qquad C_{n>0} = \frac{H_n^2(\sqrt{\lambda}) + 2nH_{n-1}^2(\sqrt{\lambda})}{2^2 n!}. \tag{17}$$

Substituting equation (16) into equations (14) and (15), executing the T-integral, and summing the geometric series of equation (13), we obtain

$$\mathcal{G}_\infty\left(p_x, p_y; |0-0|; \omega\right) = 2\sqrt{\frac{m}{\pi\omega_c}}\mathrm{e}^{-p_x^2/m\omega_c}\left[s_1\cot\left(\frac{\pi\Omega}{2}\right) + 2s_2\right], \tag{18}$$

where

$$s_1 = \sum_{n=0}^{\infty} C_n \frac{\sin\left[\frac{\pi}{2}(\Omega-2n)\right]}{\Omega - 2n}, \tag{19a}$$

$$s_2 = \sum_{n=0}^{\infty} C_n \frac{\sin^2\left[\frac{\pi}{4}(\Omega-2n)\right]}{\Omega - 2n}. \tag{19b}$$

Landau level spectral structure is evident in equation (18) with simple poles on the right-hand side for $\omega = n\omega_c + p_y^2/2m$. Considering the electron dispersion relation, equation (8), there is a plethora of modes that mix discrete Landau level electron states for motion skipping between the narrow quantum well walls (effectively involving in-plane translation) admixed with the zero-field lowest subband energy eigenstate. They are discussed in section 5 and illustrated in figures 1 and 2. Such modes are not uniformly spaced, but they do lie between each pair of adjacent Landau levels, and are undamped. Similar results have been obtained by Merkt [7].

4. Statistical thermodynamics

In addressing the statistical thermodynamics of the quantum well, we consider the thermodynamic potential, Ω (not to be confused with Ω employed in section 3 above, equations (13)–(19); Boltzmann constant $k_B \to 1$):

$$\Omega = F - \xi\langle N\rangle = -\tau\ln\mathrm{Tr}\,\mathrm{e}^{-(H_{op}-\xi N)/\tau} = -\tau W, \tag{20}$$

where F is the free energy, N is the number operator, H_{op} is the Hamiltonian, τ is temperature, ξ is the chemical potential and W is the grand potential (log of the grand partition function).

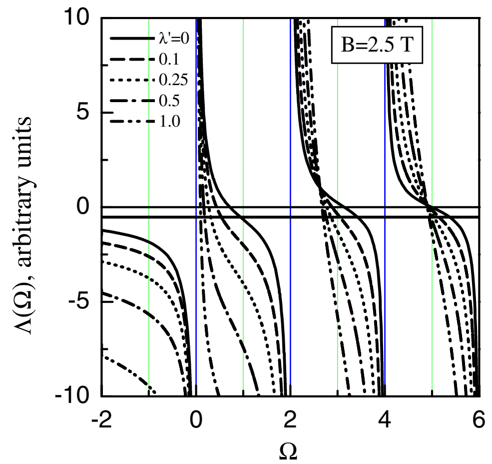

Figure 1. Schematic solutions of equation (8) for several parameter values $\lambda' = 0, 0.1, 0.25, 0.5, 1.0$ and magnetic field strength $B = 2.5$ T.

(This figure is in colour only in the electronic version)

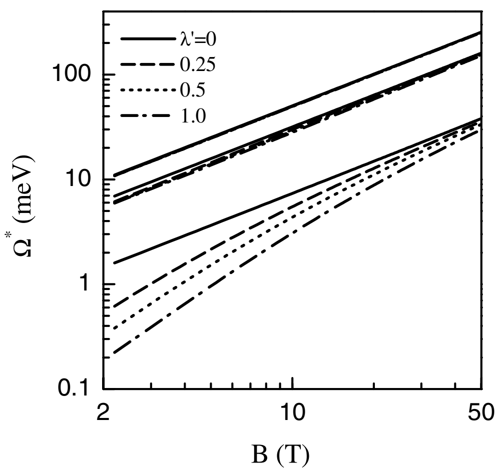

Figure 2. Eigenenergy levels, solutions of equation (8) for several parameter values $\lambda' = 0, 0.25, 0.5$ and 1.0, as functions of magnetic strength in tesla (log–log plot).

Noting that we can also write (ε_{r} are the single-particle energies) $\Omega = -\tau \sum_{\mathrm{r}} \ln(1 + \mathrm{e}^{(\xi-\varepsilon_{\mathrm{r}})/\tau})$, we have

$$\lim_{\xi\to-\infty} \Omega(\xi) = \lim_{\xi\to-\infty} W(\xi) = 0. \tag{21}$$

The magnetic moment, M, may be obtained as

$$M = -\left(\frac{\partial F}{\partial H}\right)_{\tau,V,N} = -\left(\frac{\partial \Omega}{\partial H}\right)_{\tau,V,\xi}, \tag{22}$$

and we will employ the last equality, understanding V as area for the quantum well and ξ to be held constant as well as temperature, in the differentiation with respect to magnetic field, H.

We evaluate Ω using the relation

$$\langle N \rangle = -\left(\frac{\partial \Omega}{\partial \xi}\right)_{\tau\,\text{fixed}}, \tag{23}$$

and integrating with respect to chemical potential (recall equation (21) and keep τ fixed):

$$\Omega = -\int_{-\infty}^{\xi} \mathrm{d}\xi' \, \langle N(\xi')\rangle = \mathrm{i}\int_{-\infty}^{\xi} \mathrm{d}\xi' \int \mathrm{d}^3\mathbf{r}\, G_{<}^{\xi',\tau}(\mathbf{r}, t; \mathbf{r}, t). \tag{24}$$

The last equation requires the 'lesser' part of the one-electron thermodynamic Green's function $G_{\{\lessgtr\}}^{\xi',\tau}$, which may be written in terms of its spectral weight $A(\mathbf{r}, \mathbf{r}'; \omega)$ (in position-frequency representation) as

$$G_{\{\lessgtr\}}^{\xi',\tau}(\mathbf{r}, \mathbf{r}'; \omega) = \mathrm{i}\left\{\begin{matrix} f_0(\omega) \\ -1 + f_0(\omega)\end{matrix}\right\} A(\mathbf{r}, \mathbf{r}'; \omega), \tag{25}$$

where $f_0(\omega)$ is the Fermi–Dirac distribution function. Since the spectral weight relates to the *retarded* Green's function $G(\mathbf{r}, \mathbf{r}'; \omega)$ (obtained in equation (7)) as

$$A(\mathbf{r}, \mathbf{r}'; \omega) = 2\,\mathrm{Im}\, G(\mathbf{r}, \mathbf{r}'; \omega), \tag{26}$$

we have (bear in mind $\mathbf{r}' = \mathbf{r}$ as well as $t' = t$)

$$\Omega = -2\int_{-\infty}^{\xi} \mathrm{d}\xi' \int_{-\infty}^{\infty} \mathrm{d}^3\mathbf{r} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} f_0(\omega)\, \mathrm{Im}\, G(\mathbf{r}, \mathbf{r}; \omega). \tag{27}$$

The involvement of spin in the Dyson equation (6) is readily separated as $G(T) \sim \mathrm{e}^{-\mathrm{i}\mu_0 H \sigma_3 T}$, just as for $G_\infty(T)$, and it cancels across the equation since U is independent of spin in these considerations. Correspondingly, we can view the solution of equation (7) as applicable to the spin-independent part of the retarded Green's function, in which the role of $C(\mathbf{r}, \mathbf{r}')$ (equation (2)) is subsumed in the wavenumber shifts of p_x ($p_x \to p_x - eHz/2$; $p_x \to p_x - eHz'/2$). (Note that while we could employ spin-traced Green's functions in determining the energy spectrum shifted by $\hbar\omega_c/2$ above, it would be incorrect to continue the use of the spin-traced functions here. Hence, we account for spin separately at the outset as described above.)

Employing equation (7) with $\mathbf{r}' = \mathbf{r}$, we have

$$\begin{aligned} G_{\mathrm{QW}}(\mathbf{r}, \mathbf{r}; \omega) &\equiv G(\mathbf{r}, \mathbf{r}; \omega) - G_\infty(\mathbf{r}, \mathbf{r}; \omega) \\ &= U_0 \int_{-\infty}^{\infty} \frac{\mathrm{d}p_x}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}p_y}{2\pi} \mathcal{G}_\infty\left(p_x - eHz/2, p_y; |z|; \omega\right) \\ &\quad \times \mathcal{G}_\infty\left(p_x - eHz/2, p_y; |z|; \omega\right)\left[1 - U_0 \mathcal{G}_\infty\left(p_x, p_y; |0-0|; \omega\right)\right]^{-1}, \end{aligned} \tag{28}$$

where we identify the contribution of the quantum well by subtracting G_∞, which will just yield known bulk results. Without the spin factor, we have

$$\begin{aligned} \mathcal{G}_\infty(p_x, p_y, |z - z'|; T) &= -\mathrm{i}\Theta_+(T) A_\infty(p_x, p_y, |z - z'|; T) \\ &= -\mathrm{i}\Theta_+(T) \int_{-\infty}^{\infty} \frac{\mathrm{d}p_z}{2\pi} \mathrm{e}^{\mathrm{i}p_z(z-z')} \frac{\mathrm{e}^{-\mathrm{i}p_y^2 T/2m}}{\cos(\omega_c T/2)} \exp\left[-\mathrm{i}\frac{p_x^2 + p_z^2}{m\omega_c} \tan(\omega_c T/2)\right]. \end{aligned} \tag{29}$$

In this first examination of statistical thermodynamics of the thin quantum well in a magnetic field, we address the case of low field, devoid of de Haas–van Alphen Landau quantization phenomenology, $\hbar\omega_c < 2mU_0^2 < \xi$, setting $\cos(\omega_c T/2) \to 1$ and $\tan(\omega_c T/2) \to \omega_c T/2$. Consequently ($\delta$ is a positive infinitesimal),

$$\begin{aligned} \mathcal{G}_\infty(p_x, p_y, |z - z'|; \omega) &= -\mathrm{i}\int_0^{\infty} \mathrm{d}t \int_{-\infty}^{\infty} \frac{\mathrm{d}p_z}{2\pi} \mathrm{e}^{\mathrm{i}\omega T} \mathrm{e}^{\mathrm{i}p_z(z-z')} \exp\left(-\mathrm{i}\frac{p_x^2 + p_y^2 + p_z^2}{2m} T\right) \\ &= \int_{-\infty}^{\infty} \frac{\mathrm{d}p_z}{2\pi} \frac{\mathrm{e}^{\mathrm{i}p_z(z-z')}}{\omega + \mathrm{i}\delta - (p_x^2 + p_y^2 + p_z^2)/2m}. \end{aligned} \tag{30}$$

Substitution of equation (30) into equation (28) and setting $k_x = p_x - eHz/2$ yields:

$$G_{\rm QW}(\mathbf{r},\mathbf{r};\omega) = U_0 \int_{-\infty}^{\infty} \frac{\mathrm{d}k_x}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}p_y}{2\pi} \left[\int_{-\infty}^{\infty} \frac{\mathrm{d}p_z}{2\pi} \frac{\mathrm{e}^{\mathrm{i}p_z z}}{\omega + \mathrm{i}\delta - \frac{k_x^2+p_y^2+p_z^2}{2m}} \right]^2$$

$$\times \left[1 - U_0 \int_{-\infty}^{\infty} \frac{\mathrm{d}q_z}{2\pi} \frac{1}{\omega + \mathrm{i}\delta - \frac{(k_x+eHz/2)^2+p_y^2+q_z^2}{2m}} \right]^{-1}. \qquad (31)$$

Forming the position-space integral required in equation (27) and introducing the notation $\tilde{\omega} = \omega/\xi$ and $(k_x, p_y, p_z) = p_{\rm F}(k, p, q)$, where $p_{\rm F} = \sqrt{2m\xi}$, we can also write (a is the lateral area of the quantum well):

$$\int \mathrm{d}^3\mathbf{r}\, \mathrm{Im}\, G_{\rm QW}(\mathbf{r},\mathbf{r};\omega) = U_0 a \frac{p_{\rm F}^4}{\xi^2} \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi}$$

$$\times\ \mathrm{Im} \int_{-\infty}^{\infty} \mathrm{d}z \left[\int_{-\infty}^{\infty} \frac{\mathrm{d}q}{2\pi} \frac{\mathrm{e}^{\mathrm{i}qp_{\rm F}z}}{\tilde{\omega} + \mathrm{i}\delta - (k^2+p^2+q^2)} \right]^2$$

$$\times \left\{ 1 - \frac{U_0 p_{\rm F}}{\xi} \int_{-\infty}^{\infty} \frac{\mathrm{d}q'}{2\pi} \frac{1}{\tilde{\omega} + \mathrm{i}\delta - [(k + \frac{eHz}{2p_{\rm F}})^2 + p^2 + q'^2]} \right\}^{-1}. \qquad (32)$$

Addressing the zero-field limit ($H \to 0$), it is convenient to execute the z-integral first, and then the q- and q'-integrals, with the result (see appendix B)

$$\int \mathrm{d}^3\mathbf{r}\, \mathrm{Im}\, G_{\rm QW}(\mathbf{r},\mathbf{r};\omega) = -\frac{U_0 a p_{\rm F}^3}{8\xi^2} \int_0^{\infty} \frac{\mathrm{d}r}{2\pi}$$

$$\times\ \mathrm{Re} \left\{ (\tilde{\omega} - r + \mathrm{i}\delta)^{-1} \left[\mathrm{i}\frac{U_0 p_{\rm F}}{2\xi} + (\tilde{\omega} - r + \mathrm{i}\delta)^{1/2} \right]^{-1} \right\}. \qquad (33)$$

Focusing attention on the degenerate case,

$$\int_{-\infty}^{\xi} \mathrm{d}\xi' f_0(\omega) = \Theta_+(\xi - \omega)(\xi - \omega), \qquad (34)$$

and equation (27) then yields the part of Ω associated with the quantum well, $\Omega_{\rm QW}$, as (set $x \equiv 1 - (\tilde{\omega} - r)$ and $y \equiv (1 - \tilde{\omega})^2$)

$$\Omega_{\rm QW}^0 = \frac{U_0 a p_{\rm F}^3}{32\pi^2} \int_0^{\infty} \mathrm{d}y \int_{y^{1/2}}^{\infty} \mathrm{d}x\, \mathrm{Re}[(1 - x + \mathrm{i}\delta)(\mathrm{i}s + \sqrt{1-x})]^{-1}, \qquad (35)$$

in the zero-field limit, $\Omega_{\rm QW} \to \Omega_{\rm QW}^0$. Here, we have defined $s = U_0 p_{\rm F}/2\xi$. The last factor of the x-integrand yields a real contribution only for $x < 1$, leading to the integral

$$\mathcal{I} = \int_0^{\infty} \mathrm{d}y \int_{y^{1/2}}^{1} \mathrm{d}x\, \mathrm{Re} \frac{-\mathrm{i}s + \sqrt{1-x}}{(1-x)(s^2+1-x)}, \qquad (36)$$

which may be evaluated as (see appendix B) [16]

$$\mathcal{I} = \frac{8}{s} \int_0^1 \mathrm{d}t\,(t - t^3) \arctan\left(\frac{t}{s}\right) = \frac{8}{s} \left[\frac{3s^2}{4} \arctan\left(\frac{1}{s}\right) - \left(\frac{7s}{12} - \frac{s^3}{4}\right) - \frac{1}{4}\arctan s + \frac{\pi}{8} \right]. \qquad (37)$$

The last term in equation (37), π/s, leads to a contribution to $\Omega_{\rm QW}$ which fails to vanish as $U_0 \to 0$. This would be problematic, except for the fact that we have not yet accounted for a contribution from the Dirac prescription applied to the first factor of the integrand of equation (33), namely $-\mathrm{i}\pi\delta(\tilde{\omega}-r)$, which just cancels the nonvanishing term. Thus, the zero magnetic field limit, Ω^0_{QW}, is given in the degenerate case by

$$\Omega^0_{\mathrm{QW}} = \frac{a p_{\mathrm{F}}^2 \xi}{2\pi^2}\left[\frac{3s^2}{4}\arctan\left(\frac{1}{s}\right) - \left(\frac{7s}{12} - \frac{s^3}{4}\right) - \frac{1}{4}\arctan s\right]. \tag{38}$$

Considering finite magnetic field at zero temperature, we again employ equation (32) and evaluate the q-integral as

$$\int_{-\infty}^{\infty} \mathrm{d}q \frac{\mathrm{e}^{\mathrm{i}qp_{\mathrm{F}}z}}{\tilde{\omega} + \mathrm{i}\delta - (k^2+p^2+q^2)} = -\mathrm{i}\frac{\exp\{\mathrm{i}\sqrt{\tilde{\omega}-(k^2+p^2)}\,p_{\mathrm{F}}|z|\}}{2\sqrt{\tilde{\omega}-(k^2+p^2)}}. \tag{39}$$

Again employing equation (34) in the degenerate limit, the result for Ω_{QW} given by equation (27) may be expressed as (set $\beta = eH/2p_{\mathrm{F}}^2 = \hbar\omega_{\mathrm{c}}/4\xi$; $\gamma = U_0 p_{\mathrm{F}}/2\xi$; $C = U_0 a p_{\mathrm{F}}^3/4\pi$; $x = p_{\mathrm{F}}z$; all dimensionless)

$$\Omega_{\mathrm{QW}} = C\int_0^1 \mathrm{d}\tilde{\omega}(1-\tilde{\omega})\int_{-\infty}^{\infty}\frac{\mathrm{d}k}{2\pi}\int_{-\infty}^{\infty}\frac{\mathrm{d}p}{2\pi}\,\mathrm{Im}\int_{-\infty}^{\infty}\mathrm{d}x\frac{\exp\{2\mathrm{i}\sqrt{\tilde{\omega}-k^2-p^2}|x|\}}{\tilde{\omega}-k^2-p^2}$$
$$\times\frac{1}{1+\mathrm{i}\gamma[\tilde{\omega}-(k+\beta x)^2-p^2]^{-1/2}}. \tag{40}$$

Setting $\bar{r}^2 = k^2+p^2$; $k = \bar{r}\cos\theta$, $p = \bar{r}\sin\theta$, and $\bar{q} = \tilde{\omega}-\bar{r}^2$, $d\bar{q} = -d(\bar{r}^2)$, we have an integral representation for the magnetic field dependence of the thermodynamic potential, Ω_{QW}, of the quantum well:

$$\Omega_{\mathrm{QW}} = \frac{C}{2(2\pi)^2}\int_0^1 \mathrm{d}\tilde{\omega}(1-\tilde{\omega})\int_{-\infty}^{\tilde{\omega}}\mathrm{d}\bar{q}\int_0^{2\pi}\mathrm{d}\theta\,\mathrm{Im}\int_{-\infty}^{\infty}\mathrm{d}x\frac{\exp\{2\mathrm{i}\bar{q}^{1/2}|x|\}}{\bar{q}}$$
$$\times\frac{1}{1+\mathrm{i}\gamma[\bar{q}-2\beta x\sqrt{\tilde{\omega}-\bar{q}}\cos\theta-\beta^2x^2]^{-1/2}}. \tag{41}$$

Albeit exact, the simpler appearance of equation (41) is somewhat deceptive since expansion in powers of magnetic field (β) diverges term-by-term after the zero-field limit. Such magnetic field power series divergencies are to be expected from a perusal of equation (32), since such an expansion would involve the last integrand factor expanded in powers of $\frac{eHz}{2p_{\mathrm{F}}k}$, and higher even inverse powers of k lead to divergences (we explicitly verify this in appendix C). However, higher odd powers of k indicate vanishing of the k-integral whose integrand is otherwise even in k. This, too, is to be expected since odd powers of H should be expected to vanish to accommodate the fact that this system cannot have an intrinsic magnetic moment, M, so $\lim_{H\to 0}\frac{\partial\Omega_{\mathrm{QW}}}{\partial H} = 0$. Thus, the four-fold integral of equation (41) is an even function of H, and is *not analytic* in H. Moreover, we have examined the magnetic susceptibility represented by its second derivative with respect to magnetic field, and find that its limit as $H \to 0$ does not exist (see appendix C). Equation (41)—while correct—describes a highly singular function that requires further study.

5. Discussion and conclusions

Our approach to the dynamics and statistical thermodynamics of a thin quantum well in a parallel magnetic field has been a global one, in which the Green's functions determined in equations (7) and (28) provide explicit closed-form analytic results both inside the quantum well *and* outside the quantum well. They incorporate both the localized states bound within the well as well as the extended states above the potential walls enclosing the quantum well, concisely representing *all* the eigenstates (and eigenenergies) in terms of bulk functions expressed as integrals of elementary functions. This feature offers tractability in the result which we have employed in our determination of the (grand) thermodynamic potential and magnetic response of the quantum well. Such tractability can also be advantageous in other studies. While our model $\delta(z)$-potential accommodates just one subband state in the absence of a magnetic field, such a description has proven useful in a variety of applications in which higher subbands are energetically inaccessible.

In regard to specific calculations, we have examined weak magnetic field corrections to the lowest subband energy to order ω_c^2, equation (12). These include an ω_c^2-term proportional to p_x^2 which may be interpreted in terms of an anisotropic mass shift, and there is also an ω_c^2-shift of the lowest subband energy. There is no subband energy shift of order ω_c because of the symmetry of our $\delta(z)$-potential confining the quantum well. This result is applicable to the mixing of closely packed Landau eigenstates for skipping electron motion between the narrow quantum well walls admixed with the lowest subband state of the well.

For stronger magnetic fields

$$\hbar\omega_c \gtrsim \frac{2mU_0^2}{\hbar^2}, \tag{42}$$

at which the *discrete* character of the parallel-field Landau levels is felt, the mixing of the individual Landau level electron modes with skipping between the narrow quantum well walls (effectively involving in-plane translation) admixed with the zero-field lowest subband state results in many undamped eigenenergies that lie between each pair of adjacent Landau levels; but they are not uniformly spaced. The dispersion relation for these modes and their behaviour as functions of magnetic field (in terms of the variable $\Omega = 2\Omega^*/\omega_c$, with $\Omega^* = \omega - p_y^2/2m$) are illustrated in figures 1 and 2, respectively. Our calculations are carried out for a narrow GaAs–AlGaAs-based quantum well which we model by $U(z) = U_0\delta(z)$, with the value of $U_0 = \int dz\, U(z)$ based on a potential well wall height (above the well bottom) of 250 meV and well width 10 nm, in a parallel magnetic field. The effective mass is $m = 0.067\, m_0$ and we take the 2D electron density in the quantum well as 1×10^{15} m^{-2}, corresponding to the zero-temperature Fermi energy, $E_F \cong 7$ meV. In figure 1 we plot the quantity $\Lambda(\Omega) = [s_1 \cot(\pi\Omega/2) + 2s_2]$ of equation (18) as a function of Ω, transposing the other factors of $\mathcal{G}_\infty(p_x, p_y; |0-0|; \omega)$ to the left-hand side of the dispersion relation of equation (8) which is a constant independent of Ω. The Landau-quantized quantum well eigenenergies, $\hbar\omega$, occur at the intersections of this constant, horizontal line (parallel to the horizontal axis of figure 1 and below it) with the plotted curves of $\Lambda(\Omega)$. These electron modes depend on p_x, and we illustrate this with plots for several values of the parameter $\lambda' = p_x^2/2mE_F = 0, 0.1, 0.25, 0.5$ and 1.0 for magnetic field strength $B = 2.5$ T. The multitude of modes comes about by hybridization of each individual Landau state mixing with the lowest subband level that the well has in the absence of the parallel magnetic field. These hybrid electron eigenstates of the quantum well are clearly illustrated in figure 2, in which the roots are plotted in terms of Ω^* as functions of magnetic field for $\lambda' = 0,\ 0.25, 0.5$ and 1.0.

Our analysis of the statistical thermodynamics of a thin quantum well has produced an explicit analytic expression for its (grand) thermodynamic potential in a parallel magnetic field, equation (27), as well as the thermodynamic Green's function. We have employed this in an exact determination of the thermodynamic potential of the quantum well, Ω_{QW}, in the zero-field degenerate limit in terms of elementary functions (equation (38)). In a similar analysis at finite magnetic field we provide an integral representation of the magnetic field dependence of Ω_{QW} in equation (41).

These results may have interesting implications regarding the photoconductivity experiments of [1] for high parallel magnetic fields. Furthermore, this work may serve to provide a field strength criterion for the uniqueness of the interacting levels of an emitter quantum well coupled with the main quantum well of a double-barrier resonant quantum well system (as proposed in [17, 18]), when subjected to a parallel magnetic field. Further work is in progress to extend this analysis to multiple thin quantum wells in a parallel magnetic field.

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Appendix A. Identities

Mehler's Formula is given by [15]

$$(1-t^2)^{-1/2}\exp\left(\frac{2xyt-(x^2+y^2)t^2}{1-t^2}\right)=\sum_{n=0}^{\infty}\frac{H_n(x)H_n(y)}{2^2 n!}t^n. \tag{A.1}$$

Setting $x = y$ and $t = \mathrm{e}^{\mathrm{i}z}$ ($x \geqslant 0$ and $0 \leqslant z \leqslant \pi$) we have

$$\exp\left(\frac{2x^2\mathrm{e}^{\mathrm{i}z}}{1+\mathrm{e}^{\mathrm{i}z}}\right)=\sqrt{1-\mathrm{e}^{2\mathrm{i}z}}\sum_{n=0}^{\infty}\frac{H_n^2(x)}{2^2 n!}\mathrm{e}^{\mathrm{i}nz}. \tag{A.2}$$

Introducing the fact that

$$\frac{2\mathrm{e}^{\mathrm{i}z}}{1+\mathrm{e}^{\mathrm{i}z}}=1+\mathrm{i}\tan(z/2),$$

and multiplying both sides by e^{-x^2}, it follows that

$$\exp[\mathrm{i}x^2\tan(z/2)]=\sqrt{1-\mathrm{e}^{2\mathrm{i}z}}\mathrm{e}^{-x^2}\sum_{n=0}^{\infty}\frac{H_n^2(x)}{2^2 n!}\mathrm{e}^{\mathrm{i}nz}. \tag{A.3}$$

Finally, multiplying both sides by

$$\sqrt{\cot(z/2)}=\sqrt{\frac{\mathrm{i}(1+\mathrm{e}^{\mathrm{i}z})}{\mathrm{e}^{\mathrm{i}z}-1}},$$

we obtain

$$\sqrt{\cot(z/2)}\exp[\mathrm{i}x^2\tan(z/2)]=\mathrm{e}^{-\mathrm{i}\pi/4}\mathrm{e}^{-x^2}(1+\mathrm{e}^{\mathrm{i}z})\sum_{n=0}^{\infty}\frac{H_n^2(x)}{2^2 n!}\mathrm{e}^{\mathrm{i}nz}. \tag{A.4}$$

Equations (A.2) and (A.3) can also be rewritten in the form

$$\mathrm{e}^{-\mathrm{i}x^2\cot t}=(1-\mathrm{e}^{-4\mathrm{i}t})\mathrm{e}^{-x^2}\sum_{n=0}^{\infty}D_n(x)\mathrm{e}^{-2\mathrm{i}nt}, \tag{A.5}$$

where

$$D_n(x)=(-1)^n\frac{H_n^2(x)}{2^2 n!}. \tag{A.6}$$

Appendix B. Integrals

(1) z-integral and q- and q'-integrals of equation (32) leading to (33):

$$\int_{-\infty}^{\infty} \mathrm{d}z \left[\int_{-\infty}^{\infty} \frac{\mathrm{d}q}{2\pi} \frac{\mathrm{e}^{\mathrm{i}qp_{\mathrm{F}}z}}{\tilde{\omega}+\mathrm{i}\delta-(k^2+p^2+q^2)}\right]^2 = \int_{-\infty}^{\infty} \frac{\mathrm{d}q}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tilde{q}}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}z\, \mathrm{e}^{\mathrm{i}(q+\tilde{q})p_{\mathrm{F}}z}$$
$$\times [\tilde{\omega}+\mathrm{i}\delta-(k^2+p^2+q^2)]^{-1}[\tilde{\omega}+\mathrm{i}\delta-(k^2+p^2+\tilde{q}^2)]^{-1}$$
$$= \int_{-\infty}^{\infty} \frac{dq}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\tilde{q} \frac{\delta(q+\tilde{q})}{p_{\mathrm{F}}}[\tilde{\omega}+\mathrm{i}\delta-(k^2+p^2+q^2)]^{-2}$$
$$= \frac{1}{p_{\mathrm{F}}} \int_{-\infty}^{\infty} \frac{\mathrm{d}q}{2\pi} \frac{1}{[\tilde{\omega}+\mathrm{i}\delta-(k^2+p^2+q^2)]^2} = \frac{-\mathrm{i}}{4p_{\mathrm{F}}}[\tilde{\omega}+\mathrm{i}\delta-(k^2+p^2)]^{-3/2}. \tag{B.1}$$

A similar evaluation of the last q'-integral in the denominator factor of equation (32) yields the zero-field limit in the form ($r \equiv k^2+p^2$)

$$\int \mathrm{d}^3\mathbf{r}\, \mathrm{Im}\, G_{\mathrm{QW}}(\mathbf{r},\mathbf{r};\omega) = \frac{U_0 a p_{\mathrm{F}}^3}{4\xi^2} \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi}$$
$$\times\ \mathrm{Im}\left\{\frac{-\mathrm{i}}{[\tilde{\omega}+\mathrm{i}\delta-(k^2+p^2)]^{3/2}}\left[1+\frac{\mathrm{i}U_0p_{\mathrm{F}}}{2\xi}\frac{1}{[\tilde{\omega}+\mathrm{i}\delta-(k^2+p^2)]^{1/2}}\right]^{-1}\right\}$$
$$= -\frac{U_0 a p_{\mathrm{F}}^3}{8\xi^2}\int_0^{\infty}\frac{\mathrm{d}r}{2\pi}\,\mathrm{Re}\left\{(\tilde{\omega}-r+\mathrm{i}\delta)^{-1}\left[\mathrm{i}\frac{U_0p_{\mathrm{F}}}{2\xi}+(\tilde{\omega}-r+\mathrm{i}\delta)^{1/2}\right]^{-1}\right\}. \tag{B.2}$$

(2) The integral $\mathcal{I}$:

$$\mathcal{I} = \int_0^{\infty} \mathrm{d}y \int_{y^{1/2}}^{1} \mathrm{d}x\ \mathrm{Re}\, \frac{-\mathrm{i}s+\sqrt{1-x}}{(1-x)(s^2+1-x)}$$
$$= \int_0^{\infty} \mathrm{d}y \int_{y^{1/2}}^{1} \mathrm{d}x \frac{1}{\sqrt{1-x}(s^2+1-x)} = 4\int_0^{\infty}\mathrm{d}u\, u \int_0^{\sqrt{1-u}} \frac{\mathrm{d}w}{w^2+s^2}, \tag{B.3}$$

where $u \equiv y^{1/2}$ and $w \equiv (1-x)^{1/2}$, and the upper limit of the u-integral is now seen to be unity. The w-integral is readily evaluated [16], leading to

$$\mathcal{I} = -\frac{4}{s}\int_0^1 \mathrm{d}u\, u\left[\arctan\left(\frac{s}{\sqrt{1-u}}\right)-\frac{\pi}{2}\right], \tag{B.4}$$

and setting $t = \sqrt{1-u}$ and noting the identity $\arctan x + \arctan 1/x = \pi/2$, we have [16]

$$\mathcal{I} = \frac{8}{s}\int_0^1 \mathrm{d}t\,(t-t^3)\arctan\left(\frac{t}{s}\right) = \frac{8}{s}\left[\frac{3s^2}{4}\arctan\left(\frac{1}{s}\right)-\left(\frac{7s}{12}-\frac{s^3}{4}\right)-\frac{1}{4}\arctan s+\frac{\pi}{8}\right]. \tag{B.5}$$

Appendix C. Ω_{QW} with finite magnetic field

Rewriting equation (40) with the definition $\bar{k} = k + \beta x$, we have

$$\Omega_{\mathrm{QW}} = C\int_0^1 \mathrm{d}\tilde{\omega}\,(1-\tilde{\omega})\int_{-\infty}^{\infty}\frac{\mathrm{d}\bar{k}}{2\pi}\int_{-\infty}^{\infty}\frac{\mathrm{d}p}{2\pi}\,\mathrm{Im}\int_{-\infty}^{\infty}\mathrm{d}x$$
$$\times\ \frac{\exp\{2\mathrm{i}\sqrt{\tilde{\omega}-(\bar{k}-\beta x)^2-p^2}|x|\}}{\tilde{\omega}-(\bar{k}-\beta x)^2\{1+\mathrm{i}\gamma[\tilde{\omega}-\bar{k}^2-p^2]^{-1/2}\}}. \tag{C.1}$$

Expansion to second order in powers of β yields ($\rho \equiv r^2 \equiv \bar{k}^2 + p^2$)

$$\Omega_{\mathrm{QW}} = \frac{C}{\pi}\xi^2 \int_0^1 \mathrm{d}\tilde{\omega}\,(1-\tilde{\omega}) \int_0^{\tilde{\omega}} \mathrm{d}\rho \frac{1}{(\tilde{\omega}-\rho)^{3/2} + \gamma^2(\tilde{\omega}-\rho)^{1/2}} \times \left[1 - \frac{\beta^2}{2(\tilde{\omega}-\rho)^2} - \frac{13\beta^2}{16}\frac{\rho}{(\tilde{\omega}-\rho)^3} + \mathcal{O}(\beta^3)\right], \tag{C.2}$$

where we have executed the x-integral and the angular integral in the $\bar{k}$–p plane. The β-dependent terms are clearly divergent.

Furthermore, to examine the magnetic susceptibility directly, we form

$$\frac{\partial^2}{\partial\beta^2}\int_{-\infty}^{\infty} \mathrm{d}x \frac{\exp\{2\mathrm{i}\sqrt{\tilde{\omega}-(\bar{k}-\beta x)^2 - p^2}|x|\}}{\tilde{\omega}-(\bar{k}-\beta x)^2 - p^2} = -\mathrm{i}\frac{5\bar{k}^2 + 15/4}{(\tilde{\omega}-\bar{k}^2-p^2)^{9/2}} - \mathrm{i}\frac{5/4}{(\tilde{\omega}-\bar{k}^2-p^2)^{7/2}}. \tag{C.3}$$

Correspondingly

$$\lim_{\beta\to 0}\frac{\partial^2\Omega_{\mathrm{QW}}}{\partial\beta^2} = -\frac{C}{4\pi}\int_0^1 \mathrm{d}\tilde{\omega}\,(1-\tilde{\omega})\int_0^{\tilde{\omega}} \mathrm{d}z \frac{1}{\tilde{\omega}-z+\gamma^2}\left[\frac{5z/2 + 15/4}{(\tilde{\omega}-z)^{7/2}} + \frac{5/4}{(\tilde{\omega}-z)^{5/2}}\right], \tag{C.4}$$

and this limit also does not exist, reflecting the highly singular behaviour of Ω_{QW} as a function of magnetic field.

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