Review Topics & Formulas for Unit 3



Schrodinger time-independent energy eigen equation.

$$\mathbf{H} / \boldsymbol{\omega}_m \rangle = \hbar \boldsymbol{\omega}_m / \boldsymbol{\omega}_m \rangle = \boldsymbol{\varepsilon}_m / \boldsymbol{\omega}_m \rangle \tag{9.3.1a}$$

H-eigenvalues use **r**-expansion (9.2.6) of **H** and C_6 symmetry **r**^{*p*}-eigenvalues from (8.2.9).

$$\langle k_m | \mathbf{r}^p | k_m \rangle = e^{-ipk_m a} = e^{-ipm2\pi/N} \text{ where: } k_m = m(2\pi/Na)$$

$$\langle k_m | \mathbf{H} | k_m \rangle = H \langle k_m | \mathbf{1} | k_m \rangle + S \langle k_m | \mathbf{r} | k_m \rangle + T \langle k_m | \mathbf{r}^2 | k_m \rangle + U \langle k_m | \mathbf{r}^3 | k_m \rangle + T^* \langle k_m | \mathbf{r}^4 | k_m \rangle + S^* \langle k_m | \mathbf{r}^5 | k_m \rangle$$

$$= H + S e^{-ik_m a} + T e^{-i2k_m a} + U e^{-i3k_m a} + T^* e^{i2k_m a} + S^* e^{ik_m a} \qquad (9.3.5a)$$

Bloch dispersion relation. And Bohr limit (k<< π/a) approxiamtion. Band group velocity V_{group} .

$$\hbar\omega_m = E_m = H - 2|S| \cos(k_m a) = H - 2|S| + |S|(k_m a)^2 + \dots$$
(9.3.8)
$$U_m = \frac{d\omega_m}{d\omega_m} = 2\frac{|S|}{d\omega_m} \sin(k_m a) \left(\cos^2 \frac{|S|}{d\omega_m} + \cos^2 \frac{$$

$$V_{group} = \frac{d\omega_m}{dk_m} = 2\frac{|S|}{\hbar}a\sin(k_ma) \quad \left(\equiv 2\frac{|S|}{\hbar}k_ma^2, \text{ for: } k_m <<\pi/a \right)$$
(9.3.10)

Effective mass M_{eff} inversely proportional to S. $M_{eff}(0) = \hbar^2/(2|S| a^2)$

Fourier transform of a Gaussian $e^{-(m/\Delta m)^2}$ momentum distribution is a Gaussian $e^{-(\phi/\Delta \phi)^2}$ in coordinate ϕ . $\langle m|\Psi \rangle = e^{-(m/\Delta m)^2}$ implies: $\langle \phi |\Psi \rangle = e^{-(\phi/\Delta \phi)^2}$ (9.3.14)

The relation between *momentum uncertainty* Δm and *coordinate uncertainty* $\Delta \phi$ is a *Heisenberg relation*.

$$\Delta m/2 = 1/\Delta \phi$$
, or: $\Delta m \Delta \phi = 2$ (9.3.15)

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(9.3.11a)

$$V_{group}^{Bohr}(m \leftrightarrow n) = \frac{\omega_m - \omega_n}{k_m - k_n} = \frac{(m^2 - n^2)hv_1}{(m - n)h/L} = (m + n)\frac{L}{\tau_1} = (m + n)V_1 \quad (9.3.16)$$

Predicting fractional revivals: *Farey Sum* \oplus *_F* of the rational fractions n_1/d_1 and n_2/d_2

$$t_{12-intersection} = \frac{n_2 + n_1}{d_2 + d_1} = \frac{n_2}{d_2} \oplus_F \frac{n_1}{d_1}$$
(9.3.18)

Appendix 9.A. Relative phase of peaks in a revival lattice

The first derivation here of revival amplitudes at stroboscopic time fractions $t_v = \tau(v/N)$ and kaleidescopic angular positions $\phi_{\rho} = 2\pi(\rho/N)$ assumes N is odd. At times when fraction (v/N) is reduced, all N revival peak sites hop up with identical magnitude and with particular arrangement of phases that clearly distinguishes each v/Nfrom all others. First we derive formulas for these phases as a function of site index ρ and revival time index v. (If time fraction v/N reduces to v_R/N_R , then use (v_R, N_R) in place of (v, N) to find N_R peak phases of subgroup C_{N_R} revivals.) The first step is to complete the square of exponent in sum.

$$\begin{split} \Psi_{0}\left(\phi_{\rho},t_{\nu}\right) &= \frac{1}{N} \sum_{m=0}^{N-1} e^{i\left(m \ \rho - m^{2} \nu\right)\frac{2\pi}{N}} = \frac{1}{N} \sum_{m=0}^{N-1} e^{-i\left(m^{2} \nu - m\rho + \frac{\rho^{2}}{4\nu}\right)\frac{2\pi}{N}} e^{i\frac{\rho^{2}}{4\nu}\frac{2\pi}{N}} \\ &= \frac{1}{N} \sum_{m=0}^{N-1} e^{-i\left(m\nu - \frac{\rho}{2}\right)\left(m - \frac{\rho}{2\nu}\right)\frac{2\pi}{N}} e^{i\frac{\rho^{2}}{4\nu}\frac{2\pi}{N}} \\ &= \frac{1}{N} \sum_{m=0}^{N-1} e^{-i\left(2m\nu - \rho\right)^{2}\frac{2\pi}{4\nu N}} e^{i\frac{\rho^{2}}{2\nu}\frac{2\pi}{N}} \end{split}$$
(A.1)

The integer square $(2m\nu-\rho)^2$ in the exponent is to be treated as an integer-modulo- $4\nu N$ since the phase factor repeats after that value. However, as summation index *m* runs through the integers m = 0, 1, 2, ..., N-1 it exhausts all the possible values of $(2m\nu-p)^2 - mod - 4\nu N$ for a given ν and ρ , and the values are the same no matter what we take for the range of *m*. For example, consider tables of phase index $(2m\nu-\rho)^2 - mod - 4\nu N$ for select times of $\nu=1$ and $\nu=2$ for an N=5 level excitation.

$(2mv - \rho)^2 \mod 4vN$ for $N=5$									$(2mv - \rho)_{4vN}^2 \text{for } N=5$												
v=1	m = 0	1	2	3	4	5	6		v=2	m = 0	1	2	3	4	5	6	7	8	9	10…	
$\rho = 0$	$\overline{0}$	4	16	16	4	0	4	(, , ,)	$\rho = 0$	$\overline{0}$	16	24	24	16	0	16	24	24	16	0	
1	1	1	9	5	9	1	1	(A.2a)	1	1	9	9	1	$\overline{2}\overline{5}$	1	9	9	1	25	1	(A.2b)
2	4	$\overline{0}$	4	16	16	4	0		2	4	4	36	$\overline{20}$	36	4	4	36	20			
3	9	1	1	9	5	9	1		3	9	1	$\overline{25}$	1	9	9	1					
4	16	4	$\overline{0}$	4	16	16	4		4	16	$\overline{0}$	16	24	24	16					i	

Note that *N* consecutive values for *m* give the same sum no matter whether the sum starts at m=0 or at a *sum-shift* value $m=\mu$. The idea is to shift the summation index *m* to $m-\mu$ so that a $(2m\nu-\rho)^2 -mod-4\nu N$ binomials in row- ρ can be replaced by a simple square $(2m\nu)^2 -mod-4\nu N$ monomial found in the $\rho=0$ row. This will reduce the exponent to a term independent of site-index ρ plus a Δ -term independent of summation-index *m*.

It would be nice if the Δ -term were also independent of ρ but the tables show that is asking too much! So, $\Delta = \Delta(\rho, \nu)$ and, each of the rows $\rho = 1$, ..., *N*-1 differ from the $\rho = 0$ row by a single *modular difference* $\Delta(\rho, \nu)$ in phase index which is overlined in the table and is the *single unpaired* number in each row. For example, subtracting $\Delta(1,1)=5$ -mod-20 = $(5)_{20}$ from the $(\rho=1)$ row of the $(\nu=1)$ table and shifting forward by $\mu_1=2$ gives the $(\rho=0)$ row (mod-20). The shifts needed to line up rows $\rho=1$, 2, 3, and 4 are $\mu_1=2$, $\mu_2=4$, $\mu_3=6$, and $\mu_4=8$ respectively, that is $\mu_{\rho}=\mu_1\rho$. These observations are summarized by a modular equation.

$$\left(2\left(m-\mu_{\rho}\right)\nu-\rho\right)^{2} \mod 4\nu N \equiv \left(2\left(m-\mu_{\rho}\right)\nu-\rho\right)^{2}_{4\nu N} = \left(2m\nu\right)^{2}_{4\nu N} - \Delta(\rho,\nu)$$
(A.3a)

This is supposedly valid for all values of *m* so for m=0 the equation reads

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$$\left(-2\mu_{\rho}v-\rho\right)_{4vN}^{2}=0-\Delta(\rho,v) \quad , \tag{A.3b}$$

where

Subtracting equation (A.3b) from (A.3a) gives the following, again valid for all m.

 $\mu_{\rho} = \mu_1 \rho$.

$$(2(m-\mu_{\rho})v-\rho)_{4vN}^{2} - (-2\mu_{\rho}v-\rho)_{4vN}^{2} = (2mv)_{4vN}^{2}$$
$$(4mv(-2\mu_{\rho}v-\rho))_{4vN} = (0)_{4vN} = \kappa 4vN = 0, 4vN, 8vN, \dots, 4vN(N-1)$$

Next, set m=1, and solve for the *m*-sum-shift μ_{ρ} of row ρ .

$$-8\mu_{\rho}v^{2} - 4v\rho = -\kappa 4vN = 0, -4vN, -8vN, \dots, -4vN(N-1)$$

$$2\mu_{\rho}v + \rho = \kappa N = 0, N, 2N, \dots, N(N-1) \text{ or: } \mu_{\rho} = \frac{\kappa N - \rho}{2v} = (\text{integer})_{N}$$
(A.4a)

A value $\kappa = 0, 1, 2, ..., N-1$ is selected so that *m*-sum-shift μ_{ρ} is an integer $\mu_{\rho} = 0, 1, 2, ..., N-1$, too. Substituting the resulting μ_{ρ} value in (A.3a) gives the phase modular difference Δ first defined there and in (A.3b).

$$\Delta(\rho, \nu) = -\left(2\nu\mu_{\rho} + \rho\right)_{4\nu N}^{2} = -\left(2\nu\left(\frac{\kappa N - \rho}{2\nu}\right) + \rho\right)_{4\nu N}^{2} = -\left(\kappa N\right)_{4\nu N}^{2} , \qquad (A.4b)$$

where

$$\kappa = \frac{2\nu\mu_{\rho} + \rho}{N} \,. \tag{A.4c}$$

Puttiing (A.3a) into the revival wavefunction sum (A.1) gives

$$\begin{split} \psi_{0}\left(\phi_{\rho},t_{\nu}\right) &= \frac{1}{N} \sum_{m=0}^{N-1} e^{-i\left(2m\nu-\rho\right)^{2} \frac{2\pi}{4\nu N}} e^{i\frac{\rho^{2}}{4\nu} \frac{2\pi}{N}} \\ &= \frac{1}{N} \sum_{m=0}^{N-1} e^{-i\left[\left(2m\nu\right)^{2} - \Delta(\rho,\nu)\right] \frac{2\pi}{4\nu N}} e^{i\frac{\rho^{2}}{4\nu} \frac{2\pi}{N}} \qquad \left[\text{using:}(A.3a)\right] \\ &= \frac{1}{N} \sum_{m=0}^{N-1} e^{-i\left[\left(2m\nu\right)^{2} + (\kappa N)^{2} - \rho^{2}\right] \frac{2\pi}{4\nu N}} \qquad \left[\text{using:}(A.4b)\right] \\ &= \frac{1}{N} \sum_{m=0}^{N-1} e^{-i\left[\left(2m\nu\right)^{2} + 4\mu^{2}\rho\nu^{2} + 4\mu\rho\nu\rho\right] \frac{2\pi}{4\nu N}} \qquad \left[\text{using:}(A.4b)\right] \\ &= \frac{1}{N} \sum_{m=0}^{N-1} e^{-i\left[\left(2m\nu\right)^{2} + 4\mu^{2}\rho\nu^{2} + 4\mu\rho\nu\rho\right] \frac{2\pi}{4\nu N}} \qquad \left[\text{using:}(A.4c)\right] \\ &= P(\nu)e^{\frac{-i\left[\mu^{2}\rho\nu + \mu\rho\rho\right] 2\pi}{N}} = P(\nu)e^{\frac{-i\left[\mu^{2}\rho\nu + \mu_{1}\right]\rho^{2} 2\pi}{N}} \qquad \left[\text{using:}(A.3c)\right] \quad (A.5a) \end{split}$$

The overall phase and amplitude prefactor P(v) is a Gaussian sum discussed in Appendix 9B.

$$P(\mathbf{v}) = \frac{1}{N} \sum_{m=0}^{N-1} e^{-i(2m\mathbf{v})^2 \frac{2\pi}{4\mathbf{v}N}} = \frac{1}{N} \sum_{m=0}^{N-1} e^{-i\mathbf{v}m^2 \frac{2\pi}{N}}$$
(A.5b)

Finally, the $(\rho = 1)$ *m*-sum-shift μ_1 is the first fraction $(N-1)/2\nu$, $(2N-1)/2\nu$, $(3N-1)/2\nu$, ..., or $(N^2-1)/2\nu$, to yield an integer according to (A.4a). Recall that it was assumed that *N* and ν are relatively prime, that is, have no common factors. It seems evident that the integer arithmetic behind base-*N* counter revivals is not trivial, even for the case of odd-*N*. To complete this particular *N*=5 example we find the sum-shift μ_1 at each revival time $\nu=1-4$.

(A.3c)

From the discussion of Appendix 9B come the overall prefactors $P(v=1)=1/\sqrt{5}$, $P(2)=-1/\sqrt{5}$, $P(3)=-1/\sqrt{5}$, and $P(v=1)=1/\sqrt{5}$, which are needed to complete the following N=5 revival table using (A.5).

A phasor gauge plot of the N=5 revivals (A.7) is shown in Fig. 9.4.3c.

The summation (A.1) for *even-N* is mostly the same as the above. Time index v is replaced by v/2.

$$\psi_{0}(\phi_{\rho}, t_{\nu}) = \frac{1}{N} \sum_{m=0}^{N-1} e^{-i(m\nu - \rho)^{2} \frac{2\pi}{2\nu N}} e^{i\frac{\rho^{2}}{2\nu} \frac{2\pi}{N}}, \text{ where; } t_{\nu} = \nu \frac{2\pi}{2N}, \text{ for } N \text{-even.}$$
$$= P(\nu) e^{\frac{-i\left[\mu_{\rho}^{2}\nu + 2\mu_{\rho}\rho\right]2\pi}{2N}} = P(\nu) e^{\frac{-i\left[\mu_{1}^{2}\nu + 2\mu_{1}\right]\rho^{2} 2\pi}{2N}}$$
(A.8a)

where

$$\mu_1 = \frac{\kappa N - 1}{\nu} = \text{first integer in } \frac{N - 1}{\nu}, \frac{2N - 1}{\nu}, \frac{3N - 1}{\nu}, \dots$$
(A.8b)

Again the overall phase and amplitude prefactor P(v) is a Gaussian sum discussed in Appendix B.

$$P(\mathbf{v}) = \frac{1}{N} \sum_{m=0}^{N-1} e^{-i(m\mathbf{v})^2 \frac{2\pi}{2\nu N}} = \frac{1}{N} \sum_{m=0}^{N-1} e^{-i\nu m^2 \frac{2\pi}{2N}}$$
(A.8c)

This works for odd-numerator time fractions 1/2N, 3/2N, 5/2N,...= $\nu/2N$. For the even numerator ones, we take advantage of the revival sequence $\nu/N = 1/N$, 2/N, 3/N,... for N cut in half and shifted by π . If N/2 is odd then (A. 5) is used. If N/2 is even then (A.8) is used again, but with N cut in half to N/2. Note that fractions with singlyeven denominators have zeros at $\phi=0$ and peaks at $\phi=\pm\pi$. Fractions with odd denominators have peaks at $\phi=0$ and zeros at $\phi=\pm\pi$. Fractions with doubly-even denominators have zeros at $\phi=0$ and $\phi=\pm\pi$.

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Appendix 9.B. Overall phase of peaks in a revival lattice

The evaluation of the N-term integral Gaussian sum

$$G(v) = \sum_{m=0}^{N-1} e^{-ivm^2 \frac{2\pi}{N}} = NP(v)$$
(B.1)

in the prefactor P(v)=G(v)/N given by (A.5b) is, perhaps, the least trivial part of the revival formulation. The development involves complex Gaussian integer analysis, a subject which occupied Gauss for more than the first decade of his most productive years. Here we will be content with giving a list of the results for the first few integer combinations that would be relevant for the revivals shown previously.

$$\frac{N=2}{\sum_{m=0}^{N-1}e^{-im^{2}\frac{2\pi}{N}}=0 -i\sqrt{3} (1-i)\sqrt{4} \sqrt{5} 0 -i\sqrt{7} (1-i)\sqrt{8} \sqrt{9} 0 -i\sqrt{11} (1-i)\sqrt{12}}{\sum_{m=0}^{N-1}e^{-i2m^{2}\frac{2\pi}{N}}=2 i\sqrt{3} 0 -\sqrt{5} -i\sqrt{12} -i\sqrt{7} (1-i)\sqrt{4} \sqrt{9} \sqrt{20} i\sqrt{11} 0}{\sum_{m=0}^{N-1}e^{-i3m^{2}\frac{2\pi}{N}}=0 3 (1+i)\sqrt{4} -\sqrt{5} 0 i\sqrt{7} -(1+i)\sqrt{8} -i\sqrt{27} 0 -i\sqrt{11} (1-i)6}{\sum_{m=0}^{N-1}e^{-i4m^{2}\frac{2\pi}{N}}=2 -i\sqrt{3} 4 \sqrt{5} i\sqrt{12} -i\sqrt{7} 0 \sqrt{9} -\sqrt{20} -i\sqrt{11} -i\sqrt{48}}{\sum_{m=0}^{N-1}e^{-i5m^{2}\frac{2\pi}{N}}=0 i\sqrt{3} (1-i)\sqrt{4} 5 0 i\sqrt{7} -(1-i)\sqrt{8} \sqrt{9} 0 -i\sqrt{11} -(1-i)\sqrt{12}}{\sum_{m=0}^{N-1}e^{-i6m^{2}\frac{2\pi}{N}}=2 3 0 \sqrt{5} 6 i\sqrt{7} (1+i)4 i\sqrt{27} -\sqrt{20} i\sqrt{11} 0}{\sum_{m=0}^{N-1}e^{-i7m^{2}\frac{2\pi}{N}}=0 -i\sqrt{3} (1+i)\sqrt{4} -\sqrt{5} 0 7 (1+i)\sqrt{8} \sqrt{9} 0 -i\sqrt{11} -(1+i)\sqrt{12}}{(1+i)\sqrt{12}}$$
(B.2)

Particuarly simple general results are had for the case of doubly-even integer.

$$\frac{N = 2n}{\sum_{m=0}^{N-1} e^{-im^2 \frac{2\pi}{N}}} = (1-i) (1-i)\sqrt{2} (1-i)\sqrt{3} (1-i)\sqrt{4} (1-i)\sqrt{5}$$
(B.3)

A complex vector diagram of the first few G(u) sums is shown below in Fig. 9B.1.

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Fig. 9B.1 Sums of modular squares $(m^2)_N = m^2 \mod N$ (N = 3-12).