Supplementary Information

Table S1. Summary of k-grid dependence for band energies at key symmetry points for MgB_2 with P6/mmm or P-6c2 symmetry. Standard deviations for P-6c2 calculations for k < 0.013 A^{-1} are less than 1meV.

Space Group	Pressure (GPa)	n	k ($Å^{-1}$)	G (meV)	A (meV)	E_{av} (meV)
P6/mmm	0	1	0.020	403.770	787.415	595.593
	0	1	0.010	400.000	782.440	591.220
	0	1	0.005	399.290	781.740	590.515

Space Group	Pressure (GPa)	n	k ($Å^{-1}$)	G (meV)		A(E_0) (meV)	E_{av} (meV)	ΔE1	ΔE2	2Δ	Comment
P-6c2	0	2	0.013	398.500	780.340	581.570	589.420	198.770	183.070	15.700	All degen
	0	2	0.010	398.500	780.341	581.566	589.420	198.775	183.066	15.709	All degen
	0	2	0.005	398.800	781.390	582.210	590.095	199.180	183.410	15.770	All degen
			Average	398.600	780.690	581.782	589.645	198.908	183.182	15.726	
			StdDev	0.173	0.606	0.371	0.390	0.235	0.197	0.038	

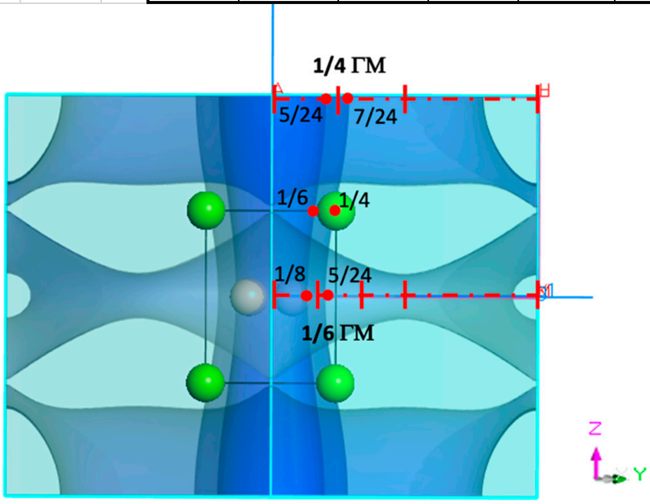

Figure S1. Fermi surfaces for MgB_2 with attributed P6/mmm symmetry. Approximate geometrical relationships for the radii of the light (inner) and heavy (outer) effective mass tubular sections are labelled (see also Figure S9 of reference [50] in the article).

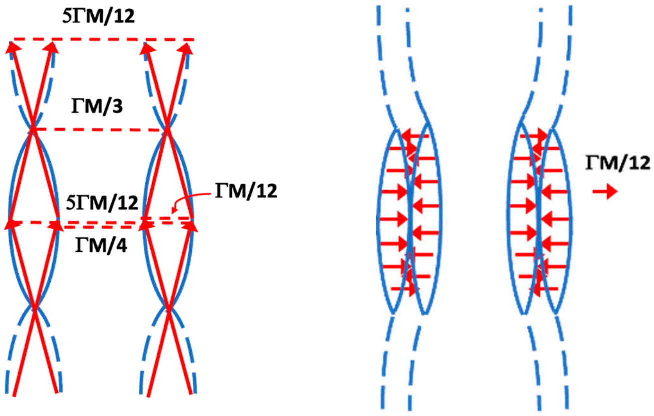

Figure S2. (a) Nesting vectors on either side of the folded light effective mass Fermi surface. Fermi surface nesting is prevalent for the double superlattice with vector approximately ΓM/3 long (see Figures 5 and 6). (b) Schematic of the folded inner and outer tubular Fermi surfaces for the double (2x), whose DFT calculated graph was shown in Figure 6. Fermi surface nesting between inner and outer tubes at short wavevector (ΓM/12) can be identified to the right.

Nesting vectors of average dimensions (approximately 5ΓM/12 long) also connect the tubular sections of light effective mass to the heavy effective mass in addition to short wavevectors that connect the same sides of each respective tubular section. These short wavevectors are approximately ΓM/12 long. Thus, ten nesting vectors, three longer horizontal (ΓM/3, ΓM/2 and 5ΓM/12 long), one short horizontal (ΓM/12 long) and six diagonals with horizontal components given by three longer horizontal nesting vectors, respectively, can be defined.

With respect to the modified tight binding equations (section 3.2), for convenience, we equate $\Delta = 2\hbar\omega$,

$$E_n(k_x, k_y, k_z) = E_0 - (2t_\perp^{\mathrm{n}} - 2\hbar\omega)\cos(ck_z) - \hbar^2\left(k_x^2 + k_y^2\right)/2m_n\ , \quad 0 \le ck_z \le \frac{\pi}{2} \tag{S1}$$

$$E_n(k_x, k_y, k_z) = E_0 - (2t_\perp^{\mathrm{n}} + 2\hbar\omega)\cos(ck_z) - \hbar^2\left(k_x^2 + k_y^2\right)/2m_n\ , \quad \frac{\pi}{2} \le ck_z \le \pi \tag{S2}$$

Since $\hbar\omega$ is relatively small compared to $2t_\perp$ and 1 in eV units, we can write $\hbar\omega \approx \sin(\hbar\omega)$,

$$E_n(k_x, k_y, k_z) = E_0 - 2t_\perp^{\mathrm{n}} cos(ck_z) + 2\, sin(\hbar\omega).\cos(ck_z) - \hbar^2\left(k_x^2 + k_y^2\right)/2m_n\ , \quad 0 \le ck_z \le \frac{\pi}{2} \tag{S3}$$

$$E_n(k_x, k_y, k_z) = E_0 - 2t_\perp^{\mathrm{n}} cos(ck_z) - 2\, sin(\hbar\omega).\cos(ck_z) - \hbar^2\left(k_x^2 + k_y^2\right)/2m_n\ , \quad \frac{\pi}{2} \le ck_z \le \pi \tag{S4}$$

These equations (i.e., Eqs. S2a & S2b) can then be written as the following combination of cosine and sine functions:

$$E_n(k_x, k_y, k_z) = E_0 - 2t_\perp^{\mathrm{n}} \cos(ck_z) + \sin(\hbar\omega + ck_z) + \sin(\hbar\omega - ck_z) - \hbar^2 \left(k_x^2 + k_y^2\right)/2m_n , \quad 0 \le ck_z \le \frac{\pi}{2} \tag{S5}$$

$$E_n(k_x, k_y, k_z) = E_0 - 2t_\perp^{\mathrm{n}} \cos(ck_z) - [\sin(\hbar\omega + ck_z) + \sin(\hbar\omega - ck_z)] - \hbar^2 \left(k_x^2 + k_y^2\right)/2m_n , \quad \frac{\pi}{2} \le ck_z \le \pi \tag{S6}$$