Symmetry and Correlation Aspects of Quantum Dynamics

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Refs.

- 1. Shenglong Xu and Congjun Wu, Phys. Rev. Lett. 120, 096401 (2018).
- 2. Wang Yang, Jianda Wu, Shenglong Xu, Zhe Wang, Congjun Wu arXiv:1702.01854.

3. Z. Wang, J. Wu, W. Yang, A. K. Bera, D. Kamenskyi, A.T.M. N. Islam, S. Xu, J. M. Law, B. Lake, C. Wu, A. Loidl, Nature 554, 219 (2018).

Introduction



<u>Crystal – a fundamental of condensed matter</u>



• 230 space groups – Fedorov, Schönflies (1891)

Crystal system: Cubic

Bravais lattice: **FCC** (face-centered cubic)

Point group: T_d or $\overline{4}3m$

Space group: O_h^7 or $Fd\overline{3}m$

Non-symmorphic symmetries: screw rotation glide reflection





Bloch Theorem (1928)

• Chemical bond (small molecule):





• Bloch band (large crystal)



$$\psi_{k,m}\left(\vec{r}\right) = e^{i\vec{k}\cdot\vec{r}}u_m(\vec{r})$$



 Origin of (band) insulator is quantum: gap due to the interference of matter wave!

Dynamics under periodic driving

• Floquet Theorem (1883)

$$H(t) = H(t+T)$$
 $\Omega = 2\pi/T$

$$\psi_{\omega}(t) = e^{-i\omega t}u(t) = e^{-i\omega t}\sum_{n}a_{n}e^{-in\Omega t}$$



Explore many-body physics via Floquet engineering



"ferro"-magnetic domain formation, universal scaling across quantum phase transition

Chin's group, Nature Physics 9, 769-774 (2013), Science 354, 606-610 (2016)

Floquet framework is NOT generic

• Temporal and spatial symmetries decoupled.

c.f. A 3D crystal is not just a 2D crystal (ab-plane) direct product with a 1D crystal (c-axis)

• Dynamic crystal \neq space crystal \otimes Floquet periodicity!

 A general framework for space-time coupled symmetries – space-time group!



Introduction



Strong correlation physics

- Central theme: spectra functions based on the Kubo formula.
 - 1. Emphasis on **low energy** physics
 - 2. Imaginary (Matsubara) frequency
 - **3. Imaginary** time evolution quantum Monte Carlo





• How can integrable models help?

High **real-frequency** spectra beyond effective low energy theory.

Multi-particle (anti)-bound states

• Resonance states in high energy physics.

• Efimov states in nuclear physics and in cold atom physics.

Chin's group, Phys. Rev. Lett. 113, 240402 (2014)





Spin dynamics in antiferromagnet

• Bethe string states (magnon anti-bond states)

SrCo₂V₂O₈ Electron spin resonance (ESR) B∥c Three-string excitations Néel-С Field-Critical ordered polarized 4 $\chi_{\pi/2}$ (ZHZ) Two-string excitations Frequency 3 (body)- string M sinon-psinon states 2 Magnons 2 (body) - string states 0 0 10 20 30 Magnetic field, B (T)

Loidl's group, Wu's group, et al, Nature 554, 219 (2018).

Quantum dynamic systems



S. L. Xu and C. Wu, Phys. Rev. Lett. 120, 096401 (2018).

<u>Dynamic "crystal" – space-time symmetries</u> • Space-time unit cell \neq space domain \otimes time domain. temporal periodicity unnecessary $V(x,t) = \cos(k_1 x - \omega_1 t)$ $+\cos(k_2x-\omega_2t)$ $V(0,t) = \cos \omega_1 t + \cos \omega_2 t$ spacial periodicity unnecessary $V(x,0) = \cos k_1 x + \cos k_2 x$ a_1 an • New framework \rightarrow space-time group. S. L. Xu and C. Wu, Phys. Rev. Lett. 120, 096401 (2018).

<u>Reciprocal lattice (momentum-energy)</u>

 $V(\vec{r}, t) = V(\vec{r} + \vec{u}_i, t + \tau_i), \quad i = 1 \dots, D + 1$



$$b_i \cdot a_j = \vec{G}_i \cdot \vec{u}_j - \Omega_i \tau_j = 2\pi \delta_{ij}$$

• Time quasi-crystal with D+1 frequencies (beyond Floquet).

The generalized Bloch-Floquet theorem $i\hbar\partial_t\psi(\vec{r},t) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)\right)\psi(\vec{r},t)$ $\psi_{\kappa m}(\vec{r},t) = e^{i(\vec{k}\cdot\vec{r}-\omega t)}u_m(\vec{r},t)$

 $\kappa = (\vec{k}, \omega)$: the (lattice) momentum-energy vector (mod B) $u_m(\vec{r}, t)$: the same space-time periodicity of $V(\vec{r}, t)$

S. L. Xu and CW, Phys. Rev. Lett. 120, 096401 (2018)

$$u_m(\vec{r},t) = \sum_B c_{m,B} e^{i(\vec{G}\cdot\vec{r} - \Omega t)}$$

 $\sum_{B'} \{ [-\Omega + \epsilon_0 (k+G)] \delta_{B,B'} + V_{B-B'} \} \ c_{m,B'} = \omega_m \ c_{m,B}$

 $B = (\vec{G}, \Omega)$ take all D+1 dim. reciprocal lattice vectors

"Space-time" group



Representations:

- $M_{\Gamma}\psi_{\kappa} = \psi_{\kappa}(\Gamma^{-1}(\vec{r},t))$ for s=1
- $M_{\Gamma}\psi_{\kappa} = \psi_{\kappa}^* (\Gamma^{-1}(\vec{r}, t))$ for s=-1 (anti-unitary)

"Space-time" non-symmorphic symm.

• If τ itself is not a symmetry \rightarrow space-time nonsymmorphic symm.





S. L. Xu and C. Wu, Phys. Rev. Lett. 120, 096401 (2018).

T. Morimoto, et al, PRB (2017)

c.f. 17 wallpaper groups in 2D



1+1 D space-time group

Only 2-fold axis allowed.

- 3,4,6-fold ones are not.
- Reflection ٠

 $m_{x}:(x,t) \rightarrow (-x,t)$

Time-reversal

$$m_t: (x, t) \to (x, -t)$$

Time-glide reflection ٠



$$g_x:(x,t)\to \left(-x,t+\frac{T}{2}\right)$$

glide time-reversal

$$g_t:(x,t) \to \left(x+\frac{a}{2},-t\right)$$



Orthorhombic :













 Cm_t





 $C2m_xm_t$

2+1 D space-time group

- No cubic crystal system.
- Two different monoclinic crystal systems.





• Classification: 275 spacetime groups in 2+1 D

Crystal System	MP Group	Bravais Lattice	G(2, 1)
Triclinic	1, 2'	Primitive	2
T-Monoclinic	11' 2 21'	Primitive	8
1 Monochine	11,2,21	Centered	5
R-Monoclinic	m m' m'm?'	Primitive	8
	110,110,110 1102	Centered	5
Orthorhombic		Primitive	68
	a 1 1a	T-Base-Centered	15
	mm2, m'm'2 mm21', m1'	R-Base-Centered	22
		Face-Centered	7
		Body-Centered	15
Tetragonal	4,41',4'	Primitive	49
Tetragonar	4'm'm, 4m'm'	Body-Centered	19
Trigonal	3,6',3m	Primitive	18
	3m', 6'm'm	Rhombohedral	7
Hexagonal	6, 61', 31' 6mm, 6m'm' 6mm1', 3m1'	Primitive	27

Space-time symmetry in 2D materials (in progress)

• Coherent lattice dynamics: chiral phonon → BN, MoS₂,WSe₂



• Realized in WSe2 by inter-valley transfer of holes through hole-phonon interaction

Xiang Zhang's group, Science 359, 579 (2018).

Space-time symmetry in 2D materials (in progress)

R: 3-fold rotation



• Blue site \rightarrow 3-fold axis

R:
$$(x, y, t) \to \left(-\frac{1}{2}x - \frac{\sqrt{3}}{2}y + \sqrt{3}, \frac{\sqrt{3}}{2}x - \frac{1}{2}y, t\right)$$

• Plaquette center: time-screw axis

S:
$$(x, y, t) \to \left(-\frac{1}{2}x + \frac{\sqrt{3}}{2}y, -\frac{\sqrt{3}}{2}x - \frac{1}{2}y, t + \frac{T}{3}\right)$$

 Central position of a red site → time-screw axis

Hu, Wu et al, in progress.

Degeneracy from space-time symmetry

• Theorem: operations for the wavevector group of \vec{k} , satisfying $g_1g_2 = T(\vec{u})g_2g_1$, with $\vec{k} \cdot \vec{u} = 2\pi p/q$ (p/q co-prime) \rightarrow q-fold degeneracy at $\kappa = (\vec{k}, \omega)$

S and R both leave K invariant: $(S \cdot R)|_{K} = \exp\left(i\frac{2\pi}{3}\right)(R \cdot S)|_{K}$

Nondegeracy with static distortion (only R)

Triple degeneracy at K (R and S)



Further developments in speculation

• Time dependent potential for phononic and photonic crystals, optical lattices for cold atoms ...

• Semi-classic transport – non-adiabatic treatment

• Time crystal -- Spontaneous discrete time translation symmetry breaking. (Nayak, Wilczek)



W. Yang, J. Wu, S. L. Xu, Z. Wang, C. Wu arXiv:1702.01854.

Z. Wang, J. Wu, W. Yang, A. K. Bera, D. Kamenskyi, A.T.M. N. Islam, S. Xu, J. M. Law, B. Lake, C. Wu, A. Loidl, Nature 554, 219 (2018).

Magnon (anti)-bound states – Bethe string states

• 1D ferromagnet: spin-flip \rightarrow magnon attraction \rightarrow bound state





Cold boson Mott insulators - bound state propagation.

I. Bloch's group, Nature 502 (2013).

Joint probability P_{ij} peaks at $j = i \pm 1$



i ⁸⁷Rb $|\uparrow\rangle = |1, -1\rangle, |\downarrow\rangle = |2, -2\rangle, \quad J \approx 54Hz$

Quasi-1D antiferromagnet SrCo₂V₂O₈



Screw chain consisting of CoO_6 octahedra running along the crystalline *c*-axis



$$H = J \sum_{n=1}^{N} \left\{ S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \Delta (S_n^z S_{n+1}^z - \frac{1}{4}) \right\} - g\mu_B h \sum_{n=1}^{N} S_n^z$$

 $J \approx 3.55 meV$, $\Delta \approx 2.04$, $g \approx 5.85$

fitted by thermodynamic property measurements: spin gap, critical field, and saturation field.

Wang, Zhe, M. Schmidt, A. K. Bera, A. T. M. N. Islam, B. Lake, A. Loidl, and J. Deisenhofer, PRB 91, no. 14 140404 (2015).

<u>Many-body physics of repulsive magnons (spin- \downarrow)</u>

• 1D spin-1/2 antiferromagnet (Ising anisotropy)



spin- $\uparrow \rightarrow \bigcirc$

spin- $\downarrow \rightarrow$ hard-core boson \rightarrow spinless fermion \bigcirc (Jordan-Wigner)

• $H > H_{c_1}$: magnetization \rightarrow dope vacancies

a snapshot of ground state

• Anti-bond states at high energies

2-string state energy cost ~ J



Measure excitations - electron spin resonance (ESR)

• Larmor precession:

$$H = -g_e \mu_B h S_z$$



H: 3500G,
$$v = \frac{\omega}{2\pi} = 9 - 10GHz$$





High real-frequency spin excitation spectra

- ESR in the longitudinal B-field
- THz light along *c*-axis: $S^{+-}(q, \omega)$ and $S^{-+}(q, \omega)$ at $q = 0, \pm \frac{\pi}{2}, \pi$.



Loidl's group, Wu's group, et al, Nature 554, 219 (2018).

Dynamic spin structure factor

• Observable: ESR and neutron spectroscopy

Fourier spectra of real-time correlation: $\langle G | S_i^a(t) S_i^{\overline{a}}(t') | G \rangle$

$$S^{a\bar{a}}(q,\omega) = 2\pi \sum_{\mu} \left| \left\langle \mu \right| S_q^{\bar{a}} \left| G \right\rangle \right|^2 \delta(\omega - E_{\mu} + E_{GS})$$

Transverse:
$$S^{+-}(q,\omega), S^{-+}(q,\omega)$$

 Each matrix element → Summation over excitations → Check saturation with sum rules.

Why Bethe Ansatz?

 All eigenstates are known not just the ground state → Spin dynamics at intermediate and high energies.

Nature of excitations manifest – good Bethe quantum numbers

- **Exact diagonalization:** very small size.
- **TEBD:** difficult to handle gapless systems.
- **QMC**: difficult to handle real frequency.
- Luttinger liquid: only applies at low energy.

Correlation functions via Bethe Ansatz (BA)

• Coordinate BA inapplicable for correlation function calculations

$$k_{1} \xrightarrow{k_{2}} k_{3} \xrightarrow{k_{3}} m! \text{ terms}$$

$$\psi = \sum_{P} A_{p_{1}p_{2}..p_{m}} e^{ik_{p_{1}}x_{1}+k_{p_{2}}x_{2}+...k_{pm}x_{m}}$$

• Algebraic Bethe ansatz – Form factor

L. A. Takhtadzhan and L. D. Faddeev *Russ. Math. Sur.* 34,11 (1979)

Many-body matrix elements \rightarrow determinants;

Dynamic spin structure factor not done before for the XXZ model via BA

N. Kitanine, J. M. Maillet and V. Terras *Nucl. Phys. B* 554, 647 (1999)

Spectra of
$$S^{+-}(q, \omega)$$

 $S^{+-}(q, \omega): \sum_{\mu} \langle G|S_i^+(t)|\mu \rangle \langle \mu|S_j^-(t')|G \rangle$

 $|\mu\rangle$: Add a spin down (•) to the ground state $\langle \mu | S_z | \mu \rangle = \langle G | S_z | G \rangle - 1$:



String states (anti-bound states)



No 4-string state contribution

Dynamic spin-structure factor $-S^{-+}(q, \omega)$ $S^{-+}(q, \omega)$: $\sum_{\mu} \langle G | S_i^-(t) | \mu \rangle \langle \mu | S_j^+(t') | G \rangle$ $| \mu \rangle$: remove a spin down (•) from the ground state $\langle \mu | S_z | \mu \rangle = \langle G | S_z | G \rangle + 1$:

No string-state contribution





<u>Transverse DSF – Evolution with magnetization</u>

N=200, *∆* = 2

S⁺⁻



Summary

• A platform for (periodical) dynamic systems for everyone.

space-time group, Bloch-Floquet theorem



• High real-frequency – identification of 3-string states – hint for high dimensional states....





Back up

Symmetry consequences on dispersions

Dispersion relation $f(k, \omega) = 0 \rightarrow$ generally multi-valued

• Winding in the Brillouin zone torus: (w_1, w_2)





• Non-spinor Kramers degeneracy by $g_t: (x, t) \rightarrow (x + \frac{a}{2}, -t)$

$$M_{g_{t}}^{2}\psi_{\kappa} = \psi_{\kappa}(x - a, t) = -\psi_{\kappa}$$
 for $\kappa = (\pi, \omega)$



Winding #: (even, 0)





Bethe Ansatz (BA)

• Many-body scattering amplitude = a product of two-particle ones.

$$\psi = A_{12} e^{ik_1x_1 + k_2x_2} + A_{21}e^{ik_1x_1 + k_2x_2}$$



periodical boundary condition: $k_i N + \sum_{j \neq i} \pi + \Theta(k_j, k_i) = 2\pi I_i$ Bethe quantum number

• Ground state energy (Heisenberg chain): $\frac{E_G}{NI} = \frac{1}{4} - ln2$

Longitudinal DSF $S^{zz}(q, \omega)$ - intensity plot $\hbar\omega/J$ $\hbar\omega/J$ $\hbar\omega/J$ π π π 2m=0.3 2m=0.1 2m=0.5 $\hbar\omega/J$ $\hbar\omega/J$ π π 2m=0.7 2m=0.9

Bethe quantum numbers											
$-\frac{M-1}{2} - S^{z} < I_{\alpha}^{(n)} < \frac{M-1}{2} + S^{z}$: N=32, M=8 (spin-down).											
-	<u>23</u> 2	$-\frac{7}{2}$	$-\frac{3}{2}$	$\frac{1}{2}$	$\frac{5}{2}$ $\frac{7}{2}$			$\frac{23}{2}$			
Ground state:	00000000						000	0			
1 $\psi\psi$ state:	0000000	ν • Ο ψ	• Ο ψ			000	000	00			
1 $\psi\psi^*$ state:	00000		\bigcirc ψ			000	000	0			
						unbou	nd part	ticles			
1 $\chi^{(2)}R$ state:	0000000	$\bigcirc \bigcirc$				000	000	С			
	00000	000			0000	0					
	Length-two str	ing									

Algebraic Bethe Ansatz

Yang-Baxter Equation:

 $R_{12}(\lambda_1, \lambda_2) R_{13}(\lambda_1, \lambda_3) R_{23}(\lambda_2, \lambda_3) = R_{23}(\lambda_2, \lambda_3) R_{13}(\lambda_1, \lambda_3) R_{12}(\lambda_1, \lambda_2)$

Monodromy matrix:

$$\mathcal{T}(\lambda) = R_{0n}(\lambda, i\frac{\eta}{2}) \dots R_{02}(\lambda, i\frac{\eta}{2}) R_{01}(\lambda, i\frac{\eta}{2}) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}_{[0]}$$

Transfer matrix and XXZ Hamiltonian:

$$T(\lambda) = \text{Tr}\mathcal{T}(\lambda)$$
 $H = \sin(i\eta)\frac{d}{d\lambda}\ln T(\lambda)|_{\lambda = i\eta/2} + \text{const.}$

Magnon creation operator:

$$\Psi(\lambda_1, \lambda_2, ..., \lambda_r) = B(\lambda_1) B(\lambda_2) ... B(\lambda_r) |\uparrow\uparrow ... \uparrow\rangle$$

L. A. Takhtadzhan and L. D. Faddeev Russ. Math. Sur. 34,11 (1979)

Algebraic Bethe ansatz and quantum inverse problem

Three key ingredients:

• Magnon creation operators

 $|\Psi(\lambda)\rangle = B(\lambda_1)B(\lambda_2)\dots B(\lambda_M)|\uparrow\uparrow\uparrow\dots\uparrow\rangle$

Monodromy matrix: $\begin{pmatrix} A & B \\ C & D \end{pmatrix}$ B: magnon creation C: magnon annihilation A+D: conserved quantity

 Quantum inverse problem (Relate local spin operators with quasi-particle operators.)
 i-1

$$\sigma_i^- = \prod_{\alpha=1}^{l-1} (A+D)(\xi_\alpha) \cdot B(\xi_i) \cdot \prod_{\alpha=l+1}^N (A+D)(\xi_\alpha)$$

• F-basis

(Simplifies quasi-particle operators.)

$$FB(\lambda)F^{-1} = \sum_{i=1}^{N} \sigma_i^- \bigotimes_{j \neq i} diagonal \ matrix \ at \ site \ j$$

Form factors can be evaluated.

Derivation of determinant formulae

 $\langle \mu | S_n^a | \lambda \rangle = \frac{\langle \Psi(\{\mu_i\}) | S_j^a | \Psi(\{\lambda_j\}) \rangle}{\sqrt{\langle \Psi(\{\mu_i\}) | \Psi(\{\mu_i\}) \rangle} \cdot \sqrt{\langle \Psi(\{\lambda_j\}) | \Psi(\{\lambda_j\}) \rangle}}$

Quantum inverse problem:

$$\sigma_{i}^{-} = \prod_{\alpha=1}^{i-1} (A+D) (\xi_{\alpha}) \cdot B(\xi_{i}) \cdot \prod_{\alpha=i+1}^{N} (A+D) (\xi_{\alpha}),$$

$$\sigma_{i}^{+} = \prod_{\alpha=1}^{i-1} (A+D) (\xi_{\alpha}) \cdot C(\xi_{i}) \cdot \prod_{\alpha=i+1}^{N} (A+D) (\xi_{\alpha}),$$

$$\sigma_{i}^{z} = \prod_{\alpha=1}^{i-1} (A+D) (\xi_{\alpha}) \cdot (A-D) (\xi_{i}) \cdot \prod_{\alpha=i+1}^{N} (A+D) (\xi_{\alpha}),$$

$$\begin{aligned} \mathbf{F}\text{-basis:} \\ \widetilde{D}_{1\dots N}(\lambda;\xi_1,\dots,\xi_N) &\equiv F_{1\dots N}(\xi_1,\dots,\xi_N) \ D_{1\dots N}(\lambda;\xi_1,\dots,\xi_N) \ F_{1\dots N}^{-1}(\xi_1,\dots,\xi_N) \\ &= \bigotimes_{i=1}^N \left(\begin{array}{c} b(\lambda,\xi_i) & 0\\ 0 & 1 \end{array} \right)_{[i]} \\ \widetilde{B}_{1\dots N}(\lambda) &= \sum_{i=1}^N \ \sigma_i^- \ c(\lambda,\xi_i) \ \bigotimes_{j\neq i} \left(\begin{array}{c} b(\lambda,\xi_j) & 0\\ 0 & b^{-1}(\xi_j,\xi_i) \end{array} \right) \end{aligned}$$

Determinant Formulas for Form Factors

$$\begin{aligned} |\langle \mu | S_q^- | \lambda \rangle|^2 &= N \delta_{q,q\{\lambda\}-q\{\mu\}} |\sin(i\eta)| \frac{\Pi_{j=1}^{M+1} |\sin(\mu_j - i\eta/2)|^2}{\Pi_{j=1}^M |\sin(\lambda_j - i\eta/2)|^2} \\ &= \Pi_{j>k=1}^{M+1} |\sin^2(\mu_j - \mu_k) - \sin^2(i\eta)|^{-1} \Pi_{j>k=1}^M |\sin^2(\lambda_j - \lambda_k) - \sin^2(i\eta)|^{-1} \\ &= \frac{|\det H^-|^2}{|\det \Phi(\{\mu\})| \ |\det \Phi(\{\lambda\})|} \end{aligned}$$

V. E. Korepin *Commun. Math. Phys.* 86, 391 (1982)
J. M. Maillet and J. Sanchez De Santos *arXiv: q-alg/9612012* (1996)
N. Kitanine, J. M. Maillet and V. Terras *Nucl. Phys. B* 554, 647 (1999)

• For string states, the formulas need to be regularized.

J. Mossel, and J-S Caux New J. Phys., 12.5 (2010)

Bethe-Gaudin-Takahashi (BGT) equations

- Reference state: all spins up. Spin-down particles act as particles.
- String states: multi-particle bound states with complex rapidities.



Sum rules

• Integrated intensity: $c_a = \pm 1, 0$, for $a = \pm, z$.

$$R_{a\bar{a}} = \frac{1}{N} \sum_{q} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} S^{a,\bar{a}}(q,\omega) = \frac{1}{4} + \frac{m}{2}c_a$$

• Transverse first frequency moment (FFM).

$$W_{\perp}(q) = \frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \,\omega \left(S^{+-}(q,\omega) + S^{-+}(q,\omega) \right) = \alpha_{\perp} + \beta_{\perp} \cos q$$
$$\alpha_{\perp} = -e_0 - \Delta \frac{\partial e_0}{\partial_{\Delta}} + mh \qquad \beta_{\perp} = (2 - \Delta^2) \frac{\partial e_0}{\partial_{\Delta}} + \Delta e_0$$

• Longitudinal first frequency moment (FFM).

$$W_{\parallel}(q) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \ \omega S^{zz}(q,\omega) = (1 - \cos q)\alpha_{\parallel} \quad \alpha_2 = -e_0 + \Delta \frac{\partial}{\partial_{\Delta}} e_0$$

Algorithm: dynamics for integrable systems



String states (anti-bound states)



• No 4-string state contribution.